
Advancing process understanding and modeling of contrail formation with emphasis on hydrogen combustion

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Zusammenfassung

Durch den Einsatz von aus erneuerbaren Energien hergestelltem Wasserstoff (H_2) könnten die mit dem Flugverkehr verbundenen CO_2 -Emissionen vollständig vermieden werden. Etwa zwei Drittel der Klimawirkung des derzeit auf fossilen Treibstoffen basierenden Flugverkehrs entfallen jedoch auf Nicht- CO_2 -Effekte, wobei langlebige Kondensstreifen-Zirren (vom Flugverkehr erzeugte Eiswolken) den größten Beitrag darstellen.

Zur Abschätzung des Strahlungsantriebs von Kondensstreifen-Zirren werden globale Zirkulationsmodelle (general circulation models, GCMs) mit integrierten Kondensstreifenmodulen eingesetzt. Kleinskalige Prozesse unterhalb der Gitterauflösung dieser Modelle können nicht explizit aufgelöst werden und müssen daher parametrisiert werden. Das betrifft die Prozesse der Kondensstreifenbildung, die innerhalb der ersten Sekunden in der Abgasfahne hinter einem Triebwerk stattfinden.

Eine zentrale Größe ist dabei die Anzahl der gebildeten Eiskristalle, die einen maßgeblichen Einfluss auf die Lebensdauer und Strahlungswirkung langlebiger Kondensstreifen hat. Für konventionelle Kerosinverbrennung, bei der Tropfenaktivierung mit anschließendem Gefrieren zu Eiskristallen hauptsächlich auf emittierten Rußpartikeln erfolgt, existiert bereits eine geeignete Parametrisierung der Eiskristallanzahl. Im Fall der Wasserstoffverbrennung sind jedoch sowohl die thermodynamischen Bedingungen aufgrund erhöhter Wasserdampfemissionen als auch die Art der Kondensationskeime grundlegend anders. Im Idealfall ist das Abgas partikelfrei, sodass sich Eiskristalle ausschließlich auf eingemischten Umgebungsaerosolen bilden. Diese fundamentalen Unterschiede erfordern eine speziell auf den Wasserstofffall zugeschnittene Parametrisierung.

Ziel der vorliegenden Arbeit ist die Entwicklung einer solchen, für den Wasserstofffall gültigen Parametrisierung. Grundlage ist ein umfassender Datensatz von Simulationen der Kondensstreifenbildung, die mit einem Boxmodell mit partikelbasierter Mikrophysik durchgeführt wurden. Anhand dieser Simulationen wird der Einfluss von Umgebungsbedingungen, Aerosoleigenschaften und Triebwerksparametern auf die Eiskristallanzahl systematisch untersucht und physikalisch interpretiert. Flache neuronale Netze werden trainiert und als Fitfunktion für die simulierte Eiskristallanzahl verwendet. Trotz ihrer einfachen Architektur sind die Netze flexibel genug, um nichtlineare Abhängigkeiten präzise abzubilden. Da ihre Anwendung nur wenige Rechenschritte erfordert, lassen sich diese Netze leicht in großskalige Modelle integrieren. Darüber hinaus stellen physikalisch motivierte analytische Skalierungen eine breite Anwendbarkeit der Parametrisierung sicher.

Des Weiteren wird der mögliche Einfluss von volatilen Partikeln untersucht, die sich aus Schmierölemissionen bilden könnten. Sowohl für Kerosin- als auch Wasserstoffverbrennung wird analysiert, unter welchen Szenarien diese Partikel die Eiskristallbildung dominieren könnten.

Die entwickelte Parametrisierung kann in großskalige Modelle integriert werden und stellt damit einen zentralen Baustein zur Abschätzung der Strahlungswirkung langlebiger Kondensstreifen-Zirren dar, die von einer möglichen zukünftigen wasserstoffbetriebenen Flugzeugflotte erzeugt würden. Darüber hinaus könnte die präsentierte Methodik in Kombination mit dem erarbeiteten theoretischen Verständnis genutzt werden, um eine vergleichbare Parametrisierung für nachhaltige Treibstoffe (sustainable aviation fuels, SAFs) zu erarbeiten.

Abstract

The use of hydrogen (H_2) produced from renewable energy sources could eliminate aviation-related CO_2 emissions entirely. For present-day aviation based on fossil fuels, however, roughly two-thirds of the climate impact are attributable to non- CO_2 effects, with the largest contribution arising from long-lived contrail cirrus (ice clouds generated by aviation).

The radiative forcing of contrail cirrus is estimated using general circulation models (GCMs) with integrated contrail modules. As small-scale processes below the grid resolution of these models cannot be resolved explicitly, they must be parameterized. This includes the processes governing contrail formation that occur within the first seconds in the exhaust plume behind an aircraft engine.

A key quantity is the number of ice crystals formed, as it strongly influences the lifetime and radiative impact of long-lived contrails. For conventional kerosene combustion, droplet activation followed by freezing into ice crystals occurs primarily on emitted soot particles. A suitable parameterization of ice crystal number already exists for this case. For hydrogen combustion, however, both the thermodynamic conditions due to increased water vapor emissions and the nature of the condensation nuclei differ fundamentally. In the ideal case, the exhaust is particle-free, so that ice crystals form exclusively on entrained ambient aerosol particles. These fundamental differences require a parameterization specifically tailored to hydrogen combustion.

The aim of this work is to develop such a parameterization for the hydrogen combustion case. The parameterization is based on a comprehensive dataset of contrail formation simulations performed with a box model including particle-based microphysics. Using these simulations, the influence of ambient conditions, aerosol properties, and engine parameters on ice crystal number is systematically investigated and physically interpreted. Shallow neural networks are trained and used as a fitting function to represent the simulated ice crystal number. Despite their simple architecture, these networks are sufficiently flexible to accurately represent nonlinear dependencies. Since their application requires only a small number of computational operations, they can be readily integrated into large-scale models. Physically motivated analytical scalings further ensure the broad applicability of the parameterization.

In addition, the potential influence of volatile particles that may form from lubrication oil emissions is investigated. The scenarios under which these particles may dominate ice crystal formation are analyzed for both kerosene and hydrogen combustion.

The parameterization developed can be integrated into large-scale models and thus provides a basis for estimating the radiative impact of contrail cirrus produced by a potential future fleet of hydrogen-powered aircraft. Moreover, the methodology presented together with the theoretical understanding gained could be used to derive a comparable parameterization for sustainable aviation fuels (SAFs).

List of publications

Co-authorship:

- Bier, A., Unterstrasser, S., **Zink, J.**, Hillenbrand, D., Jurkat-Witschas, T., and Lottermoser, A.: Contrail formation on ambient aerosol particles for aircraft with hydrogen combustion: a box model trajectory study, *Atmos. Chem. Phys.*, 24, 2319–2344, <https://doi.org/10.5194/acp-24-2319-2024>, 2024
Contributions: extending the box model code (e.g., refining the SIP merging algorithm described in Appendix A); developing the theoretical background for Sec. 3.2.2 and drafting that section; updating figures during revision; partially responding to reviewer comments.

This dissertation is submitted as a cumulative thesis and is based on the following first-author studies (appended to this thesis and abbreviated P1–4):

- **P1.** **Zink, J.**, Unterstrasser, S., and Burkhardt, U.: Contrail formation for aircraft with hydrogen combustion - Part 1: A systematic microphysical investigation, *Atmos. Chem. Phys.*, 26, 3125–3143, <https://doi.org/10.5194/acp-26-3125-2026>, 2026
Contributions: conceptualizing; performing, analyzing, and interpreting box model simulations; producing all tables and figures; writing (first draft, editing, and reviewing); responding to reviewer comments.
- **P2.** **Zink, J.** and Unterstrasser, S.: Contrail formation for aircraft with hydrogen combustion - Part 2: Engine-related aspects, *Atmos. Chem. Phys.*, 26, 3145–3165, <https://doi.org/10.5194/acp-26-3145-2026>, 2026
Contributions: conceptualizing; literature research; developing the theoretical framework; analyzing CFD data; extending the box model code; performing, analyzing, and interpreting box model simulations; producing all tables and figures; writing (first draft, editing, and reviewing); responding to reviewer comments.
- **P3.** **Zink, J.**, Weiß-Rehm, C., Unterstrasser, S., and Burkhardt, U.: Contrail formation for aircraft with hydrogen combustion - Part 3: A neural-network-based parameterization of ice crystal number, *EGUsphere* [preprint], <https://doi.org/10.5194/egusphere-2026-1088>, 2026 [under review for ACP]
Contributions: conceptualizing; performing, analyzing, and interpreting box model simulations; training and evaluating neural networks; producing all tables and figures except Fig. 8; writing (first draft, editing, and reviewing).
- **P4.** **Zink, J.**, Unterstrasser, S., and Jurkat-Witschas, T.: On the Potential Role of Lubrication Oil Particles in Contrail Formation for Kerosene and Hydrogen Combustion, *J. Geophys. Res.*, 130, e2025JD043487, <https://doi.org/10.1029/2025jd043487>, 2025
Contributions: conceptualizing; literature research; extending the box model code; performing, analyzing, and interpreting box model simulations; producing all tables and figures; writing (first draft, editing, and reviewing); responding to reviewer comments.

Disclaimer: Parts of this thesis are rephrased passages from the publications. Although the author has made an effort to avoid copying text verbatim, some sections may still closely resemble the original wording.

List of abbreviations

Abbreviation	Meaning
CFD	Computational Fluid Dynamics
CN	Condensation Nucleus
CO ₂	Carbon Dioxide
ECHAM	EC from ECMWF and HAM for Hamburg
ECHAM-CCMod	ECHAM with Contrail Cirrus Module
ECMWF	European Centre for Medium-Range Weather Forecasts
ERF	Effective Radiative Forcing
EULAG	Eulerian-Lagrangian Fluid Solver
GCM	General Circulation Model
GHG	Greenhouse Gas
HDN	Homogeneous Droplet Nucleation
H ₂	Molecular Hydrogen
H ₂ O	Water
H ₂ SO ₄	Sulfuric Acid
HNO ₃	Nitric Acid
IN	Ice Nucleus
IPCC	Intergovernmental Panel on Climate Change
ISSR	Ice-supersaturated Region
LCM	Lagrangian Cloud Module
LES	Large Eddy Simulation
NO _x = NO + NO ₂	Nitrogen Oxides
O ₂	Molecular Oxygen
RadMod	Radial Model
RANS	Reynolds-Averaged Navier-Stokes
SAF	Sustainable Aviation Fuel
SIP	Simulation Particle
SO _x = SO ₂ + SO ₃	Sulfur Oxides
UNFCCC	United Nations Framework Convention on Climate Change

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Chapter 1

Introduction

1.1 Motivation

1.1.1 Hydrogen economy

Global climate change represents one of the most pressing challenges of the 21st century, primarily driven by the continuous increase in anthropogenic greenhouse gas (GHG) emissions. These emissions originate mainly from fossil fuel combustion (in heat and electricity generation, transportation, and the buildings sector), industrial processes, agriculture, and land-use changes (IPCC, 2021). In line with the Paris Agreement (UNFCCC, 2015), limiting the global average temperature rise to well below 2 °C with efforts to limit it to 1.5 °C above pre-industrial levels is necessary to minimize the risk of the most severe and partially irreversible consequences of climate change (IPCC, 2023). This includes extreme weather events (e.g., heatwaves, heavy precipitation, droughts, intense tropical cyclones), rising sea levels, biodiversity loss, and threats to food and water security, with serious impacts on human health, living conditions, economic and social stability, and the resilience of critical infrastructure. To keep global warming within the Paris Agreement thresholds, rapid and sustained reductions in GHG emissions across all sectors are required, with net-zero carbon dioxide (CO₂) emissions achieved around mid-century (IPCC, 2023). In this multi-sector decarbonization effort, hydrogen (H₂) could play a pivotal role.

A hydrogen economy envisions H₂ as a clean and versatile energy carrier replacing fossil fuels in transportation, industry, and power generation (Staffell et al., 2019). This transition requires extensive infrastructure for production, storage, distribution, and end-use technologies such as fuel cells and gas turbines (Tashie-Lewis and Nnabuife, 2021). Hydrogen produced via electrolysis powered by renewable energy sources (green hydrogen) does not generate carbon emissions during production (Dincer and Acar, 2015; Nikolaidis and Poullikkas, 2017; Ajanovic et al., 2022). Moreover, when hydrogen is used in gas turbines or fuel-cell systems, it undergoes the reaction



producing no direct greenhouse gas emissions other than water vapor.

However, hydrogen is not without environmental risks. Combusting hydrogen in air can lead to the formation of nitrogen oxides (NO_x) from atmospheric nitrogen,

contributing to air pollution and ozone formation. In addition, hydrogen leakage can indirectly contribute to global warming by extending the atmospheric lifetime of methane and increasing concentrations of tropospheric ozone and stratospheric water vapor (Ocko and Hamburg, 2022; Hauglustaine et al., 2022; Warwick et al., 2023). These secondary effects highlight the need to assess the full climate implications of a hydrogen-based energy system to support its effective and sustainable deployment.

1.1.2 Use of hydrogen in aviation

Two main concepts are being investigated for the potential future use of hydrogen in aviation (Tiwari et al., 2024; Soleymani et al., 2024; Richardson, 2025). The first concept involves H_2 fuel cells, in which the chemical energy of the fuel is converted into electrical energy. This electrical energy powers electric motors that drive propellers to generate thrust. The second concept is direct H_2 combustion in gas turbine engines. Here, the energy released during combustion is used either to drive a propeller (in a turboprop configuration) or to produce a high-velocity exhaust jet for thrust (in turbofan engines). Propeller-driven aircraft (fuel cell or turboprop) operate most efficiently at lower flight speeds and altitudes and would therefore be well suited for regional and short-haul missions. In contrast, turbofan engines enable higher cruise speeds and altitudes, making them more appropriate for medium- and long-haul operations.

The potential use of hydrogen in aviation introduces several technical and infrastructural challenges. Because H_2 has a low volumetric energy density in its gaseous form, it must be liquefied to achieve a practical storage density for aircraft. This requires cooling it to around 20 K, which in turn necessitates specialized liquefaction facilities and cryogenic infrastructure at airports (Hoelzen et al., 2022). Onboard, the liquid H_2 must be stored in well-insulated cryogenic tanks. Even in its liquid state, H_2 has roughly four times lower volumetric energy density than conventional jet fuel, meaning that approximately four times more tank volume is required to store the same amount of usable energy. These larger tanks also add weight and occupy space within the airframe, potentially reducing payload or range unless aircraft are redesigned (Tiwari et al., 2024; Soleymani et al., 2024).

1.1.3 Non- CO_2 effects of aviation

Despite the challenges outlined in Sect. 1.1.2, hydrogen could play a crucial role in decarbonizing the aviation sector in the long term (Airbus, 2020) by eliminating direct CO_2 emissions. The climate effect of CO_2 emissions can be quantified with comparatively high confidence. Once emitted, CO_2 remains in the atmosphere for centuries, is mixed nearly uniformly on global scales, and absorbs infrared radiation in well-characterized spectral bands. Consequently, the effective radiative forcing (ERF) from aviation CO_2 emissions can be estimated with high confidence (Lee et al., 2021). ERF is defined as the change in Earth’s energy balance at the top of the atmosphere caused by a perturbation, after rapid atmospheric adjustments have taken place but before the surface temperature responds.

However, the climate impact of aviation extends beyond CO_2 emissions, with non- CO_2 effects contributing substantially to total ERF (Lee et al., 2021). These non- CO_2

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effects include (i) NO_x emissions that influence ozone, methane, and stratospheric water vapor (e.g., Sausen et al., 2005; Lee et al., 2009; Frömming et al., 2012; Pitari et al., 2015), (ii) water vapor emissions in the stratosphere (e.g., Gauss, 2003; Ponater et al., 2006; Frömming et al., 2012; Wilcox et al., 2012), (iii) aerosol–radiation interactions (e.g., Sausen et al., 2005; Righi et al., 2013; Gettelman and Chen, 2013), (iv) aerosol–cloud interactions (e.g., Penner et al., 2018; Righi et al., 2021, 2025), and (v) contrails formed in ice-supersaturated regions (ISSRs) (e.g., Burkhardt and Kärcher, 2011; Chen and Gettelman, 2013; Bock and Burkhardt, 2016; Schumann et al., 2015).

The net ERF associated with these non- CO_2 effects is estimated to be positive, meaning that it contributes to climate warming. For present-day aviation, these effects account for roughly two-thirds of the total climate impact, with contrails representing the largest contributor. However, this estimate is subject to considerable uncertainty.

Contrails form and persist for minutes to hours only under specific temperature and humidity conditions in the upper troposphere and exhibit strong spatial and temporal variability. Their radiative impact depends on atmospheric conditions, flight routes, time of day, and season. Furthermore, their evolution involves complex microphysical processes, including interactions with natural cirrus clouds. As a result, the ERF associated with contrails remains uncertain and is assessed with low confidence (Lee et al., 2021, 2023).

A rigorous assessment of alternative propulsion concepts, such as H_2 combustion, therefore requires a robust understanding of all processes involved. This includes detailed knowledge of the mechanisms governing initial contrail formation and the subsequent development of persistent, long-lived contrails.

1.1.4 Contrail life cycle and impact of early processes

The evolution of a single contrail is typically divided into three regimes (Paoli and Shariff, 2016) (Fig. 1.1). In the *jet regime*, intense turbulence caused by strong shear between the jet and its surroundings leads to rapid mixing of the hot and humid exhaust with the much colder ambient air. Under suitable ambient conditions, transient supersaturation is generated and ice crystals can form on aerosol particles within a few seconds (e.g., Kärcher and Yu, 2009; Lewellen, 2020; Bier et al., 2022, 2024; Yu et al., 2024). These ice crystals become trapped within the counter-rotating wing-tip vortices. This marks the *vortex regime*, in which the vortices generated by lift descend due to their mutual induction (Spalart, 1998; Gerz et al., 2002). The associated adiabatic compression and heating during this descent lead to partial sublimation of the ice particles (Sussmann and Gierens, 1999; Unterstrasser et al., 2008; Kleine et al., 2018). In addition, baroclinic instabilities within the descending primary wake cause detrainment and the formation of a secondary wake near the emission altitude (Lewellen and Lewellen, 1996; Unterstrasser et al., 2014). After approximately five minutes, the vortices break up. This phase is sometimes referred to as an additional *dissipation regime*, which is, however, often not explicitly separated from the preceding vortex regime. Following this breakup, the contrail enters the *dispersion regime*, during which it evolves into a cirrus cloud (Schumann, 2012; Lewellen, 2014; Unterstrasser et al., 2017a). This stage is characterized by spreading due to vertical wind shear, ice particle growth or sublimation, and sedimentation. Under favorable atmospheric conditions, this regime can

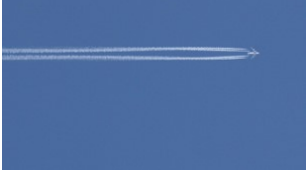
	Jet regime	Vortex regime	Dispersion regime
			
Time scale	Seconds	Minutes	Hours
Physical processes	Turbulent mixing of hot, humid exhaust air with cold ambient air; Ice crystal formation	Interaction of ice crystals with descending vortices; Partial loss of ice crystals	Contrail spreading; Ice crystal growth/sublimation; Sedimentation processes

Figure 1.1: Contrail life cycle and governing physical processes. Credits: DLR (CC BY-NC-ND 3.0, left and middle photo) and S. Unterstrasser (right photo).

persist for several hours before the contrail cirrus finally dissolves (Jensen et al., 1998; Haywood et al., 2009; Laken et al., 2012; Bier et al., 2017).

The direct contribution of the jet and vortex regimes to the overall lifetime-integrated radiative effect of a contrail is typically small (Unterstrasser and Gierens, 2010a). However, the microphysical and dynamical processes occurring during these early phases have a long-lasting impact on the properties and life cycle of the contrail cirrus cloud (Burkhardt et al., 2018). Consequently, these initial processes exert a significant indirect impact on the overall radiative effect of the contrail (Bier and Burkhardt, 2022).

While the total ice mass after vortex breakup is of minor importance (Unterstrasser and Gierens, 2010b; Lottermoser and Unterstrasser, 2025), the number of ice crystals at this stage strongly and nonlinearly influences the integrated radiative impact of the resulting contrail cirrus under a given set of meteorological conditions (Unterstrasser and Gierens, 2010b; Lewellen, 2014; Burkhardt et al., 2018; Lottermoser and Unterstrasser, 2025). If, for example, the initial number of ice crystals is reduced, the ice crystals are on average larger, assuming the same total amount of water vapor is consumed from the environment. For a given total ice mass, fewer and larger ice crystals tend to decrease the contrail's optical depth compared to many smaller ice crystals (Lottermoser and Unterstrasser, 2026). Moreover, larger ice crystals sediment more rapidly, which reduces the lifetime of a contrail cirrus cloud. However, the lifetime is not solely controlled by microphysical sedimentation but is also influenced by dynamical processes in the surrounding environment, which affect the persistence of an ISSR (Bier et al., 2017; Hofer and Gierens, 2025).

1.1.5 Aim of the thesis

As outlined in Sect. 1.1.4, the number of ice crystals at vortex breakup is the quantity that has a long-lasting impact on contrail cirrus properties and their radiative effect. Accurately representing this quantity in large-scale models is therefore essential. Large-scale models, including general circulation models (GCMs) with integrated

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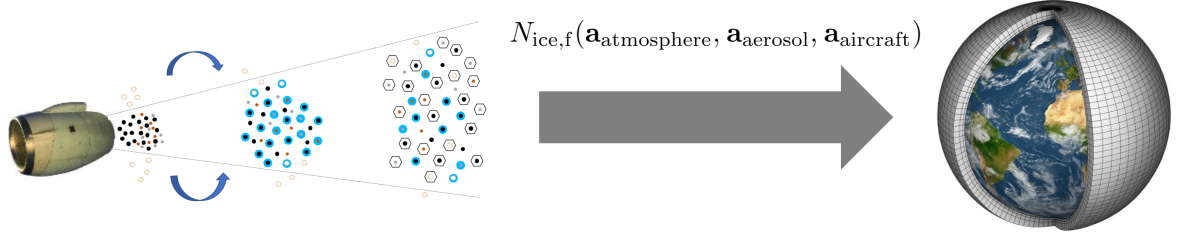


Figure 1.2: The parameterization for the number of ice crystals represents the small-scale processes of ice crystal formation through a functional relationship that can be implemented in large-scale models. The right schematic was produced by ChatGPT.

contrail modules ([Burkhardt and Kärcher, 2009; Gettelman and Chen, 2013; Bock and Burkhardt, 2016; Schumann et al., 2015]), are used to estimate the radiative forcing of the contrail coverage from global upper-tropospheric air traffic. These models, however, cannot explicitly resolve the early small-scale processes occurring during the jet and vortex regimes. Therefore, contrails are typically initialized after vortex breakup, and the earlier processes must be parameterized, i.e., expressed through simplified mathematical relationships.

For conventional kerosene combustion, both a parameterization for the initial number of ice crystals formed ([Kärcher et al., 2015]) and a parameterization for the loss of ice crystals during the vortex phase ([Unterstrasser, 2016]) have been developed. These parameterizations have been implemented in the GCM with contrail module ECHAM-CCMod ([Bier and Burkhardt, 2019, 2022]). Recently, the parameterization for ice crystal loss has been extended to include scenarios with hydrogen propulsion ([Lottermoser and Unterstrasser, 2025]). To date, a parameterization for the contrail formation stage does not exist for H_2 propulsion.

The aim of this thesis is to address this gap by developing a new parameterization for the H_2 combustion case. The parameterization should provide a functional relationship for the final number of ice crystals formed $N_{ice,f}$ (i.e., the number when contrail formation is finished) that is suitable for implementation in large-scale models (illustrated in Fig. 1.2). Specifically, the functional relationship

$$N_{ice,f} = N_{ice,f}(a_{atmosphere}, a_{aerosol}, a_{aircraft}) \quad (1.2)$$

should incorporate the dependence on variables that influence contrail ice crystal formation: $a_{atmosphere}$ denotes a set of variables characterizing the background atmosphere (e.g., ambient temperature), $a_{aerosol}$ represents properties (e.g., number concentration, size distribution) of aerosol particles that act as precursors for the ice crystal formation and $a_{aircraft}$ comprises aircraft-related parameters (e.g., engine size).

The development of such a parameterization requires a solid understanding of the underlying processes of contrail formation, as well as appropriate modeling approaches to represent them. The subsequent sections of this introductory part therefore provide the relevant background information. This includes a brief description of the theory of contrail formation (Sect. 1.2) and an overview of approaches for modeling contrail formation (Sect. 1.3). Furthermore, Sect. 1.4 provides a brief description of the contrail formation model used, which forms the basis for the development of the parameteri-

zation. The introductory part concludes with a refinement of the overarching goal by formulating four research questions (Sect. 1.5), each of which is addressed in one of the four publications P1-P4.

1.2 Theory of contrail formation

Hot, humid exhaust air (called the plume) mixes with cold ambient air downstream of an aircraft engine under isobaric conditions. Under suitable ambient conditions, this mixing process can lead to transient water supersaturation, providing favorable conditions for the formation of contrail ice crystals. The following subsections provide a brief review of the fundamental microphysical and thermodynamic principles of contrail formation, with an emphasis on the changes that occur when switching from conventional kerosene to hydrogen combustion.

1.2.1 Microphysics

The commonly accepted scientific understanding of contrail formation is that aerosol particles present in the plume activate into liquid droplets, which subsequently freeze homogeneously into ice crystals (Kärcher, 2018) (illustrated in Fig. 1.3). This formation pathway is supported by the fact that the majority of upper-tropospheric aerosol particles, including those originating from aircraft emissions, readily act as condensation nuclei (CN). In contrast, ice nuclei (IN) are comparatively rare, with concentrations typically orders of magnitude lower than those of CN (e.g., Rogers et al., 1998; Beer et al., 2022). The level of supersaturation required for droplet activation depends on particle size, through the Kelvin (curvature) effect, and on particle hygroscopicity (see Sect. 1.4.3).

For conventional kerosene combustion, the dominant CN are soot particles formed through incomplete combustion and coated with other emission products (Kärcher and Yu, 2009; Kleine et al., 2018). Soot particles are emitted in the size range $\sim 10\text{--}100\text{ nm}$ with numbers $10^{14}\text{--}10^{15}$ per kilogram of fuel burned (Moore et al., 2017).

In addition, ultrafine volatile particles (radii $\sim 1\text{--}10\text{ nm}$) form prior to contrail formation from gaseous emissions (Kärcher, 2018). These particles are expected to significantly contribute to ice crystal formation under conditions where the soot number is reduced and high supersaturations are encountered in the exhaust plume (Kärcher and Yu, 2009; Yu et al., 2024). Volatile particles mainly form from condensable vapors generated when combustion by-products (sulfur oxides (SO_x), nitrogen oxides (NO_x), and unburned hydrocarbons) are oxidized to sulfuric acid, nitric acid, and low-volatile organic compounds. These volatile particles initially appear in two modes: a charged mode, formed on ionized molecules (chemi-ions) with numbers up to 10^{17} per kilogram of fuel burned, and a neutral mode that remains too small to influence ice crystal formation (Yu and Turco, 1997; Haverkamp et al., 2004). Ground-based measurements (R.C. Miake-Lye (Aerodyne Research), personal communication), in-flight measurements (Dischl et al., 2025) as well as simulation results (Yu et al., 2024) suggest that the number of volatile particles originating from combustion products is strongly influenced by the fuel's sulfur content.

1.2 Theory of contrail formation

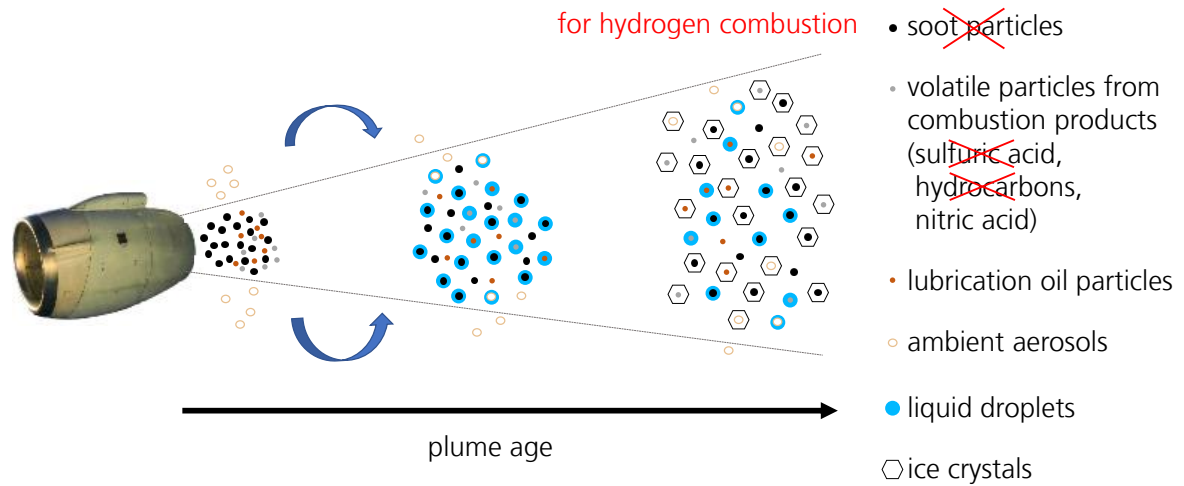


Figure 1.3: Schematic illustration of the microphysical pathway of ice crystal formation in the expanding exhaust plume behind an aircraft engine. Aerosol particles activate into liquid droplets, which then freeze homogeneously into ice crystals. Soot particles, sulfuric acid –the main contributor to volatile particle formation in kerosene combustion cases– and hydrocarbons are absent in hydrogen exhaust plumes.

Another non-combustion source of volatile particles is lubrication oil. Lubrication oil is used to cool, seal, and reduce friction in moving parts of the engine. Lubrication oil systems are typically sealed recirculating systems (Linke-Diesinger, 2010). Controlled venting and minor leakages through worn seals can release oil mist, which contributes to particulate matter in the exhaust (Yu et al., 2010, 2012; Fushimi et al., 2019; Yu et al., 2019; Ungeheuer et al., 2021). Laboratory studies have shown that heating lubrication oil to high temperatures causes it to evaporate and subsequently renucleate, producing large numbers of small particles (Ungeheuer et al., 2022). Consequently, a large number of small oil particles is expected in the exhaust of engine configurations where venting occurs near the hot sections at the engine exit. Moreover, Ponsonby et al. (2024) demonstrated in a laboratory experiment that lubrication oil particles can activate into liquid droplets, which subsequently freeze into ice crystals.

In addition to soot and volatile particles, ambient aerosols represent a third type of particle that can act as CN in the exhaust plume. These ambient particles are gradually entrained into the plume, with their number depending on the background aerosol concentration. Ambient aerosols exhibit large variability in number concentration, size distribution, and chemical composition (Petzold et al., 2002; Minikin et al., 2003; Hermann et al., 2003; Borrmann et al., 2010; Kaiser et al., 2019; Brock et al., 2021). Typically, their total number present in the plume during ice crystal formation is 1-2 orders of magnitude lower than the soot number for conventional kerosene combustion.

In the case of H_2 combustion, soot particles, sulfur compounds, and unburned hydrocarbons are absent. However, volatile particles originating from emitted NO_x or from lubrication oil could still be present in hydrogen exhaust plumes. Another possible pathway for ice crystal formation is homogeneous droplet nucleation (HDN). HDN is the process in which small droplets form directly from the vapor phase without the

involvement of condensation nuclei. HDN requires high relative humidities ($\gtrsim 500\%$) (Wölk and Strey, 2001), which are generally not encountered in kerosene exhaust plumes but could occur within hydrogen exhaust plumes at low ambient temperatures (Bier et al., 2024). In the ideal scenario, the exhaust is entirely particle-free, and HDN plays a negligible role in the H_2 combustion case. In that case, ice crystal formation would rely solely on ambient aerosols entrained into the exhaust plume.

1.2.2 Thermodynamics

Assuming a well-mixed exhaust plume and neglecting the kinetic energy of the jet, the partial pressure of water vapor in the plume and the plume temperature follow a mixing line in the absence of microphysical processes (Fig. 1.4). This line represents how these quantities evolve from the engine exit conditions toward ambient conditions during the isobaric mixing process. The slope of this mixing line can be expressed as

$$G = \frac{EI_v c_p p_a}{\epsilon Q(1 - \eta)} , \quad (1.3)$$

where EI_v denotes the mass-specific water vapor emission index of the fuel, Q the specific combustion heat (lower calorific heating value of the fuel), c_p the specific heat capacity at constant pressure, p_a the ambient pressure, $\epsilon = 0.622$ the ratio of the molar masses of dry air and water vapor, and η the overall efficiency of propulsion (Schumann, 1996). The slope G influences the Schmidt–Appleman threshold temperature Θ_G (Schmidt, 1941; Appleman, 1953; Schumann, 1996). This threshold temperature Θ_G corresponds to the ambient temperature at which the mixing line is tangent to the water saturation curve for a given ambient relative humidity over water $RH_{\text{wat},a}$ (Fig. 1.4). When the ambient temperature is below Θ_G , transient supersaturation occurs during the mixing process, enabling plume particles to activate into liquid droplets.

Replacing kerosene with hydrogen increases the energy-specific water vapor emission index EI_v/Q by roughly a factor of 2.6 (Table 1.1), resulting in a steeper mixing line (Fig. 1.4). This steeper slope leads to an increase in Θ_G by around 10 K (Fig. 1.5). Since the level of supersaturation encountered depends on how far the ambient temperature lies below Θ_G , higher and longer-lasting supersaturation levels occur in a hydrogen plume than in a conventional kerosene plume under the same ambient conditions.

While the Schmidt–Appleman threshold temperature provides a criterion for whether liquid droplets may form, ice crystal formation requires that these droplets freeze homogeneously (Sect. 1.2.1). Droplets that do not freeze will evaporate shortly after the transient water-supersaturated plume becomes subsaturated again (if the ambient air were

Table 1.1: Water vapor emission index EI_v and specific combustion heat Q for kerosene (second column) and hydrogen combustion (third column), along with their ratios (last column). Values are taken from Table 1 in Schumann (1996).

parameter	kerosene	hydrogen	ratio
$EI_v / (\text{kg kg}^{-1})$	1.25	8.94	7.15
$Q / (\text{MJ kg}^{-1})$	43.0	120.	2.79
$EI_v/Q / (\text{kg MJ}^{-1})$	0.0291	0.0745	2.56

1.2 Theory of contrail formation

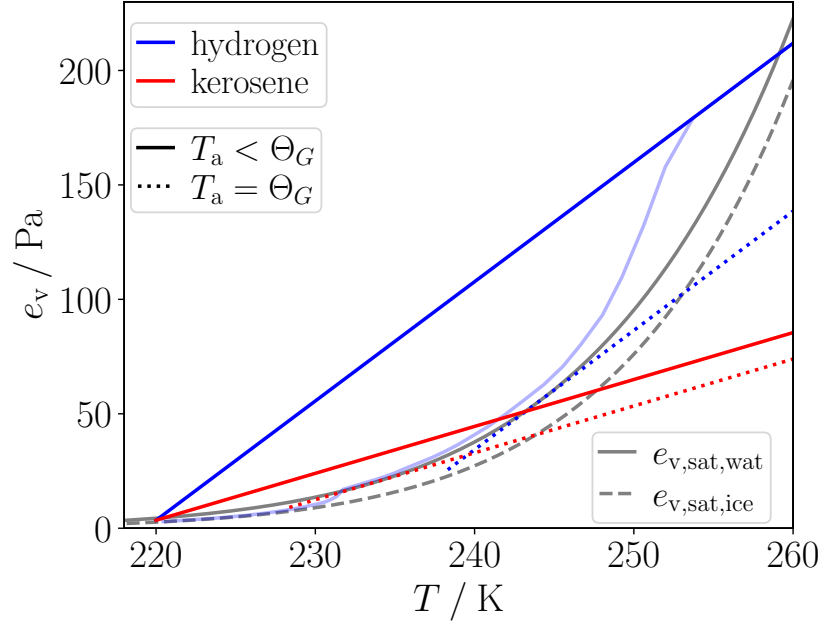


Figure 1.4: Mixing lines (partial pressure of water vapor in the plume e_v vs plume temperature T) are depicted for both hydrogen and kerosene combustion cases for the ambient pressure $p_a = 260 \text{ hPa}$, ambient relative humidity over water $RH_{\text{wat},a} = 80 \%$ and overall efficiency of propulsion $\eta = 0.4$. Shown are threshold cases with ambient temperatures $T_a = \Theta_G$ such that the mixing line just touches the saturation curve over water $e_{v,\text{sat},\text{wat}}$ for the given $RH_{\text{wat},a}$ value. Additionally, cases with a lower ambient temperature of $T_a = 220 \text{ K}$ are displayed. The transparent blue curve serves as an exemplary illustration of the evolution with microphysical water vapor depletion.

supersaturated with respect to water, natural cirrus clouds would likely already have formed). For kerosene combustion, the homogeneous freezing temperature is typically above Θ_G (Fig. 1.5). This means that under conditions where droplet formation happens, these droplets will freeze into ice crystals. In contrast, the homogeneous freezing temperature is typically below Θ_G in hydrogen combustion cases. This means that scenarios exist in which droplets form but do not freeze into ice crystals. Consequently, in the case of H_2 combustion, the binary question of whether ice crystals form is governed mainly by the homogeneous freezing process rather than by the Schmidt–Appleman threshold temperature. Nevertheless, the degree to which the ambient temperature lies below Θ_G remains a key factor, as it determines the supersaturation levels encountered.

In addition to the requirement that the ambient temperature must be below both the Schmidt–Appleman threshold temperature and the homogeneous freezing temperature of supercooled droplets, the contrail must form within an ISSR ($RH_{\text{ice},a} \geq 100 \%$) to evolve into a persistent cirrus cloud. For $RH_{\text{ice},a} < 100 \%$, the ice crystals will sublime shortly after their formation.

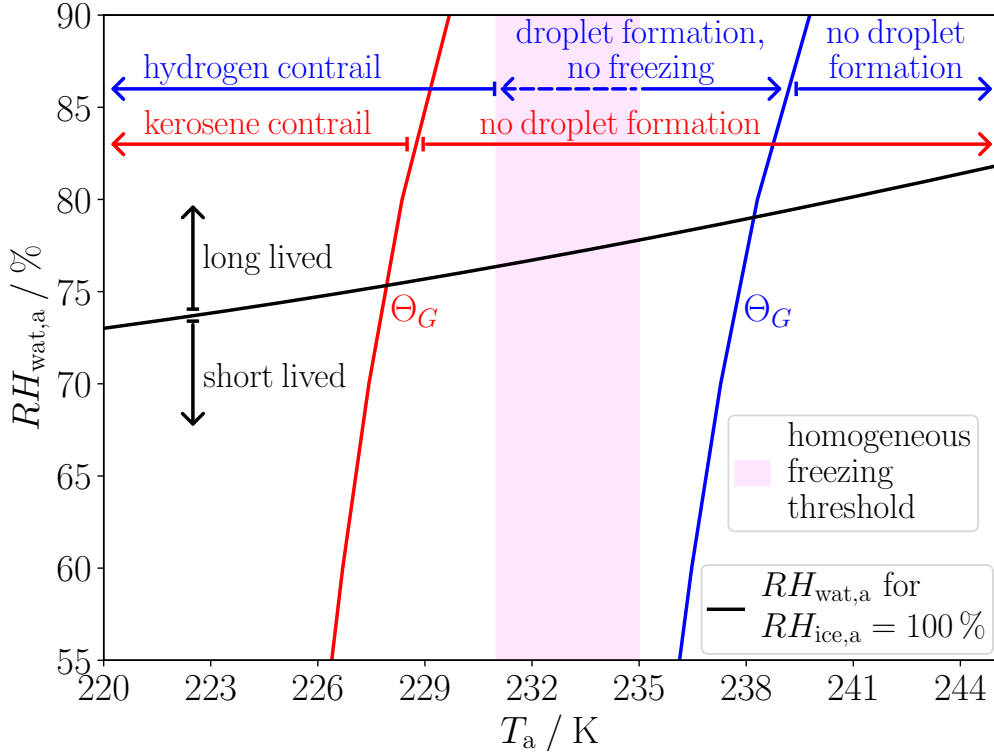


Figure 1.5: Thermodynamic criteria for contrail formation illustrated in a phase space spanned by ambient relative humidity over water $RH_{\text{wat},a}$ and ambient temperature T_a . Schmidt-Appleman threshold temperatures Θ_G are depicted for both kerosene (red curve) and hydrogen (blue curve) combustion cases for the ambient pressure $p_a = 260$ hPa and overall efficiency of propulsion $\eta = 0.4$. If the ambient temperature T_a is below Θ_G , aerosol particles can activate into droplets. Moreover, the range of homogeneous freezing temperatures for supercooled droplets is indicated. Below the homogeneous freezing temperature, droplets freeze into ice crystals. Furthermore, the black line shows where the ambient relative humidity over ice equals $RH_{\text{ice},a} = 100\%$. For a relative humidity above this line, a formed contrail will be persistent.

1.3 Approaches for modeling contrail formation

As outlined in Sect. 1.1.5, the objective of this work is to develop a parameterization for the number of ice crystals formed in H_2 combustion scenarios. This motivates the use of an approach that allows for a systematic exploration of how the number of ice crystals depends on atmospheric conditions, aerosol properties, and aircraft parameters. To this end, existing approaches for modeling contrail formation are reviewed.

The simplest models of contrail formation rely solely on the thermodynamic principles outlined in Sect. 1.2.2. While such models can predict the conditions under which contrails form for different propulsion systems (Richardson, 2025), they do not provide information on the number of ice crystals formed. In a more advanced approach, Kärcher et al. (2015) developed a microphysical model that predicts the ice crystal number based on first principles. They reformulated and simplified the governing equations such that an analytical expression for the number of ice crystals could be deduced.

1.3 Approaches for modeling contrail formation

In other approaches, the microphysics of contrail formation is simulated with time-resolved numerical models. Sect. 1.3.1 summarizes the dynamical frameworks used in these models, and Sect. 1.3.2 provides an overview of the methods used to represent aerosol particles and hydrometeors (droplets and ice crystals).

1.3.1 Dynamical representation

The dynamically most detailed representations are provided by three-dimensional (3D) large-eddy simulations (LES) (e.g., Paoli et al., 2008, 2013; Garnier et al., 2014; Vancassel et al., 2014; Lewellen, 2020; Afkari et al., 2025). LES explicitly resolve the largest turbulent eddies, while smaller, unresolved motions are represented through subgrid-scale parameterizations. Owing to their high computational cost, LES studies typically cover only a limited number of simulations and often employ simplified microphysical schemes.

A less computationally demanding alternative is offered by 3D Reynolds-averaged Navier-Stokes (RANS) models (e.g., Khou et al., 2015, 2017; Cantin et al., 2022), which resolve only the mean flow field, while turbulent fluctuations are parameterized through closure schemes. The simplest dynamical representation is provided by 0D box models (e.g., Kärcher and Yu, 2009; Bier et al., 2022, 2024; Yu et al., 2024).

In 0D models, the microphysics is computed offline without coupling to the dynamics. Instead, dilution is externally prescribed, governing the plume’s mass increase and cooling over time. This external dilution can be based on analytical formulations (e.g., Schumann et al., 1998) or on data derived from a-priori LES or RANS simulations. The main advantage of this approach lies in its low computational cost, which enables extensive parameter studies across a broad range of emission parameters, aerosol properties, and ambient conditions with a detailed microphysical model.

At their simplest, 0D models prescribe dilution along a single average trajectory, thereby neglecting any spatial heterogeneity within the plume. A more advanced multi-0D approach accounts for plume heterogeneity by using an ensemble of independent trajectories, where each trajectory represents a certain fraction of the plume’s mass/volume (Bier et al., 2022). However, since each trajectory is modeled separately, diffusive exchange between neighboring trajectories remains neglected. To bridge this gap, Lottermoser and Unterstrasser (2024) developed the 1D framework RadMod, which serves as an intermediate solution between computationally demanding 3D models and dynamically simplified 0D approaches. Thus far, only the dynamical component of RadMod has been described.

In a comprehensive study, Lewellen (2020) compared LES and 0D box model simulations of contrail formation for kerosene combustion. In both approaches, the same sophisticated microphysical model was employed. Across a range of simulated conditions, the 0D model was found to generally overpredict ice crystal numbers compared to LES results when ice crystal formation occurred on emitted particles with high number concentrations. This is attributed to missing mixing processes between air parcels of different ages in 0D box models. In contrast, close agreement was observed in scenarios where the number of emitted particles was low or when ice crystals formed primarily on entrained ambient aerosols.

1.3.2 Eulerian field variables vs. Lagrangian particle tracking

The representation of aerosol particles and hydrometeors in contrail formation models is commonly based on one of two conceptual approaches (Unterstrasser et al., 2012). The first is an Eulerian framework, in which prognostic equations for number and mass concentrations are solved on a grid (two-moment bulk schemes). In the simplest case, bulk models assume that all particles of a given type have the same size (monodisperse distribution), which keeps computational cost low. More advanced bulk schemes prescribe a fixed functional form of the particle size distribution, such as a log-normal distribution with a specified width. However, since these models only predict the zeroth and first moments (number and mass), the shape of the size distribution does not evolve in time.

To allow a time-evolving size spectrum, spectral (bin) models divide the size distribution into multiple bins and solve separate prognostic equations for each bin. While this approach captures the evolution of the size distribution, it substantially increases the number of prognostic variables and therefore the computational cost.

An alternative to the Eulerian framework is the Lagrangian particle-based approach, in which aerosol particles and hydrometeors are represented by simulation particles (SIPs), sometimes also referred to as super-droplets (Shima et al., 2009; Grabowski et al., 2019). Each SIP is advected with the flow and represents a number of physical particles with identical properties. The microphysical processes act directly on these SIPs.

Although more computationally demanding than simple bulk schemes, the Lagrangian approach offers several advantages: First, the particle size distribution emerges and evolves naturally from the SIP ensemble without requiring a prescribed shape. Second, since SIPs are tracked at discrete positions, numerical diffusion associated with the grid-based advection of scalar concentration fields in Eulerian models is avoided. Third, the Lagrangian formulation provides a clear separation between particle dynamics and microphysics: particle positions are governed by trajectory equations, while changes in particle properties are described by separate microphysical equations. In contrast, Eulerian approaches typically combine transport and microphysical source and sink terms within a single prognostic partial differential equation. This combined treatment can lead to numerical artifacts, such as artificial shock and rarefaction waves (Wacker and Seifert, 2001), or unphysical broadening of particle size distributions due to numerical diffusion (Morrison et al., 2018).

1.4 LCM box model

Among the approaches discussed in Sect. 1.3, box-model frameworks enable a detailed representation of microphysical processes at low computational cost, thereby facilitating extensive sensitivity studies. They are particularly suitable for scenarios in which ice crystal formation is dominated by entrained ambient aerosol particles (Sect. 1.3.1), as assumed for most H_2 combustion cases considered in this work. Based on these considerations, the box-model variant of the Lagrangian Cloud Module (LCM) is used to generate the data that form the basis for developing the parameterization of ice crystal number in H_2 combustion scenarios.

1.4 LCM box model

The LCM was initially introduced by Sölch and Kärcher (2010) and employs a particle-based approach. Two variants of LCM have been used in the past. The first is fully coupled to the fluid solver EULAG (Smolarkiewicz and Margolin, 1997, 1998; Smolarkiewicz et al., 2014). It has been used for studies of natural cirrus clouds (Sölch and Kärcher, 2011; Unterstrasser et al., 2017b) as well as contrails during both the vortex regime (Unterstrasser and Sölch, 2010; Unterstrasser, 2014) and the dispersion regime (Unterstrasser et al., 2017a). The second variant represents the box model implementation. This version has served as a tool to evaluate the numerical performance and convergence of particle-based algorithms for depositional growth and nucleation (Unterstrasser and Sölch, 2014) as well as collisional growth processes (Unterstrasser et al., 2017c, 2020).

More recently, Bier et al. (2022, 2024) extended the box-model variant to include the physics of contrail formation on both soot and ambient aerosol particles. For conventional kerosene combustion with ice crystal formation on soot particles, the LCM box model was compared to and validated against other models (Bier et al., 2022). The following sections summarize the version of the box-model framework employed in Bier et al. (2024) for simulations of contrails from H₂ combustion. This box-model version serves as the starting point for the present work and is used in all publications, with further extensions described in publications P2 and P4.

1.4.1 Initialization

The box model is initialized at the engine exit by specifying the corresponding conditions (exit area, exit temperature, exit jet speed). In addition, fuel/engine properties (water vapor emission index, combustion heat, fuel flow, overall efficiency of propulsion) and ambient conditions (temperature, pressure, relative humidity) are defined as input parameters.

The formation of soot and volatile particles is not explicitly modeled. Instead, size distributions for the different particle types are specified at initialization. The specific form of the size distribution is not fixed, but typically a lognormal distribution is used. The corresponding number density function in radius space is given by

$$n(r) = \frac{N}{\sqrt{2\pi}} \frac{1}{\ln(\sigma)} \frac{1}{r} \exp \left[-\frac{1}{2} \left(\frac{\ln(r/\bar{r})}{\ln(\sigma)} \right)^2 \right]. \quad (1.4)$$

Here, N denotes the total number, $\bar{r}$ the geometric mean radius, and σ the geometric width.

A SIP ensemble sampling the size distribution is generated following the algorithm described in Appendix A of Unterstrasser and Sölch (2014). Each SIP carries information such as its weight (i.e., the number of physical particles it represents), particle type, phase, radius, and the associated liquid or ice water mass.

As ambient aerosols are entrained over time, a single SIP ensemble cannot be specified at initialization. Instead, a new SIP ensemble is generated at each time step during the contrail formation process. Due to the continuous creation of SIPs, their number would rapidly increase. Therefore, a SIP merging algorithm, described in Appendix A of Bier et al. (2024), is applied.

1.4.2 Plume dilution

The evolution of plume dilution, which determines the increase in plume mass, is externally prescribed. The overall dilution can be expressed as

$$\begin{aligned}\mathcal{C}(t) &= \frac{\mathcal{C}_E + 1}{\mathcal{D}(t)} \\ &\approx \frac{\mathcal{C}_E}{\mathcal{D}(t)},\end{aligned}\tag{1.5}$$

where $\mathcal{C}_E$ is the air-to-fuel ratio and $\mathcal{D}$ is the dilution factor. The air-to-fuel ratio describes the mixture of ambient air and fuel mass at the engine exit and is given by

$$\mathcal{C}_E = \frac{Q(1 - \eta)}{c_p(T_E - T_a)}\tag{1.6}$$

with the engine exit temperature T_E . For kerosene combustion, air-to-fuel ratios are on the order of 50-70 (Kärcher et al., 2015). These ratios may be even higher for hydrogen combustion, as the mass-specific heat of combustion is larger by a factor of 2.79 (Table 1.1) and therefore less fuel is needed for the same amount of energy. These large values justify neglecting the fuel mass in the approximation made in Eq. (1.5). The value of the dilution factor $\mathcal{D}$ is one at the engine exit and gives the mass fraction of exhaust air in a plume parcel downstream of the engine. Hence, it is a monotonically decreasing function with time (downstream position).

From the evolution of $\mathcal{D}$, the entrainment rate

$$\omega(t) = -\frac{d \ln \mathcal{D}}{dt}\tag{1.7}$$

can be derived. Using ω , the evolution of the water vapor mass fraction χ_v and temperature T is governed by

$$\frac{d\chi_v}{dt} = -\omega(t)(\chi_v(t) - \chi_{v,a}) + S_{PH}(t)\tag{1.8a}$$

$$\frac{dT}{dt} = -\omega(t)(T(t) - T_a) + S_{LH}(t).\tag{1.8b}$$

Here, $\chi_{v,a}$ and T_a denote the ambient levels, while S_{PH} and S_{LH} represent source/sink terms due to phase transitions and the associated latent heat exchange. By using the same ω in both equations, the same diffusivity for mass and heat is assumed. This is justified by the fact that mixing is dominated by turbulence within a strong jet.

By relating

$$e_v = \frac{p_a}{\epsilon} \chi_v,\tag{1.9}$$

the partial pressure of water vapor e_v and temperature T evolve along the mixing line with slope G (Eq. (1.3)) in the absence of microphysical processes ($S_{PH} = S_{LH} = 0$). The entrainment rate ω specifies the speed of dilution.

Due to the increase in plume mass over time, the effective plume cross-sectional area increases from its value at the engine exit. The effective area is defined as

$$\hat{A}(t) = A(t) \frac{U_{\text{tot}}(t)}{U_\infty},\tag{1.10}$$

1.4 LCM box model

where A is the actual plume cross-sectional area and U_{tot} is the total jet speed, given by the sum of the aircraft speed U_{∞} and the excess jet speed U_{jet} relative to the ambient air. The effective area accounts for the axial divergence of the jet and is representative of the plume volume (see Sect. 3.2.2 in [Bier et al., 2024](#)). The increase in effective area over time is expressed as

$$\hat{A}(t) = \hat{A}_{\text{E}} \frac{T(t)}{T_{\text{E}} \mathcal{D}(t)} , \quad (1.11)$$

where $\hat{A}_{\text{E}}$ denotes the value at the engine exit, and the temperature ratio reflects density changes during plume dilution under isobaric mixing conditions.

The dilution state downstream of the engine also controls how many ambient aerosol particles are present in the plume. The number of entrained ambient aerosol particles per meter of flightpath is given by

$$N_{\text{aer}}(t) = n_{\text{aer}} \frac{T_{\text{a}} \hat{A}_{\text{E}}}{T_{\text{E}}} (\mathcal{D}^{-1}(t) - 1) \quad (1.12)$$

with the ambient aerosol number concentration n_{aer} .

Equations [\(1.5\)](#)–[\(1.12\)](#) can be understood as describing the average plume conditions (average trajectory approach). In this approach, the equations are evaluated using an average dilution factor $\bar{\mathcal{D}}$. Alternatively, the equations can also be applied to multiple trajectories, where each trajectory represents a fraction of the plume’s mass/volume (trajectory ensemble approach). The initial area $\hat{A}_{\text{E},k}$ of the k -th trajectory represents a portion of the total exit area $\hat{A}_{\text{E}}$, and the temporal evolution of the plume quantities is governed by the individual dilution factor $\mathcal{D}_k$. The box model is run separately for each trajectory, and the results of the sub-simulations are combined in the post-processing, where extensive quantities (e.g., ice crystal number) are summed and intensive quantities (e.g., plume temperature) are averaged in a mass-weighted manner (see Supplement of [Bier et al., 2022](#)).

1.4.3 Droplet activation and growth

The equilibrium saturation ratio over a spherical solution droplet is described by the Köhler curve ([Petters and Kreidenweis, 2007](#)), given by

$$S_{\text{K}} = a_{\text{wat}} \cdot \exp \left(\frac{2 \hat{\sigma} M_{\text{wat}}}{R T \rho_{\text{wat}} r_{\text{wet}}} \right) . \quad (1.13)$$

The first term is the water activity (solute effect) and the second term is the Kelvin term (curvature effect) with the surface tension of the solution droplet $\hat{\sigma}$, the molar mass of water M_{wat} , the universal gas constant R , the temperature T , the mass density of water ρ_{wat} , and the wet radius r_{wet} . In κ -Köhler theory ([Petters and Kreidenweis, 2007](#)), the water activity is expressed as

$$a_{\text{wat}} = \frac{r_{\text{wet}}^3 - r_{\text{d}}^3}{r_{\text{wet}}^3 - r_{\text{d}}^3(1 - \kappa)} \quad (1.14)$$

with the particle dry radius r_{d} and the hygroscopicity parameter κ , which is a measure of the ability of an aerosol particle to take up water. For aerosol particles that consist

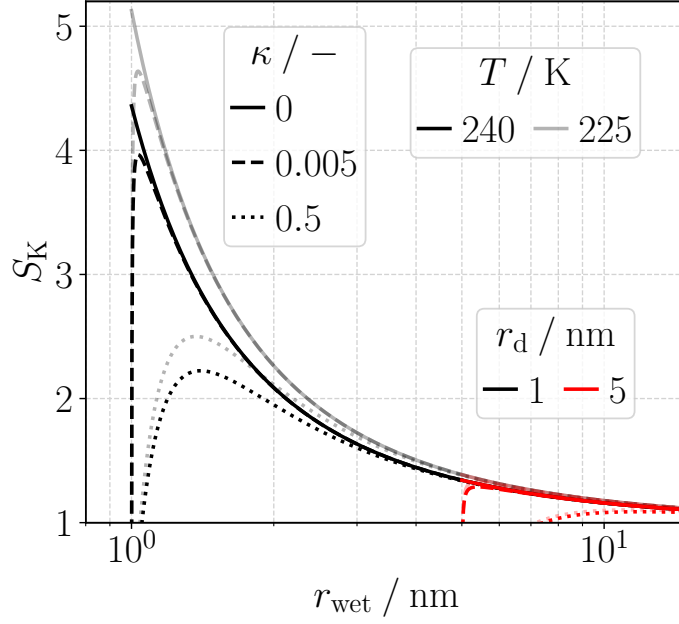


Figure 1.6: Equilibrium saturation ratio S_K over a droplet with wet radius r_{wet} according to κ -Köhler theory for different hygroscopicities κ (line style), two plume temperatures T (transparency) and dry radii r_d (color). Taken from publication [P4](#), licensed under CC BY 4.0.

of multiple components, an effective κ value is derived as a volume-weighted average across the individual species ([Petters and Kreidenweis, 2007](#)). For insoluble but wettable particles ($\kappa = 0$), the Köhler curve reduces to the Kelvin curve (Fig. [1.6](#)). Higher κ values lower the maximum of the Köhler curve.

When the plume saturation ratio starts to rise, hygroscopic water uptake of (partially) soluble aerosol particles occurs until the maximum of S_K is exceeded. Beyond the maximum, the solution droplet experiences a supersaturated environment and therefore can grow until the supersaturation is depleted. Thus, a particle is said to be activated into a liquid droplet when the plume saturation ratio has exceeded the maximum of S_K .

For spherical droplets, the single droplet mass growth equation is given by ([Kulmala, 1993](#))

$$\dot{m}_{\text{wat}} = \frac{4\pi r_{\text{wet}}(e_v - e_{K,\text{wat}})}{\frac{R_v T}{D_v} \beta_m^{-1} + \frac{e_{K,\text{wat}} L_c^2}{R_v K T^2} \beta_t^{-1}}. \quad (1.15)$$

Here, e_v is the actual water vapor pressure, and $e_{K,\text{wat}}$ is the product of the saturation vapor pressure over a flat water surface $e_{v,\text{sat},\text{wat}}$ and the equilibrium saturation ratio over a solution droplet surface S_K . R_v is the specific gas constant of water vapor, D_v the binary diffusion coefficient of air and water vapor, L_c is the specific latent heat for condensation/evaporation and K the conductivity of air. β_m and β_t are correction factors for non-continuum effects in mass and heat transfer, respectively, accounting for the transition between the continuum and free-molecular regimes ([Fuchs and Sutugin, 1971](#)).

1.5 Research questions

1.4.4 Homogeneous freezing and ice crystal growth

The homogeneous freezing temperature of supercooled solution droplets is calculated according to Appendix B in Bier et al. (2024) via

$$T_{\text{frz}} = T_{\text{frz},0}(V_{\text{wat}}, \dot{T}) - \Delta T(a_{\text{wat}}) . \quad (1.16)$$

The first term, $T_{\text{frz},0}$, represents the freezing temperature of a pure water droplet ($a_{\text{wat}} = 1$). It is parameterized following Kärcher et al. (2015) based on Riechers et al. (2013) and it varies with droplet water volume V_{wat} and cooling rate $\dot{T}$. The second term, $\Delta T(a_{\text{wat}})$, is a correction term based on O and Wood (2016) and accounts for the decrease in T_{frz} with decreasing water activity a_{wat} (e.g., Koop et al., 2000). Equation (1.16) is individually evaluated for each SIP. If the plume temperature falls below T_{frz} , all droplets represented by the SIP are assumed to freeze into ice crystals.

The mass change of a single ice crystal is given by (Mason, 1971)

$$\dot{m}_{\text{ice}} = \frac{4\pi C r_{\text{ice}} D_v \beta_v^{-1} (e_v - e_{\text{K,ice}})}{\frac{D_v \beta_v^{-1} L_d e_{\text{K,ice}}}{K \beta_k^{-1} T} \left(\frac{L_d}{R_v T} - 1 \right) + R_v T} . \quad (1.17)$$

Here, C is the shape factor, set to one under the assumption of spherical ice crystals, which are typically found in young contrails (Schröder et al., 2000). r_{ice} is the equivalent volume radius, and L_d the specific latent heat for deposition/sublimation. $e_{\text{K,ice}}$ is the product of the saturation vapor pressure over a flat ice surface $e_{v,\text{sat,ice}}$ and the Kelvin term for the assumed spherical ice crystal. β_v and β_k are transitional correction factors (Pruppacher and Klett, 1996).

1.5 Research questions

Building on the background information provided in Sects. 1.2–1.4, the overarching aim of this thesis –namely, to develop a parameterization for the number of ice crystals formed in H_2 combustion scenarios (Sect. 1.1.5)– can now be further specified by formulating guiding research questions.

For the development of the parameterization, the contrail is assumed to form in clear-sky conditions behind a turbofan engine, i.e., for combustion-based propulsion (Sect. 1.1.2). Furthermore, it is assumed that the exhaust from hydrogen combustion is initially particle-free and that HDN is negligible, such that ice crystals form exclusively on entrained ambient aerosol particles (Sect. 1.2.1). Under these assumptions, the simplified dynamical representation of a box model is considered appropriate (Sect. 1.3.1). As motivated in the introductory sentences of Sect. 1.4, the outcome of the LCM box model therefore serves as the basis for constructing the parameterization.

The assumption of particle-free exhaust and negligible HDN is critically discussed across the publications P1–P3. In addition, publication P4 explicitly deals with the potential role of lubrication oil particles in ice crystal formation. On this basis, the central research questions of this thesis are formulated as follows:

- *Q1: How do ambient conditions and the properties of ambient aerosol particles influence the microphysics of contrail ice crystal formation in hydrogen combustion scenarios?*

- *Q2: Which parameters related to aircraft engines significantly influence the ice crystal formation process in hydrogen combustion scenarios?*
- *Q3: How can the large simulation database created to address Q1 and Q2, together with the gained physical understanding, be condensed into a parameterization of ice crystal number for hydrogen combustion?*
- *Q4: In which scenarios would lubrication oil particles dominate ice crystal formation?*

Chapter 2

Summary of specific results and conclusions

Each of the four central research questions [Q1](#)–[Q4](#) is addressed in one of the publications [P1](#)–[P4](#). This chapter summarizes the content, main results, and conclusions of each publication. A few (simplified) key figures are presented. More detailed descriptions, methodological information, and supporting figures and tables are available in the respective publications. For orientation, references to the publications are given in the form $\{Px \text{ Sect. } y\}$, where x denotes the publication number and y the section number.

2.1 Microphysical aspects

Research question [Q1](#) is addressed in publication [P1](#), which builds upon and extends the work presented in [Bier et al. \(2024\)](#). The LCM box model is used to perform a large set of simulations covering a wide range of atmospheric conditions and aerosol properties, allowing for a systematic exploration of how ice crystal formation depends on these variables. Several additional aspects are investigated that were not considered in the earlier study.

Among these is an assessment of the role of coarse-mode particles (diameter $\gtrsim 1 \mu\text{m}$) $\{P1 \text{ Sect. } 3.1.1\}$. These particles are found to have neither a direct nor an indirect effect on the ice crystal number, owing to their typically much lower number concentrations compared to coexisting nucleation-mode ($\lesssim 20 \text{ nm}$), Aitken-mode ($\sim 20\text{--}100 \text{ nm}$), or accumulation-mode ($\sim 100\text{--}1000 \text{ nm}$) particles. Consequently, coarse-mode particles can be safely neglected in a parameterization of ice crystal number.

Furthermore, it is shown that the number of ice crystals formed in the presence of multiple coexisting aerosol populations can be accurately approximated by a weighted-mean approach based on single-population simulations $\{P1 \text{ Sect. } 3.1.2\}$ (Fig. [2.1](#)). Here, each aerosol population represents a set of particles characterized by a monomodal size distribution and a given hygroscopicity. The weighted-mean approach is expressed as

$$\hat{N}_{\text{ice,f}} = \sum_i \frac{n_{\text{aer},i}}{n_{\text{aer,tot}}} N_{\text{ice,f},i}(n_{\text{aer,tot}}) , \quad (2.1)$$

where $\hat{N}_{\text{ice,f}}$ denotes the approximated total ice crystal number and $N_{\text{ice,f},i}(n_{\text{aer,tot}})$ the

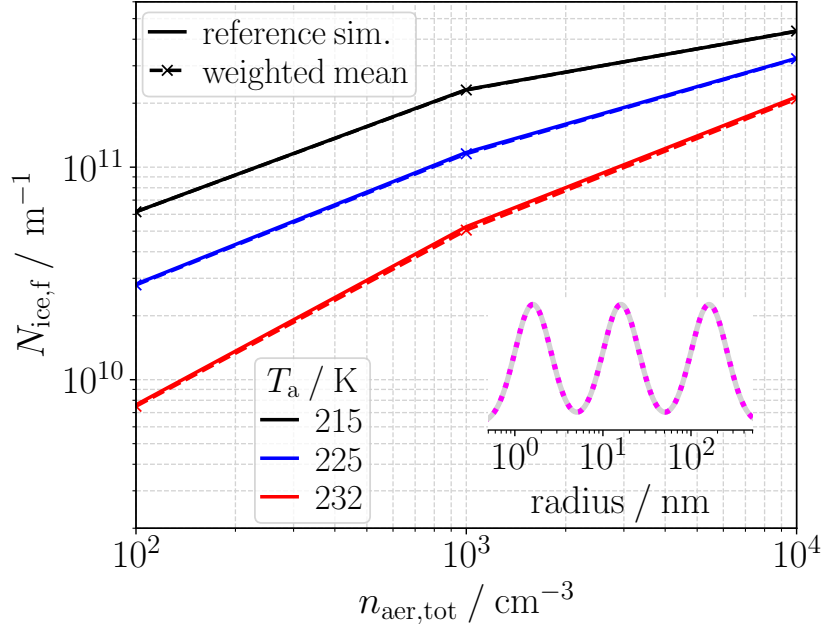


Figure 2.1: Weighted-mean approach for six ambient aerosol populations. Displayed is the final number of ice crystals formed $N_{\text{ice},f}$ as a function of total aerosol number concentration $n_{\text{aer,tot}}$ for different ambient temperatures T_a . The six populations comprise three geometric mean radii $\bar{r}_{\text{d,aer}} = \{2, 20, 200\}$ nm each combined with two hygroscopicities $\kappa_{\text{aer}} = \{0.05, 0.5\}$ (illustrated by the inset; the solid grey and the dotted magenta lines indicate the two hygroscopicities). Each population is assumed to contribute one sixth to the total aerosol number concentration. Reference simulations including all six aerosol populations in a single simulation (solid lines) are compared to the weighted-mean approach according to Eq. (2.1) (dashed lines with markers). Taken from publication [P1], licensed under CC BY 4.0.

number of ice crystals formed on population i in single-population simulations assuming the total aerosol number concentration $n_{\text{aer,tot}}$ of all populations instead of the actual concentration $n_{\text{aer},i}$. Due to the success of the weighted-mean approach, ice crystal formation only needs to be parameterized as a function of the properties of a single aerosol population. The effects of multiple coexisting aerosol populations are then captured through weighted combinations of single-population results. This reduces the dimensionality of the parameter space and avoids the curse of dimensionality (Bellman, 1957) without loss of generality.

In addition, a conservative offline estimate suggests that homogeneous droplet nucleation (HDN) may become relevant only at very low ambient temperatures ($T_a \lesssim 210$ K) {P1 Sect. 3.2}. At higher temperatures, this process can safely be neglected.

Finally, a database of more than 20,000 simulations provides a systematic coverage of the parameter space {P1 Sect. 3.3}. Across the parameter space investigated, ambient temperature and aerosol number concentration emerge as the dominant controlling factors for the ice crystal number. Moreover, for the subspace defined by $T_a \leq 225$ K and $10 \text{ nm} \leq \bar{r}_{\text{d,aer}} \leq 100 \text{ nm}$, the number of ice crystals formed becomes nearly independent of ambient relative humidity as well as size and hygroscopicity of the ambient aerosol

2.2 Engine-related aspects

particles. This finding enables the development of a parameterization with reduced complexity in this sub-regime (Sect. 2.3).

2.2 Engine-related aspects

Research question Q2 is investigated in publication P2, which extends the focus beyond microphysical processes to include the role of engine-related parameters. A theoretical framework is developed to describe how these parameters influence the engine exit conditions and the thermodynamic evolution of the exhaust plume. This framework is incorporated into the LCM box model. Simulations are then performed to identify which engine-related parameters significantly influence ice crystal formation in hydrogen combustion scenarios.

Building on classical thermodynamic theory {P2 Sect. 2.1} (see also Sects. 1.2.2 and 1.4.2), the study examines how variations in overall efficiency of propulsion {P2 Sect. 2.2}, ambient conditions, engine size, and exit jet speed {P2 Sect. 2.3} shape engine exit conditions and dilution speed. Furthermore, a framework is presented that extends beyond classical thermodynamic theory {P2 Sect. 2.4}. Turbofan engines generate thrust through both a core flow, where combustion occurs, and a bypass flow ducted around the core. While excess water vapor above ambient levels is confined to the core, excess total enthalpy (static enthalpy plus kinetic energy) is found in both streams. Consequently, water vapor and enthalpy have different distributions at the engine exit. In contrast to classical assumptions of well-mixed core and bypass flows and complete kinetic energy dissipation at the onset of contrail formation, the framework explicitly treats kinetic energy dissipation and the entrainment of total enthalpy from the bypass into the core plume.

The theoretical considerations are neither limited to a specific fuel type nor dependent on microphysical processes, i.e., they do not rely on the nature of the ice-forming particles. In P2, their impact on ice crystal formation is, however, examined exclusively for hydrogen combustion with contrail formation on entrained ambient aerosol particles. The box model is set up accordingly, incorporating dilution data from several independent CFD simulations of different engine configurations {P2 Sect. 3}.

Sensitivity simulations show that changes in engine exit conditions and dilution speed arising from variations in ambient temperature have a negligible impact on the number of ice crystals formed {P2 Sect. 4.1}. Therefore, these effects can be safely disregarded in a parameterization.

Furthermore, deviations in overall efficiency of propulsion η from a reference value η^* can be represented by a scaling relation that expresses the sensitivity of $N_{\text{ice,f}}$ to η through its dependence on the ambient pressure p_a {P2 Sect. 4.2}. Specifically, prescribing p_a and η yields a similar ice crystal number as using the reference overall efficiency η^* while adjusting the pressure according to

$$p_{a,\text{adj}} = p_a \frac{1 - \eta^*}{1 - \eta} . \quad (2.2)$$

As a consequence, the central part of the parameterization only needs to represent the dependence of $N_{\text{ice,f}}$ on ambient pressure, while variations in η can be accounted for through the pressure adjustment.

2. Summary of specific results and conclusions

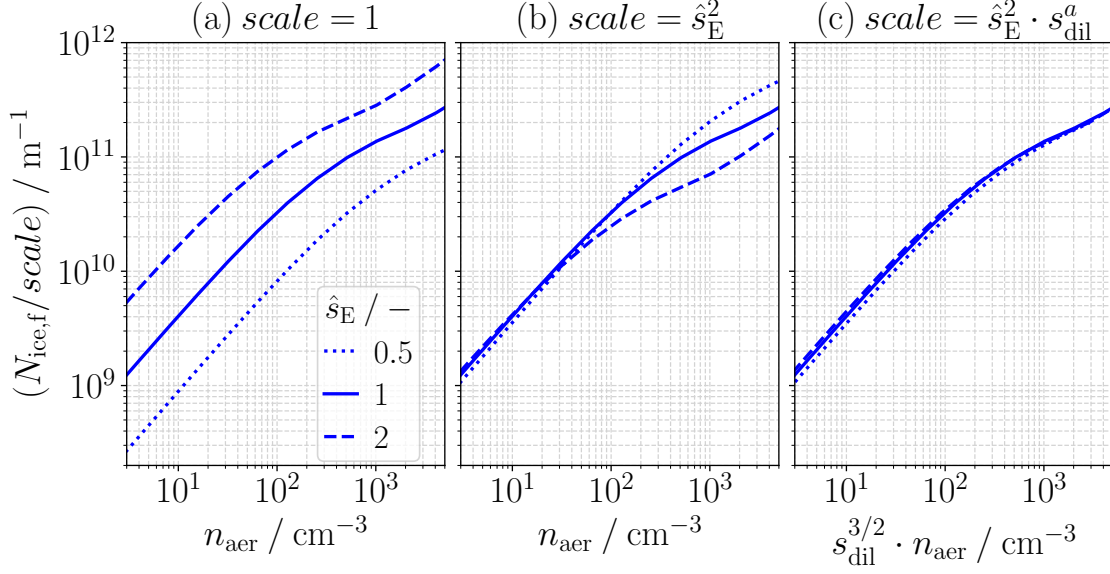


Figure 2.2: Final number of ice crystals formed $N_{\text{ice},f}$ for scenarios in which the engine exit radius is scaled by $\hat{s}_E$ (different line styles). Shown are (scaled) $N_{\text{ice},f}$ values as a function of (scaled) aerosol number concentration n_{aer} at the ambient temperature $T_a = 225$ K. (a) Unscaled data. (b) Normalization by the scale of the effective exit area. (c) Scaling according to Eq. (2.3) with $s_{\text{dil}} = \hat{s}_E$.

An additional scaling is proposed to account for changes in engine size and exit jet speed $\{P2 \text{ Sects. 4.3 and 4.4}\}$. It is expressed as

$$\frac{N_{\text{ice},f}}{\hat{s}_E^2 \cdot s_{\text{dil}}^a} \sim f\left(s_{\text{dil}}^{3/2} \cdot n_{\text{aer}}\right) . \quad (2.3)$$

Here, $\hat{s}_E$ is a geometric scaling factor, such that $\hat{s}_E^2$ represents the scaling of the effective exit area relative to a reference configuration. The factor s_{dil} accounts for variations in dilution speed associated with changes in engine size or exit jet speed. The exponent a is temperature-dependent. The function f depends on ambient conditions and aerosol properties, but not explicitly on engine size or exit jet speed.

Normalizing the ice crystal number only by the scale of the effective exit area shows that dilution speed influences $N_{\text{ice},f}$ (Fig. 2.2b). When the full scaling according to Eq. (2.3) is applied, the curves corresponding to different engine sizes collapse (Fig. 2.2c). This demonstrates that scenarios with different engine sizes or exit jet speeds can be scaled to each other. Consequently, the central part of the parameterization only needs to represent ice crystal formation for a reference engine configuration, while deviations can be accounted for using Eq. (2.3).

The explicit treatment of kinetic energy dissipation and the entrainment of enthalpy initially contained in the bypass flow is found to have a negligible impact on the final number of ice crystals formed on entrained ambient aerosol particles $\{P2 \text{ Sect. 4.5}\}$. This result can be explained by the continuous entrainment of these aerosol particles: by the time enough particles have been entrained and activated to substantially deplete the available water vapor, core and bypass flows are already well mixed and most kinetic

2.3 Neural-network-based parameterization of ice crystal number

energy has dissipated into heat. Consequently, the classical thermodynamic theory of contrail formation is sufficient when ice crystals form on entrained ambient aerosol particles, and the parameterization does not require additional variables representing kinetic energy or bypass effects.

The implications of the outlined findings are discussed in the context of existing literature {P2 Sect. 5}. In particular, emphasis is placed on identifying which conclusions are specific to contrail formation on entrained ambient aerosol particles and on how the results may differ when emitted particles (e.g., as in kerosene combustion) contribute to ice crystal formation –an aspect that is also highlighted in the concluding section {P2 Sect. 6}.

2.3 Neural-network-based parameterization of ice crystal number

Publication P3 addresses research question Q3 by synthesizing insights gained in P1 and P2 into a final parameterization of ice crystal number. To this end, a neural-network-based approach is developed that emulates the output of the underlying box-model simulations. The development is based on a comprehensive training dataset comprising more than 20,000 simulations introduced in P1, complemented by an independent verification dataset of more than 5,000 additional simulations {P3 Sect. 2.1}.

To represent ice crystal formation across different physical regimes, three shallow neural networks are trained {P3 Sect. 2.2}. A first regression model, termed *FullNet*, is trained on the full training dataset, where the simulated ice crystal number satisfies $N_{\text{ice},f} > 0$ {P3 Sect. 2.2.1}. This model can be applied across the entire parameter space covered by the training data.

Given that the ice crystal number becomes nearly independent of relative humidity as well as aerosol particle size and hygroscopicity within the subspace defined by $T_a \leq 225 \text{ K}$ and $10 \text{ nm} \leq \bar{r}_{d,\text{aer}} \leq 100 \text{ nm}$ (Sect. 2.1), a second regression model, termed *ReducedNet*, is introduced. It is trained for this regime and uses a reduced set of input variables. Owing to its reduced complexity and network size, ReducedNet serves as a lightweight alternative to FullNet within this regime.

At high ambient temperatures ($T_a > 230 \text{ K}$), aerosol particles may activate into liquid droplets without subsequently freezing. If droplets do not freeze, they will evaporate shortly after their formation (Sect. 1.2.2). To account for this binary behavior, a dedicated classification model, termed *ClassificationNet*, is trained to predict whether or not ice crystal formation occurs {P3 Sect. 2.2.2}.

For the regression models, the error distributions obtained for the training and verification datasets are in close agreement, indicating that the models generalize well without significant overfitting {P3 Sect. 3.1}. Median relative errors of parameterized ice crystal numbers relative to box model-simulated values are below 10 %. For the ClassificationNet, both false-negative and false-positive rates remain below 2 %. Upper-tropospheric profiles comparing parameterized and simulated ice crystal numbers additionally confirm the consistency between the neural-network-based parameterization and the underlying box-model simulations {P3 Sect. 3.2}.

The neural networks provide the ice crystal number for a single aerosol population and

2. Summary of specific results and conclusions

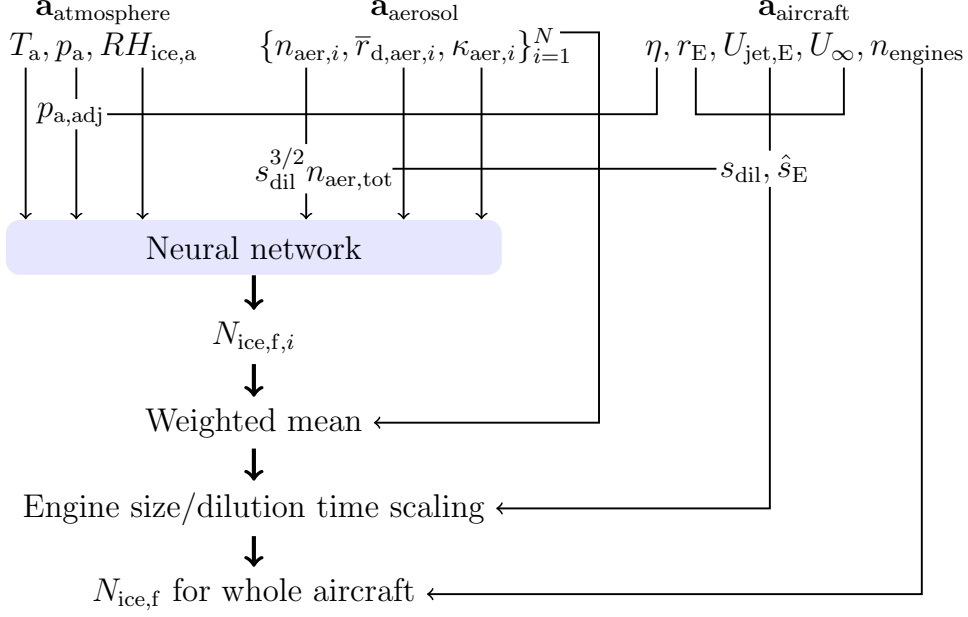


Figure 2.3: Schematic overview of how various variables enter the parameterization of $N_{ice,f}$. In the core, the neural-network-based approach returns $N_{ice,f,i}$ for a single aerosol population and a reference engine. The dependence on the overall efficiency of propulsion is accounted for by adjusting the ambient pressure according to Eq. (2.2). On top of the neural network, the weighted-mean approach (Eq. (2.1)) accounts for multiple coexisting aerosol populations. By suitable scaling (Eq. (2.3)), the parameterization incorporates the effects of deviations in engine size and jet speed from the reference engine, with associated changes in dilution speed. See text for a description of variable names.

reference engine (Fig. 2.3). The parameterization is generalized {P3 Sect. 3.3} by incorporating several scaling relations derived in P1 and P2 (Eqs. (2.1), (2.2), and (2.3)). A practical guide on how to apply the final parameterization is provided {P3 Appendix A}. Taken together, the final functional relationship can be expressed as {P3 Sect. 5}

$$\begin{aligned}
 N_{ice,f} &= N_{ice,f}(\mathbf{a}_{atmosphere}, \mathbf{a}_{aerosol}, \mathbf{a}_{aircraft}) \\
 &= N_{ice,f}(T_a, p_a, RH_{ice,a}, \{n_{aer,i}, \bar{r}_{d,aer,i}, \kappa_{aer,i}\}_{i=1}^N, \eta, r_E, U_{jet,E}, U_\infty, n_{engines}) \quad (2.4) \\
 &\approx N_{ice,f}(T_a, p_a, RH_{ice,a}, \{n_{aer,i}, \bar{r}_{d,aer,i}, \kappa_{aer,i}\}_{i=1}^N, \eta, m_{C,tot}, n_{engines}) .
 \end{aligned}$$

It incorporates input variables characterizing the background atmosphere, **a_{atmosphere}** (ambient temperature T_a , pressure p_a , and relative humidity over ice $RH_{ice,a}$). Furthermore, it includes properties **a_{aerosol}** of multiple aerosol populations i (number concentration $n_{aer,i}$, geometric mean radius $\bar{r}_{d,aer,i}$, and hygroscopicity $\kappa_{aer,i}$). Finally, it contains aircraft-related parameters **a_{aircraft}** (overall efficiency of propulsion η , engine core exit radius r_E , core exit excess jet speed $U_{jet,E}$, aircraft speed U_∞ , and number of engines $n_{engines}$). If information on engine size and jet speed is unavailable, an approximation based on the total fuel consumption of the aircraft, $m_{C,tot}$, can be applied.

The newly developed parameterization is compared with the analytical model of Kärcher et al. (2015) {P3 Sect. 4.1}. The latter model was originally developed for

2.4 Potential role of lubrication oil particles

soot-rich kerosene combustion conditions and was not designed for application to hydrogen combustion scenarios. However, it has recently been adapted and applied to such scenarios (Pettersson et al., 2025). The comparison demonstrates that a database of time-resolved simulations is essential for realistically capturing the full ice crystal formation process on entrained ambient aerosol particles. It is therefore not recommended to apply the parameterization of Kärcher et al. (2015) to scenarios where ice crystal formation is dominated by ambient aerosol particles. As highlighted by the comparison, the reliance of the developed parameterization on a comprehensive database of time-resolved simulations is a key strength {P3 Sect. 4.2} (see also Sect. 3.1).

2.4 Potential role of lubrication oil particles

Publication P4 questions the main assumption of the developed parameterization that ambient aerosol particles are the sole precursors of ice crystals in hydrogen combustion scenarios. Under this assumption, ice crystal numbers are typically reduced by a factor of 10–100 compared to conventional kerosene cases (Bier et al., 2024; P1; P2). Challenging this assumption, publication P4 extends the box model to include lubrication oil particles and explores a broad set of scenarios with different numbers and sizes of these particles, for which the impact on ice crystal formation is analyzed. Scenarios are investigated for both hydrogen and kerosene combustion, including cases where soot emissions are strongly reduced compared to present-day values.

The study is motivated by ground-based measurements behind dedicated engines as well as laboratory experiments that point to lubrication oil as a potential source of volatile particles in exhaust plumes {P4 Sect. 1} (see also Sect. 1.2.1). A simple conceptual framework is introduced to relate the emitted oil volume rate to the resulting oil particle number, assuming that a fraction of the oil evaporates in hot exhaust regions and subsequently renucleates to form a population of small particles {P4 Sect. 2.1}. The analysis shows that even tiny amounts of oil (a few milliliters per hour or even less) can produce particle numbers comparable to or even exceeding present-day soot levels when the newly formed particles are only a few nanometers in size. For comparison, typical oil emissions from the venting system are on the order of a few hundred milliliters per hour (Linke-Diesinger, 2010; Decker et al., 2024), depending on engine type and thrust setting.

A hierarchy of scenarios with increasing complexity is investigated {P4 Sect. 3}. The analysis begins with idealized simulations that include only oil particles {P4 Sect. 3.1}. Although such conditions are unlikely to occur in reality, they help to isolate the activation behavior of oil particles and provide a reference for interpreting more realistic cases. Additional particle types are then introduced that compete with the oil particles for the available water vapor {P4 Sect. 3.2}. Soot particles are considered for kerosene combustion cases and ambient aerosols are incorporated for hydrogen combustion cases. In a final set of scenarios, volatile particles that mainly originate from combustion products are added as a third type {P4 Sect. 3.3}. For hydrogen combustion, these represent scenarios where nitric acid could contribute to volatile particle formation.

The many scenarios explored demonstrate that the properties (number, size, and hygroscopicity) of each particle type involved ultimately determine which type signif-

2. Summary of specific results and conclusions

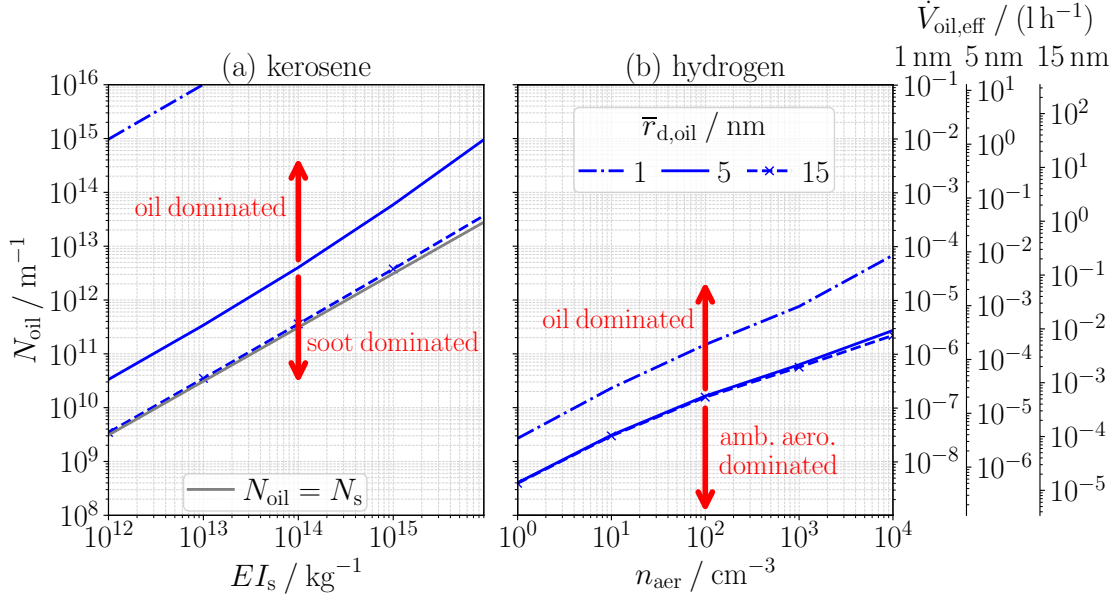


Figure 2.4: Transition curves where both particle types contribute equally to the number of ice crystals for (a) oil and soot particles for kerosene combustion and (b) oil particles and ambient aerosols for hydrogen combustion at the ambient temperature $T_a = 225 \text{ K}$. For a given geometric mean dry radius $\bar{r}_{\text{d,oil}}$ (indicated by the line style), each line separates an oil-particle-dominated regime from a (a) soot- or (b) ambient-aerosol-dominated regime. The transition is illustrated for $\bar{r}_{\text{d,oil}} = 5 \text{ nm}$ at (a) a soot emission index $EI_s = 10^{14} \text{ kg}^{-1}$ and (b) an ambient aerosol number concentration $n_{\text{aer}} = 10^2 \text{ cm}^{-3}$. The grey line in (a) indicates where the emitted oil particle number equals the number of emitted soot particles. The additional y-axes show the amount of oil $\dot{V}_{\text{oil,eff}}$ required to yield N_{oil} particles per meter of flight path that are log-normally distributed with specified $\bar{r}_{\text{d,oil}}$ and $\sigma_{\text{oil}} = 1.6$.

icantly contributes to ice crystal formation. As a consequence, the resulting picture is complex, and measurements at cruise altitude are necessary to determine which of the presented scenarios are representative under soot-poor and hydrogen combustion conditions.

Despite this complexity, a clear message emerges *{P4 Sects. 4 and 5}*: in soot-poor kerosene cases or in hydrogen cases, many scenarios point to oil-dominated ice crystal formation, with ice crystal numbers comparable to or exceeding present-day values in soot-rich scenarios. Remarkably, only tiny amounts of oil may be sufficient to produce oil-dominated ice crystal formation (Fig. 2.4). Such conditions are expected to arise when the venting system releases oil close to the hot core exit, allowing entrainment into high-temperature regions that promote evaporation and renucleation. If the venting is located far away from the hot zones, the emitted oil may be entrained into the plume only when it has already cooled down, preventing the oil from evaporating. The oil particles are then expected to be large in size (hundreds of nanometers) and correspondingly low in number. A careful consideration of the placement of the venting system is therefore essential. Otherwise, the 10–100-fold reduction in ice crystal number for hydrogen combustion becomes unlikely.

Chapter 3

Overarching conclusions and outlook

A simulation-based parameterization has been developed that provides the number of contrail ice crystals formed in the exhaust plume of engines burning hydrogen. Such a parameterization is essential for the initialization of large-scale models that estimate the radiative forcing of contrails from a possible future fleet of hydrogen-powered aircraft. This chapter summarizes the overarching conclusions of the developed framework by outlining its key strengths and limitations (Sect. 3.1), followed by an outlook on ongoing research and future perspectives (Sect. 3.2).

3.1 Strengths and limitations of the developed parameterization

The parameterization builds directly on time-resolved contrail formation simulations performed with the LCM box model, which incorporates detailed microphysics. The underlying physical processes influencing ice crystal formation, in particular the roles of ambient conditions, ambient aerosol properties, and engine-related parameters, have been examined comprehensively in P1 and P2 (addressing research questions Q1 and Q2). In P3, this physical understanding and the resulting large simulation database have been condensed into a neural-network-based parameterization of ice crystal number (thus answering research question Q3). Shallow neural networks serve solely as fitting functions for the simulation outputs, with median relative errors below 10 %. Apart from this fitting error, the parameterization faithfully reproduces the time-resolved model results and introduces no further assumptions beyond those made in the LCM box model itself. In combination with the derived scaling relations, the neural networks provide a generalized framework that captures the (nonlinear) dependence of the ice crystal number on multiple variables. Owing to their shallow architecture, the networks require only a short sequence of arithmetic operations {P3 Sect. 2.2}, yet they are sufficiently flexible to represent the underlying nonlinearities.

The networks are trained on a systematically constructed simulation database without weighting the data according to the joint probability distribution of ambient conditions, aerosol properties, and air-traffic patterns. This design choice ensures that

the parameterization remains broadly applicable, enabling its use across a wide range of potential future scenarios. In this way, it accommodates uncertainties in climate projections, future ambient aerosol loading, and the evolution of air traffic.

The simple architecture of the shallow neural networks greatly facilitates their implementation in large-scale models. In contrast to multidimensional lookup tables, which require significantly more storage and also interpolation between tabulated values, the neural-network approach provides a compact and efficient means of integrating detailed box-model results into global models.

The parameterization has already been implemented in ECHAM-CCMod by C. Weiß-Rehm and U. Burkhardt, with first applications suggesting that the estimated contrail radiative forcing for hydrogen combustion scenarios differs substantially from that for conventional kerosene combustion (further details will be presented in the PhD thesis by C. Weiß-Rehm). During this implementation process, it became clear that the neural-network framework can be updated with little effort. Once an appropriate simulation database is available, retraining the neural networks takes only a few minutes on a local machine. Updating the neural networks in large-scale models is equally straightforward and requires nothing more than replacing the weight matrices.

Concerning the limitations, the current parameterization relies exclusively on a single model. Although the LCM box model has been compared with other models for conventional kerosene combustion (Bier et al., 2022), corresponding studies for H₂ combustion are largely absent. To the author’s knowledge, apart from the approach by Pettersson et al. (2025), no other publications on contrail formation from H₂ combustion are currently available. This scarcity of independent work introduces a clear validation gap. Physical parameterizations within the box model that become particularly important for H₂ combustion therefore represent a notable source of uncertainty.

An example is the treatment of homogeneous freezing of supercooled droplets. The employed parameterization (Sect. 1.4.4) is based on laboratory experiments conducted under conditions typical of natural cirrus formation, which are characterized by lower turbulence and smaller cooling rates than those present in aircraft exhaust plumes. Its applicability to contrail formation therefore remains uncertain. Measurements at temperatures where our simulations suggest a strong influence of homogeneous freezing (ambient temperatures $\gtrsim 230$ K) would be particularly valuable for validation. In the first demonstrator in situ flight experiment (see Sect. 3.2), however, contrail measurements were conducted only below 230 K.

Another key source of uncertainty concerns the potential role of volatile particles (Sects. 1.2.1 and 2.4). Although P4 addresses research question Q4 by identifying a range of scenarios in which lubrication oil particles may dominate ice crystal formation, it remains unclear which of these scenarios are representative at cruise conditions. Accordingly, the contribution of particles originating from lubrication oil or from NO_x emissions to ice crystal formation remains poorly constrained.

3.2 Ongoing research and future perspectives

A key task for future studies is therefore to better characterize the entrainment of lubrication oil into the hot exhaust sections, as well as its evaporation and renucleation

3.2 Ongoing research and future perspectives

at cruise conditions. If additional model studies or measurements indicate that the impact of oil is unavoidable, the parameterization needs to be updated accordingly. This may be the case for engine configurations in which locating the venting system sufficiently far from the hot core flow is not technically feasible. The scenarios explored in [P4](#) therefore need to be constrained through representative in situ measurements, and improved knowledge is required on how the impact varies across different engine types.

A second area requiring further investigation concerns the particle formation from nitric acid. An update of the parameterization will be necessary if model results or measurements show that nitric acid can efficiently nucleate new particles even in the absence of sulfuric acid (Sect. [1.2.1](#)). This formation pathway is currently being investigated by a French research team at ONERA within the EU project [HYDEA](#) ([2023](#)).

Another open point is to refine the estimate of the importance of HDN in the H_2 combustion case. HDN has recently been implemented into the box model in a parallel PhD project on H_2 fuel-cell systems by D. Hillenbrand. As a next step, the extended model should be applied to the low-temperature cases for which the offline estimate [{P1 Sect. 3.2}](#) suggests a potential relevance of HDN. Such simulations would clarify whether HDN actually plays a role under these conditions.

In December 2024, the first demonstrator experiment for H_2 combustion took place ([Blue Condor](#)). In this campaign, a glider was equipped with a small turbojet engine (an engine with only a core flow and no bypass) operated on hydrogen. In-flight emission and contrail measurements were performed by a chaser aircraft carrying dedicated instrumentation. For direct comparison, a second glider equipped with an identically sized turbojet engine but operating on kerosene was flown in parallel.

The campaign was supported during the conception and execution phases by simulations and theoretical expertise. Owing to the characteristics of the demonstrator engine, the dilution behavior as well as the thermodynamic criteria for contrail formation (Sect. [1.2.2](#)) differ from those expected for larger engines. Therefore, the LCM box model was adapted to the specific experimental setup by incorporating dedicated dilution data and adjusting the initial conditions accordingly.

Currently, the measurements and model simulations are being compared, and the results will be published in a dedicated scientific paper. The comparison also examines to what extent the measurements obtained for the demonstrator engine can be scaled to larger engines expected for future hydrogen-powered aircraft. In this context, the theoretical understanding developed in publication [P2](#) provides valuable guidance.

In addition to the measurement results obtained during the Blue Condor campaign, a further future opportunity for validating the H_2 contrail formation simulations is offered by the project [KlimaRAT](#) ([2025](#)). Within this project, the controlled generation of contrails in a wind tunnel operated at pressure and temperature conditions representative of cruise altitude is foreseen. Experimental setups are planned that reflect boundary conditions relevant to hydrogen combustion.

Building on the experience gained from developing the parameterization for H_2 combustion, a future perspective is to create an analogous parameterization for sustainable aviation fuels (SAFs), which are likely to be adopted earlier than hydrogen combustion in commercial aviation ([Airbus](#)). SAFs are produced from renewable feedstocks such as waste oils, biomass, agricultural residues, municipal solid waste, or captured carbon

3. Overarching conclusions and outlook

combined with green hydrogen. They can be used in today’s aircraft with minimal modifications and could therefore serve as a near-term alternative to conventional jet fuel. Their lower aromatic content typically reduces soot number emissions (Moore et al., 2017; Bräuer et al., 2021; Voigt et al., 2021; Märkl et al., 2024). However, model results (Kärcher and Yu, 2009; Yu et al., 2024) and measurements (Dischl et al., 2025) show that volatile particles also contribute to ice crystal formation in soot-poor regimes, with the volatile particle number strongly depending on the fuel’s sulfur content. This contribution of volatile particles is currently not included in the contrail initialization of ECHAM-CCMod.

Since the workflow for training neural networks and integrating the resulting parameterizations into ECHAM-CCMod is established (Sect. 3.1), the main task is to generate a suitable database of contrail formation simulations for SAFs. This includes revisiting how volatile particles are treated in the LCM box model, which currently uses a prescribed size distribution at initialization (Sect. 1.4.1). A more complete approach would explicitly model their formation (e.g., Yu et al., 2024).

Moreover, when volatile particles contribute to ice crystal formation, engine-related aspects should be re-examined to determine which conclusions and scaling relations derived for contrail formation on entrained ambient aerosols remain valid (revisiting research question Q2). However, a simplified 0D box model may not sufficiently cover all relevant dynamical aspects at high volatile particle numbers (Sect. 1.3.1). A promising alternative is the 1D RadMod framework (Lottermoser and Unterstrasser, 2024), which is currently coupled to LCM by W. F. Thi. This model accounts for radial plume heterogeneity with online microphysics and is still expected to have a relatively low computational cost. Ultimately, the most realistic representation would come from LES. Therefore, coupling the contrail formation microphysics of LCM to EULAG or another LES code could be another future direction. While LES is not suited for running a large number of simulations, it could deliver valuable benchmark cases for RadMod.

Another important avenue for future research is to move beyond the implicit assumption in the simulation setup that contrails form in clear-sky conditions (Sect. 1.5). Recent work by Petzold et al. (2025) suggests that most contrails actually develop within pre-existing natural cirrus. Contrail formation embedded in existing cirrus remains largely unexplored, and its long-lasting influence on the microphysical and radiative properties of the natural clouds is unclear. Understanding these interactions will be essential for assessing potential differences across fuel types (conventional kerosene, SAF, H₂).

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P1. Contrail formation for aircraft with hydrogen combustion - Part 1: A systematic microphysical investigation



Contrail formation for aircraft with hydrogen combustion – Part 1: A systematic microphysical investigation

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Abstract. The number of ice crystals formed during the contrail's jet phase has a long-lasting impact on the life cycle and radiative forcing of contrail cirrus clouds. For conventional kerosene combustion, suitable parameterizations for early ice crystal number have been developed and employed in general circulation models that are used to estimate the climate impact of contrail cirrus. However, a parameterization for the number of ice crystals formed is lacking for hydrogen combustion. To develop such a parameterization, we present a comprehensive set of contrail formation simulations using the particle-based Lagrangian Cloud Module in a box model approach. Unlike kerosene combustion, no soot particles are emitted. Thus, ice crystals are assumed to form on ambient aerosols entrained into the exhaust plume. The total number of entrained particles primarily governs the nonlinear depletion of water vapor. Consequently, the impact of coarse-mode particles is negligible due to their low abundance. Additionally, ice crystal formation from multiple aerosol populations can be reconstructed from single-population simulations using population-specific properties (size and hygroscopicity) and the total number concentration. We also identify atmospheric conditions where homogeneous droplet nucleation can be safely neglected as potential ice formation pathway. Based on more than 20 000 simulations covering a broad range of atmospheric conditions and aerosol properties, we identify a regime where ice crystal formation becomes nearly independent of ambient relative humidity, aerosol size, and hygroscopicity. Our results provide a basis for a data-driven parameterization of ice crystal number in contrails from hydrogen combustion, to be presented in a companion paper.

1 Introduction

1.1 Motivation

A hydrogen economy envisions the widespread use of hydrogen as a clean energy carrier, replacing fossil fuels in sectors such as transportation, industry, and power generation (Staffell et al., 2019). The successful implementation of a hydrogen economy requires large-scale infrastructure for hydrogen production, storage, distribution, and end-use technologies such as fuel cells or gas turbines (Tashie-Lewis and Nnabuike, 2021). Hydrogen produced via electrolysis using renewable energy (commonly referred to as green hydrogen) is free of carbon emissions during its production (Dincer and Acar, 2015; Nikolaidis and Poullikkas, 2017; Ajanovic et al., 2022). Furthermore, hydrogen used in gas turbines or fuel-

cell systems produces no direct greenhouse gas emissions except water vapor.

Despite its potential to have net-zero greenhouse gas emissions, the use of hydrogen is not without environmental concerns. One of the risks involves hydrogen leakage, which can indirectly contribute to global warming by extending the atmospheric lifetime of methane and increasing tropospheric ozone and stratospheric water vapor levels (Ocko and Hamburg, 2022; Hauglustaine et al., 2022; Warwick et al., 2023).

Two concepts are being explored for a potential future use of hydrogen in aviation (Tiwari et al., 2024; Soleymani et al., 2024; Richardson, 2025). One is hydrogen fuel-cell propulsion, where the fuel's chemical energy is converted into electricity that drives propeller-based systems. The other is direct hydrogen combustion in gas turbines, which provide thrust

either through a propeller (turboprop) or a high-velocity exhaust jet (turbofan). Propeller systems operate most efficiently at lower speeds and altitudes and could therefore be suited to regional or short-haul flights, whereas turbofan engines enable higher cruise speeds and altitudes and might also be applied to medium- and long-haul missions.

The use of hydrogen in aviation comes with several challenges. On the ground, it requires the development of dedicated production, liquefaction, and storage infrastructure at airports, which demands significant investment and logistical coordination (Hoelzen et al., 2022). Onboard the aircraft, hydrogen's low volumetric energy density necessitates larger and heavily modified fuel tanks, reducing payload capacity or flight distance unless aircraft are redesigned (Tiwari et al., 2024; Soleymani et al., 2024). Cryogenic storage of liquid hydrogen to minimize its volume adds another technical complexity.

Despite these challenges, hydrogen could play a role in decarbonizing aviation in the long term. However, the climate impact of aviation extends beyond CO₂ emissions, with non-CO₂ effects such as nitrogen oxides (NO_x) emissions and contrails contributing to the overall radiative forcing. According to Lee et al. (2021), these non-CO₂ effects currently account for over half of aviation's total effective radiative forcing, although this estimate is associated with a large uncertainty. Therefore, to properly assess a potential new aviation technology such as hydrogen combustion from the perspective of non-CO₂ effects, a solid understanding of all relevant processes is required. This includes an understanding of processes ranging from the contrail formation to the impacts of long-lived contrails.

The life cycle of individual contrails is typically divided into three regimes (Paoli and Shariff, 2016): During the *jet regime*, hot exhaust air rapidly mixes with the cold ambient air and ice crystals form under suitable conditions (e.g., Schumann, 1996; Kärcher and Yu, 2009; Lewellen, 2020; Bier et al., 2022, 2024; Yu et al., 2024). During the *vortex regime*, contrails increase in vertical extent as parts of the ice crystals become trapped within the descending wake vortices. Adiabatic heating resulting from this downward motion causes partial loss of ice crystals (Sussmann and Gierens, 1999; Unterstrasser et al., 2008; Kleine et al., 2018). After vortex-breakup, the *dispersion regime* follows associated with the transition into contrail cirrus (Schumann, 2012; Lewellen, 2014; Unterstrasser et al., 2017a). This regime is marked by contrail spreading due to vertical wind shear, ice crystal growth/sublimation, and ice crystal sedimentation. For suitable ambient conditions, this regime can last several hours until dissolution of the contrail cirrus cloud (Jensen et al., 1998; Haywood et al., 2009; Laken et al., 2012; Bier et al., 2017).

The direct contributions to the contrail's total lifetime-integrated radiative effect during the jet and vortex regimes are typically small (Unterstrasser and Gierens, 2010a). However, early processes occurring in these phases have a sub-

stantial impact on the properties and life cycle of the contrail cirrus cloud (Burkhardt et al., 2018). Consequently, these initial processes exert a significant indirect influence on the overall radiative effect associated with a contrail (Bier and Burkhardt, 2022). While the total ice mass after the vortex break-up has a low impact, the number of ice crystals at this stage strongly and non-linearly influences the radiative effect of the contrail cirrus cloud for a given set of meteorological conditions (Unterstrasser and Gierens, 2010b; Lottermoser and Unterstrasser, 2025).

The idealized study of a single contrail's life cycle provides helpful insights into the relevant physical processes that influence its radiative impact. However, it cannot deliver an estimate of the radiative impact of the globally-distributed contrail coverage, which varies across time and space. This requires a realistic representation of aircraft traffic and the interaction of the contrails with the background atmosphere. For such purposes, general circulation models (GCM) have been extended to include a parameterization for contrail cirrus (Burkhardt and Kärcher, 2009; Gettelman and Chen, 2013; Bock and Burkhardt, 2016; Schumann et al., 2015). However, due to the coarse spatial and temporal resolution in a GCM, early processes during the jet and vortex phases can not be resolved. Therefore, contrails are typically initialized after the vortex break-up, while earlier processes need to be parameterized. For conventional kerosene combustion, a parameterization for contrail ice crystal formation (Kärcher et al., 2015), valid for the soot-rich regime, and a parameterization for the ice crystal loss during the wake vortex phase (Unterstrasser, 2016) have been implemented in the contrail initialization within ECHAM-CCMod (Bier and Burkhardt, 2019, 2022). Moreover, the parameterization for the ice crystal loss has been recently extended to also include hydrogen combustion scenarios (Lottermoser and Unterstrasser, 2025) and has been implemented in ECHAM-CCMod in the meantime. To date, a suitable parameterization for the number of ice crystals formed during the jet phase does not exist for hydrogen-powered aircraft.

1.2 Scope and outline of the study

Our overarching goal is to develop a parameterization for the final number of ice crystals formed for aircraft with hydrogen combustion, suitable for implementation in GCMs and other large-scale contrail models. Specifically, we seek a functional relationship of the form

$$N_{\text{ice},f} = N_{\text{ice},f}(a_{\text{atmosphere}}, a_{\text{aerosol}}, a_{\text{aircraft}}), \quad (1)$$

where $a_{\text{atmosphere}}$ denotes a set of variables characterizing the background atmosphere (e.g., ambient temperature), a_{aerosol} represents properties of ambient aerosols (number concentration, size distribution and solubility) and a_{aircraft} includes aircraft-related parameters (e.g., engine size).

Our objective is to identify a functional relationship that balances simplicity with physical fidelity. In other words, we

aim to capture the impact of the key processes that govern ice crystal formation in a form that is simple enough to be easily applied in other models (level of complexity, computing time, ease of implementation). In Parts 1 and 2 of a trilogy of papers, we systematically explore a broad parameter space and address aspects that have not been explored before to gain a deep insight into the physical processes influencing the ice crystal formation. This allows us to select the set of variables that constitute the inputs to the parameterization of $N_{\text{ice},f}$.

While a previous $N_{\text{ice},f}$ parameterization of contrail formation (Kärcher et al., 2015) used a first-principles-based concept, the current work across Parts 1 to 3 employs a hybrid approach. It combines a data-driven advanced regression method to fit a multidimensional database of contrail formation simulations with analytical scaling relations. To keep the number of dimensions in the simulation database as small as possible, we identify conditions under which the sensitivity to specific variables is negligible, and also employ analytical scaling relations derived from sensitivity simulations.

In Part 1, we focus on the roles of atmospheric variables $a_{\text{atmosphere}}$ and aerosol properties a_{aerosol} . Aircraft-related parameters a_{aircraft} are addressed in Part 2. The final parameterization, synthesizing insights from Parts 1 and 2, will be presented in Part 3.

In the current study, we first provide background information on contrail formation for the hydrogen combustion case (Sect. 2.1) and on the properties of ambient aerosol particles (Sect. 2.2), followed by a short review of the contrail formation model employed in the study (Sect. 2.3). This model is then used to investigate further (micro-)physical aspects that were not addressed in a previous publication by Bier et al. (2024). This includes the potential role of coarse mode particles in the contrail formation process (Sect. 3.1.1), a suitable scaling relation capturing the influence of multiple co-existing aerosol populations on the number of ice crystals (Sect. 3.1.2) and an investigation of the potential importance of the homogeneous droplet nucleation process (Sect. 3.2). We then present a large data set of simulations systematically scanning the relevant parameter space (Sect. 3.3) before we discuss the generality and limitations of our results and their relation to conventional kerosene contrails (Sect. 4). The study concludes with a discussion of our findings in the light of the design of a $N_{\text{ice},f}$ parameterization (Sect. 5).

2 Background and model description

2.1 Contrail formation for the hydrogen combustion case

During the jet phase, the mixing of the hot and humid exhaust (called the plume) with cold ambient air can lead to transient water supersaturation for suitable ambient conditions. In the absence of microphysical processes, the partial pressure of water vapor in the plume and the plume temperature evolve along the so-called mixing line (Fig. 1), whose slope can be

determined by

$$G = \frac{EI_v c_p p_a}{\epsilon Q(1 - \eta)}. \quad (2)$$

In Eq. (2), EI_v is the mass-specific water vapor emission index, Q the combustion heat (lower calorific value), c_p is the specific heat capacity at constant pressure, p_a the ambient pressure, $\epsilon = 0.622$ the ratio of molar masses of dry air and water vapor and η the overall efficiency of propulsion (Schumann, 1996). The slope of the mixing line influences the Schmidt–Appleman threshold temperature (Schmidt, 1941; Appleman, 1953; Schumann, 1996). The Schmidt–Appleman threshold temperature Θ_G is defined as the ambient temperature for which the mixing line just touches the saturation curve over water for a given ambient relative humidity over water $RH_{\text{wat},a}$ (Fig. 1). (Note that in some previous studies, e.g., Kärcher et al., 2015 and Ponsonby et al., 2025, Θ_G denotes the threshold temperature assuming ambient air at water saturation ($RH_{\text{wat},a} = 100\%$). Here, it refers to the threshold temperature for the actual ambient relative humidity, following the naming convention of Bier et al., 2024.) If the ambient temperature is below Θ_G , transient water supersaturation is generated during the mixing process and plume particles may activate into liquid droplets.

Burning hydrogen instead of kerosene results in a higher energy-specific water vapor emission index EI_v/Q of about 2.6 (Schumann, 1996; Bier et al., 2024), thus leading to a steeper slope of the mixing line (Fig. 1). This steeper slope leads to higher and longer-lasting supersaturations compared to conventional kerosene combustion for the same ambient conditions, influencing the contrail formation process (Bier et al., 2024). In particular, the formation of ice crystals is limited by the homogeneous freezing temperature of super-cooled droplets, which is typically lower than the classical Schmidt–Appleman threshold temperature in the hydrogen combustion case (Fig. 1). Nevertheless, the extent to which the ambient temperature is below the Schmidt–Appleman threshold temperature still plays an important role, as it determines both the maximum plume supersaturation and the duration of supersaturated conditions, thereby controlling the activation of aerosol particles into liquid droplets.

For conventional kerosene combustion, soot particles are the dominant condensation nuclei for liquid droplet activation, with subsequent freezing into ice crystals (Kärcher and Yu, 2009; Kleine et al., 2018). In addition, volatile particles originating from condensable gaseous species (sulfuric acid, nitric acid, organics) (Kärcher et al., 2000) may contribute to ice crystal formation at high supersaturations, i.e., at low ambient temperatures. A recent study by Yu et al. (2024) hints at the importance of the sulfur content in the fuel for volatile particle formation. Soot particles and sulfur are absent in the hydrogen combustion case. Therefore, other particles acting as condensation nuclei may contribute significantly to ice crystal formation. In this study, we assume that the ice crystals form on entrained ambient aerosols. To date,

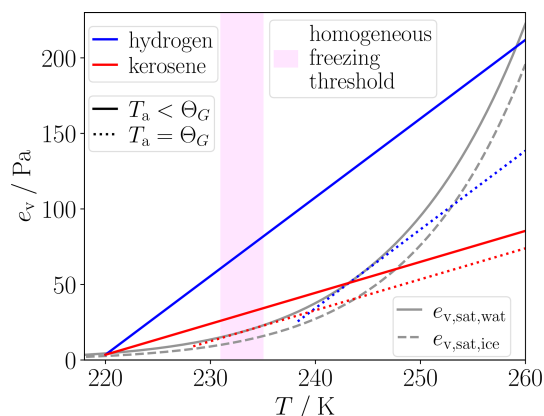


Figure 1. Mixing lines (partial pressure of water vapor in the plume e_v vs plume temperature T) are depicted for both hydrogen and kerosene combustion cases for the ambient pressure $p_a = 260$ hPa, ambient relative humidity over water $RH_{\text{wat},a} = 80\%$ and overall efficiency of propulsion $\eta = 0.4$. Shown are threshold cases with ambient temperatures $T_a = \Theta_G$ such that the mixing line just touches the saturation curve over water $e_{v,\text{sat},\text{wat}}$ for the given $RH_{\text{wat},a}$ value. Additionally, cases with a lower ambient temperature of $T_a = 220$ K are displayed. Moreover, the range of homogeneous freezing temperatures for supercooled droplets is indicated.

it is unclear whether volatile particles originating from emitted NO_x with associated formation of nitric acid or from lubrication oil (Ungeheuer et al., 2022; Ponsonby et al., 2024; Zink et al., 2025) are abundant enough at cruise altitude to dominate ice crystal formation. Due to the higher supersaturations encountered in the hydrogen combustion case, an additional pathway to ice crystal formation could be homogeneous droplet nucleation (HDN). HDN is the process where small droplets form out of the vapor phase without any condensation nucleus involved. For this process, high relative humidities ($\gtrsim 500\%$) are a prerequisite (Wölk and Strey, 2001). Assuming the exhaust air is particle-free and the HDN process is negligible, entrained ambient aerosols are the only precursors of the ice crystal formation. Bier et al. (2024) showed that, at the same ambient temperature and pressure and for typical aerosol number concentrations (Sect. 2.2), the resulting ice crystal number is reduced by roughly one to two orders of magnitude compared to soot-rich kerosene combustion cases.

2.2 Properties of ambient aerosol

Aerosol particles in the atmosphere are typically classified into four modes based on particle diameter (Petzold and Kärcher, 2012): nucleation mode (diameter $\lesssim 20$ nm), Aitken mode (~ 20 – 100 nm), accumulation mode (~ 100 – 1000 nm), and coarse mode ($\gtrsim 1$ μm). Nucleation mode particles form by gas-to-particle conversion, where supersaturated vapors (e.g., sulfuric acid, ammonia, nitric acid, and low-volatility organic compounds) nucleate homogeneously

or on existing ions (Yu et al., 2010a). Sources of these vapors in the upper troposphere (UT) include both natural and anthropogenic emissions, which are transported from lower altitudes to the UT by deep convection or large-scale atmospheric lifting (e.g., Hermann et al., 2003). Another direct source is aircraft emissions (e.g., Righi et al., 2021, 2023).

Aitken mode particles form by the growth of nucleation mode particles via condensation of vapors and coagulation of smaller particles. Some Aitken particles can also originate directly from combustion sources, such as aviation soot. Growth of Aitken particles via continued condensation and coagulation leads to the formation of accumulation mode particles. The direct contribution of aircraft emissions to the accumulation mode is typically small (Petzold et al., 1999). Unlike secondary aerosols that originate from gas-to-particle conversion, coarse mode particles are mechanically-induced primary aerosols (e.g., sea salt, dust, volcanic ash), which are transported to the UT mainly by deep convection or volcanic eruptions.

The various chemical components, ranging from highly soluble components like sulfuric acid or inorganic salts to weakly/insoluble particles like freshly emitted soot, leads to a wide range of aerosol particle solubilities (Kaiser et al., 2019). The solubility of an aerosol particle depends on its mixing state (Riemer et al., 2019). Both modeled and observed total aerosol number concentrations in the UT exhibit strong seasonal and geographic variability (Petzold et al., 2002; Minikin et al., 2003; Hermann et al., 2003; Borrmann et al., 2010; Kaiser et al., 2019; Brock et al., 2021). These studies report nucleation and Aitken mode particle number concentrations in the UT ranging from $\sim 10^2$ to $\sim 10^4$ cm^{-3} . Number concentrations of accumulation mode particles are typically lower, ranging from $\sim 10^1$ to $\lesssim 10^3$ cm^{-3} . Due to the larger size, however, the accumulation mode typically contains more mass than the nucleation and Aitken modes. Except in extreme scenarios, such as volcanic eruptions, coarse mode particle concentrations in the UT are generally several orders of magnitude lower, with number concentrations typically well below 1 cm^{-3} (Kaiser et al., 2019; Beer et al., 2020; Brock et al., 2021).

The strong influence of anthropogenic emissions on aerosol number concentrations in the UT introduces additional variability in future projections, as a potential reduction in emissions could result in a cleaner atmosphere. Such a reduced aerosol load was observed during the BLUESKY campaign during the COVID-19 lockdown (Voigt et al., 2022).

2.3 LCM box model

This section serves as a short review of the used model. Detailed explanations and underlying equations can be found in Bier et al. (2022, 2024).

The Lagrangian Cloud Module (LCM) was first described in Sölch and Kärcher (2010) and uses a particle-based ap-

proach (also known as super-droplet method, Shima et al., 2009; Grabowski et al., 2019). Two variants of LCM exist: The first is fully coupled to the fluid solver EULAG and was used to simulate natural cirrus clouds (Sölch and Kärcher, 2011; Unterstrasser et al., 2017b) as well as contrails during the vortex phase (Unterstrasser and Sölch, 2010; Unterstrasser, 2014) and the dispersion phase (Unterstrasser et al., 2017a). The second LCM variant is a box model version with simplified prescribed dynamics. It was for example used to evaluate the numerical implementation and convergence of particle-based algorithms of depositional growth and nucleation (Unterstrasser and Sölch, 2014) and collisional growth (Unterstrasser et al., 2017c, 2020).

Bier et al. (2022, 2024) expanded the LCM box model version by contrail formation physics on soot and ambient aerosols, respectively. In this version, aerosol particles and hydrometeors (liquid droplets and ice crystals) are represented by simulation particles (SIPs). Each SIP represents a certain number of physical particles with identical properties. Each SIP carries information such as particle type, particle phase (dry, liquid, or ice), radius, and the associated liquid or ice water mass.

In this box model version, the dilution is either analytically prescribed or obtained from a previously performed CFD simulation. The dilution governs plume expansion, cooling, and humidity evolution. Moreover, the dilution state determines the total number of entrained ambient aerosol particles for a given ambient aerosol number concentration. The contrail microphysics is then calculated in a time-resolved manner in an offline approach without feedback on the plume dynamics. The microphysical processes considered include hygroscopic growth of aerosol particles and activation into water droplets (described by κ -Köhler theory, Petters and Kreidenweis, 2007), condensational droplet growth, homogeneous freezing of supercooled droplets, depositional ice crystal growth, and latent heat release/consumption during phase transitions. The employed parameterization for homogeneous freezing (described in Appendix B of Bier et al., 2024) accounts for the dependence of the freezing process on droplet water volume and cooling rate (Kärcher et al., 2015), as well as for freezing-point depression caused by dissolved solutes (Koop et al., 2000; O and Wood, 2016). The employed parameterization shows a strong decrease in the freezing fraction toward 235 K, consistent with laboratory experiments (e.g., Murray et al., 2010; O and Wood, 2016; Tarn et al., 2021; Ponsonby et al., 2024). We therefore apply a temperature threshold at 235 K and assume that supercooled droplets do not freeze into ice crystals for $T_a \geq 235$ K.

In this study, we use the same box model version with its numerical setup as Bier et al. (2024) to simulate contrail formation on entrained ambient aerosols for hydrogen combustion. As dilution data, we use 1000 trajectories, which are a representative merged subset from the 25000 FLUDILES trajectories. These trajectories were obtained from a large-eddy simulation of the exhaust plume evolution downstream

of a CFM56 engine representative for an A340-300 aircraft (Vancassel et al., 2014). Each trajectory represents a fraction of the plume volume/mass. The box model is run for each trajectory separately and results are presented as sums over all trajectories for extensive quantities (e.g., total ice crystal number) and as mass-weighted averages for intensive quantities (e.g., plume temperature).

We use the set of baseline values listed in Table 1 (denoted by the asterisks), which are prescribed in the model setup if not stated differently. The prescribed water vapor emission index EI_v^* and specific combustion heat Q^* for hydrogen combustion are fixed throughout the whole study. Other parameters that are not listed in Table 1 (ambient temperature T_a , aerosol number concentration n_{aer}) are varied in each subsection of Sect. 3 and their prescribed values are explicitly stated there.

Compared to the setup in Bier et al. (2024), we use a higher value for the overall efficiency of propulsion of $\eta^* = 0.4$ (increased from 0.36), reflecting a projection towards more efficient engines. The impact of varying the overall efficiency of propulsion on contrail formation is discussed in detail in Part 2 (Zink and Unterstrasser, 2026) of this paper series. Additionally, we correct a discrepancy made in Bier et al. (2024) regarding the geometric width of the log-normal aerosol size distribution. While a value of $\sigma_{aer} = 1.6$ was reported, the actual value used in their simulations was $\sigma_{aer} = 1.69$ (see Sect. A). Although the exact value of the geometric width has a negligible effect on the results (Fig. A1), we have corrected the bug and now use the true value of $\sigma_{aer} = 1.6$ as reported in our setup.

3 Results

3.1 Multiple aerosol populations

As outlined in Sect. 2.2, the ambient aerosol size distribution consists of multiple modes. We introduce the term *aerosol population*, which refers to a set of aerosol particles characterized by a specific mono-modal size distribution and hygroscopicity. The total aerosol can then be a composition of multiple populations (expressed as a superposition of lognormal size distributions).

Clearly, to obtain a realistic picture of ice crystal formation on ambient aerosols, multiple aerosol populations should be considered. At the same time, this comes at the cost of increased complexity due to the larger number of parameters involved. In this section, we present means of reducing the number of parameters, with emphasis placed on the governing physical processes.

3.1.1 Impact of coarse mode particles

As written in Sect. 2.2, coarse mode particles are typically several orders of magnitude fewer in number compared to co-existing nucleation, Aitken, or accumulation mode particles.

Table 1. Baseline values of ambient pressure p_a^* , ambient relative humidity $\text{RH}_{\text{ice},a}^*$, aircraft speed U_∞^* , water vapor emission index EI_v^* , specific combustion heat Q^* , overall efficiency of propulsion η^* , exit temperature T_E^* , exit area A_E^* , exit excess jet velocity $U_{\text{jet},E}^*$ (total jet speed minus aircraft speed), geometric mean radius of aerosol particles $\bar{r}_{\text{d,aer}}^*$, geometric width σ_{aer}^* and hygroscopicity κ_{aer}^* .

background conditions	$p_a^* = 260 \text{ hPa}$, $\text{RH}_{\text{ice},a}^* = 115 \%$, $U_\infty^* = 250 \text{ m s}^{-1}$
fuel/engine properties	$EI_v^* = 8.94 \text{ kg kg}^{-1}$, $Q^* = 120 \text{ MJ kg}^{-1}$, $\eta^* = 0.4$
engine exit conditions	$T_E^* = 580 \text{ K}$, $A_E^* = 0.25\pi \text{ m}^2$, $U_{\text{jet},E}^* = 230 \text{ m s}^{-1}$
aerosol properties	$\bar{r}_{\text{d,aer}}^* = 20 \text{ nm}$, $\sigma_{\text{aer}}^* = 1.6$, $\kappa_{\text{aer}}^* = 0.5$

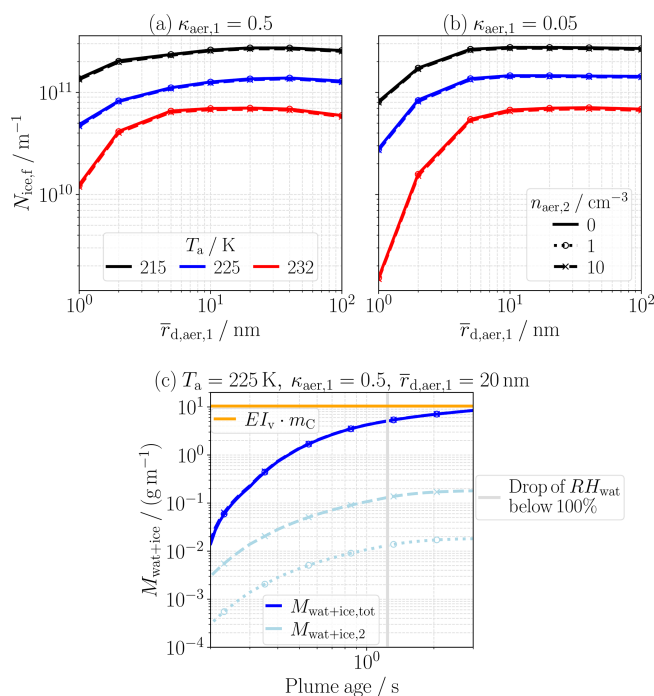


Figure 2. (a)–(b) Impact of coarse mode particles ($\bar{r}_{\text{d,aer},2} = 2000 \text{ nm}$, $\kappa_{\text{aer},2} = 0.05$) on the final number of ice crystals formed $N_{\text{ice},f}$. In all simulations, the total aerosol number concentration is $n_{\text{aer,tot}} = n_{\text{aer},1} + n_{\text{aer},2} = 1000 \text{ cm}^{-3}$ with varying $n_{\text{aer},2}$ values (different line styles). Shown are results as a function of the geometric mean radius of the smaller aerosol mode $\bar{r}_{\text{d,aer},1}$ for different ambient temperatures T_a (different colors) and different hygroscopicity combinations (panel). (c) Illustrative example of the evolution of depleted water-vapor mass on droplets and ice crystals. Shown are both the total depleted mass and the portion attributed to coarse-mode particles. The orange horizontal line marks the emitted water-vapor mass corresponding to the fuel consumption of $m_C \approx 1.17 \text{ g m}^{-1}$. The vertical gray line indicates the time at which the plume relative humidity with respect to water falls below 100 %, marking the approximate end of droplet activation.

Due to their low abundance, a significant direct contribution to the total ice crystal number is not expected. However, due to their large size and thus low Kelvin barrier, they can activate into water droplets at lower supersaturations. This raises

the question of whether their earlier activation could indirectly influence the activation behavior of smaller particles by changing the water vapor concentration within the plume and therefore the final number of ice crystals formed $N_{\text{ice},f}$ (i.e., the number when ice crystal formation is finished).

To investigate this, we performed simulations using a bimodal size distribution that includes a coarse mode with a geometric mean radius of $\bar{r}_{\text{d,aer},2} = 2000 \text{ nm}$, and a smaller mode with geometric mean radius $\bar{r}_{\text{d,aer},1}$ (Fig. 2). The coarse mode is assumed to be weakly soluble (hygroscopicity $\kappa_{\text{aer},2} = 0.05$), while the smaller mode is considered either highly soluble ($\kappa_{\text{aer},1} = 0.5$) or weakly soluble ($\kappa_{\text{aer},1} = 0.05$). Simulations were performed with a total aerosol number concentration of $n_{\text{aer,tot}} = n_{\text{aer},1} + n_{\text{aer},2} = 1000 \text{ cm}^{-3}$, comparing scenarios with $n_{\text{aer},2} = \{1, 10\} \text{ cm}^{-3}$ against those without coarse mode particles ($n_{\text{aer},2} = 0 \text{ cm}^{-3}$).

Across all scenarios, the presence of coarse mode particles does not result in a noticeable change in the ice crystal number (Fig. 2). Due to their low relative abundance and the continuous entrainment of aerosols into the plume over time, they are not abundant enough to significantly deplete the water vapor at an early stage to hinder the smaller-sized particles in their activation. Indeed, the amount of water vapor taken up by the few coarse mode particles is negligible compared to the total water vapor available in the plume (emitted water-vapor mass plus entrained ambient moisture) during droplet and ice crystal formation (Fig. 2c). This low importance of coarse mode particles was also found for other values of $n_{\text{aer,tot}}$, $\kappa_{\text{aer},2}$ and dilution speed (not shown). Therefore, if the coarse mode particles are two or more orders of magnitude fewer in number than another particle mode – as is typically the case in the UT (see Sect. 2.2) – we can safely neglect them in the ice crystal formation process.

3.1.2 Scaling relation for multiple aerosol populations

The results in Sect. 3.1.1 show that an aerosol population can be neglected in the ice-crystal formation process when its number concentration is much lower than that of a co-existing population. We now investigate situations in which the number concentrations of co-existing populations are comparable.

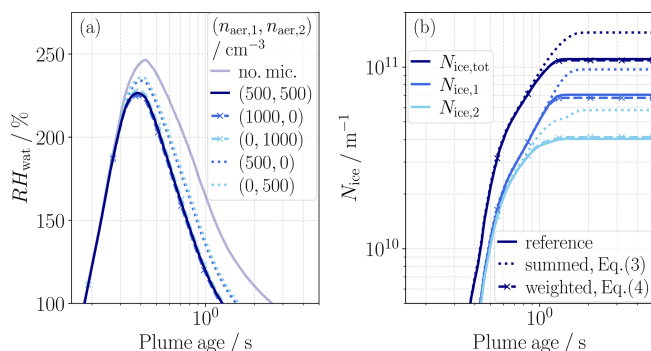


Figure 3. Evolution of (a) plume relative humidity RH_{wat} and (b) ice crystal number N_{ice} at an ambient temperature of $T_a = 225$ K for a case with two aerosol populations ($n_{\text{aer},1} = n_{\text{aer},2} = 500 \text{ cm}^{-3}$, $\kappa_{\text{aer},1} = \kappa_{\text{aer},2} = 0.5$, $\bar{r}_{\text{d,aer},1} = 20 \text{ nm}$, $\bar{r}_{\text{d,aer},2} = 2 \text{ nm}$). (a) Shown is the RH_{wat} evolution from a simulation excluding microphysical water-vapor depletion (transparent line), together with the evolution when both aerosol populations are included simultaneously (dark-blue line). Also shown are simulation results including only one population at a time, using its respective properties and either its actual number concentration or the total number concentration (different colors and line styles). (b) Displayed are the total ice crystal number $N_{\text{ice,tot}}$ and the contributions from the two aerosol populations, $N_{\text{ice},1}$ and $N_{\text{ice},2}$. Additionally, the approximations obtained from Eqs. (3) and (4) are shown.

We begin with an illustrative example that includes two aerosol populations ($n_{\text{aer},1} = n_{\text{aer},2} = 500 \text{ cm}^{-3}$, $\kappa_{\text{aer},1} = \kappa_{\text{aer},2} = 0.5$, $\bar{r}_{\text{d,aer},1} = 20 \text{ nm}$, and $\bar{r}_{\text{d,aer},2} = 2 \text{ nm}$). Water-vapor depletion by activated aerosols alters the evolution of the plume relative humidity RH_{wat} compared to simulations excluding microphysical water-vapor depletion (shown by the difference between the transparent and opaque dark-blue lines in Fig. 3a). The evolution of RH_{wat} is almost the same in simulations where both populations are included simultaneously and in simulations where only one population is included but assigned the total number concentration (Fig. 3a). In contrast, simulations that include only one population with its actual number concentration reach higher RH_{wat} values because the depletion of water vapor that would occur through activation of the second population is not accounted for.

As a consequence, attempting to reproduce the impact of multiple co-existing populations on the final ice crystal number by simply summing

$$\tilde{N}_{\text{ice,f}} = \sum_i N_{\text{ice,f},i}(n_{\text{aer},i}) \quad (3)$$

overestimates the actual number of ice crystals formed (Fig. 3b). Here, $\tilde{N}_{\text{ice,f}}$ is the approximated total ice crystal number and $N_{\text{ice,f},i}(n_{\text{aer},i})$ is the ice crystal number obtained from a simulation that includes only population i with its respective number concentration $n_{\text{aer},i}$.

In another approach, Bier et al. (2024) attempted to replicate simulations with two co-existing aerosol populations by

prescribing a single population with total number concentration and averaged properties (size, hygroscopicity) of the two. Their findings revealed substantial differences from the actual ice crystal number when nucleation-mode particles are involved.

Alternatively, we test a different scaling approach, where we perform separate simulations for each aerosol population i . In each of these simulations, only population i is included, characterized by its log-normal size distribution and hygroscopicity. Instead of using the actual number concentration $n_{\text{aer},i}$ of this population, we prescribe the total aerosol number concentration $n_{\text{aer,tot}}$. We then apply a weighted-mean approach

$$\hat{N}_{\text{ice,f}} = \sum_i \frac{n_{\text{aer},i}}{n_{\text{aer,tot}}} \cdot N_{\text{ice,f},i}(n_{\text{aer,tot}}), \quad (4)$$

where i goes over all aerosol populations. In Eq. (4), $\hat{N}_{\text{ice,f}}$ is the approximated total ice crystal number and $N_{\text{ice,f},i}(n_{\text{aer,tot}})$ the simulated number of ice crystals formed on population i with assumed total aerosol number concentration $n_{\text{aer,tot}}$.

This weighted-mean approach reasonably reproduces the ice crystal number of the reference simulation in which both aerosol populations are included simultaneously (Fig. 3b). Its success can be attributed to the fact that it is the total number of entrained aerosols that primarily drives the competition for the available water vapor (Fig. 3a). In the hydrogen combustion case, supersaturation levels become sufficiently high for all early entrained aerosol particles – including the nucleation mode particles – to activate into droplets. Toward the end of the supersaturated period, however, the newly entrained small-sized particles do not overcome the Kelvin barrier and therefore do not activate into droplets. As a result, fewer ice crystals eventually form on the nucleation-mode particles (Fig. 3b). Nevertheless, the evolution of plume relative humidity is mainly controlled by the total number of the earlier activated aerosols.

After the illustrative example (Fig. 3), we now explore a broader set of simulations involving two co-existing aerosol populations. We prescribe a total number concentration $n_{\text{aer,tot}} = 1000 \text{ cm}^{-3}$ with varying ratios $n_{\text{aer},1} : n_{\text{aer},2}$ for various combinations of aerosol properties and different ambient temperatures (Fig. 4). We confirm for $n_{\text{aer},1} : n_{\text{aer},2} = 1$ (as done by Bier et al., 2024) that simulations using a single aerosol population with total number concentration and average properties can reproduce the reference simulations well, except in cases where one geometric mean radius is smaller and the other larger than $\sim 5 \text{ nm}$ (Fig. 4a–d). For the latter cases, the weighted-mean approach strongly reduces the deviations from the reference simulations. The weighted-mean approach works well for equal partitions of the two number concentrations (Fig. 4a–d) as well as for unequal partitions (Fig. 4e–f). In fact, the approach works better the more strongly the two number concentrations differ, as then the contribution of the population with lower concentration becomes less and less important (similarly to the coarse mode

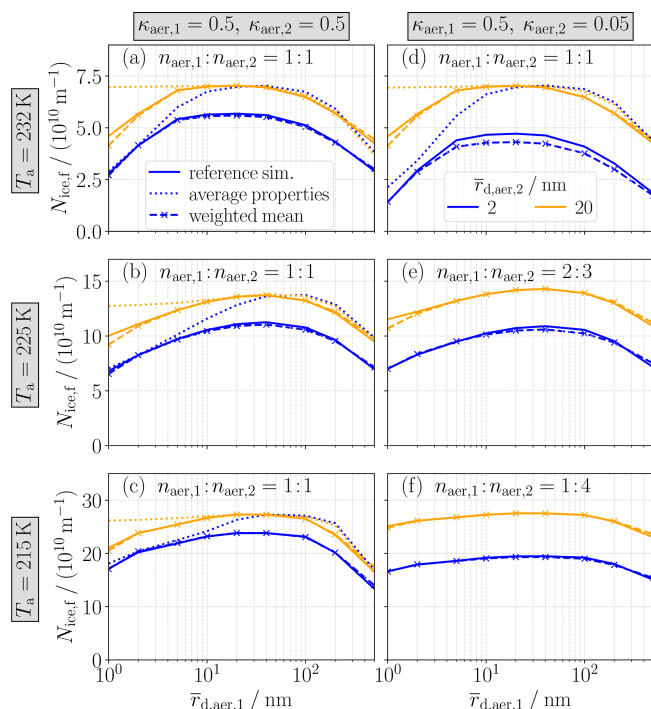


Figure 4. Weighted-mean approach for two ambient aerosol populations. Shown is the total number of ice crystals formed $N_{ice,f}$ as a function of the geometric mean radius of the first population $\bar{r}_{d,aer,1}$. The color of the curves indicates the geometric mean radius of the second population $\bar{r}_{d,aer,2}$. Each row corresponds to a different ambient temperature T_a and the two columns are for two different combinations of hygroscopicities $\kappa_{aer,1}$ and $\kappa_{aer,2}$. Results are shown for a total aerosol number concentration $n_{aer,tot} = n_{aer,1} + n_{aer,2} = 1000 \text{ cm}^{-3}$, the ratio of the two concentrations is displayed in each panel. Reference simulations including both aerosol populations in a single simulation (solid lines) are compared to the weighted-mean approach according to Eq. (4) (dashed lines with marker). For concentration ratios of 1 : 1, results for simulations including a single aerosol population with average geometric mean radius and average hygroscopicity are displayed additionally (dotted lines).

particles, Sect. 3.1.1). For the examples shown in Fig. 4, the weighted-mean approach yields a median relative error of 0.74 %, with the errors ranging from a minimum of 0.003 % to a maximum of 9.95 %.

So far, we restricted our analysis to two co-existing aerosol populations and to a fixed total number concentration of $n_{aer,tot} = 1000 \text{ cm}^{-3}$. In the following, we show that the scaling approach (Eq. 4) is generally applicable for multiple co-existing aerosol populations and different total number concentrations $n_{aer,tot}$. To do so, we perform simulations incorporating in total six aerosol populations, obtained by combining three monomodal size distributions (geometric mean radii $\bar{r}_{d,aer} = \{2, 20, 200\} \text{ nm}$) with two hygroscopicities ($\kappa_{aer} = \{0.05, 0.5\}$), such that each population represents a monomodal size distribution with an assigned hygroscopicity.

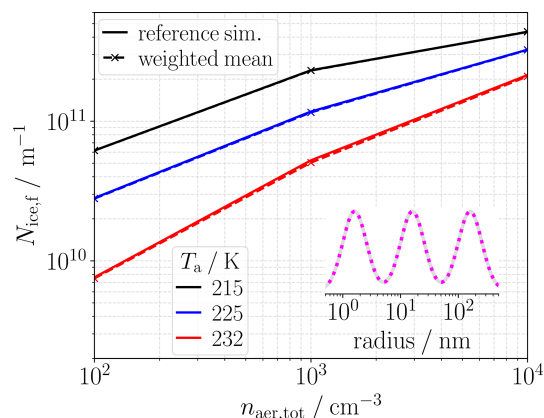


Figure 5. Weighted-mean approach for six ambient aerosol populations. Displayed is the final number of ice crystals formed $N_{ice,f}$ as a function of total aerosol number concentration $n_{aer,tot}$ for different ambient temperatures T_a . The six populations comprise three geometric mean radii $\bar{r}_{d,aer} = \{2, 20, 200\} \text{ nm}$ each combined with two hygroscopicities $\kappa_{aer} = \{0.05, 0.5\}$ (illustrated by the inset; the solid gray and the dotted magenta lines indicate the two hygroscopicities). Each population is assumed to contribute one sixth to the total aerosol number concentration. Reference simulations including all six aerosol populations in a single simulation (solid lines) are compared to the weighted-mean approach according to Eq. (4) (dashed lines with marker).

icity. We prescribe different $n_{aer,tot}$ with each population assumed to contribute one sixth to the total number concentration. These simulations can be accurately reproduced using the weighted-mean approach (Eq. 4) across all investigated ambient temperatures (Fig. 5), demonstrating the broad applicability of this scaling method. For the examples shown in Fig. 5, the weighted-mean approach yields a median relative error of 0.86 %, with the errors ranging from a minimum of 0.08 % to a maximum of 3.65 %.

The success of the weighted-mean approach – attributed to the fact that the total number of entrained aerosol particles primarily drives water vapor depletion – implies that only the dependence of $N_{ice,f}$ on the properties of a single population needs to be represented. The effect of the co-existence of multiple populations can then be emulated by this approach. This reduces the dimensionality of the parameter space and avoids the curse of dimensionality (Bellman, 1957) without loss of generality.

3.2 Importance of homogeneous droplet nucleation

As described in Sect. 2.1, homogeneous droplet nucleation (HDN) with subsequent freezing into ice crystals could be another contrail ice formation pathway. For this process, high supersaturations are needed. In the hydrogen combustion case, high plume relative humidities are encountered at low ambient temperatures, with increasing peak values with decreasing ambient temperatures (Fig. 3b in Bier et al., 2024)

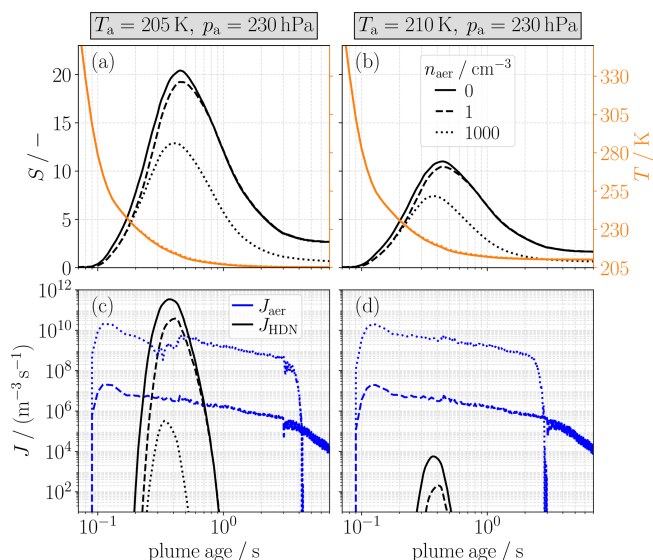


Figure 6. (a)–(b) Time evolution of saturation ratio S (black curves) and plume temperature T (orange curves) for different ambient aerosol number concentrations (indicated by the linestyle). (c)–(d) Nucleation rates on ambient aerosols J_{aer} according to Eq. (5) (blue curves) and homogeneous droplet nucleation rates J_{HDN} obtained by inserting the time evolutions S and T into Eq. (7) (black curves). The two columns are for two different ambient temperatures T_a for the same ambient pressure p_a .

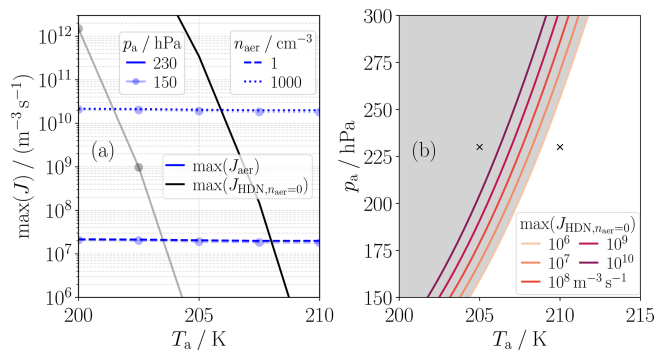


Figure 7. (a) Maxima of nucleation rates $\max(J)$ as a function of ambient temperature T_a for two ambient pressures p_a (indicated by transparency and dotted marker). Depicted are the maximum nucleation rates connected with ambient aerosols $\max(J_{\text{aer}})$ (blue lines) for two aerosol number concentrations n_{aer} (different linestyles) and the maximum rates of homogeneous droplet nucleation obtained when moving along the mixing line $\max(J_{\text{HDN}, n_{\text{aer}}=0})$ (black lines). (b) Isolines for maxima of homogeneous droplet nucleation rates obtained when moving along the mixing line for different T_a and p_a combinations. The two black crosses indicate the combinations of T_a and p_a used in the two columns of Fig. 6.

hinting towards a potential importance of the HDN process at low ambient temperatures.

Here, we try to assess the relative importance of the HDN process using an offline approach. To do so, we first evalu-

ate the time-dependent nucleation rate on entrained ambient aerosols from the box model simulations via

$$J_{\text{aer}}(t) = \frac{N_{\text{act}}(t) - N_{\text{act}}(t - \delta t)}{\delta t \cdot \hat{A}(t)} \quad (5)$$

with the box model time step δt , the effective plume area $\hat{A}$ and the number of already activated aerosols per meter of flightpath

$$N_{\text{act}}(t) = N_{\text{drop}}(t) + N_{\text{ice}}(t) \quad (6)$$

as sum of droplet number N_{drop} and ice particle number N_{ice} . We compare this nucleation rate J_{aer} to potential homogeneous nucleation rates. For this we use the empirical nucleation rate (Wölk and Strey, 2001; Wölk et al., 2002)

$$J_{\text{HDN}} = J_{\text{BD}} \exp \left(A + \frac{B}{T} \right) \quad (7)$$

with the empirical constants $A = -27.56$ and $B = 6500 \text{ K}$ and the classical Becker–Döring nucleation rate

$$J_{\text{BD}} = \sqrt{\frac{2\sigma}{\pi m}} v \left(\frac{e_v}{k_B T} \right)^2 \exp \left\{ \frac{-16\pi v^2 \sigma^3}{3(k_B T)^3 (\ln S)^2} \right\} \quad (8)$$

in units $\text{m}^{-3} \text{s}^{-1}$. In Eq. (8), σ is the surface tension of the critical cluster of water molecules, m is the mass of a water molecule, v is the molecular volume, k_B is the Boltzmann constant, T is the temperature, and $S = e_v / e_{v, \text{sat, wat}}$ is the saturation ratio (relative humidity given as ratio and not in percentage) with the actual partial pressure of water vapor e_v and the equilibrium partial vapor pressure over a flat water surface $e_{v, \text{sat, wat}}$.

In our offline approach, we evaluate $J_{\text{HDN}}(t)$ via Eq. (7) by using the time series $T(t)$ and $S(t)$ as obtained from existing box model simulations. For simulations with microphysics switched off (ambient aerosol number concentration $n_{\text{aer}} = 0 \text{ cm}^{-3}$), the evolution of T and S over time is governed solely by dilution along the mixing line. For $n_{\text{aer}} > 0 \text{ cm}^{-3}$, the temperature evolution differs minimally due to latent heating from phase transitions. The evolution of the saturation ratio S is strongly affected by the choice of the n_{aer} value due to the water vapor depletion by activated aerosols (Fig. 6a–b).

Since our offline approach does not consider water vapor consumption by homogeneously nucleated droplets, it tends to overestimate J_{HDN} at later times t . Furthermore, it does not determine whether clusters formed at a given time are stable and grow or whether they evaporate thereafter. However, as this approach tends to overestimate J_{HDN} , it allows for a conservative estimate of the importance of the HDN process.

At the ambient temperature $T_a = 205 \text{ K}$, the encountered saturation ratios S are high (Fig. 6a), and thus also the rates J_{HDN} for low ambient aerosol number concentrations n_{aer}

(Fig. 6c). At these low n_{aer} , the maximum of the calculated rates J_{HDN} exceeds the maximum of the rates J_{aer} . However, when ambient aerosols are more abundant with substantial depletion of the water vapor, the calculated rates J_{HDN} become several orders of magnitude lower than the corresponding rates J_{aer} (dotted lines for $n_{\text{aer}} = 1000 \text{ cm}^{-3}$ in Fig. 6c).

At an higher ambient temperature ($T_{\text{a}} = 210 \text{ K}$), the encountered supersaturations S are lower (Fig. 6b), resulting in J_{HDN} values that remain several orders of magnitude below the rates J_{aer} , even for low n_{aer} (Fig. 6d). In addition, the maxima of J_{HDN} occur much later than those of J_{aer} . Consequently, indirect effects such as a significant activation suppression of ambient aerosols due to the water vapor depletion by a few spontaneously nucleated droplets are highly unlikely (based on the same reasoning as for the coarse-mode particles discussed in Sect. 3.1.1).

After displaying the time evolution of nucleation rates for the two example cases (Fig. 6), we now extend our analysis to a broader set of scenarios. For these scenarios, we evaluate the maxima of the nucleation rates (Fig. 7a). Although these values represent instantaneous rates, they serve as a robust indicator of the integrated total number (Appendix B). The maximum of J_{aer} is almost independent of ambient temperature T_{a} and pressure p_{a} at low ambient temperatures and scales nearly linearly with ambient aerosol number concentration n_{aer} (Fig. 7a and Fig. B1). In contrast, the maximum of J_{HDN} depends non-linearly on the supersaturation and is therefore highly sensitive to both T_{a} and p_{a} .

As the highest potential J_{HDN} values occur in the absence of ambient aerosols ($n_{\text{aer}} = 0 \text{ cm}^{-3}$), we use these rates for a most conservative estimate. In particular, we evaluate the maxima of the rates $J_{\text{HDN}, n_{\text{aer}}=0}$ for various combinations of p_{a} and T_{a} . Isolines of $\max(J_{\text{HDN}, n_{\text{aer}}=0})$ are shown in Fig. 7b. Since the maxima of J_{aer} are at least one order of magnitude above $10^6 \text{ m}^{-3} \text{ s}^{-1}$ for aerosol number concentrations $n_{\text{aer}} \geq 1 \text{ cm}^{-3}$ (Fig. 7a), we choose the isoline $\max(J_{\text{HDN}, n_{\text{aer}}=0}) = 10^6 \text{ m}^{-3} \text{ s}^{-1}$ as a conservative boundary for an estimation where HDN may be important. This boundary can be approximated by

$$p_{\text{a}}(T_{\text{a}}) = a \cdot T_{\text{a}}^2 + b \cdot T_{\text{a}} + c \quad (9)$$

with $a = 1.04 \cdot 10^2 \text{ Pa K}^{-2}$, $b = -4.14 \cdot 10^4 \text{ Pa/K}$, and $c = 4.12 \cdot 10^6 \text{ Pa}$.

If a $p_{\text{a}} - T_{\text{a}}$ pair lies to the right/below of this boundary (white region in Fig. 7b), we can be very sure that HDN does not play a significant role as the nucleation rates on the ambient aerosols are substantially higher regardless of the ambient aerosol number concentration. In the gray region of Fig. 7b, it remains uncertain whether HDN may significantly contribute to droplet formation. This depends on the aerosol number concentration and requires an explicit, time-resolved simulation of relative humidity and temperature evolution, along with the kinetics of droplet cluster growth/evaporation.

Equation (9) remains valid when the ambient relative humidity deviates from the baseline value $RH_{\text{ice}, \text{a}}^* = 115 \%$, as

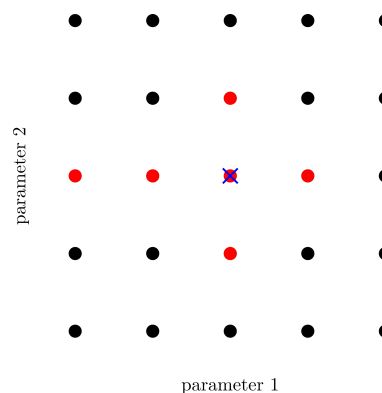


Figure 8. Schematic depiction of the difference between a one-at-a-time approach and the simulation setup used in the current study. Starting from a set of baseline values (blue cross), the values of a single parameter are varied in a one-at-a-time approach while all other parameters are kept constant (red dots). In the current study, we set up simulations for all possible combinations of parameter values (black dots).

such a deviation only causes a slight shift of the mixing line and has compared to a change in T_{a} and p_{a} only a minor effect on the maximum supersaturation.

3.3 Systematic investigation

3.3.1 Simulation data base

Bier et al. (2024) primarily used a one- or two-at-a-time approach to investigate the main sensitivities of the number of ice crystals formed $N_{\text{ice}, \text{f}}$ to different parameters. This method involves starting from a set of baseline values and varying one or two parameters at a time while keeping all others fixed. The goal of this section is to explore the parameter space more systematically. First, we expand the range of parameter values beyond those considered by Bier et al. (2024). Second, instead of varying one or two parameters at a time, we perform simulations for all possible combinations of parameter values (schematically illustrated in Fig. 8 for two parameters). This approach results in a total of $n_{\text{sim}} = \prod_i n_i$ simulations, where n_i denotes the number of values explored for parameter i . For the parameter values listed in Table 2, this leads to more than $n_{\text{sim}} > 20\,000$ simulations. This systematic investigation enables us to make general statements about the sensitivity of $N_{\text{ice}, \text{f}}$ to different parameters across various regions of the parameter space. Moreover, the resulting comprehensive dataset provides a suitable basis for a data-driven parameterization approach. Alternative sampling strategies, such as Latin hypercube sampling, could reduce the number of simulations required. However, since the computational cost of the box model is low, we can afford to use the full-factorial sampling strategy.

Ambient temperatures are specified over a broad range, prescribed linearly in 5 K steps from $T_{\text{a}} = 210 \text{ K}$ to $T_{\text{a}} =$

230 K. We use a finer resolution for $T_a \geq 230$ K to capture the non-linear dependence on the homogeneous freezing process in this temperature range.

The range of prescribed ambient pressures reflects a wide altitude range for possible aircraft traffic. Clearly, as we performed simulations for all possible combinations of ambient temperature and pressure, highly unlikely atmospheric scenarios are also part of the dataset. Nonetheless, ambient pressure primarily influences supersaturation levels at a given ambient temperature through its effect on the slope of the mixing line (Eq. 2). Thus, even the less likely combinations represent extrapolations that still capture the primary influence of ambient pressure on the contrail formation process and do not deteriorate the representation of contrail formation under more realistic atmospheric conditions. In addition, a small subset of temperature–pressure combinations in the dataset falls into a regime where the estimate presented in Sect. 3.2 suggests that HDN cannot be excluded as a potential contributor to ice formation. As HDN is not included in the simulations, the corresponding ice crystal numbers for these conditions are therefore subject to higher uncertainty.

We only consider ice (super-)saturated conditions ($\text{RH}_{\text{ice},a} \geq 100\%$) as only contrails formed under these conditions will persist for a longer time. For the chosen upper limit ($\text{RH}_{\text{ice},a} = 140\%$), the environment is sub-saturated with respect to water for all investigated ambient temperatures (e.g., $\text{RH}_{\text{ice},a} = 140\%$ corresponds to $\text{RH}_{\text{wat},a} \approx 80\%$ at $T_a = 210$ K and to $\text{RH}_{\text{wat},a} \approx 96\%$ at $T_a = 234.5$ K). If the environment were supersaturated with respect to water, natural clouds would be anyway present. Even under water sub-saturated conditions, aerosols may grow hygroscopically large enough to freeze and initiate natural cirrus formation in some scenarios. However, this study does not address contrail formation in the presence of existing natural cirrus, and we therefore assume a cloud-free background in all simulations.

As the impact of multiple coexisting aerosol populations can be inferred from individual simulations, each including only one of the populations with a suitably adjusted number concentration (Sect. 3.1.2), it is sufficient to explore the dependence on the properties of single aerosol populations systematically. The prescribed aerosol number concentrations span several orders of magnitude, representing the large variability in the atmosphere. As the number of ice crystals formed is only weakly dependent on the geometric width (Fig. A1), this parameter is held constant at $\sigma_{\text{aer}} = 1.6$ across all simulations (Brock et al., 2021; Bier et al., 2024). In contrast, the geometric mean radius is varied using an approximately logarithmic spacing, covering the full range from small nucleation mode particles to large accumulation mode particles. Based on the findings in Sect. 3.1.1, we do not cover coarse mode particles. The nearly logarithmic spacing provides enhanced resolution in linear space for the small-sized particles to capture the non-linear influence of the Kelvin effect on the droplet activation. Finally, pre-

scribed aerosol hygroscopicity values span several orders of magnitude to account for the diverse solubilities of potential aerosol species (see Table 1 in Petters and Kreidenweis, 2007).

3.3.2 Systematic evaluation of the ice crystal number

In this section, we present the results of the $n_{\text{sim}} > 20\,000$ simulations in a condensed manner. As a first step, we investigate the mean dependence of the final number of ice crystals formed $N_{\text{ice},f}$ on the various parameters. To do so, we look at all simulations that use a specific value k of the parameter i , and calculate the arithmetic mean of $N_{\text{ice},f}$ across these n_{sim}/n_i simulations, where n_i is the number of values considered for parameter i .

This analysis confirms several findings already reported by Bier et al. (2024). The mean number of ice crystals decreases with increasing ambient temperature T_a (Fig. 9a), owing to lower and shorter-lasting supersaturation at higher temperatures. Above $T_a \sim 230$ K, a pronounced nonlinear decline in ice crystal number is observed, attributed to the large freezing time scales of supercooled droplets at those temperatures. Unlike conventional contrail formation on soot particles in soot-rich regimes, where ice crystal numbers saturate at low ambient temperatures, our results show a continuous increase in ice crystal number with decreasing T_a due to continuous entrainment of ambient aerosols into the plume and prolonged supersaturation at lower temperatures.

Higher ambient pressure p_a results in increased ice crystal numbers (Fig. 9b), driven by enhanced supersaturation caused by a steeper slope of the mixing line (Eq. 2). The mean ice crystal number shows only a weak dependence on ambient relative humidity, with a slight increase with increasing $\text{RH}_{\text{ice},a}$ (Fig. 9c).

The mean number of ice crystals formed strongly depends on the background aerosol number concentration n_{aer} (Fig. 9d). At low n_{aer} , the relationship is approximately linear, whereas saturation effects become apparent for high n_{aer} . For $\bar{r}_{d,\text{aer}} \lesssim 10$ nm, the mean ice crystal number increases with increasing geometric mean radius (Fig. 9e), driven by the nonlinear Kelvin effect. Between $\bar{r}_{d,\text{aer}} \gtrsim 10$ nm and $\bar{r}_{d,\text{aer}} \lesssim 100$ nm, the dependence is weak. Since Bier et al. (2024) only investigated values up to $\bar{r}_{d,\text{aer}} = 70$ nm, they did not report the decrease in ice crystal number observed for $\bar{r}_{d,\text{aer}} \gtrsim 100$ nm. This decline is due to the freezing-point depression of solution droplets, which will be discussed in more detail further below. In this mean-based analysis, the aerosol hygroscopicity κ_{aer} has only a minor impact on the ice crystal number (Fig. 9e).

To gain deeper insight, we refine our analysis by still considering a specific value k of parameter i , while additionally grouping the data by the n_j values of a co-parameter j . Within each subgroup, we compute the arithmetic mean over the $n_{\text{sim}}/(n_i \cdot n_j)$ simulations and plot the obtained n_j mean values as colored dots in Fig. 9, where the color denotes the

Table 2. Box model simulations for all possible combinations of listed parameter values are performed.

parameter	values
ambient temperature T_a (K)	210, 215, 220, 225, 230, 232.5, 234.5
ambient pressure p_a (hPa)	150, 230, 320, 400
ambient relative humidity over ice $RH_{ice,a}$ (%)	100, 115, 125, 140
aerosol number concentration n_{aer} (cm^{-3})	1, 10, 100, 1000, 10000
aerosol geometric mean radius $\bar{r}_{d,aer}$ (nm)	1, 2, 5, 10, 20, 40, 100, 200, 500
aerosol hygroscopicity κ_{aer} (–)	0.01, 0.05, 0.25, 1.25

co-parameter used for grouping. The spread of the dots indicates how sensitive the ice crystal number is to the considered co-parameter at a given parameter value k .

This analysis confirms that ambient aerosol number concentration and ambient temperature are the most influential parameters throughout the examined parameter space. Furthermore, the extent of the dots reveals that the ice crystal number is significantly sensitive to $RH_{ice,a}$ only when $T_a \gtrsim 230$ K (Fig. 9a). Additionally, this analysis indicates that the hygroscopicity κ_{aer} becomes influential for $\bar{r}_{d,aer} \lesssim 10$ nm and $\bar{r}_{d,aer} \gtrsim 100$ nm (Fig. 9e). This is caused by two distinct physical processes: A higher hygroscopicity κ_{aer} reduces the critical supersaturation required for droplet activation. This becomes important when the Kelvin effect is strong, i.e., for small-sized particles. Conversely, a higher κ_{aer} value lowers the freezing temperature of supercooled droplets. While the freezing behavior of weakly soluble activated aerosols is similar to that of pure supercooled droplets, the presence of soluble material within a supercooled droplet inhibits the initiation of the freezing process (Koop et al., 2000). This means that some well-soluble aerosols activate into droplets but do not freeze. This suppression becomes more pronounced for larger dry particle radii due to the higher solute content for a given water content.

All together, this systematic investigation shows that the number of ice crystals is almost independent of ambient relative humidity, ambient aerosol size, and hygroscopicity for the parameter subspace defined by $T_a \leq 225$ K and $10 \text{ nm} \leq \bar{r}_{d,aer} \leq 100$ nm. This conclusion is supported by an analysis restricted to this subspace, as shown in Fig. 10.

4 Discussion

In this section, we place our findings in a broader context and critically assess their generality, associated uncertainties, and relation to conventional kerosene contrails. All conclusions are based on a systematically conducted model study using the LCM box model with contrail formation assumed on entrained ambient aerosol particles. The LCM box model has previously been compared to other contrail formation models for ice crystal formation on emitted soot particles in kerosene combustion cases (Bier et al., 2022). Clearly, such validation for kerosene contrails does not extend to the mi-

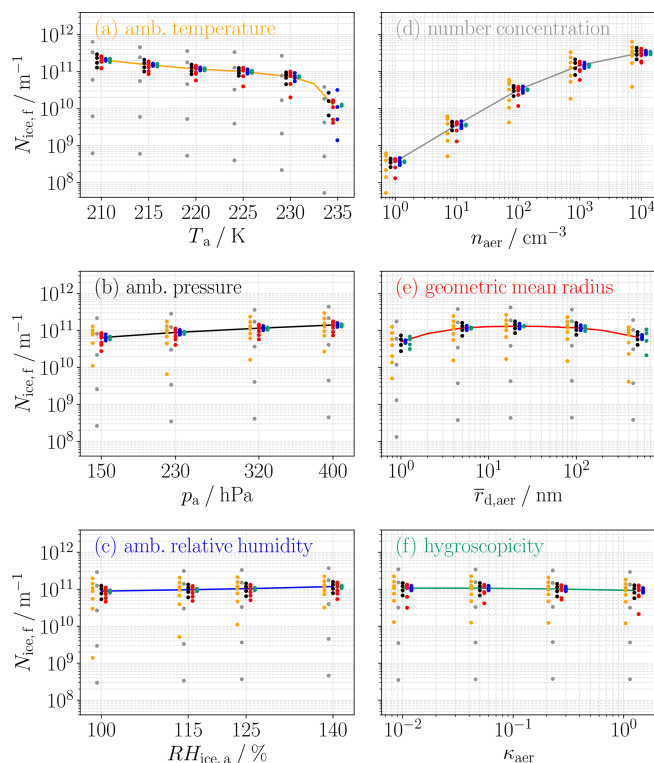


Figure 9. Mean dependence of the final number of ice crystals formed $N_{ice,f}$ on the various parameters (different colored solid lines in each panel). The colored dots show the mean $N_{ice,f}$ calculated within subgroups grouped by the specific parameter value at the x -axis and by the values of a co-parameter. Different colors indicate the various co-parameters, with the corresponding parameter ranges taken from Table 2. The dots for the different co-parameters correspond to the parameter value at the center but are shifted for visualization purposes. In (a), the dependence on the co-parameters is not displayed for $T_a = 232.5$ K and in (e) the dependence on the co-parameters is only displayed for each second geometric mean radius.

crophysical processes that are particularly relevant for hydrogen combustion. This is, for example, the case at temperatures for which kerosene contrails do not form and where homogeneous freezing plays a crucial role. A step toward obtaining measurement data under hydrogen combustion conditions has been taken with the first demonstrator experi-

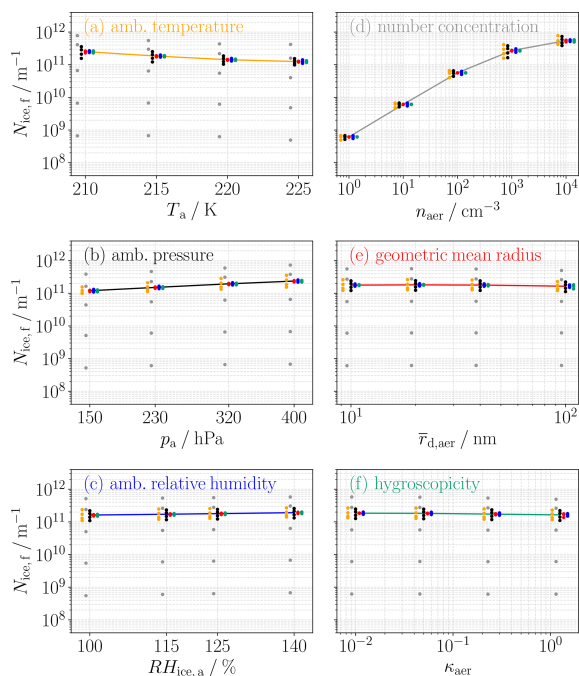


Figure 10. Same as Fig. 9, but for the subspace defined by $T_a \leq 225$ K and $10 \text{ nm} \leq \bar{r}_{d,\text{aer}} \leq 100 \text{ nm}$.

ment (Blue Condor, 2025). Still, the very limited measurement database constitutes a clear validation gap. Despite this limitation, the conclusions derived in this study are grounded in physical process understanding rather than being specific to the particular model setup.

In our simulations, we did not vary the prescribed dilution, which controls plume cooling and humidity evolution. Changes in dilution speed are expected if engine size or jet speed is changed (Lewellen, 2020). While the dilution speed influences the absolute number of ice crystals formed (see Part 2; Zink and Unterstrasser, 2026), the conclusions drawn here are not affected, which is further elaborated in the subsequent paragraphs.

Because few coarse-mode particles have a negligible influence on the water vapor budget, their role remains unimportant even if additional particle types (e.g., lubrication oil particles) were to contribute to ice crystal formation in hydrogen combustion cases. Water-vapor depletion is dominated by the far more numerous other particles in the plume, leaving coarse-mode particles unable to exert a significant effect, even under slower dilution scenarios. Coarse-mode particles would only become relevant if their number concentrations were of a similar order of magnitude to those of the other involved particle populations, which is typically not the case (Sect. 2.2).

The dilution state not only controls plume temperature and humidity but also determines the number of particles entrained into the plume for a given ambient aerosol number concentration. Because the total number of already entrained

and activated aerosol particles primarily governs water-vapor depletion (Sect. 3.1.2), the weighted-mean approach remains valid across different dilution scenarios. However, the weighted-mean approach is not expected to be generally applicable to particle types other than entrained ambient aerosols. In particular, it cannot represent the competition between emitted soot particles and volatile particles that form prior to contrail formation in kerosene combustion cases. Owing to the Kelvin effect, small volatile particles can only activate into droplets at sufficiently high plume supersaturations, that is, when ambient temperatures are well below the Schmidt–Appleman threshold temperature (Kärcher and Yu, 2009; Yu et al., 2024; Ponsonby et al., 2025). Beyond this thermodynamic constraint, the activation of volatile particles is additionally influenced by interactions with the soot particles. Since all particles are present in the plume from the onset of contrail formation, the largest soot particles activate first. Depending on their number, they can substantially deplete the water vapor and thereby partially or fully suppress the activation of smaller volatile particles. Consequently, water-vapor competition is controlled not only by the total particle number but also by the particle properties (size, hygroscopicity), in contrast to what we found for continuously entrained ambient aerosol populations in the hydrogen combustion case.

Using a conservative offline estimate, we identified a large region of parameter space in which HDN can safely be neglected (white region in Fig. 7b). Because this assessment is based on conservative order-of-magnitude considerations, it remains robust against uncertainties in dilution speed. The identified region would also remain valid if other particle types in addition to ambient aerosols were to contribute to water-vapor depletion, which would further suppress the conditions favorable for HDN. For combinations of temperature and pressure in which HDN may potentially become relevant in hydrogen combustion (grey region in Fig. 7b), its actual importance cannot be assessed within the present framework and requires simulations in which HDN is included online. For conventional kerosene combustion, the approximately 2.6-times lower energy-specific water vapor emission index leads to substantially reduced supersaturation, making HDN highly unlikely even at low temperatures and justifying its omission in previous kerosene studies.

Moreover, the regime identified in Sect. 3.3.2, in which $N_{\text{ice},f}$ is only weakly sensitive to particle properties, is a consequence of microphysical processes. In particular, both the Kelvin effect and freezing-point depression are negligible within this regime. The low sensitivity of $N_{\text{ice},f}$ to $\text{RH}_{\text{ice},a}$ for $T_a \lesssim 225$ K is consistent with findings for conventional kerosene contrails well below the Schmidt–Appleman threshold temperature (e.g., Fig. 4c in Bier et al., 2022). Changes in $\text{RH}_{\text{ice},a}$ only slightly shift the mixing line and therefore have a weaker impact on the supersaturations encountered than changes in ambient temperature or pressure.

Section 3.3.2 presents a comprehensive analysis of ice crystal number assuming formation on entrained ambient aerosol particles. An additional particle source may arise from lubrication oil released from engine breather vents (Yu et al., 2010b, 2012; Decker et al., 2024), with its impact depending strongly on where the oil is injected into the exhaust plume. If venting occurs close to the hot core flow, high temperatures promote evaporation and subsequent renucleation in the cooling plume. This produces a nucleation-mode particle population (Ungeheuer et al., 2022) that typically forms well before contrail formation begins. These particles can activate into liquid droplets and subsequently freeze into ice crystals (Ponsonby et al., 2024). In contrast, if the breather flow is emitted farther from hot engine sections, the oil is expected to be entrained into the water-vapor plume only after the exhaust has substantially cooled. Under these conditions, the resulting particles are expected to remain relatively large (hundreds of nanometers) and low in number, contributing little to the total ice crystal number.

Recent work by Zink et al. (2025) demonstrates that even very small lubrication oil emissions (on the order of a few milliliters per hour or even less) can generate substantial particle numbers when evaporation and renucleation occur. In many scenarios they investigated, ice crystal formation is dominated by oil particles rather than by entrained ambient aerosol. Lubrication oil emissions therefore represent a potentially important but highly configuration-dependent particle source whose relevance for contrail formation may vary substantially across engine designs. Technical design choices may thus play a key role in determining their importance for contrail formation in hydrogen combustion cases.

5 Conclusions

In this section, we summarize the key findings of our study and discuss their implications for the development of an upcoming parameterization for the number of ice crystals formed. We conducted simulations using the particle-based LCM box model to investigate contrail formation on entrained ambient aerosol particles for hydrogen combustion. Our focus was on microphysical processes, with the main findings being:

- Coarse-mode particles typically do not need to be accounted for, as their much lower number concentrations compared to coexisting nucleation, Aitken, or accumulation mode particles result in a negligible depletion of the available water vapor. Consequently, they exert neither a significant direct nor indirect influence on ice crystal formation.
- We showed that the ice crystal number formed on multiple aerosol populations can be approximated by a weighted-mean approach based on simulations that include only a single population. The success of this

weighted-mean approach is physically explained by the fact that the total number of entrained aerosol particles largely governs the competition for the available water vapor. Therefore, it is sufficient to suitably parameterize the dependence of the ice crystal number on the properties of a single population. The ice crystal number formed on multiple populations with different properties can then be obtained by this weighted-mean approach.

- We provided a formula for a conservative boundary dividing the parameter space into regions where homogeneous droplet nucleation can safely be neglected and regions where this process might play a role in ice crystal formation. For a parameterization based on contrail formation on ambient aerosol particles, the boundary can serve as a first indication of whether neglecting homogeneous droplet nucleation is justified for a specific use case.
- A systematic investigation confirmed that ambient temperature and aerosol number concentration are the most important predictors for the number of ice crystals formed. Moreover, we showed that for the subspace defined by $T_a \leq 225$ K and $10 \text{ nm} \leq \bar{r}_{d, \text{ aer}} \leq 100 \text{ nm}$, the final number of ice crystals formed becomes nearly independent of ambient relative humidity as well as the size and hygroscopicity of ambient aerosol particles. This finding enables the development of a parameterization with reduced complexity within this sub-regime.

The microphysical investigations presented here are complemented by the study of Zink et al. (2025), which explores the potential role of lubrication oil particles in ice crystal formation. In Part 2 of the paper series (Zink and Unterstrasser, 2026), we present findings that focus on engine-related aspects rather than on microphysical processes of contrail formation. Finally, in the forthcoming Part 3, we will introduce a parameterization based on a neural network that has been trained with the full set of simulation results. It is designed to meet the constraints and practical needs for implementation in a general circulation model or other large-scale contrail models. These models can then be used to estimate the radiative impact of contrails from a fleet of aircraft with hydrogen combustion.

Appendix A

The lognormal particle-size distribution reads

$$n(r) = \frac{N}{\sqrt{2\pi}} \frac{1}{\ln \sigma_r} \frac{1}{r} \exp \left[-\frac{1}{2} \left(\frac{\ln r / \bar{r}}{\ln \sigma_r} \right)^2 \right], \quad (\text{A1})$$

where r is the particle radius, $n(r)$ the number density, N the total number, $\bar{r}$ the geometric mean radius and $\sigma_r > 1$ the

geometric width. The geometric width σ_m of a corresponding mass distribution is related to σ_r by

$$\sigma_r = \sigma_m^k, \quad (\text{A2})$$

where $k = 1/3$ for spherical particles. In the box model, σ_m is used internally. By mistake, Bier et al. (2024) used the relation $\sigma_{r,\text{wrong}} = k \cdot \sigma_m$ instead of Eq. (A2), resulting in incorrect values shown in their Fig. 5d. The correct values $\sigma_{r,\text{correct}}$ are then given by

$$\sigma_{r,\text{correct}} = (3 \cdot \sigma_{r,\text{wrong}})^{1/3}. \quad (\text{A3})$$

These corrected values are displayed in Fig. A1.

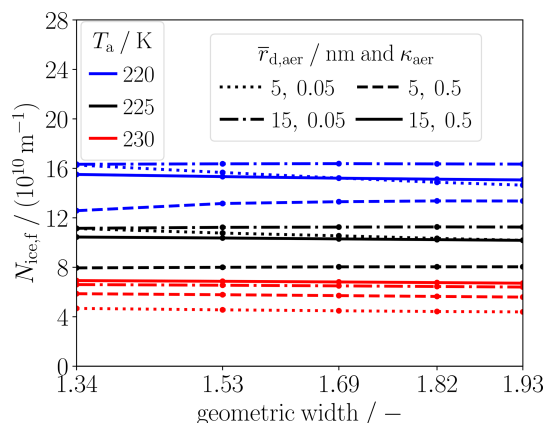


Figure A1. Corrected Fig. 5d of Bier et al. (2024). Depicted is the final number of ice crystals formed $N_{\text{ice},f}$ as a function of the geometric width of the background aerosol distribution. Simulation results are shown for different ambient temperatures T_a and different combinations of geometric mean radius $\bar{r}_{d,\text{aer}}$ and hygroscopicity κ_{aer} for the number concentration $n_{\text{aer}} = 600 \text{ cm}^{-3}$. In the original figure, wrong values of the geometric width are displayed on the x-axis.

Appendix B

Figure B1 demonstrates that evaluating the maximum nucleation rate, as done in Sect. 3.2, provides a robust indicator of the integrated total number. Shown are results for the ambient temperature and pressure combinations used in Fig. 7a. The maximum nucleation rate on entrained ambient aerosols scales nearly linearly with the ambient aerosol number concentration for the evaluated conditions. This maximum therefore indicates the order of magnitude of the integrated total number. Moreover, under the assumption that plume relative humidity and temperature evolve along the mixing line, a nearly linear relationship between the maximum homogeneous nucleation rate and the integrated number is evident.

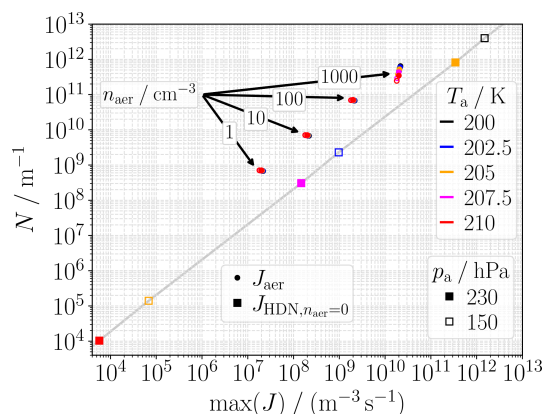


Figure B1. Maximum of nucleation rate $\max(J)$ and integrated number $N = \int J(t) \hat{A}(t) dt$ for different combinations of ambient temperature T_a (indicated by color) and pressure p_a (filled vs. unfilled markers). Results are presented for droplet activation on ambient aerosols (circle markers), obtained from box-model simulations using several aerosol number concentrations n_{aer} . Moreover, results are shown for the HDN rates that would arise if the plume relative humidity and temperature evolved along the mixing line (square markers). These results are connected by the grey line.

Data availability. The box-model simulation results, together with the plotting scripts required to reproduce the figures presented in this study, are available in a Zenodo repository (<https://doi.org/10.5281/zenodo.17977711>, Zink, 2025).

Author contributions. JZ: Conceptualization, Data curation, Formal analysis, Investigation, Methodology, Software, Validation, Visualization, Writing – original draft, Writing – review and editing. SU: Conceptualization, Methodology, Funding acquisition, Software, Supervision, Project Administration, Writing – review and editing. UB: Discussion

Competing interests. The contact author has declared that none of the authors has any competing interests.

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P2. Contrail formation for aircraft with hydrogen combustion - Part 2: Engine-related aspects



Contrail formation for aircraft with hydrogen combustion – Part 2: Engine-related aspects

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Abstract. The number of ice crystals formed in nascent contrails strongly influences contrail-cirrus life cycle and radiative forcing. Previous studies on contrails from hydrogen combustion focused on microphysical processes that affect the ice crystal number. These studies, however, paid less attention to engine-related aspects. To fill this gap, we investigate how the exhaust plume evolution is thermodynamically influenced by (i) the overall efficiency of propulsion, (ii) the engine exit conditions due to varying ambient conditions, (iii) the engine size and exit jet speed, and (iv) the explicit treatment of kinetic energy dissipation and entrainment of enthalpy initially contained in the bypass flow of a turbofan engine. Based on simulations with the box model version of the Lagrangian Cloud Module, we investigate how these aspects influence the contrail formation process and derive suitable (scaling) relations for the number of ice crystals $N_{\text{ice},f}$ formed on entrained ambient aerosols for hydrogen combustion. We find that the impact of a change in overall efficiency can be mimicked by adjusting the ambient pressure. Moreover, results from scenarios with different engine sizes or jet speeds can be scaled onto each other. Furthermore, for contrail formation on entrained ambient aerosols, a simplified modeling approach is sufficient, assuming that all emitted combustion heat is contained as static enthalpy in the core flow at engine exit. These relations help to derive an expression of $N_{\text{ice},f}$ through a functional relationship that relies on a reduced set of input parameters, while ensuring a generalized parameterization of $N_{\text{ice},f}$ in contrails from hydrogen combustion.

1 Introduction

1.1 Motivation

Aviation's total radiative forcing arises not only from CO₂ emissions but also significantly from non-CO₂ effects, including nitrogen oxide (NO_x) emissions and the formation of persistent contrail cirrus clouds (Lee et al., 2021). The estimation of the contrail cirrus' radiative impact requires a realistic representation of contrails in large-scale models. Therefore, the general circulation model (GCM) ECHAM has been expanded by the contrail module CCMoD (Burkhardt and Kärcher, 2009; Bock and Burkhardt, 2016). Due to the coarse resolution of GCMs, small-scale processes in the early stages of contrails can not be explicitly resolved and therefore have to be parameterized. The early ice crystal number is the key quantity of young contrails, which strongly influences

the later contrail cirrus properties, life cycle and radiative forcing (Unterstrasser and Gierens, 2010; Lewellen, 2014; Burkhardt et al., 2018; Lottermoser and Unterstrasser, 2025). For kerosene combustion, parameterizations have been developed for both the initial number of ice crystals formed (Kärcher et al., 2015) and the loss of ice crystals due to wake vortex interaction (Unterstrasser, 2016). These parameterizations have been successfully implemented in CCMoD (Bier and Burkhardt, 2019, 2022). To assess the radiative impacts of contrails from alternative aviation technologies such as hydrogen combustion, these parameterizations need to be revised. Recently, Lottermoser and Unterstrasser (2025) extended the wake vortex loss parameterization to hydrogen combustion scenarios. However, a parameterization for the initial number of ice crystals formed is still lacking for hydrogen combustion cases.

1.2 Previous research

Contrail formation theories/models range from binary decisions on whether contrails form or not (Schmidt, 1941; Appleman, 1953; Schumann, 1996; Richardson, 2025), to time-squeezed microphysical models (Kärcher et al., 2015), to fully time-resolved microphysical models. In the latter models, the dynamical representation ranges from 3D large-eddy simulations (LES) (e.g., Paoli et al., 2008, 2013; Garnier et al., 2014; Vancassel et al., 2014; Lewellen, 2020; Afkari et al., 2025) and 3D Reynolds-Averaged Navier-Stokes (RANS) models (e.g., Khou et al., 2015, 2017; Cantin et al., 2022), to 0D box models (e.g., Kärcher and Yu, 2009; Bier et al., 2022, 2024; Yu et al., 2024). A 0D box model approach uses an offline approach, meaning that the microphysics is calculated without feedback on the dynamics. Instead, the dilution, which describes plume expansion, cooling, and humidity evolution, is externally prescribed. This can be either through analytical formulations (e.g., Schumann et al., 1998) or based on output from prior performed LES or RANS simulations. The big advantage of these 0D box models is their low computational cost due to their simplified dynamic representation, which allows exploring a large parameter space of emission, aerosol and meteorological parameters with a detailed microphysical contrail formation model. At their minimal computational cost, when relying on an average trajectory, 0D models neglect any plume heterogeneity. The plume heterogeneity is accounted for when an ensemble of trajectories (so-called multi-0D approach as described in Bier et al., 2022) is used, but as long as the box model is run for each trajectory separately, diffusive processes between nearby trajectories are neglected. Therefore, Lottermoser and Unterstrasser (2024) introduced the 1D framework RadMod as a compromise between computational expensive 3D models with detailed dynamical core and low-cost 0D box models with strongly simplified dynamics. So far, only the dynamical component of this 1D framework has been described.

Previous studies on contrail formation from hydrogen combustion showed that microphysical processes strongly control the number of contrail ice crystals formed (Bier et al., 2024; Zink et al., 2025, 2026). For a comprehensive understanding of contrail formation, however, it is also essential to consider how engine characteristics influence the microphysical processes. This includes a realistic representation of how various aspects of commercial turbofan engines affect contrail formation, as well as how these influences may change with advancements in modern and future engine technologies.

Turbofan engines generate thrust through two streams: a core flow, where combustion takes place, and a bypass flow ducted around the core (Walsh and Fletcher, 2004). The overall efficiency of propulsion represents the fraction of the fuel's combustion heat converted into the work rate performed by the thrust (Schumann, 2000; Schumann et al.,

2000). The overall efficiency of propulsion depends on the flight state (Poll and Schumann, 2024) and can be expressed as the product of the thermal efficiency and the propulsive efficiency. Thermal efficiency measures the proportion of combustion heat converted into power delivered by the engine core. According to the second law of thermodynamics, this value is always less than one. Thermal efficiency has increased over the years due to higher overall pressure ratios and higher turbine inlet temperatures (Yin and Rao, 2020). Current values are around ~ 0.45 , with a practical upper limit near ~ 0.55 due to physical limitations (e.g., material properties) and constraints on NO_x emissions (Yin and Rao, 2020). Propulsive efficiency measures how effectively core delivered power is converted into thrust. Some energy inevitably remains as kinetic energy in the exhaust, so this efficiency also remains below one. The values of propulsive efficiency have increased over the years, with current values around ~ 0.8 , and are expected to increase to approximately ~ 0.85 (Yin and Rao, 2020). This increase over the years is primarily due to the adoption of higher bypass ratios, which is the ratio of the bypass to core mass flow. A higher bypass ratio means that a larger mass of air is accelerated at a lower velocity reducing the kinetic energy in the exhaust. Bypass ratios have increased from approximately ~ 2 in the 1960s, to ~ 4 – 6 in the 1980s, to ~ 8 – 10 in the 2000s, and up to around ~ 12 in the 2010s with the advent of geared turbofans (Gloeckner and Rodway, 2017; Alves et al., 2020). Future ultra-high bypass ratio engines may reach values up to ~ 20 (Gloeckner and Rodway, 2017). However, as the bypass ratio increases, so does the fan diameter, which leads to increased aerodynamic drag and installation challenges (Magrini et al., 2020), imposing a practical upper limit. To overcome this technical limit, a potential future technology could be the use of open rotor fans with bypass ratios $\gtrsim 30$ (Gloeckner and Rodway, 2017), and theoretical propulsive efficiencies of up to ~ 0.95 (Yin and Rao, 2020).

In a comprehensive study, Lewellen (2020) investigated contrail formation for kerosene combustion using a LES and an average 0D box model approach. As part of this study, Lewellen investigated the impact of engine size on dilution speed and developed a corresponding scaling law for the number of ice crystals formed on ambient aerosols. To the best of the authors' knowledge, the influence of engine size has not yet been studied for hydrogen combustion. This aspect could, however, be of particular relevance, as hydrogen-powered aviation is expected to be introduced first in regional, short- and medium-haul aircraft with smaller engines, and potentially later extended to long-haul aircraft equipped with larger engines (Tiwari et al., 2024; Soleymani et al., 2024).

By comparing a wide range of simulations, Lewellen (2020) also found that a 0D box model approach generally overestimates ice crystal numbers relative to LES results when simulating contrail formation on emitted particles with high numbers. In contrast, box model results closely match

the LES outcomes for low particle numbers or contrail formation on entrained ambient aerosols (which is the case in our setups). Hence, a 0D box model approach is deemed appropriate for our study, which deals with contrail formation on entrained ambient aerosols for hydrogen combustion.

1.3 Scope and outline of the study

Here we literally repeat the according subsection “Scope and outline of the study” of Part 1 (see Sect. 1.2 in Zink et al., 2026): Our overarching goal is to develop a parameterization for the final number of ice crystals formed for aircraft with hydrogen combustion, suitable for implementation in GCMs and other large-scale contrail models. Specifically, we seek a functional relationship of the form

$$N_{\text{ice},f} = N_{\text{ice},f}(a_{\text{atmosphere}}, a_{\text{aerosol}}, a_{\text{aircraft}}), \quad (1)$$

where $a_{\text{atmosphere}}$ denotes a set of variables characterizing the background atmosphere (e.g., ambient temperature), a_{aerosol} represents properties of ambient aerosols (number concentration, size distribution and solubility) and a_{aircraft} includes aircraft-related parameters (e.g., engine size).

Our objective is to identify a functional relationship that balances simplicity with physical fidelity. In other words, we aim to capture the impact of the key processes that govern ice crystal formation in a form that is simple enough to be easily applied in other models (level of complexity, computing time, ease of implementation). In Parts 1 and 2 of a trilogy of papers, we systematically explore a broad parameter space and address aspects that have not been explored before to gain a deep insight into the physical processes influencing the ice crystal formation. This allows us to select the set of variables that constitute the inputs to the parameterization of $N_{\text{ice},f}$.

While a previous $N_{\text{ice},f}$ parameterization of contrail formation (Kärcher et al., 2015) used a first-principles-based concept, the current work across Parts 1 to 3 employs a hybrid approach. It combines a data-driven advanced regression method to fit a multidimensional database of contrail formation simulations with analytical scaling relations. To keep the number of dimensions in the simulation database as small as possible, we identify conditions under which the sensitivity to specific variables is negligible, and also employ analytical scaling relations derived from sensitivity simulations.

In Part 1, we focus on the roles of atmospheric variables $a_{\text{atmosphere}}$ and aerosol properties a_{aerosol} . Aircraft-related parameters a_{aircraft} are addressed in Part 2. The final parameterization, synthesizing insights from Parts 1 and 2, will be presented in Part 3.

In the current study, we incorporate the leading effects of engine-related aspects into the simulations. In Sect. 2 we provide the theoretical background about the extensions made to our used box model (described in Sect. 3). We then investigate the impact of these aspects on the number of ice crystals formed (Sect. 4) before we discuss the findings in the light

of existing literature and propose possibilities for future research (Sect. 5). Finally, we conclude with a discussion of how our findings can be used in the development of a generalized parameterization of ice crystal number (Sect. 6).

2 Theoretical considerations

In this section, we describe how various engine-related aspects influence the thermodynamic evolution of the exhaust plume. These considerations are not restricted to the specific model used. Nevertheless, they motivate and inform the extensions made to our box model (described in Sect. 3). Furthermore, the considerations are valid for both hydrogen and kerosene combustion and do not involve microphysics, making them, for example, independent of assumptions about the type of ice-forming particles.

In a first step, we shortly summarize the most relevant equations describing the classical thermodynamic contrail formation theory (Sect. 2.1). We then present theoretical estimates of how changes in overall efficiency of propulsion (Sect. 2.2), ambient temperature and pressure as well as jet velocity and size (Sect. 2.3) influence the jet dilution and plume thermodynamics. Finally, we introduce a framework that allows to consider the effect of the initial separation of the exhaust into a core and bypass flow on the plume thermodynamical evolution in our box model (Sect. 2.4).

2.1 Classical thermodynamic theory

We review and present the equations necessary for understanding the considerations in the subsequent sections. Detailed derivations and explanations can be found in Bier et al. (2022, 2024).

Fuel is combusted in an aircraft engine to produce thrust, propelling the aircraft forward in accordance with Newton’s third law of motion. In this context, the overall efficiency of propulsion (Schumann, 2000)

$$\eta = \frac{FU_{\infty}}{\dot{m}_F Q} \quad (2)$$

is defined as the ratio of work rate performed by the thrust F at aircraft speed U_{∞} and the chemical energy supplied by the fuel, which is determined by the fuel flow rate $\dot{m}_F$ and the mass-specific heat of combustion Q (also known as lower calorific value). The remaining part of the chemical energy $\dot{m}_F Q(1 - \eta)$, which does not contribute to generating the thrust, is contained in the exhaust air in the form of excess total enthalpy above ambient levels. The total enthalpy is the sum of static enthalpy and kinetic energy. Additionally, the combustion of fuel adds water vapor to the core exhaust, quantified by the fuel-dependent water vapor (mass) emission index EI_v .

We refer to the core exhaust as plume and to individual parts of it as plume parcels. Each plume parcel mixes with

cold ambient air downstream of the engine. Classical thermodynamic contrail formation theory assumes that the core and bypass air of a turbofan engine are fully mixed by the time contrail formation begins (or, equivalently, that the emitted enthalpy is entirely contained within the core flow at the engine exit). Additionally, it assumes a stagnant exhaust plume, such that the entire kinetic energy is presumed to have been dissipated into heat at the onset of contrail formation. Furthermore, the theory assumes the same entrainment rate ω for both enthalpy and mass, implying a Lewis number of one. This assumption is generally reasonable, as turbulent diffusion is expected to dominate over molecular diffusion under contrail formation conditions within a strong jet. The entrainment rate is defined as

$$\omega(t) = -\frac{d \ln \mathcal{D}}{dt}, \quad (3)$$

where $\mathcal{D}$ is the dilution factor. The value of $\mathcal{D}$ is one at the engine exit and gives the mass fraction of core air in a plume parcel downstream of the engine (hence, it is a monotonically decreasing function with time/downstream position).

In addition to the stated assumptions, an isobaric mixing process is assumed. Furthermore, when relating static enthalpy and temperature, the slight temperature dependence of the specific heat capacity at constant pressure c_p is neglected (Schumann, 1996). The temperature evolution of a plume parcel is then governed by (Kärcher, 1995)

$$\frac{dT}{dt} = -\omega(t)(T(t) - T_a) + S_{LH}(t). \quad (4)$$

In Eq. (4), T_a is the ambient temperature and S_{LH} denotes a source/sink term accounting for the microphysical latent heat release/consumption during phase transitions. Analogously, the equation for the plume parcel's water vapor mass fraction χ_v is expressed as

$$\frac{d\chi_v}{dt} = -\omega(t)(\chi_v(t) - \chi_{v,a}) + S_{PH}(t), \quad (5)$$

where $\chi_{v,a}$ is the ambient level and S_{PH} is a source/sink term due to phase changes. The plume parcel's water vapor mass fraction χ_v and partial water vapor pressure e_v are related by (Schumann, 1996)

$$e_v = \frac{p_a}{\epsilon} \chi_v \quad (6)$$

with the ambient pressure p_a and the ratio of molar masses of dry air and water vapor $\epsilon = 0.622$.

Equations (4) to (6) lead for each plume parcel in the absence of microphysical processes ($S_{LH} = S_{PH} = 0$) to a universal mixing line in an $e_v - T$ diagram. The slope of this mixing line is determined by (Schumann, 1996)

$$G = \frac{EI_v c_p p_a}{\epsilon Q(1 - \eta)}. \quad (7)$$

The entrainment rate ω just tells how fast the thermodynamic quantities describing the plume parcel's state evolve along this line.

At engine exit, the exhaust is already a mixture of ambient air and fuel mass, which is described by the air-to-fuel ratio

$$C_E = \frac{Q(1 - \eta)}{c_p(T_E - T_a)}, \quad (8)$$

with T_E denoting the exit temperature. The time-dependent overall dilution of a plume parcel is then defined as

$$\begin{aligned} \mathcal{C}(t) &= \frac{C_E + 1}{\mathcal{D}(t)} \\ &\approx \frac{C_E}{\mathcal{D}(t)}, \end{aligned} \quad (9)$$

where the fuel mass is neglected in the approximation due to the typically large air-to-fuel ratios. For kerosene combustion, air-to-fuel ratios are on the order of 50–70 (Kärcher et al., 2015). These ratios may be even higher for hydrogen combustion, as the mass-specific heat of combustion is larger by a factor of 2.79 (Bier et al., 2024) and therefore less fuel is needed for the same amount of energy.

The fuel mass flow rate can be expressed as

$$\dot{m}_F = \frac{p_a \hat{A}_E U_\infty}{R_d T_E C_E} \quad (10)$$

with the specific gas constant R_d and effective core exit area

$$\hat{A}_E = A_E \frac{U_{\text{tot},E}}{U_\infty}. \quad (11)$$

The effective core exit area $\hat{A}_E$ combines the true physical exit area A_E with the ratio between total exit jet speed $U_{\text{tot},E}$ and aircraft speed U_∞ . The total jet speed $U_{\text{tot},E}$ is the sum of excess jet speed $U_{\text{jet},E}$ with respect to the ambient air and the aircraft speed U_∞ . The effective area accounts for the axial divergence of the jet and is representative of a plume parcel's volume (see Sect. 3.2.2 in Bier et al., 2024 for details). Using $\hat{A}_E$, the number of entrained ambient aerosols per meter of flightpath is given by

$$N_{\text{aer}}(t) = n_{\text{aer}} \frac{T_a \hat{A}_E}{T_E} (\mathcal{D}^{-1}(t) - 1), \quad (12)$$

where n_{aer} is the ambient aerosol number concentration.

2.2 Variation of overall efficiency

We aim to study the impact of varying supersaturations that arise from the influence of η on the slope G of the mixing line (Eq. 7). Clearly, an increase in η reflects technological advancements in engine configuration (Sect. 1.2). Here, we do not explicitly address the underlying causes of varying efficiencies among different engines (e.g., differences in engine design such as bypass ratios or jet velocities), and we

therefore neglect their potential influence on exhaust plume dynamics and the associated dilution. Such a dilution time scaling is proposed in Sect. 2.3 for other purposes. Instead, our focus is to investigate the thermodynamic influence of η on the formation of ice crystals. To this end, we present a physically consistent model setup as follows.

We assume the same ambient conditions and the same flight Mach number but an engine that is more/less efficient, i.e., a change of overall efficiency from a reference value η^* to another value η . According to Eq. (2) this implies that the fuel flow has to be adjusted to

$$\dot{m}_F = \frac{\eta^*}{\eta} \dot{m}_F^* \quad (13)$$

to maintain the thrust. We now assume that the core mass flow is preserved, as then the plume's mass and number of entrained ambient particles (Eq. 12) stay the same for a given dilution state downstream of the engine. From preserving the core mass flow, a change in the air-to-fuel ratio

$$C_E = \frac{\eta}{\eta^*} C_E^* \quad (14)$$

follows. In combination with Eq. (8) this implies a change in core engine exit temperature

$$T_E = \frac{\eta^*(1-\eta)}{\eta(1-\eta^*)} (T_E^* - T_a) + T_a, \quad (15)$$

where T_a is the ambient temperature. Equations (13) to (15) together with Eq. (10) imply a change in the core exit effective area

$$\hat{A}_E = \frac{T_E}{T_E^*} \hat{A}_E^*. \quad (16)$$

2.3 Dilution time scaling

The length and velocity scale of a free turbulent round jet are the nozzle exit radius r_E and exit velocity $U_{\text{jet},E}$, respectively (Pope, 2000). We write down the Reynolds-averaged mean momentum equation in polar-coordinates (Kärcher and Fabian, 1994; Lottermoser and Unterstrasser, 2024), which reads in non-dimensional form

$$\hat{\rho} \hat{U} \frac{\partial \hat{U}}{\partial \hat{x}} + \hat{\rho} \hat{V} \frac{\partial \hat{U}}{\partial \hat{r}} = \frac{\hat{D}_T}{\hat{r}} \frac{\partial}{\partial \hat{r}} \left(\hat{\rho} \hat{r} \frac{\partial \hat{U}}{\partial \hat{r}} \right) \quad (17)$$

with the scaled axial velocity $\hat{U} = U/U_{\text{jet},E}$, radial velocity $\hat{V} = V/U_{\text{jet},E}$, axial coordinate $\hat{x} = x/r_E$, radial coordinate $\hat{r} = r/r_E$, density $\hat{\rho} = \rho/\rho_0$, and turbulent viscosity $\hat{D}_T = D_T/(r_E U_{\text{jet},E})$.

Since $\hat{D}_T \approx \text{const.}$ (Pope, 2000), solving Eq. (17) together with the continuity equation, temperature equation, and equation of state gives a universal solution for the scaled variables. Looking at a time increment

$$dt = \frac{dx}{U} = \frac{d\hat{x}}{\hat{U}} \frac{r_E}{U_{\text{jet},E}} \quad (18)$$

and setting $d\hat{x} = d\hat{x}^* \cdot 1$ and $\hat{U} = \hat{U}^* \cdot 1$ (due to the universal solution for the scaled variables), it follows the relation

$$dt = \frac{U_{\text{jet},E}^*}{U_{\text{jet},E}} \cdot \frac{r_E}{r_E^*} \cdot dt^* = s_{\text{shear}} \cdot s_E \cdot dt^* = s_{\text{dil}} \cdot dt^*, \quad (19)$$

where asterisks symbols denote reference values. In Eq. (19) we use the definitions

$$s_{\text{shear}} := U_{\text{jet},E}^*/U_{\text{jet},E} \quad (20a)$$

$$s_E := r_E/r_E^* \quad (20b)$$

$$s_{\text{dil}} := s_{\text{shear}} \cdot s_E. \quad (20c)$$

This dilution time scaling (Eq. 19) was first proposed by Lewellen (2020). By using $U_{\text{jet},E}$ as velocity scale, we implicitly assume a strong jet speed regime (Chu et al., 1999), where the jet dynamics are similar to a setup without relative movement between jet source (here aircraft engine) and environment. Far downstream of the aircraft engine, however, when the jet has been decelerated, the dilution is influenced by the coflow velocity U_∞ (Chu et al., 1999; Kärcher and Fabian, 1994; Enjalbert et al., 2009; Lottermoser and Unterstrasser, 2024). Moreover, $\hat{D}_T \approx \text{const.}$ might be only a valid assumption when a self-similar flow has been established (Pope, 2000; Lottermoser and Unterstrasser, 2024). In addition, the dynamical influence of a bypass flow is not explicitly treated in the above derivation. Nevertheless, as suggested by Lewellen (2020), Eq. (19) may contain the leading factors of a dilution time scaling. In the analysis of our simulation results, the scaling properties presented so far will help to reveal underlying and possibly hidden relations between seemingly different scenarios.

2.3.1 Impact of ambient conditions on engine exit conditions

In many cases, we set up box model simulations using ambient conditions (ambient temperature T_a and ambient pressure p_a) that differ from those used in the Computational Fluid Dynamics (CFD) simulations (T_a^* and p_a^*) from which the dilution factor is extracted. The ambient conditions, in turn, influence the engine exit conditions and jet dilution speed. To account for this, we follow the procedure recommended by Lewellen (2020). He suggests preserving temperature and pressure ratios, Mach numbers, and overall efficiency following common industry practice (Volponi, 1998; Kurzke, 2003; Walsh and Fletcher, 2004). This leads to the scaling relations summarized in Table 1. Note that the scaling refers to total temperatures and pressure values (defined in Appendix A). However, neglecting the slight dependency of the adiabatic index κ on the temperature, this holds also for static temperature and pressure values.

We use the scaling relations in Table 1 to prescribe the engine exit conditions in the box model (e.g., $T_E = T_a/T_a^* \cdot T_E^*$). The velocity scale follows from preserving Mach numbers together with the fact that the speed of sound scales with $T^{1/2}$. According to this velocity scale $(T_a/T_a^*)^{1/2}$ and Eq. (19), the dilution time scales as

$$s_{\text{dil}} = s_{\text{shear}} = \left(\frac{T_a^*}{T_a} \right)^{1/2}. \quad (21)$$

2.3.2 Engine size scaling

Assuming an otherwise comparable engine (unchanged temperatures, pressures, velocities, bypass ratio, overall efficiency of propulsion, and cruise conditions), but scaling the exit radius r_E by a factor s_E leads to the following scaling relations (Lewellen, 2020): The exit area scales with s_E^2 , and accordingly also the fuel flow and thrust if everything else stays the same. Moreover, the dilution time scales with $s_{\text{dil}} = s_E$ (Eq. 19). Although s_{dil} has the same value as s_E in this consideration, we explicitly distinguish between them to disentangle the geometric effect from the effect on the dilution.

Clearly, scaling the same engine in size is a rather academically-driven approach and physical and technical limitations have to be considered in real-world engine design (see Lewellen, 2020 for details). Nevertheless, the leading impact of engine size on the number of ice crystals formed can be studied with this approach.

2.4 Treatment of bypass flow and kinetic energy dissipation

As the combustion takes place in the core of a turbofan engine, excess water vapor at the engine exit is only contained in the core flow. However, part of the chemical energy released during combustion is used to drive the fans. Due to the work performed on the fluid by the blades, the bypass air contains excess static enthalpy and kinetic energy above ambient levels. Consequently, water vapor and total enthalpy are distributed differently at the engine exit of a turbofan engine.

Richardson (2025) investigated contrail formation criterion for various propulsion systems. Assuming that the core and bypass of a turbofan are already well-mixed at engine exit, this mixed exhaust is already supersaturated in his investigated hydrogen combustion case (see his Fig. 4b). As this well-mixed state is one of the assumptions of the classical thermodynamic contrail formation theory (Sect. 2.1), this approach becomes insufficient when simulating the time-resolved contrail formation process. Therefore, a more sophisticated modeling approach is needed accounting for the initial separation of emitted total enthalpy into the core and bypass flow.

2.4.1 Revised temperature equation

The goal of this section is to derive a revised temperature equation when two main assumptions of the classical thermodynamic theory (Sect. 2.1) are dropped: The first assumption is that all kinetic energy has been completely converted into heat at the onset of contrail formation and the second is that the core and bypass air of a turbofan engine are already fully mixed at this stage.

To describe the initial separation of emitted total enthalpy into the core and bypass flow, we introduce the (time-constant) scalar factor

$$\begin{aligned} \beta &= \frac{E_{\text{tot,core}} \dot{m}_{\text{core}}}{E_{\text{tot,core}} \dot{m}_{\text{core}} + E_{\text{tot,bypass}} \dot{m}_{\text{bypass}}} \\ &= \frac{E_{\text{tot,core}}}{E_{\text{tot,core}} + E_{\text{tot,bypass}} \cdot b} \end{aligned} \quad (22)$$

with the core and bypass mass flows $\dot{m}_{\text{core}}$, $\dot{m}_{\text{bypass}}$, the bypass ratio $b = \dot{m}_{\text{bypass}}/\dot{m}_{\text{core}}$ and the mass-specific total enthalpies at engine exit

$$\begin{aligned} E_{\text{tot},y} &= E_{\text{static},y} + E_{\text{kin},y} \\ &= c_p(T_{E,y} - T_a) + \frac{1}{2}(U_{\text{tot},E,y} - U_\infty)^2, \end{aligned} \quad (23)$$

which are evaluated in a frame of reference fixed to the ambient air (Schumann, 2000). In Eq. (23), y denotes core or bypass, c_p is the specific heat capacity at constant pressure, $T_{E,y}$ denotes exit temperature, T_a is the ambient temperature and $U_{\text{tot},E,y}$ is the sum of excess jet velocity $U_{\text{jet},E,y}$ and freestream velocity U_∞ . Note that the calculation of the static enthalpy with $c_p(T_{E,y} - T_a)$ is a simplification of the formula $\int_{T_a}^{T_{E,y}} c_p(\tilde{T}) d\tilde{T}$ neglecting the temperature-dependency of c_p (Schumann, 1996) and assumes that the static pressure at engine exit has already relaxed to the ambient pressure.

The factor β can take values between zero and one. The term $\beta \dot{m}_F Q(1 - \eta)$ is the part of emitted combustion heat that is contained in the core flow at the engine exit. The remaining part $(1 - \beta) \dot{m}_F Q(1 - \eta)$ is contained in the bypass flow distributed over a b times larger air mass.

Therefore, downstream of the engine, three air masses with initially different properties mix: Hot core air containing excess water vapor, moderately heated bypass air without a water vapor add-on, and cold ambient air with the ambient moisture level. Each air parcel downstream of the engine contains a specific fraction of each of the three air masses. Since excess water vapor (the prerequisite for contrails) is only contained in the core flow, we define an air parcel that contains core air as a 'plume parcel'. This is in accordance with the definition of the dilution factor $\mathcal{D}$ as mass fraction of core air.

We define the time-dependent factor

$$\gamma(t) := \frac{1}{b} \frac{B(t)}{\mathcal{D}(t)} \quad (24)$$

Table 1. Scales for varying ambient conditions. The subscript “a” stands for ambient. Asterisk denote reference values at which the CFD simulation was performed.

variable	temperatures	pressures	densities	velocities	fuel flow
scale	T_a/T_a^*	p_a/p_a^*	$(p_a/p_a^*) \cdot (T_a^*/T_a)$	$(T_a/T_a^*)^{1/2}$	$p_a/p_a^* \cdot (T_a/T_a^*)^{1/2}$

as the ratio between the fraction of bypass air in the plume parcel $\mathcal{B}$, and the fraction of core air in the plume parcel $\mathcal{D}$ normalized by the bypass ratio b . It holds $\gamma = 0$ at core engine exit and $\gamma \rightarrow 1$, when core and bypass air are well mixed. With the definition of γ , we can write down the equation for the plume parcel’s mass-specific total enthalpy for an isobaric mixing process as

$$\begin{aligned}
 E_{\text{tot}}(t) &:= c_p(T(t) - T_a) + E_{\text{kin}}(t) \\
 &= \frac{Q(1-\eta) \cdot [\beta + (1-\beta)\gamma(t)] - h_a}{\mathcal{C}(t)} \\
 &\approx \frac{Q(1-\eta) \cdot [\beta + (1-\beta)\gamma(t)]}{\mathcal{C}(t)} \quad (25)
 \end{aligned}$$

with the plume parcel’s static temperature T , kinetic energy E_{kin} and the overall dilution $\mathcal{C}$ (Eq. 9). Here, we neglect the ambient static enthalpy h_a on the right-hand side of Eq. (25) (as done in Schumann, 1996). Furthermore, we just write E_{kin} instead of the explicit form as done in Eq. (23) for reasons explained in Sect. 2.4.2. According to Eq. (25), the plume parcel’s mass-specific total enthalpy is determined by the diluted mass-specific core enthalpy $\beta Q(1-\eta)/\mathcal{C}$ and by the diluted mass-specific bypass enthalpy $(1-\beta)Q(1-\eta)\gamma/\mathcal{C}$, which has been gradually mixed into the plume parcel.

Evaluation of Eq. (25) at core engine exit (denoted by the subscript “E”, the subscript “core” is omitted in the following) gives the air-to-fuel ratio

$$\mathcal{C}_E = \frac{\beta Q(1-\eta)}{c_p(T_E - T_a) + E_{\text{kin},E}}. \quad (26)$$

Note that compared to Eq. (8), the factor β and $E_{\text{kin},E}$ arise additionally in Eq. (26).

Isolating the term $Q(1-\eta)$ in Eqs. (25) and (26) and equating both equations, leads to the generalized state equation of plume temperature

$$\begin{aligned}
 T(t) &= T_a - \frac{E_{\text{kin}}(t)}{c_p} + \mathcal{D}(t) \cdot \left[(T_E - T_a) + \frac{E_{\text{kin},E}}{c_p} \right] \\
 &\quad \cdot \frac{\beta + (1-\beta)\gamma(t)}{\beta} \quad (27)
 \end{aligned}$$

at any time instance. Taking the logarithmic derivative in time of Eq. (27) leads together with the definition of the entrainment rate (Eq. 3) to the general ODE for plume temperature

$$\begin{aligned}
 \frac{dT}{dt} &= \left[-\omega(t) + \frac{(1-\beta) \frac{d\gamma}{dt}}{\beta + (1-\beta)\gamma(t)} \right] \\
 &\quad \cdot \left[T(t) - T_a + \frac{E_{\text{kin}}(t)}{c_p} \right] - \frac{1}{c_p} \frac{dE_{\text{kin}}}{dt} + S_{\text{LH}}(t) \\
 &= -\hat{\omega}(t) \left[T(t) - T_a + \frac{E_{\text{kin}}(t)}{c_p} \right] - \frac{1}{c_p} \frac{dE_{\text{kin}}}{dt} \\
 &\quad + S_{\text{LH}}(t) \quad (28)
 \end{aligned}$$

with $\hat{\omega} = \omega - (1-\beta) d\gamma/dt [\beta + (1-\beta)\gamma]^{-1}$. In Eq. (28), we added a source/sink term S_{LH} accounting for the micro-physical latent heat release/consumption during phase transitions.

Compared to Eq. (4), Eq. (28) includes two additional physical processes. Firstly, the adapted entrainment rate $\hat{\omega}$ includes the effect of the gradual entrainment of the enthalpy initially contained in the bypass. Secondly, it accounts for the entrainment of bypass kinetic energy into the plume and for the viscous heating within the plume via the derivative of kinetic energy. As soon as core and bypass air are well mixed ($\gamma \rightarrow 1$, $d\gamma/dt \rightarrow 0$) and the kinetic energy has dissipated into heat ($E_{\text{kin}} \rightarrow 0$, $dE_{\text{kin}}/dt \rightarrow 0$), Eq. (28) reduces to Eq. (4). Since water vapor is released only in the core flow, the differential equation for the water vapor mass fraction χ_v is fully described by Eq. (5) without adaptations needed.

As stated in Sect. 2.1, the classical thermodynamic theory leads to a universal mixing line for all plume parcels. In contrast, when considering explicitly the mixing of core and bypass air (Eq. 28), each plume parcel can follow a distinct mixing curve determined by the time evolution of $\mathcal{D}$, γ and E_{kin} . However, each mixing curve converges towards the universal mixing line when core and bypass air are well-mixed and kinetic energy has dissipated into heat downstream of the engine.

Therefore, we intend to compare simulations incorporating the general ODE for plume temperature (Eq. 28) to the more simplified approach, where we assume that all emitted combustion heat is already contained in form of static enthalpy in the core at engine exit, i.e., a stagnant plume with $\tilde{\beta} = 1$ and $\tilde{E}_{\text{kin},E} = 0$. If we kept the same core exit temperature, this would imply a higher air-to-fuel ratio (Eq. 26 with $\tilde{\beta} = 1$ and $\tilde{E}_{\text{kin},E} = 0$) and would wholly neglect the kinetic energy and the enthalpy contained in the bypass flow at engine exit. Therefore, a physically more reasonable approach is to prescribe the same air-to-fuel ratio $\tilde{\mathcal{C}}_E = \mathcal{C}_E$,

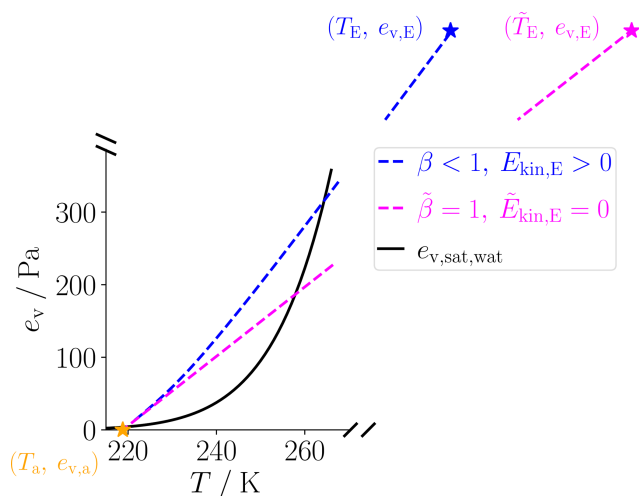


Figure 1. Exemplary mixing curve (plume partial pressure of water vapor e_v vs. temperature T) with an explicit treatment of kinetic and bypass energy (blue) compared to the universal mixing line for a stagnant plume (magenta), where the emitted combustion heat is assumed to be contained in form of static enthalpy in the core flow at engine exit. Stars denote exit and ambient conditions, respectively. The exit temperature for the stagnant plume has to be adjusted after Eq. (29) to ensure the same energy input into the system. The black curve depicts the saturation water vapor pressure over water. While this figure is intended to serve as an illustrative example, it is based on the values taken from the RANS data presented in Sect. 2.4.2.

which means a change in core exit temperature

$$\tilde{T}_E = T_a + \frac{T_E - T_a}{\beta} + \frac{E_{\text{kin},E}}{c_p \beta}. \quad (29)$$

In this approach, the total enthalpy input into the system is the same as for the case with explicit treatment of the bypass flow and kinetic energy. The effective core exit area, however, has to be adjusted according to Eq. (16) to have the same core air mass flow into the system, such that the number of entrained aerosols is the same in both approaches (Eq. 12). These two approaches are illustrated in Fig. 1 for an average trajectory (see Sect. 2.4.2 for a proper definition).

2.4.2 Evaluation with RANS data

Airbus provided us with RANS simulation data for an isolated generic turbofan engine burning hydrogen and flying at an ambient temperature $T_a = 218.8 \text{ K}$, ambient pressure $p_a = 238.42 \text{ hPa}$ with an aircraft speed $U_\infty = 231 \text{ m s}^{-1}$. For the simulation they used the compressible multi-species finite volume solver FLUSEPA, developed by the Ariane-Group (Brenner, 1991; Pont et al., 2017). Passive tracers have been seeded into the core and bypass flow to track the fractions of the different air masses (core, bypass, ambient) within each grid box at any downstream position. We obtained a 3D volume of data covering both core and bypass

flow, starting just downstream of the engine exit and ranging up to a downstream distance of about 300 m.

Pressure levels above the background are encountered near the engine exit (Fig. 2a). Since these fluctuations are relaxed to the background when contrail formation starts, the assumption of an isobaric mixing process during contrail formation is justified. Nevertheless, in order to evaluate enthalpy flows near the engine exit, we calculate potential temperature, “potential” density, and “potential” velocity as

$$T_{\text{pot}} = T \left(\frac{p_a}{p} \right)^{R_d/c_p} \quad (30a)$$

$$\rho_{\text{pot}} = \frac{p_a}{R_d T_{\text{pot}}} \quad (30b)$$

$$U_{\text{tot,pot}} = \frac{\rho}{\rho_{\text{pot}}} U_{\text{tot}} \quad (30c)$$

using the gas constant of air R_d and the specific heat capacity at constant pressure c_p . These potential variables are free of those pressure fluctuations near the engine exit (Lewellen, 2020). The potential temperature is the temperature of an air parcel that results when it is adiabatically compressed/expanded to ambient pressure (in atmospheric physics, typically the surface pressure is used as reference, here p_a is the reference pressure). The definition of potential density follows from the ideal gas law. By using potential velocity values, the mass flows are maintained. These potential variables reduce to the actual temperature T , density ρ , and velocity U_{tot} when pressure equals the ambient pressure p_a .

With these potential variables, we evaluate the integrated total enthalpy flow

$$\begin{aligned} \dot{E}_{\text{tot}}(x) &= \dot{E}_{\text{static}}(x) + \dot{E}_{\text{kin}}(x) \\ &= \sum_i \left[c_p (T_{\text{pot},i} - T_a) + \frac{1}{2} (U_{\text{tot,pot},i} - U_\infty)^2 \right] \\ &\quad \cdot \rho_{\text{pot},i} A_i U_{\text{tot,pot},i}, \end{aligned} \quad (31)$$

where i goes over all grid boxes of interest with cross-sectional area A_i at a certain downstream distance x . Evaluation of Eq. (31) over the whole exhaust, i.e., grid boxes where fractions of bypass and/or core air are contained, confirms that kinetic energy is dissipated into heat, yet the total enthalpy flow is a conserved quantity (Fig. 2b). The core plume enthalpy flow (grid boxes with core air fractions), however, increases with downstream distance until the bypass energy is fully entrained into the plume at $x \approx 60 \text{ m}$. Moreover, the kinetic energy flow within the core plume increases within the first $x \approx 40 \text{ m}$ meaning that the entrainment of kinetic energy from the bypass flow into the plume exceeds the viscous dissipation within the plume. From the total enthalpy flows $\dot{E}_{\text{tot}}$ and $\dot{E}_{\text{tot,plume}}$ near the engine exit, we estimate $\beta \approx 0.62$. Furthermore, we estimate the core exit temperature $T_{\text{pot,E}} \approx 564 \text{ K}$, the total core jet velocity $U_{\text{tot,pot,E}} \approx 428 \text{ m s}^{-1}$ and core radius $r_E \approx 0.33 \text{ m}$. Moreover, we estimate the bypass ratio b from the ratio of the

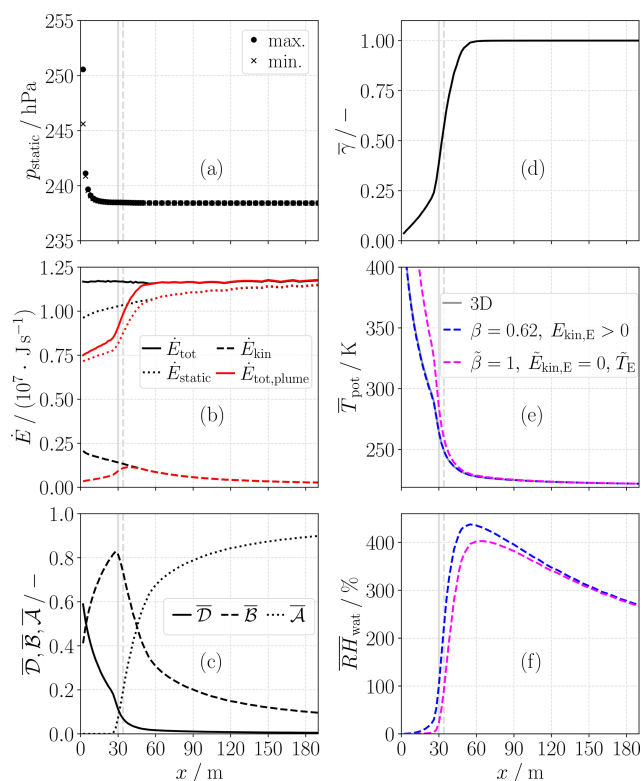


Figure 2. Evaluation of RANS data for the Airbus Turbofan engine as a function of downstream distance x with boundary conditions as listed in Table 2. **(a)** Maximum and minimum static pressure p_{static} . **(b)** Total enthalpy flow $\dot{E}_{\text{tot}}$ as sum of static enthalpy flow $\dot{E}_{\text{static}}$ and kinetic energy flow $\dot{E}_{\text{kin}}$ evaluated over the whole exhaust air, i.e., bypass and core air (black). The red curves show the total enthalpy flow and its partition evaluated within the plume defined via the core air. **(c)** Mean fractions of core air (dilution factor) $\bar{D}$, bypass air $\bar{B}$ and ambient air $\bar{A}$ within the plume. **(d)** Mean $\bar{\gamma}$ factor defined in Eq. (24). **(e)** Mean plume (potential) temperature $\bar{T}_{\text{pot}}$ extracted from the 3D field (grey curve) and calculated with the generalized state equation of plume temperature Eq. (27) (blue dashed curve) inserting mean quantities $\bar{E}_{\text{kin}}$, $\bar{D}$ and $\bar{\gamma}$. The magenta curve shows the temperature evolution where the emitted combustion heat is assumed to be contained as static enthalpy in the core flow at engine exit with adjusted exit temperature after Eq. (29). **(f)** Mean plume relative humidity over water $\bar{RH}_{\text{wat}}$ for the latter two scenarios in **(e)** calculated with mean quantities assuming a dry environment. For the two scenarios, the grey vertical lines indicate the onset of plume supersaturation $\bar{RH}_{\text{wat}} > 100\%$ and subsequent contrail formation (the same lines are depicted in each panel).

fractions $\bar{B}$ and $\bar{D}$ far downstream of the engine when core and bypass air are well-mixed. We use the estimated value as a normalization constant in the definition of γ (Eq. 24).

We calculate the average of a mass-specific quantity ξ (tracer mass fraction, momentum, static enthalpy, kinetic energy, ...) as mass flow weighted average over the core plume at a certain downstream distance x , i.e.,

$$\bar{\xi} = \frac{\sum_i \rho_{\text{pot},i} A_i U_{\text{tot,pot},i} \xi_i}{\sum_i \rho_{\text{pot},i} A_i U_{\text{tot,pot},i}}. \quad (32)$$

This type of averaging ensures that the (tracer) mass flows and energy flows calculated with average values correspond to the total flows in the 3D field. Generally, i goes over all grid boxes involving core air, i.e., $\mathcal{D}_i > 0$. However, the physical diffusion processes are partially obscured by numerical diffusion. Therefore, we define at each downstream location x a relative threshold δ for the plume boundary and consider the set of grid boxes that fulfill

$$\{i \mid \mathcal{D}_i(x) > \delta \cdot \max(\mathcal{D}(x))\}. \quad (33)$$

Per default, we set $\delta = 0.01$, but we also tested the impact of other choices (Sect. 4.5).

It is not necessarily true, that $\bar{E}_{\text{kin}} = \frac{1}{2}(\bar{U}_{\text{tot,pot}} - U_{\infty})^2$. Here, $\bar{U}_{\text{tot,pot}}$ is obtained by substituting $\xi_i = U_{\text{tot,pot},i}$ into Eq. (32). Instead, the correct calculation of the average kinetic energy $\bar{E}_{\text{kin}}$ is done by setting $\xi_i = \frac{1}{2}(U_{\text{tot,pot},i} - U_{\infty})^2$ in Eq. (32). These correctly calculated $\bar{E}_{\text{kin}}$ values have to be inserted into Eq. (28) when an average plume trajectory is considered. For such an average plume trajectory, we convert a downstream distance x to an average plume age

$$t(x) = \int_0^x d\tilde{x} / \bar{U}_{\text{tot,pot}}(\tilde{x}). \quad (34)$$

Core and bypass air mix near the engine exit (Fig. 2c). In the analysed CFD data, the core air fraction $\bar{D}$ is initially already less than one, and the bypass air fraction $\bar{B}$ larger than zero, as the first data slice is available at a downstream position slightly behind the core engine exit. In the first meters behind the engine exit, core air dilution is primarily driven by the shear between the core and bypass flow. However, before the bypass fraction $\bar{B}$ reaches its maximum at ≈ 30 m, ambient air is already contained in the plume and a noticeable increase in the dilution speed of the core air $\bar{D}$ is visible. This change in dilution speed indicates that the shear resulting from the velocity difference between the core plume and the ambient air is becoming more relevant. As this change in dilution speed occurs before the onset of microphysics, the initially reduced shear between the core and bypass flows may not have a significant influence on the contrail formation process - at least in our bulk approach with an average trajectory. However, as the bypass air is not fully contained in the core plume at the start of contrail formation ($\bar{\gamma}$ is less than one in Fig. 2d), the thermodynamics (Eq. 28) may have an impact.

The average temperature evolutions agree when calculated in two ways (Fig. 2e): directly from the 3D field by setting $\xi_i = T_{\text{pot},i}$ in Eq. (32) and by evaluating Eq. (27) inserting average quantities $\bar{E}_{\text{kin}}$, $\bar{D}$ and $\bar{\gamma}$. This justifies the approach

and its assumptions outlined in Sect. 2.4.1, in particular the assumptions of a constant c_p and the same dilution factors $\mathcal{D}$ /entrainment rates ω for enthalpy and mass. The initially higher mean plume temperature for a stagnant plume with the emitted combustion heat assumed to be contained in the core flow at the engine exit (Fig. 2e), leads to lower mean plume relative humidity values compared to the case with complete treatment of kinetic and bypass energy (Fig. 2f). The temperature and relative humidity evolutions converge when the bypass and core air are mixed, and kinetic energy has dissipated into heat.

3 Box model setup

We use the Lagrangian Cloud Module (LCM) in the box model version described in detail in Bier et al. (2024) and extended by the various aspects outlined in Sect. 2. In the particle-based LCM box model, aerosol particles and hydrometeors (droplets and ice crystals) are represented by simulation particles (SIPs). The time-resolved microphysical processes on these SIPs are simulated offline without feedback on the dynamics. Instead, dilution is prescribed analytically or using data from a previously performed CFD simulation. We incorporated dilution data from multiple sources into the box model, each briefly summarized in this section. The ambient and engine exit conditions under which the different CFD datasets were produced are provided in Table 2.

3.1 FLUDILES

The dilution is derived from a LES conducted for a single uninstalled CFM56 engine representative of an A340-300 aircraft. From this LES, Vancassel et al. (2014) generated an ensemble of 25 000 trajectories, each representing a fraction of the plume's mass/volume. Bier et al. (2024) then used a suitably merged subset of 1000 trajectories for their box model simulations. In our simulations, we utilize both this 1000-trajectory ensemble and a single average trajectory, which represents the mass-weighted average of the ensemble (see Supplement in Bier et al., 2022). The dilution factor is determined from the data by treating the temperature as a passive tracer. In the trajectory ensemble approach, box model simulations are performed for each member and results are presented as sum over all trajectories for extensive variables (e.g., ice crystal number) and as mass-weighted average for intensive variables (e.g., temperature). For the average trajectory approach, a single box model simulation is performed.

3.2 Lewellen

We use the average dilution factor obtained from a temporal LES simulation for an isolated engine representative of a B737 aircraft (Lewellen, 2020). The dilution factor is determined by an exhaust-weighted average (see Sect. 2d in

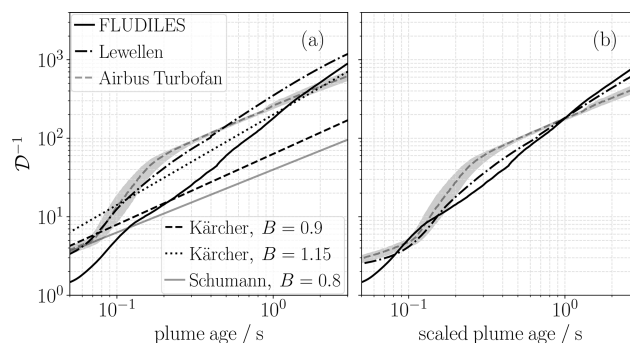


Figure 3. (a) Inverse dilution factor for average trajectories derived from various data sources. For the Airbus Turbopan, the dashed line represents the case where $\delta = 0.01$ is set in Eq. (33). The boundaries of the shaded region correspond to $\delta = 0.05$ and $\delta = 0.002$, respectively. The solid gray line is calculated with the Kärcher formula (Eq. 35) with an exponent $B = 0.8$ as proposed by Schumann et al. (1998). (b) Inverse dilution factors after scaling the core exit radius and exit velocity to the values of the FLUDILES engine (Table 2) with associated dilution time scaling (Eq. 19).

Lewellen (2020) for details). These dilution data have previously been used alternatively to the FLUDILES data in Bier et al. (2022).

3.3 Airbus Turbopan

We use the average dilution factor obtained from the RANS data we obtained from Airbus. In addition to the average dilution factor $\bar{\mathcal{D}}$ we also incorporated the extracted β , $\bar{\gamma}$ and $\bar{E}_{\text{kin}}$. Details have been described in Sect. 2.4.2. The engine is designed for a Short-Medium Range (SMR) scenario (a A320 like aircraft).

3.4 Analytical Kärcher formula

We use the analytical formula presented in Kärcher et al. (2015), which reads

$$\mathcal{D}(t > \tau_m) = \left(\frac{\tau_m}{t} \right)^B \quad (35)$$

and $\mathcal{D} = 1$ for $t \leq \tau_m$ with $\tau_m \approx 0.01$ s. The exponent B determines the dilution speed with a default value set to $B = 0.9$ after Kärcher (1999). Setting $B = 1.15$ leads to a dilution evolution more comparable to the other data sources (Fig. 3a).

The time series of $\mathcal{D}$ differ substantially between the various CFD data sources (Fig. 3a). Consistent with our theoretical understanding, the dilution data show a much smaller spread after the dilution time scaling based on the engine size and jet speed (Eq. 19) is applied (Fig. 3b).

In the result section (Sect. 4) the box model initializations differ depending on the purpose of each section. Therefore, we briefly summarize the settings at the beginning of each subsection. When not stated differently, we use the

Table 2. Ambient temperature T_a , ambient pressure p_a , flight velocity U_∞ , core engine exit excess jet velocity $U_{\text{jet,E}}$, core engine exit temperature T_E and core exit radius r_E for which the various CFD data were produced.

CFD data	T_a/K	p_a/hPa	$U_\infty/\text{m s}^{-1}$	$U_{\text{jet,E}}/\text{m s}^{-1}$	T_E/K	r_E/m
FLUDILES	220	240	250 (Mach 0.84)	230	580	0.50
Lewellen	218.8	238.4	237 (Mach 0.80)	≈ 245	≈ 580	≈ 0.30
Airbus Turbofan	218.8	238.4	231 (Mach 0.78)	≈ 197	≈ 564	≈ 0.33

FLUDILES trajectory ensemble as dilution data and the baseline values listed in Table 3 as model setup. The prescribed baseline properties of ambient aerosol particles correspond to highly-soluble Aitken-mode particles. Ambient aerosol particle sizes, solubility, and number concentrations show large variability in the atmosphere (Petzold et al., 2002; Minikin et al., 2003; Hermann et al., 2003; Borrmann et al., 2010; Kaiser et al., 2019; Brock et al., 2021). In Part 1 (Zink et al., 2026), we systematically examined how these properties influence droplet activation and the subsequent homogeneous freezing of droplets into ice crystals. Although the primary focus of the current study is on engine-related parameters, we nonetheless examine a variety of ambient aerosol scenarios, covering a wide range of number concentrations (Sect. 4).

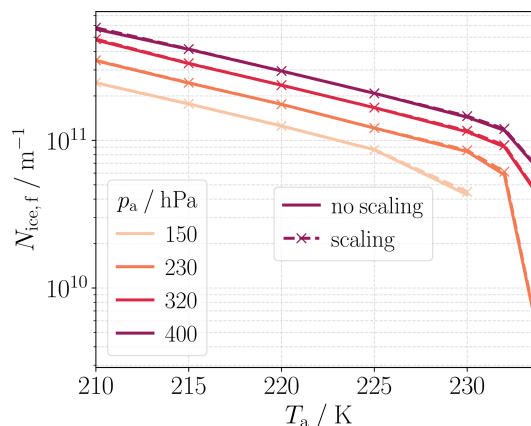
4 Results

In this section, we analyze how the different aspects described in Sect. 2 affect the contrail formation on ambient aerosols for hydrogen combustion. Specifically, we look at their impact on the final number of ice crystals formed $N_{\text{ice,f}}$, which is the ice crystal number when contrail formation is finished. Furthermore, we develop appropriate scaling relations of $N_{\text{ice,f}}$. These scaling relations allow to describe the sensitivity to selected parameters by simple analytical expressions, which are easily incorporated in the $N_{\text{ice,f}}$ parameterization.

4.1 Impact of engine exit conditions for changing ambient temperature on $N_{\text{ice,f}}$

In Sect. 2.3.1, we presented scaling relations describing how engine exit conditions and dilution speed vary with ambient temperature and pressure changes. The linear scaling of density and fuel flow with ambient pressure (Table 1 and Eq. 10) has already been consistently applied in previous box model simulations by Bier et al. (2022, 2024). In these studies, however, they held the engine exit temperature T_E constant and did not adjust the dilution speed when they changed the ambient temperature. Here, we investigate whether neglecting these changes significantly affect $N_{\text{ice,f}}$.

The FLUDILES data were produced with an ambient temperature $T_a^* = 220\text{ K}$ and an exit temperature $T_E^* = 580\text{ K}$ (Table 2). If the ambient temperature $T_a = 210\text{ K}$ is specified,

**Figure 4.** Impact of engine exit conditions for varying ambient temperature T_a on the number of ice crystals formed $N_{\text{ice,f}}$. Simulation results for scaled engine exit temperature (Table 1) and scaled dilution time (Eq. 21) with $T_a^* = 220\text{ K}$ are compared to simulations with fixed exit temperature $T_E = T_E^* = 580\text{ K}$ and without dilution time scaling applied. Results are shown for $N_{\text{ice,f}} > 0$.

the scaling suggested in Sect. 2.3.1 results in $T_E \approx 554\text{ K}$ and $s_{\text{dil}} \approx 1.02$. For $T_a = 232\text{ K}$ these two values are $T_E \approx 612\text{ K}$ and $s_{\text{dil}} \approx 0.97$. However, the difference in the number of ice crystals formed is negligible between simulation runs with the scalings applied and simulation runs with fixed $T_E = T_E^* = 580\text{ K}$ and without dilution time scaling (Fig. 4). Therefore, we can safely neglect these scaling relations in subsequent analyses and instead prescribe the same exit temperature and the same unscaled dilution regardless of the actual ambient temperature.

4.2 Scaling relation for $N_{\text{ice,f}}$ for variation of overall efficiency

This subsection analyses how $N_{\text{ice,f}}$ changes with variations of the overall efficiency of propulsion η and how $N_{\text{ice,f}}(\eta)$ can be expressed in terms of $N_{\text{ice,f}}(\eta^*)$ for a fixed reference value η^* . In a first step, we perform sensitivity studies with the FLUDILES trajectory ensemble, where a variation of η is reflected by corresponding adaptations of the engine exit conditions (as outlined in Sect. 2.2). From theoretical considerations, a higher η value implies a steeper mixing line and higher and longer-lasting supersaturation. Consistent with this, Fig. 5 shows increasing ice crystal numbers $N_{\text{ice,f}}$ with

Table 3. Baseline values of ambient pressure p_a^* , ambient relative humidity $\text{RH}_{\text{ice},a}^*$, aircraft speed U_∞^* , water vapor emission index EI_v^* , mass-specific heat of combustion Q^* , overall efficiency of propulsion η^* , exit temperature T_E^* , exit area A_E^* , exit excess jet velocity $U_{\text{jet},E}^*$, geometric mean radius of aerosol particles $\bar{r}_{\text{d,aer}}^*$, geometric width σ_{aer}^* , hygroscopicity κ_{aer}^* and number concentration n_{aer}^* .

background conditions	$p_a^* = 260 \text{ hPa}$, $\text{RH}_{\text{ice},a}^* = 115 \%$, $U_\infty^* = 250 \text{ m s}^{-1}$
fuel/engine properties	$\text{EI}_v^* = 8.94 \text{ kg kg}^{-1}$, $Q^* = 120 \text{ MJ kg}^{-1}$, $\eta^* = 0.4$
engine exit conditions	$T_E^* = 580 \text{ K}$, $A_E^* = 0.25\pi \text{ m}^2$, $U_{\text{jet},E}^* = 230 \text{ m s}^{-1}$
aerosol properties	$\bar{r}_{\text{d,aer}}^* = 20 \text{ nm}$, $\sigma_{\text{aer}}^* = 1.6$, $\kappa_{\text{aer}}^* = 0.5$, $n_{\text{aer}}^* = 1000 \text{ cm}^{-3}$

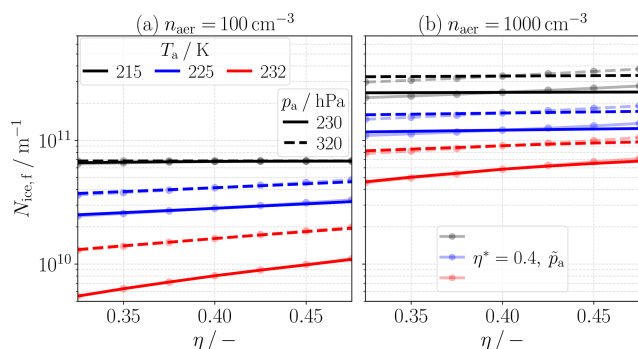


Figure 5. Influence of a variation of overall efficiency η on the number of ice crystals formed $N_{\text{ice},f}$ for three ambient temperatures T_a (different color), two ambient pressures p_a (different line styles) and two ambient aerosol number concentrations n_{aer} (different panel). Transparent lines show simulation results for fixed overall efficiency of propulsion $\eta^* = 0.4$ but adjusted ambient pressure $\tilde{p}_a$ after Eq. (36).

increasing η . Clearly, $N_{\text{ice},f}$ itself and the change of it with η depend on the meteorological background conditions. In situations with high plume supersaturations and large $N_{\text{ice},f}$ values (i.e., lower ambient temperature and higher ambient pressure), a change in η has less pronounced effect on $N_{\text{ice},f}$. For an higher ambient temperature ($T_a = 232 \text{ K}$), however, an increase in η leads to a noticeable increase in $N_{\text{ice},f}$.

The slope G of the mixing line depends on both, the overall efficiency of propulsion and the ambient pressure (Eq. 7). The value pair η and p_a corresponds to the the same slope as the value pair η^* and $\tilde{p}_a$ with the definition

$$\tilde{p}_a = p_a \frac{1 - \eta^*}{1 - \eta}. \quad (36)$$

Therefore, we try to mimic the effect of a variation of the overall efficiency by fixing its value to $\eta^* = 0.4$ but adjusting the ambient pressure after Eq. (36). In the box model setup of this simulation series with $\eta^* = 0.4$, we fix the exit temperature to $T_E^* = 580 \text{ K}$, neglecting the impact of the ambient temperature on the exit condition (Sect. 4.1) while maintaining consistency with the scaling relations presented in Sect. 2.2. Consequently, the exit conditions for the tuple (η, p_a) are different from the tuple $(\eta^*, \tilde{p}_a)$, meaning the two approaches start from different points on the mixing

line. For an ambient temperature $T_a = 225 \text{ K}$, the engine exit temperature is $T_E = 665 \text{ K}$ for $\eta = 0.35$, and $T_E = 514 \text{ K}$ for $\eta = 0.45$ using Eq. (15).

For the aerosol number concentration $n_{\text{aer}} = 100 \text{ cm}^{-3}$, the approximation with η^* and $\tilde{p}_a$ works almost perfectly (Fig. 5a). For $n_{\text{aer}} = 1000 \text{ cm}^{-3}$, the approximation slightly overestimates the ice crystal number for η values above and slightly underestimates it for values below $\eta^* = 0.4$ (Fig. 5b). The deviations come from the fact that the ambient pressure goes into other calculations within the box model (e.g., mean free path of air molecules, diffusion coefficient of water vapor) and that the starting points on the mixing line are different. However, as the deviations are only marginal, this suggests a low sensitivity of $N_{\text{ice},f}$ on the exact engine exit conditions.

In summary, changes in overall efficiency of propulsion can be well approximated by adjusting the ambient pressure. Therefore, when developing a parameterization for the number of ice crystals formed, it will be sufficient to represent the pressure dependence accurately.

4.3 Scaling relations for $N_{\text{ice},f}$ for different engine sizes

In the following, we investigate the effect of the engine size r_E on contrail formation and propose scaling relations between engine size and the number of ice crystals formed $N_{\text{ice},f}$. To do so, we perform box model simulations based on the FLUDILES trajectory ensemble. While keeping all other parameters fixed, the core exit radius r_E is scaled by the factor s_E (see definition in Eq. 20b). According to Sect. 2.3, this involves also a change of the dilution time scale by a factor s_{dil} (Eq. 19). While the scaling factors s_E and s_{dil} refer to different aspects of the problem, in our particular case, where only r_E is varied and $s_{\text{shear}} = 1$, s_{dil} takes the value of s_E .

The (effective) plume area at engine exit scales as $\hat{A}_E \propto s_E^2$. If the engine size variation had only this trivial geometric effect and the plume dilution time scale had no effect on contrail formation, then a first-order estimate would give $N_{\text{ice},f} \propto \hat{A}_E \propto s_E^2$. This first-order estimate holds, if the normalized ice crystal numbers $N_{\text{ice},f}/s_E^2$ are independent of s_E and lie on a universal curve for different s_E values. Figure 6a reveals that this is approximately the case for low aerosol number concentrations n_{aer} at ambient temperatures $T_a \lesssim 230 \text{ K}$. However, the curves corresponding to the differ-

ent s_E values start to deviate at higher aerosol number concentrations. A slower dilution leads to lower (scaled) $N_{ice,f}$ values because aerosol particles that are entrained and activated into ice crystals at an early stage have more time to consume the water vapor. While these early-activated ice crystals grow, they reduce the supersaturation, preventing later-entrained aerosols from being activated into ice crystals.

Lewellen (2020) derived a scaling relation by considering the time interval during which a plume parcel can potentially activate aerosols and the time interval required for ice crystals to grow large enough to deplete the available water vapor significantly. In our application, this scaling is expressed as (see Appendix B)

$$\frac{N_{ice,f}}{s_E^2 \cdot s_{dil}^a} \sim f(s_{dil}^{3/2} \cdot n_{aer}) \quad (37)$$

with $a = -3/2$ and f being a function that depends on ambient conditions and aerosol properties but not explicitly on the engine size/dilution speed. This means that the curves for different s_E values should collapse when the scaling is applied. Indeed, this scaling approach works reasonably well for temperatures $T_a \lesssim 230$ K (Fig. 6b). However, for $T_a = 233$ K, the curves for the different s_E values do not collapse, hinting that another timescale might become important at high ambient temperatures (which is not relevant in kerosene combustion scenarios, for which this scaling was originally developed).

We will extend the existing scaling approach by considering the limiting factor of droplet freezing. Aerosols that are activated into water droplets have to grow large enough before the freezing process is triggered (Bier et al., 2024). The duration between droplet activation and freezing into ice crystals depends on the time point at which an aerosol particle is entrained into the plume, specifically on the prevailing plume temperature, plume supersaturation, and their subsequent evolution. As a first-order estimate, we use the time difference between the first droplet activations and the first ice crystal formations in our simulations as a proxy for the freezing timescale δt_{frz} (Table 4). We compare this timescale δt_{frz} to the maximum possible duration of water supersaturation $\delta t_{supersat}$. In the absence of microphysical processes, the latter depends on dilution speed and scales linearly with s_{dil} . In Table 4, we present the average of $\delta t_{supersat}$ over all trajectories for a prescribed value of $s_{dil} = 1$.

At low ambient temperatures, supersaturations are high and long-lasting. With increasing T_a , however, $\delta t_{supersat}$ decreases. In contrast, δt_{frz} is short at low ambient temperatures and increases with increasing ambient temperature. Hence, the relative importance of δt_{frz} grows with increasing temperature. This means that, at high ambient temperatures, a substantial portion of aerosols that are entrained and activated into droplets at a later stage are unable to freeze before the relative humidity over water falls below 100 %. These droplets evaporate subsequently. Clearly, this is more pronounced for faster dilution, i.e., shorter $\delta t_{supersat}$, which ex-

plains the relative order of the three curves for $T_a = 233$ K in Fig. 6b.

However, these three curves are shifted by an approximately constant factor. This allows the freezing time scale to be accounted for by adapting the exponent a in Eq. (37). We propose maintaining $a = -3/2$ up to $T_a = 230$ K, followed by a linear increase with ambient temperature, specifically,

$$a = \begin{cases} -\frac{3}{2} & \text{for } T_a \leq 230 \text{ K} \\ \frac{1}{6}(T_a/\text{K} - 239) & \text{for } 230 \text{ K} < T_a \leq 235 \text{ K.} \end{cases} \quad (38)$$

This adapted scaling approach performs reasonably for temperatures $T_a \lesssim 233$ K (Fig. 6c). For $T_a = 234$ K, however, the symmetry breaks between the decelerated dilution ($s_{dil} = s_E = 2$) and the accelerated dilution ($s_{dil} = s_E = 0.5$). Whereas for $s_{dil} = 2$ the scaling still works reasonably well, the (scaled) $N_{ice,f}$ values are lower for $s_{dil} = 0.5$. This means that the function f introduced in Eq. (37) becomes dependent on the dilution speed, thus limiting the applicability of the scaling approach above $T_a \sim 233$ K.

4.4 Impact of different dilution data on $N_{ice,f}$

In Sect. 3, we described several data sets to prescribe the dilution in the box model. In the following, we investigate the influence of the dilution data on our model results.

In a first step, we compare results for the FLUDILES trajectory ensemble and the average trajectory (as already done by Bier et al. (2022) for contrail formation on soot particles for kerosene combustion). Both approaches yield a comparable number of ice crystals $N_{ice,f}$ when the ambient temperature T_a is below ~ 230 K (Fig. 7). At higher temperatures, however, $N_{ice,f}$ values for the ensemble approach tend to be higher than for the average trajectory approach. Furthermore, scenarios exist where no ice crystals form in the average trajectory, whereas $N_{ice,f}$ is larger than zero in the ensemble approach. How large the discrepancies between the two approaches are depends on the peak plume supersaturation (e.g., affected by ambient pressure, Fig. 7a–b) and on the aerosol properties (Fig. 7a, c, d). The key factor in understanding these differences is the interplay between the timescale of supersaturation $\delta t_{supersat}$ and freezing δt_{frz} (Sect. 4.3). In the ensemble approach, the 1000 members dilute at different speeds. Some trajectories dilute more slowly, allowing more droplets to grow sufficiently to freeze into ice crystals. In contrast, the freezing is more of a binary process in the single average trajectory approach, resulting in lower or zero ice crystal number at the same temperature.

The different dilution data were produced for different engine characteristics and background conditions (Table 2). However, we only extract the information on dilution (in terms of $\mathcal{D}$ and ω) and the information on engine size and jet speed in the subsequent analysis. Particularly, we still rely on classical contrail formation theory and do not consider the thermodynamic influence of the bypass flow and kinetic

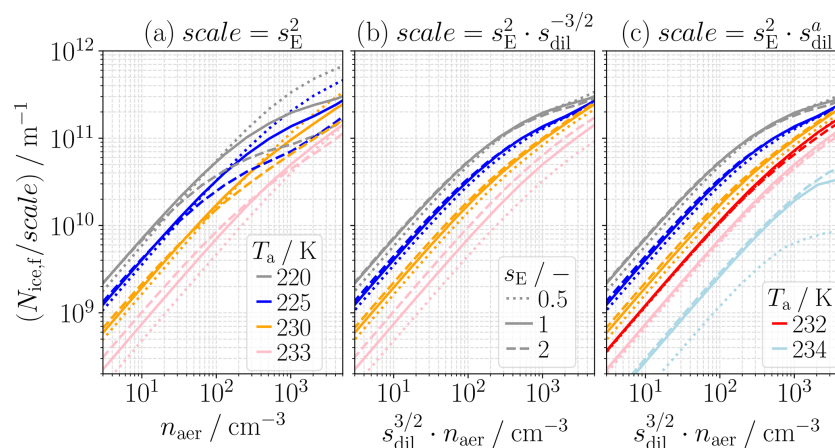


Figure 6. Scaling relations for the number of ice crystals formed $N_{\text{ice},f}$ for different engine sizes s_E (different line styles). Shown are scaled $N_{\text{ice},f}$ values as a function of (scaled) aerosol number concentration n_{aer} for different ambient temperatures T_a (different colors). **(a)** Normalization by scale of engine exit area. **(b)** Scaling after Lewellen (2020) with $s_{\text{dil}} = s_E$. **(c)** Adapted scaling with variable exponent a after Eq. (38).

Table 4. Average duration of water supersaturation $\delta t_{\text{supersat}}$ without microphysics and proxy for freezing timescale δt_{frz} for different ambient temperatures T_a for the FLUDILES trajectory data set with $s_{\text{dil}} = 1$.

T_a / K	220	225	230	231	232	233
$\delta t_{\text{supersat}}$ / s	6.5	2.3	1.4	1.2	1.1	1.0
δt_{frz} / s	< 0.1	< 0.1	0.1–0.2	0.1–0.2	0.3–0.4	0.4–0.5

energy dissipation. This will be investigated in Sect. 4.5. In each simulation setup we use the same exit temperature $T_E = 580$ K and overall efficiency $\eta = 0.4$, obviously neglecting differences among the engines. However, it disentangles the impact of those values from the influence of the dilution on $N_{\text{ice},f}$. Moreover, we intend to use the theoretically derived dilution time scaling (Sect. 2.3) with associated scaling of $N_{\text{ice},f}$ (Eq. 37) neglecting any further details in the configuration of the engines.

Since the number of entrained particles (Eq. 12) and thus the number of ice crystals formed is proportional to the effective core exit area $\hat{A}_E$ (Eq. 11), we use the geometric scale $\hat{s}_E^2 = \hat{A}_E / \hat{A}_E^*$ to make the results for the different-sized engines comparable. We use the FLUDILES engine as reference, thus $\hat{A}_E^*$ refers to its effective core area. Relating the effective core areas instead of the physical core areas (as done with the scale s_E^2 in Sect. 4.3) additionally accounts for the different ratios of total jet and aircraft velocities in the CFD data. The dilution time scale s_{dil} , however, is still determined with Eq. (19) using s_E and s_{shear} . As the FLUDILES engine is treated as reference, the associated values are $\hat{s}_E = s_{\text{dil}} = 1$ for this engine. Moreover, we set $\hat{s}_E = s_{\text{dil}} = 1$ for the Kärcher dilution as the analytical formula does not contain an explicit dependence on engine size or jet speed. Instead, the dilution speed is governed by the exponent B in Eq. (35).

Simulations using the default Kärcher dilution ($B = 0.9$ in Eq. 35), yield significantly different ice crystals numbers compared to those using the FLUDILES dilution (Fig. 8a). This difference arises from the markedly slower dilution speed (Fig. 3). However, when a faster dilution with $B = 1.15$ is used (Fig. 8b), the resulting ice crystal numbers are similar to those from the FLUDILES simulations. This suggests that the exact shape of the dilution curve over time (Fig. 3) is of lesser importance for the final number of ice crystals formed.

The faster Lewellen dilution (Fig. 3) caused by the smaller core radius (Table 2), leads to higher (scaled) $N_{\text{ice},f}$ values at high aerosol number concentrations (Fig. 8c). When the scaling after Eq. (37) is applied, the resulting curves for a given ambient temperature align reasonably well (Fig. 8d), demonstrating the consistency of the scaling approach across different dilution scenarios.

The scaling performs somewhat less ideally for the Turbofan dilution data (Fig. 8f). Especially for $T_a = 215$ K, the scaled curves have slightly different shapes. This may be partially attributed to the dynamic influence of the bypass flow on the dilution speed. Additionally, droplets do not freeze in the Airbus Turbofan case for $n_{\text{aer}} \gtrsim 1000 \text{ cm}^{-3}$ at $T_a = 232$ K in contrast to the FLUDILES simulations. Nevertheless, the scaling after Eq. (37) based on core exit conditions still accounts for the leading impact of the dilution speed on $N_{\text{ice},f}$.

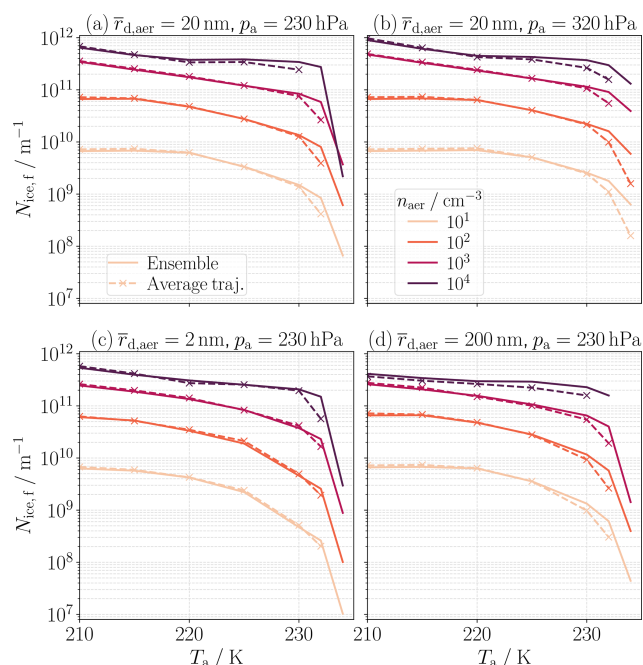


Figure 7. Comparison of FLUDILES ensemble (solid) and average trajectory (dashed) approaches. Shown are the number of ice crystals formed $N_{ice,f}$ as a function of ambient temperature T_a for different aerosol number concentrations n_{aer} (different colors). Each panel depicts results for a different combination of aerosol geometric mean radius $\bar{r}_{d,aer}$ and ambient pressure p_a . Results are shown for $N_{ice,f} > 0$.

Moreover, $N_{ice,f}$ is only weakly sensitive on the exact choice of the plume boundary in Eq. (33) (Fig. 8e–f).

4.5 Impact of bypass flow and kinetic energy dissipation on $N_{ice,f}$

Using the Airbus Turbofan dilution data, we investigate the impact on the number of ice crystals formed for the two approaches outlined in Sect. 2.4.1. The first approach explicitly considers the thermodynamics of the bypass flow, including kinetic energy effects. The second, simplified approach assumes that the whole emitted combustion heat is contained as static enthalpy in the core flow at the engine exit. In the former approach we prescribe the estimated exit conditions for the Airbus Turbofan data (Table 2 and $\beta = 0.62$) and use the extracted time evolutions of $\bar{D}$, $\bar{E}_{kin}$ and $\bar{\gamma}$ (Sect. 2.4.2). In the latter approach we make use of only $\bar{D}$ and prescribe the adjusted exit temperature $\tilde{T}_E$ after Eq. (29). Using the same $T_E = 564$ K for all ambient temperatures leads to $\tilde{T}_E = 809$ K for $T_a = 215$ K and $\tilde{T}_E = 798$ K for $T_a = 232$ K.

The former approach leads to initially higher plume supersaturation (Fig. 9a) and thus to a slightly earlier onset of droplet activation (Fig. 9b). However, this has little influence on the final number of ice crystals formed (Fig. 9b–d). This insignificant impact is due to the continuous entrainment of

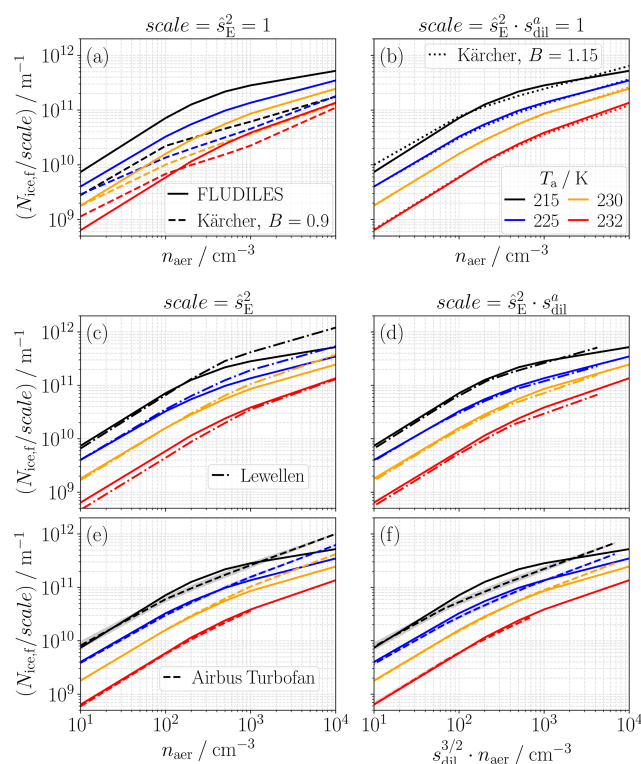


Figure 8. Impact of different dilution data on the number of ice crystals formed $N_{ice,f}$. In the left column, $N_{ice,f}$ is normalized by the scale of the effective engine exit area $\hat{s}_E^2$. In the right column, the scaling after Eqs. (37) and (38) is applied. For the FLUDILES and the Kärcher dilution, it holds $\hat{s}_E = s_{dil} = 1$. In each panel, $N_{ice,f}$ is plotted for the FLUDILES average trajectory (solid lines) as a function of (scaled) aerosol number concentration n_{aer} for different ambient temperatures T_a (different colors). In each row, results for a second dilution type (indicated by the line style) are compared to the FLUDILES results. For the Airbus Turbofan (panels e–f), the dashed line shows the simulation results where $\delta = 0.01$ is set in Eq. (33). The boundaries of the shaded regions correspond to $\delta = 0.05$ and $\delta = 0.002$, respectively. Results are shown for $N_{ice,f} > 0$.

ambient aerosols into the core plume over time. Since we assume that aerosols sucked into the bypass duct are not destroyed there, both approaches yield the same time evolution of entrained aerosols (Fig. 9b), governed by the core air dilution factor $\mathcal{D}$ (Eq. 12). Due to the continuous entrainment process, activated aerosols become abundant enough to significantly deplete the water vapor (difference between opaque and transparent curves in Fig. 9a) only at a stage when the relative humidity profiles of both approaches have already converged. This convergence occurs once the bypass and core flows have mixed and most of the kinetic energy has been converted into heat. Consequently, aerosols entrained after this point experience similar thermodynamic conditions in both modeling approaches, leading to similar ice crystal numbers.

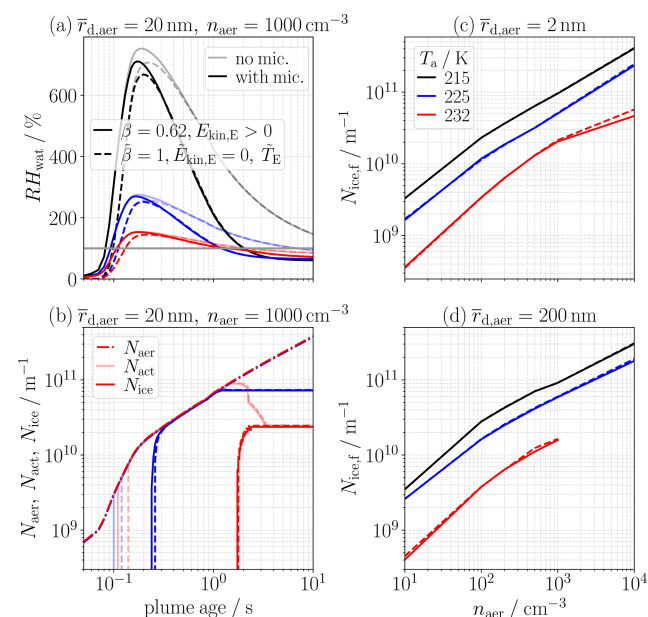


Figure 9. Results of box model simulations with the Airbus Turbofan dilution data. Compared are simulations with explicit thermodynamic treatment of bypass flow and kinetic energy (solid lines) to simulations that assume a stagnant exhaust plume with the emitted heat contained in the core flow at the engine exit (dashed lines). **(a)** Time evolution of relative humidity over water RH_{wat} without microphysical water vapor depletion (transparent lines) and with microphysics (opaque lines) for different ambient temperatures T_a (different colors). **(b)** Number of entrained aerosols N_{aer} (dashed-dotted lines), number of activated aerosols N_{act} (transparent lines) and number of ice crystals N_{ice} (opaque lines) as a function of plume age. For the sake of clarity, lines for $T_a = 215$ K are not shown. **(c–d)** Final number of ice crystals formed $N_{\text{ice},f}$ as a function of aerosol number concentration n_{aer} for two geometric mean radii $\bar{r}_{d,\text{aer}}$. Results are shown for $N_{\text{ice},f} > 0$.

5 Discussion

The following section discusses the presented findings in relation to existing literature. Based on this discussion, key implications are highlighted and possible directions for future research are proposed.

Schumann et al. (1997) pursued a similar idea to the approach outlined in Sect. 2.4. For kerosene combustion, they performed a large-eddy simulation that treated the core and bypass flow separately. They compared the temperature and partial pressure of water vapor of different plume parcels to the limiting mixing line of a core plume parcel that penetrates the bypass flow without significant interaction, thereby mixing directly with the cold ambient air. Their findings suggest that contrails could form under conditions where the classical Schmidt–Appleman theory (Schmidt, 1941; Appleman, 1953; Schumann, 1996) would not predict their formation.

Due to the higher energy-specific water vapor emission index in the hydrogen combustion case, the Schmidt–

Appleman threshold temperature is not the decisive criterion for ice crystal formation, as this threshold temperature is typically higher than the homogeneous freezing temperature of supercooled droplets (Bier et al., 2024). Moreover, the penetrative mixing proposed by Schumann et al. (1997) is not necessarily needed for the onset of contrail formation for modern turbofan engines: In the hydrogen combustion case, a plume parcel becomes already supersaturated with respect to water at an inverse dilution factor $\mathcal{D}^{-1} \sim 10$ (Fig. 2c). Clearly, the exact value depends on the specific engine exit and ambient conditions. This means that when the bypass ratio is higher than the inverse dilution factor value needed to cause supersaturation (which can be the case for modern high-bypass fans), the mixing of core and bypass air alone is sufficient to generate this supersaturation. As stated in the introductory part of Sect. 2.4, this is also evident in the study by Richardson (2025) (his Fig. 4b). Nevertheless, in the Airbus Turbofan data, ambient air is already contained in the plume before the bypass air is thoroughly mixed into the core plume (Fig. 2c–d). This supports the findings by Schumann et al. (1997) and leads to even higher supersaturation and thus promotes the onset of ice crystal formation.

Previous studies (Schumann, 1996; Richardson, 2025) have derived an explicit formula for a mixing curve accounting for the kinetic energy in the plume. In their representations, the shape of the mixing curve is fully determined by the exit and ambient conditions and does not depend on the dilution speed. In their approaches, they assume that the exhaust is well-mixed at the engine exit, with the mean axial velocity that decreases linearly with the dilution. The kinetic energy is then computed based on this mean velocity. Such an approach is appropriate when the radial profile of axial velocity is assumed to be uniform or has a shape that does not change over time (i.e., a self-similar profile, Pope, 2000). However, the initial separation of total enthalpy into the core and bypass flow does not allow for such a treatment. The mixing of three air masses (core, bypass, ambient) with different properties results in a mixing curve that explicitly depends on the time evolution of a plume parcel's $\mathcal{D}$, γ and E_{kin} . Clearly, the time-evolution of these quantities is influenced by the specific engine design, e.g., by the bypass ratio.

Additionally, Richardson (2025) examined cases with both constant and temperature-dependent specific heat capacities. The differences, however, are marginal compared to the changes we observe when the entrainment of bypass enthalpy is explicitly treated.

For entrained ambient aerosols, we have demonstrated that a simplified modeling approach is sufficient for turbofan engines (Sect. 4.5). This simplified approach assumes that the emitted combustion heat is fully contained as static enthalpy in the core flow at the engine exit. However, the simplified modeling approach might be insufficient if measurements at cruise altitude indicate a dominant contribution of emitted particles to ice crystal formation. In the hydrogen combustion case, possible sources of such particles are nitric acid

formed through oxidation of NO_x emissions or lubrication oil (Ungeheuer et al., 2022; Ponsonby et al., 2024; Zink et al., 2025). For engines where the lubrication system vents near the core flow, a large number of small particles can form when oil evaporates in the hot sections and subsequently re-nucleates in the cooling plume (Ungeheuer et al., 2022). This re-nucleation process is expected to be completed well before contrail formation begins. Consequently, unlike ambient aerosols that are entrained into the plume over time, these particles are already present or have formed prior to contrail formation. A significant water vapor depletion by ice crystals formed on emitted particles typically occurs at an earlier stage (e.g., Fig. 3a in Zink et al., 2025) than in the case of ice crystal formation on ambient aerosols. At this stage, the bypass and core may not yet be thoroughly mixed, and the kinetic energy may not have been fully converted into heat. The higher possible supersaturations encountered compared to the simplified approach (Figs. 2f, 9a) might have an impact on the activation fractions. For conventional kerosene combustion, a recent study employing large-eddy simulations with a coupled microphysical model showed that the bypass flow influences the early contrail properties up to ~ 0.6 s (Afkari et al., 2025). However, the final freezing fraction of soot particles is unaffected by the different bypass ratios they investigated.

Results from a large-eddy simulation showed that the mixing of different-aged plume parcels is a crucial process to be considered for ice crystal formation on emitted particles with high numbers (Lewellen, 2020). This process, however, is not represented in a simplified average box model approach. Therefore, if emitted particles dominate ice crystal formation, it may be beneficial to examine different parts of the core plume, specifically different trajectories that represent a certain fraction of the plume mass/volume. For a turbofan, each trajectory may follow an individual mixing curve depending on the individual time evolution of $\mathcal{D}$, γ and E_{kin} (Eq. 28). Such a trajectory ensemble, however, might only be beneficial when communication among the trajectories is included, accounting for the diffusive transport of water vapor and hydrometeors. Otherwise, the ice crystal number might be overestimated, as discussed in Bier et al. (2022).

For entrained ambient particles and kerosene combustion, Lewellen (2020) showed that neglecting the plume heterogeneity is not critical, and using an average box model approach yields ice crystal numbers comparable to those observed in large-eddy simulations. In addition, the LES results revealed a low sensitivity to different turbulence realizations. Our findings suggest that this low sensitivity on the exact mixing history is also valid for hydrogen combustion with contrail formation on ambient aerosols: Although the engine size scaling was initially applied to a single engine (Sect. 4.3), the associated dilution time scaling works also reasonable for dilution data from different sources (Sect. 4.4). These dilution data have different origins, utilizing various model approaches (RANS, LES, analytical) with

different initial and boundary conditions, and differ in how the dilution factor is extracted (from temperature, core air fraction, or analytical). All these factors influencing the details of the time evolution of the dilution factor are of minor importance for the final number of ice crystals formed. Indeed, the sensitivity to microphysical processes is much greater than the remaining differences observed among the various dilution data after the dilution time scaling has been applied (Fig. 3).

Moreover, the fact that the FLUDILES trajectory ensemble and average trajectory approaches yield similar ice crystal numbers, at least for temperatures where the homogeneous freezing timescale plays a secondary role (Fig. 7), additionally hints at the low sensitivity on the plume heterogeneity. The fact that the ice crystal numbers for these two approaches deviate for temperatures $T_a \gtrsim 230$ K hints that the plume heterogeneity may be important when the homogeneous freezing significantly influences the number of ice crystals. The trajectory ensemble without inter-trajectory communication, however, may not capture the entire physics. Therefore, forward approaches should be either to incorporate the communication into the FLUDILES trajectory data set or to investigate the homogeneous freezing dependency with RadMod (Lottermoser and Unterstrasser, 2024) coupled to LCM.

6 Conclusions

We extended the LCM box model by integrating several aspects related to the aircraft engine. This extended version was then used to simulate contrail formation on entrained ambient aerosols for hydrogen combustion. The results provide a basis for parameterizing the number of ice crystals formed $N_{\text{ice},f}$. Such a parameterization can be integrated into a general circulation model or any other large-scale contrail model to assess the radiative impacts of contrails originating from a fleet of aircraft with hydrogen combustion.

The key findings of our study are:

- Changes in engine exit conditions and dilution speed due to changing ambient temperature have a negligible effect on the formation of ice crystals. These influences can be safely disregarded in a parameterization.
- A change in overall efficiency of propulsion has approximately the same effect on the thermodynamic plume evolution as flying at a different pressure level while keeping the overall efficiency fixed. Consequently, an accurate representation of the ambient pressure dependence inherently accounts for the dependence on overall efficiency. Therefore, we can express the sensitivity of $N_{\text{ice},f}$ to the overall efficiency through its sensitivity to the ambient pressure.
- The ice crystal numbers resulting from different-sized engines and different exit jet speeds can be scaled to

each other. Therefore, it is sufficient to accurately represent $N_{\text{ice},f}$ for one reference engine size and jet speed. The ice crystal number for another-sized engine with a different jet speed can then be obtained by appropriate scaling.

- It is sufficient to assume that the whole emitted combustion heat is contained as static enthalpy in the core flow at engine exit. This simplified approach yields similar ice crystal numbers as the approach with explicit treatment of kinetic energy dissipation and entrainment of enthalpy initially contained in the bypass flow of a turbofan engine.

We note that these conclusions are valid for contrail formation on entrained ambient aerosols and not all conclusions are necessarily also true for kerosene combustion or scenarios where ice crystals form predominantly on plume particles (i.e., those particles originating from emitted species).

In case other ice crystal formation pathways in the hydrogen combustion case turn out to dominate over the formation on ambient aerosol (e.g., if lubrication oil enters the hot exhaust regions, where it may evaporate and subsequently form a distribution of small particles with high numbers), simulations incorporating these potential nuclei would need to be conducted to reassess the aforementioned conclusions.

Appendix A

The total temperature (or stagnation temperature) T_{tot} and the static temperature T_{static} are related via (Walsh and Fletcher, 2004)

$$T_{\text{tot}} = T_{\text{static}} \left(1 + \frac{\kappa - 1}{2} Ma^2 \right). \quad (\text{A1})$$

Neglecting the slight temperature dependence of the adiabatic index κ and preserving the Mach number Ma , scaling T_{tot} by a factor c means that also the static temperature T_{static} scales with this factor c .

The total pressure p_{tot} and static pressure p_{static} for a compressible isentropic flow are related by (Walsh and Fletcher, 2004):

$$p_{\text{tot}} = p_{\text{static}} \left(1 + \frac{\kappa - 1}{2} Ma^2 \right)^{\frac{\kappa}{\kappa - 1}} \quad (\text{A2})$$

As for the temperatures, Eq. (A2) implies that total and static pressures scale the same way (assuming constant κ).

Appendix B

Lewellen (2020) introduced two timescales: The first is the time interval during which a plume parcel can potentially activate aerosols, which he called τ_{mix} and has basically the same meaning as $\delta t_{\text{supersat}}$ we used in Sect. 4.3. For this

timescale it holds $\tau_{\text{mix}} \propto s_{\text{dil}}$. The second is the time interval needed for the ice crystals to grow large enough to substantially consume the water vapor, for which Lewellen (2020) used the phase relaxation time scale τ_{fc} after Khvorostyanov and Sassen (1998). It holds $\tau_{\text{fc}} \propto (\bar{r}_{\text{ice}} n_{\text{aer}})^{-1}$ and since the mean radius of the ice crystals scales as $\bar{r}_{\text{ice}} \propto n_{\text{aer}}^{-1/3}$, it follows $\tau_{\text{fc}} \propto n_{\text{aer}}^{-2/3}$. Lewellen (2020) showed that when plotting the apparent ice particle emission index normalized by the aerosol number concentration $\text{EI}_{\text{ice}}/n_{\text{aer}}$ against any function of the ratio of those two timescales, e.g., $(\tau_{\text{mix}}/\tau_{\text{fc}})^{3/2} \propto s_{\text{dil}}^{3/2} n_{\text{aer}}$, the curves for different engine sizes/dilution speeds collapse. Mathematically this can be expressed as

$$\frac{\text{EI}_{\text{ice}}}{n_{\text{aer}}} \sim g(s_{\text{dil}}^{3/2} n_{\text{aer}}), \quad (\text{B1})$$

where g is a function that depends on ambient conditions and aerosol properties but not on the engine size/dilution speed. Since $N_{\text{ice},f} \propto s_{\text{E}}^2 \text{EI}_{\text{ice}}$, it exists a function $\tilde{g}$ fulfilling

$$\frac{N_{\text{ice},f}}{s_{\text{E}}^2 n_{\text{aer}}} \sim \tilde{g}(s_{\text{dil}}^{3/2} n_{\text{aer}}). \quad (\text{B2})$$

Multiplication of Eq. (B2) with $s_{\text{dil}}^{3/2} n_{\text{aer}}$ and introducing the function $f(x) = x \tilde{g}(x)$ leads to Eq. (37) with $a = -3/2$.

Data availability. The box-model simulation results, together with the plotting scripts required to reproduce the figures presented in this study, are available in a Zenodo repository (<https://doi.org/10.5281/zenodo.17978328>, Zink, 2025).

Author contributions. JZ: Conceptualization, Data curation, Formal analysis, Investigation, Methodology, Software, Validation, Visualization, Writing – original draft, Writing – review & editing. SU: Conceptualization, Methodology, Funding acquisition, Software, Supervision, Project Administration, Writing – review & editing.

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P3. Contrail formation for aircraft with hydrogen combustion - Part 3: A neural-network-based parameterization of ice crystal number



Contrail formation for aircraft with hydrogen combustion - Part 3: A neural-network-based parameterization of ice crystal number

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Abstract. Contrail cirrus clouds are a major contributor to the climate impact of aviation. Large-scale models, such as general circulation models (GCMs) with an integrated contrail module, are used to estimate the radiative forcing of these clouds. However, small-scale processes cannot be explicitly resolved in these models and must therefore be parameterized. In this study, we develop a novel parameterization for the number of contrail ice crystals formed on ambient aerosols entrained into the exhaust plume behind aircraft burning hydrogen. The continuous entrainment of ambient aerosols, combined with higher supersaturation in hydrogen exhaust plumes, results in longer-lasting ice crystal formation than in conventional kerosene combustion, where ice crystals predominantly form on emitted soot. We construct the parameterization from a comprehensive database of time-resolved contrail formation simulations conducted with the Lagrangian Cloud Module in a box model approach. Shallow neural networks are used to reproduce the simulation outcome, complemented by analytical scaling relations to extend the applicability of the parameterization. The parameterization incorporates dependencies on ambient conditions, ambient aerosol properties and aircraft-related parameters. We compare the new parameterization with an existing one originally developed for conventional kerosene combustion that treats ice crystal formation as a single nucleation pulse. The comparison reveals that the assumption of a nucleation pulse is not reasonable for hydrogen combustion scenarios. We find it essential to base the parameterization on time-resolved simulations, as this realistically captures ice crystal formation on continuously entrained ambient aerosols.

1 Introduction

1.1 Motivation

Aviation currently contributes about 3.5 % to the anthropogenic radiative impact on climate (Lee et al., 2021). More than half of this impact arises from non-CO₂ effects, with contrail cirrus clouds being the dominant contributor to the radiative forcing (Lee et al., 2021; Kärcher, 2018; Paoli and Shariff, 2016). To quantify their radiative forcing, general circulation models (GCMs) have been extended with contrail modules (Burkhardt and Kärcher, 2009; Gettelman and Chen, 2013; Schumann et al., 2015; Bock and Burkhardt, 2016). Since processes occurring on scales below the grid resolution cannot be resolved, cloud processes need to be parameterized within GCMs. This applies to cloud microphysics in general and, in particular, to the early stages of contrail formation and the interaction of young contrails with the lift-induced wake vortices. The key quantity during the



25 early contrail stage is the number of ice crystals, which strongly influences the evolution and the radiative effect of persistent contrail cirrus (Unterstrasser and Gierens, 2010; Lewellen, 2014; Bier et al., 2017; Burkhardt et al., 2018; Lottermoser and Unterstrasser, 2025).

For conventional kerosene combustion, parameterizations have been developed for both the formation of ice crystals (Kärcher et al., 2015) and their loss due to wake vortex interactions (Unterstrasser, 2016). These parameterizations have been imple-
30 mented into the GCM with contrail parameterization, ECHAM-CCMod (Bier and Burkhardt, 2019, 2022). Since, thermodynamics and microphysics are substantially different for hydrogen combustion scenarios (Bier et al., 2024; Zink et al., 2025a), these parameterizations must be adapted or newly developed. Recently, Lottermoser and Unterstrasser (2025) extended the ice crystal loss parameterization to account for scenarios with hydrogen-powered aircraft. The present study introduces a new parameterization for the number of ice crystals formed in the exhaust plume of aircraft burning hydrogen.

35 1.2 Scope and outline of the study

Here we literally repeat the according subsection "Scope and outline of the study" of Part 1 (see Sect. 1.2 in Zink et al. (2025a)):
"Our overarching goal is to develop a parameterization for the final number of ice crystals formed for aircraft with hydrogen combustion, suitable for implementation in GCMs and other large-scale contrail models. Specifically, we seek a functional relationship of the form

$$40 \quad N_{\text{ice},f} = N_{\text{ice},f}(\mathbf{a}_{\text{atmosphere}}, \mathbf{a}_{\text{aerosol}}, \mathbf{a}_{\text{aircraft}}) , \quad (1)$$

where $\mathbf{a}_{\text{atmosphere}}$ denotes a set of variables characterizing the background atmosphere (e.g., ambient temperature), $\mathbf{a}_{\text{aerosol}}$ represents properties of ambient aerosols (number concentration, size distribution and solubility) and $\mathbf{a}_{\text{aircraft}}$ includes aircraft-related parameters (e.g., engine size).

Our objective is to identify a functional relationship that balances simplicity with physical fidelity. In other words, we aim
45 to capture the impact of the key processes that govern ice crystal formation in a form that is simple enough to be easily applied in other models (level of complexity, computing time, ease of implementation). In Parts 1 and 2 of a trilogy of papers, we systematically explore a broad parameter space and address aspects that have not been explored before to gain a deep insight into the physical processes influencing the ice crystal formation. This allows us to select the set of variables that constitute the inputs to the parameterization of $N_{\text{ice},f}$.

50 While a previous $N_{\text{ice},f}$ parameterization of contrail formation (Kärcher et al., 2015) used a first-principles-based concept, the current work across Parts 1 to 3 employs a hybrid approach. It combines a data-driven advanced regression method to fit a multidimensional database of contrail formation simulations with analytical scaling relations. To keep the number of dimensions in the simulation database as small as possible, we identify conditions under which the sensitivity to specific variables is negligible, and also employ analytical scaling relations derived from sensitivity simulations.

55 In Part 1, we focus on the roles of atmospheric variables $\mathbf{a}_{\text{atmosphere}}$ and aerosol properties $\mathbf{a}_{\text{aerosol}}$. Aircraft-related parameters $\mathbf{a}_{\text{aircraft}}$ are addressed in Part 2. The final parameterization, synthesizing insights from Parts 1 and 2, will be presented in Part 3."



The parameterization developed in the present study is based on neural networks, which serve as fitting functions for the outcomes of the contrail formation simulations. Our target quantity is the final number of ice crystals formed, i.e., the number when ice crystal formation is completed in our simulations. In previous studies, we distinguished the final number $N_{\text{ice},f}$ from the time-dependent number $N_{\text{ice}}(t)$. Since we only consider the final number here, we omit the subscript “f” throughout the paper, except in this introduction and in the conclusion (Sect. 5).

Sections 2.1 to 3.1 provide technical details on the configuration, training, and evaluation of the neural networks. Readers mainly interested in the final results with physical discussion may continue directly with Sect. 3.2, where we compare upper-tropospheric profiles of simulated and parameterized ice crystal numbers. Sect. 3.3 summarizes scaling relations derived in Parts 1 and 2, which are used to generalize the parameterization (with a practical step-by-step cookbook of how to employ the parameterization presented in Appendix A). In Sect. 4.1, we compare our approach with an existing parameterization that was originally developed for kerosene combustion but is applied here to hydrogen combustion. Finally, we discuss strengths and limitations of the developed parameterization in Sect. 4.2 before concluding in Sect. 5.

2 Data and Methods

2.1 Training and verification data

Our database consists of contrail formation simulations performed with the Lagrangian Cloud Module (LCM) in a box model approach (Bier et al., 2022, 2024). In this approach, dilution, which governs plume expansion and cooling, is prescribed externally. The microphysics is then calculated in a time-resolved manner without feedback on the plume dynamics. In the particle-based LCM, aerosol particles and hydrometeors (liquid droplets and ice crystals) are represented by simulation particles (SIPs), with each SIP corresponding to a certain number of real physical particles.

We use simulation results covering all possible combinations of variable values listed in Table 1. This results in a dataset with $\prod_{i=1}^6 n_i > 20,000$ entries, where n_i denotes the number of values sampled for variable i . A physical description of this dataset is given in Zink et al. (2025a). This gridded dataset is used to train a regression neural network (Sect. 2.2.1). Using the gridded data ensures that the model is trained within well-defined variable bounds set by the minimum and maximum values of each input variable.

To evaluate the model performance on an independent data set that was not used for training, we generate an additional $\prod_{i=1}^6 (n_i - 1) > 5,000$ simulations at randomly sampled points located between the grid points (Fig. 1). This dataset serves to assess how well the trained model performs in-between the gridded *training data*. In our study, we refer to this entire off-grid dataset as the *verification dataset*. Following standard machine learning practice, we divide it equally into two subsets: a *validation set*, used for hyperparameter tuning during training (see Sect. 2.2.1 for details), and a *testing set*, used only for evaluating the best performing model. While the term verification is common in physical modeling, validation and testing are the conventional terms in machine learning to describe these specific roles.



Table 1. LCM box model simulation results for all possible combinations of listed variable values are used as training dataset. For the verification dataset, simulations were performed for random data points between the gridded data points (Fig. 1). Parameters that were not varied are also listed (indicated with asterisks).

variable	values
ambient temperature T_a / K	210, 215, 220, 225, 230, 232.5, 234.5
ambient pressure p_a / hPa	150, 230, 320, 400
ambient relative humidity over ice $RH_{ice,a}$ / %	100, 115, 125, 140
aerosol number concentration n_{aer} / cm^{-3}	1, 10, 100, 1000, 10000
aerosol geometric mean radius $\bar{r}_{d,aer}$ / nm	1, 2, 5, 10, 20, 40, 100, 200, 500
aerosol hygroscopicity κ_{aer} / –	0.01, 0.05, 0.25, 1.25
fixed parameters	
aerosol geometric width $\sigma_{aer}^* = 1.6$	water vapor emission index $EI_v^* = 8.94 \text{ kg kg}^{-1}$
specific combustion heat $Q^* = 120 \text{ MJ kg}^{-1}$	overall propulsion efficiency $\eta^* = 0.4$
aircraft speed $U_\infty^* = 250 \text{ m s}^{-1}$	excess jet velocity $U_{jet,E}^* = 230 \text{ m s}^{-1}$
core exit radius $r_E^* = 0.5 \text{ m}$	core exit temperature $T_E^* = 580 \text{ K}$

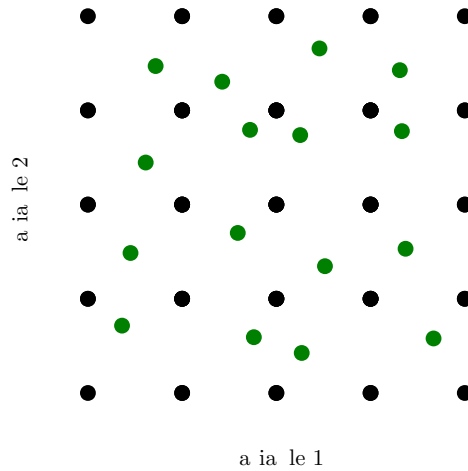


Figure 1. Schematic illustration of training (black) and verification (green) datasets.

2.2 Design of neural networks for parameterizing the ice crystal number

90 Neural networks provide a flexible framework for capturing nonlinear relationships, without requiring an explicit analytical form. This makes them particularly well suited for approximating intricate dependencies that classical fitting methods might

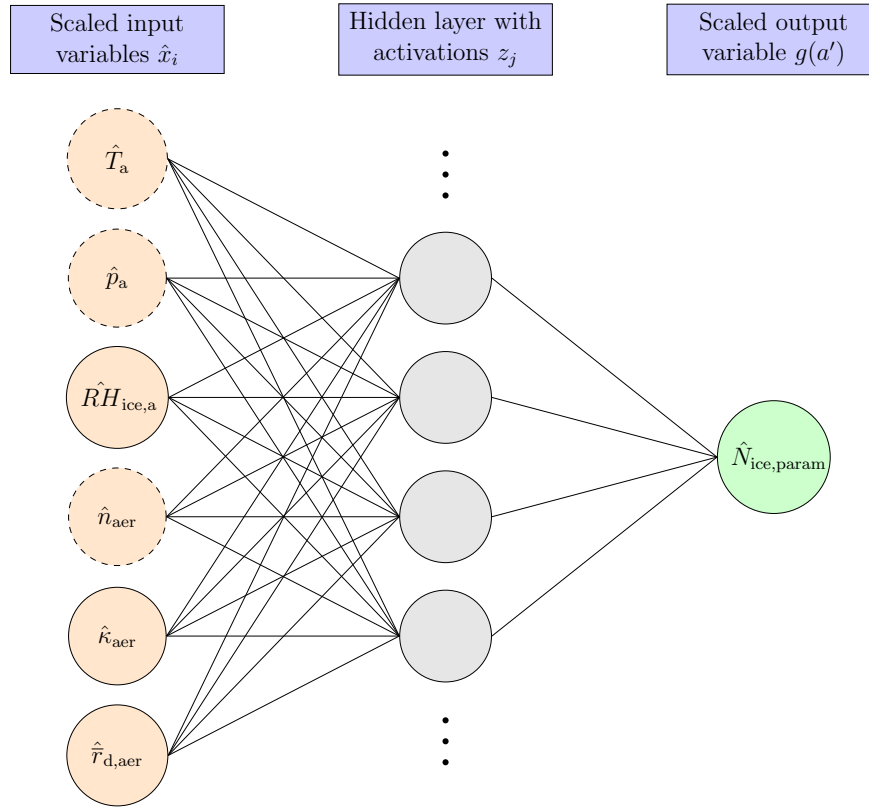


Figure 2. Schematic depiction of the employed Multilayer Perceptron. For both the FullNet and ClassificationNet, all depicted input variables are used. The ReducedNet uses only the input variables marked by dashed circles.

struggle to represent. For this reason, we chose a shallow, fully connected feedforward artificial neural network, known as a Multilayer Perceptron (MLP), to approximate the number of ice crystals as a function of the predictors listed in Table 1. To limit the total number of trainable parameters (fit parameters/coefficients), we restrict the architecture to a single hidden layer (Fig. 2).

The corresponding calculations are given by (Bishop, 2019)

$$a_j = \sum_{i=1}^{n_{inputs}} \hat{x}_i w_{ij} + \beta_j \quad (2a)$$

$$z_j = f(a_j) \quad (2b)$$

$$a' = \sum_{j=1}^{n_{nodes}} z_j w'_j + \beta' \quad (2c)$$

$$\hat{N}_{ice,param} = g(a') \quad (2d)$$



For each hidden-layer node j , the (scaled) inputs $\hat{x}_i$ are linearly combined (Eq. (2a)) using the weights w_{ij} and biases β_j . In classical regression approaches, w_{ij} and β_j would be named fit parameters/coefficients. The resulting pre-activation values a_j are then passed through a nonlinear activation function f (Eq. (2b)), yielding the hidden-layer activations z_j . These activations are again linearly combined (Eq. (2c)) and passed through the (possibly nonlinear) output activation function g (Eq. (2d)) to
105 produce the network output $\hat{N}_{ice,param}$. This sequence of operations applies to both a regression network (Sect. 2.2.1) and a classification network (Sect. 2.2.2), with $\hat{N}_{ice,param}$ having different interpretations in each case.

2.2.1 Regression neural network

In a regression neural network, $\hat{N}_{ice,param}$ is a continuous variable representing the (scaled) number of ice crystals as a function of the scaled inputs $\hat{x}_i$. The inputs x_i are scaled to $\hat{x}_i$ to improve training efficiency and enhance the performance of the
110 resulting model. As a first scaling step, all inputs describing aerosol properties (number concentration, geometric mean radius, hygroscopicity) are log-transformed

$$\tilde{x}_i = \log_{10}(x_i) \quad (3)$$

to account for the several orders of magnitude spanned by their prescribed values. The remaining inputs (ambient temperature, ambient pressure, ambient relative humidity) are left unchanged at this step ($\tilde{x}_i = x_i$). After this initial transformation, all
115 resulting inputs $\tilde{x}_i$ are standardized according to

$$\hat{x}_i = \frac{\tilde{x}_i - \mu_{\tilde{x}_i}}{\sigma_{\tilde{x}_i}}, \quad (4)$$

where $\mu_{\tilde{x}_i}$ and $\sigma_{\tilde{x}_i}$ are the mean and standard deviation of the input variable ranges. This standardization ensures that all inputs have comparable magnitudes and variability.

In addition to the scaling of the input variables, we also include a scaling of the output variable $\hat{N}_{ice}$, which can vary over
120 several orders of magnitude (Zink et al., 2025a). Since the mean squared error is used as the loss function during training (see Eq. (8)), cases with low ice crystal numbers would contribute very little to the overall (absolute) error if no output scaling were applied. Consequently, these low-number cases might be neglected during optimization of the weights and biases. To avoid this, we apply a 'hybrid' output transformation: Below a tuneable critical constant $N_{ice,crit}$, a logarithmic scaling is used, while above it, a linear approximation applies. Using the logistic function (Fig. 3a)

$$\sigma(y) = \frac{1}{1 + e^{-\alpha(y-y_0)}} \quad (5)$$

these two regimes are smoothly connected by a sigmoidal transition (Fig. 3b), expressed as

$$\hat{N}_{ice} = [1 - \sigma(y)] \log_{10}(y) + \sigma(y)[cy + d] \quad (6)$$

with $y = N_{ice}/N_{ice,crit}$. In our case, $y_0 = 1$ and α is a tuning parameter. The parameters $c = 1/\ln(10)$ and $d = -c$ in Eq. (6) ensure a smooth and differentiable transition between the logarithmic and linear regimes as $\alpha \rightarrow \infty$. This hybrid transformation
130 accounts for low ice crystal numbers without loss of accuracy in the high-number range, where the linear approximation is valid.

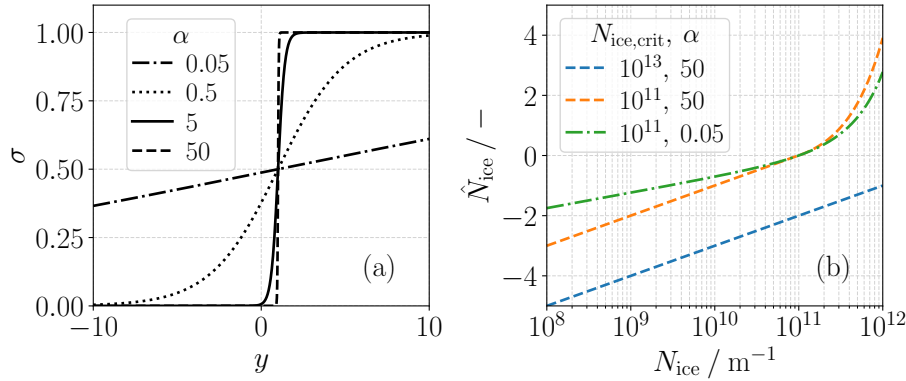


Figure 3. (a) Logistic function (Eq. (5)) for different α values and (b) hybrid coordinate transformation (Eq. (6)) for different $N_{ice,crit}$ and α values.

In summary, the trained neural network predicts the scaled values $\hat{N}_{ice,param}$ from the scaled inputs $\hat{x}_i$ (Fig. 2). The final ice crystal number $N_{ice,param}$ is then obtained by applying the inverse transformation of Eq. (6).

In a regression problem, the output activation function g is typically the identity. If the activation function of the hidden layer f were also the identity, the entire neural network would effectively reduce to a classical multiple linear regression model. However, to capture the nonlinear relationship between the ice crystal number and the inputs, a nonlinear function f is needed. We experimented with several common nonlinear activation functions (Tanh, Logistic function, Softmax, ReLU, Leaky ReLU, ELU). We found that the choice of activation function has only a minor impact on the final model performance. Consequently, we select the rectified linear unit (ReLU) defined as

$$f(a_j) = \max(0, a_j) \quad (7)$$

due to its simplicity and low computational cost.

During the training process, the loss function

$$\mathcal{L}_\gamma(\mathbf{w}; \beta) = \frac{1}{N} \sum_{k=1}^N \left(\hat{N}_{ice,param}(\hat{\mathbf{x}}_k; \mathbf{w}; \beta; \gamma) - \hat{N}_{ice,sim,k} \right)^2 + \lambda \|\mathbf{w}\|^2 \quad (8)$$

is minimized by computing its gradients with respect to the weights and biases via the backpropagation algorithm, and updating the weights and biases using the gradient descent rule (Bishop, 2019). This update procedure is repeated over multiple iterations, called epochs. In Eq. (8), the first term represents the mean squared error between the scaled training data $\hat{N}_{ice,sim,k}$ and the neural network predictions $\hat{N}_{ice,param}(\hat{\mathbf{x}}_k; \mathbf{w}; \beta; \gamma)$. Here, $\hat{\mathbf{x}}_k$ is the vector of scaled input variables $\hat{x}_i$ for simulation k , $\mathbf{w}$ denotes the collection of all weights (matrix elements w_{ij} and vector elements w'_j), β represents the biases (vector elements β_j and scalar β') and γ stands for a set of hyperparameters. The second term acts as a regularization penalty, with $\|\mathbf{w}\|^2$ being the squared Euclidean norm of the weights (i.e., the sum of squares of all weights) and λ the regularization parameter. This term prevents excessively large weights and thus helps to prevent overfitting to the training data (Bishop, 2019). We trained the



network for 300 epochs and selected the weights and biases from the epoch with the lowest validation loss as the final model parameters. We found that training beyond 300 epochs does not yield further improvements.

While Eq. (8) is used internally during the training process, we evaluate the final model performance after applying the inverse transformation of Eq. (6), i.e., on the unscaled data. For this evaluation, we use the absolute percentage error (APE),
155 defined as

$$\text{APE}_k = \frac{|N_{\text{ice,param},k} - N_{\text{ice,sim},k}|}{N_{\text{ice,sim},k}} \cdot 100\% \quad (9)$$

where $N_{\text{ice,sim},k}$ and $N_{\text{ice,param},k}$ are the simulated and parameterized values for simulation k , respectively. We then summarize the errors across the dataset of interest by computing the median absolute percentage error

$$\text{MdAPE} = \text{Median}(\{\text{APE}_k\}) \quad (10)$$

160 We use Eq. (10) as the criterion for selecting the best-performing model. This final model consists of the trained weights and biases together with a set of optimized hyperparameters. Hyperparameters are model constraints that are specified a-priori and not updated during training. Consequently, different models can be trained and compared, each with a distinct set of hyperparameters. In our case, the hyperparameters of interest include the number of hidden layer nodes n_{nodes} , the regularization parameter λ , and the hybrid-coordinate parameters $N_{\text{ice,crit}}$ and α . The model with the set of hyperparameters
165 minimizing Eq. (10) on the validation set is chosen as the final model.

In the end, we provide two regression neural networks: The *FullNet* is trained on all cases with $N_{\text{ice,sim}} > 0$ and uses the six predictors listed in Table 1. It is applicable across the full range of training data. The *ReducedNet* is trained only within the subspace defined by $T_a \leq 225 \text{ K}$ and $10 \text{ nm} \leq \bar{r}_{\text{d,aer}} \leq 100 \text{ nm}$. In this regime, the number of ice crystals formed is largely independent of ambient relative humidity, aerosol size, and aerosol hygroscopicity (Zink et al., 2025a). Consequently,
170 the ReducedNet uses only three predictors (marked by dashed circles in Fig. 2): ambient temperature, ambient pressure, and aerosol number concentration.

2.2.2 Classification neural network

In several simulations for ambient temperatures $T_a > 230 \text{ K}$, aerosols activate into liquid droplets but none of these droplets freeze into ice crystals ($N_{\text{ice,sim}} = 0$). In cases where ice crystals form in this temperature range, their numbers are typically in
175 the range from $\sim 10^8 \text{ m}^{-3}$ to $\sim 10^{11} \text{ m}^{-3}$, resulting in an abrupt transition from zero to large ice crystal numbers depending nonlinearly on the inputs. This discontinuous behavior is challenging to capture using a single regression model, as it would require a complex network with a large number of fit parameters to resolve the sharp jump accurately. To manage this, the regression model FullNet is trained only on samples with strictly positive ice crystal numbers ($N_{\text{ice,sim}} > 0$). For these cases, the dependence of ice crystal number on the inputs is smoother and can be approximated well by the regression network
180 without excessive model complexity. To explicitly separate the binary nature of ice formation from the continuous variation in ice crystal number, we introduce a classification network (hereinafter named as *ClassificationNet*). This network is trained to separate between cases with $N_{\text{ice,sim}} = 0$ and $N_{\text{ice,sim}} > 0$.



The simulated ice crystal number is converted into a binary variable via

$$\tilde{N}_{\text{ice,sim}} = \begin{cases} 1 & \text{if } N_{\text{ice,sim}} > 0 \\ 0 & \text{otherwise.} \end{cases} \quad (11)$$

185 The output activation function g of the ClassificationNet is the logistic function (Eq. (5)) and the resulting output $\hat{N}_{\text{ice,param}}$, ranging from zero to one, is interpreted as the probability that ice crystals form for a given set of inputs $\hat{\mathbf{x}}$. During the training, the regularized binary-cross entropy loss

$$\mathcal{L}_{\gamma}(\mathbf{w}; \beta) = -\frac{1}{N} \sum_{k=1}^N \left[\tilde{N}_{\text{ice,sim},k} \log \left(\hat{N}_{\text{ice,param}}(\hat{\mathbf{x}}_k; \mathbf{w}; \beta; \gamma) \right) + (1 - \tilde{N}_{\text{ice,sim},k}) \log \left(1 - \hat{N}_{\text{ice,param}}(\hat{\mathbf{x}}_k; \mathbf{w}; \beta; \gamma) \right) \right] + \lambda \|\mathbf{w}\|^2 \quad (12)$$

is minimized by updating the network weights $\mathbf{w}$ and biases β . The first term inside the summation penalizes misclassifications
190 when ice crystals have formed in the simulation (false negatives), while the second term penalizes misclassifications when no ice crystals are present (false positives). As for the regression network, the regularization term $\lambda \|\mathbf{w}\|^2$ prevents overfitting by discouraging excessively large weight values.

In the regression task, the continuous variation of ice crystal numbers (for values greater than zero) allows effective training on a gridded dataset by fitting a smooth curve. In the binary classification problem, however, the target variable takes only
195 two values, so no meaningful interpolation between grid points is possible. Therefore, we combine all gridded and off-gridded data described in Sect. 2.1 for $T_a \geq 230$ K ($> 10,000$ simulations) and randomly split the combined dataset into training, validation, and test sets with proportions of 70 %, 15 %, and 15 %, respectively. Furthermore, the combined dataset contains more simulations with $\tilde{N}_{\text{ice,sim}} = 1$ (~ 83 %). To balance the classes during training, we randomly subsample the training set with $\tilde{N}_{\text{ice,sim}} = 1$ to match the number of simulations with $\tilde{N}_{\text{ice,sim}} = 0$, which helps prevent the model from being biased
200 toward the majority class.

The probabilistic network output $\hat{N}_{\text{ice,param}}$ is finally converted into a binary variable

$$\tilde{N}_{\text{ice,param}} = \begin{cases} 1 & \text{if } \hat{N}_{\text{ice,param}} \geq 0.5 \\ 0 & \text{otherwise.} \end{cases} \quad (13)$$

With this binary variable, we evaluate the false negative rate

$$\text{FNR} = \frac{\sum(\tilde{N}_{\text{ice,param}} = 0 \mid \tilde{N}_{\text{ice,sim}} = 1)}{\sum(\tilde{N}_{\text{ice,sim}} = 1)} \cdot 100\% \quad (14)$$

205 and the false positive rate

$$\text{FPR} = \frac{\sum(\tilde{N}_{\text{ice,param}} = 1 \mid \tilde{N}_{\text{ice,sim}} = 0)}{\sum(\tilde{N}_{\text{ice,sim}} = 0)} \cdot 100\% \quad (15)$$

as an evaluation of the model performance.



3 Results

3.1 Hyperparameter tuning

210 In this section, we briefly summarize the optimization process for the hyperparameters n_{nodes} , λ , $N_{\text{ice,crit}}$, and α . Starting from an initial set of values, we vary one hyperparameter at a time while keeping the others fixed, selecting the value that yields the best performance. We then proceed to optimize the next hyperparameter using the best values found so far. After cycling through all hyperparameters, we repeat the process starting again from the first. We found that only a few such cycles are necessary before further iterations no longer produce a significant reduction in error.

215 Fig. 4 illustrates the hyperparameter tuning for the FullNet. The MdAPE initially decreases sharply with increasing number of nodes n_{nodes} for both the training and validation sets (Fig. 4a). The validation set exhibits a local minimum at $n_{\text{nodes}} = 43$, beyond which no significant improvement is observed. Hence, this value is chosen to avoid unnecessarily increasing the total number of fit parameters (Eqs. (2a)–(2d)).

For the regularization parameter λ , the validation set shows a minimum in MdAPE at $\lambda = 10^{-3}$, with increasing error
220 toward both higher and lower values (Fig. 4b). Interestingly, the training error also increases as λ decreases, which is somewhat unexpected since the training error is typically lowest for $\lambda = 0$. This behavior can be explained by the fact that the loss function applied on the scaled data during training (Eq. (8)) differs from the error metric we use to evaluate the final model performance on the unscaled data (Eq. (10)).

Regarding $N_{\text{ice,crit}}$, the MdAPE is high at low values (Fig. 4c) due to large errors in low ice crystal number cases when
225 the linear regime extends over a wide range in the hybrid coordinate transformation (Eq. (6)). The error decreases until $N_{\text{ice,crit}} \sim 10^{11} \text{ m}^{-1}$, with a slight dependence on the choice of α . Although the pair $N_{\text{ice,crit}} = 3 \cdot 10^{11} \text{ m}^{-1}$ and $\alpha = 0.5$ yields a marginally lower MdAPE than $N_{\text{ice,crit}} = 10^{11} \text{ m}^{-1}$ and $\alpha = 5$, we select the latter pair to maintain the linear regime over a broader range of ice crystal numbers.

The advantage of the hybrid-coordinate transformation becomes particularly clear when considering only cases with $N_{\text{ice,sim}} >$
230 10^{11} m^{-1} . The MdAPE of these cases is reduced from 10.9% to 7.1% for the validation set when switching from a fully logarithmic scaling ($N_{\text{ice,crit}} \rightarrow \infty$) to the hybrid-coordinate transformation with $N_{\text{ice,crit}} = 10^{11} \text{ m}^{-1}$ and $\alpha = 5$.

We performed the same hyperparameter tuning for the ReducedNet (considering also the MdAPE) and for the ClassificationNet (considering FNR and FPR). The final selected values are summarized in Table 2, together with the corresponding
235 errors for the training, validation, and testing datasets. The close agreement between training and validation errors indicates no significant overfitting to the training data. The similarity between validation and testing errors demonstrates strong generalization of the developed models.

This is further supported by the cumulative distribution functions (CDFs) of the APE for the regression networks, which show that the distributions for the training set and the verification set (validation and testing sets together) are very similar (Fig. 5). For the subspace defined by $T_a \leq 225 \text{ K}$ and $10 \text{ nm} \leq \bar{r}_{\text{d,aer}} \leq 100 \text{ nm}$ the CDFs for the ReducedNet and the FullNet
240 are nearly identical up to the ~ 80 th percentile of the APE. This is notable given the ReducedNet has a strongly reduced total number of weights and biases (Table 2). Beyond the 80th percentile of the error distribution, the FullNet exhibits slightly

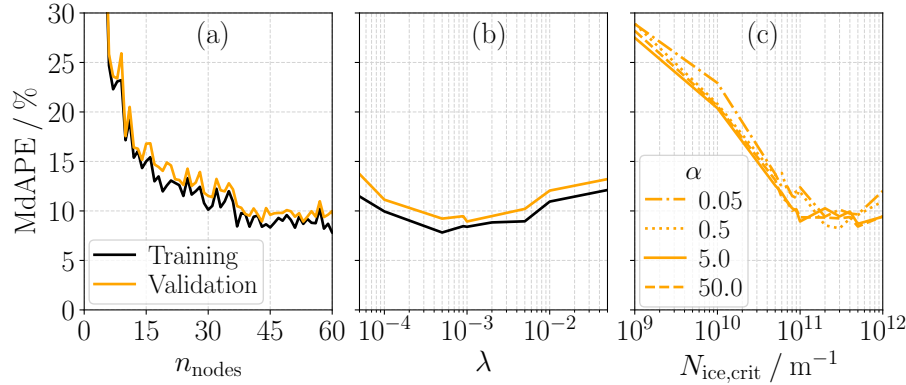


Figure 4. Median absolute percentage error (MdAPE) for the FullNet for the training (black) and validation (orange) dataset as a function of (a) node number n_{nodes} (b) regularization parameter λ and (c) hybrid-coordinate parameters $N_{\text{ice,crit}}$ and α . For the sake of clarity, only results for the validation data are depicted in (c). The hyperparameters are fixed to $n_{\text{nodes}} = 43$, $\lambda = 10^{-3}$, $N_{\text{ice,crit}} = 10^{11} \text{ m}^{-1}$ and $\alpha = 5$ except in the panel where they are varied.

Table 2. Best found hyperparameters, total number of fit coefficients (weights and biases) n_{coeff} , and corresponding training, validation and testing error for the different neural network types.

Network type	n_{nodes}	λ	$N_{\text{ice,crit}} / \text{m}^{-1}$	α	n_{coeff}	error (training/validation/testing)
FullNet	43	10^{-3}	10^{11}	5	345	MdAPE = 8.0/8.7/8.5%
ReducedNet	11	$9 \cdot 10^{-3}$	10^{11}	5	56	MdAPE = 5.5/5.0/5.2%
ClassificationNet	9	10^{-4}	-	-	73	FNR = 1.9/1.8/1.9% FPR = 1.5/1.4/1.3%

smaller errors than the ReducedNet within this subspace. This difference arises because near the defined boundaries of the subspace, the ice crystal number becomes increasingly sensitive to the input variables omitted in the ReducedNet. Omitting these sensitivities leads to slightly larger errors. Hence, applying the ReducedNet instead of the FullNet for the given subspace is a trade-off between the potential gain in computational speed and the accuracy of the parameterized values.

3.2 Upper-tropospheric profiles of simulated and parameterized ice crystal number

Table 3. Combination of ambient temperature and pressure values according to the International Standard Atmosphere (e.g., Etling, 2008).

altitude / km	8.2	8.6	9.0	9.4	9.8	10.2	10.6	11.0	12.2	13.2
T_a / K	234.85	232.25	229.65	227.05	224.45	221.85	219.25	216.65	216.65	216.65
p_a / hPa	345.81	326.16	307.42	289.56	272.55	256.36	240.96	226.32	187.30	159.97

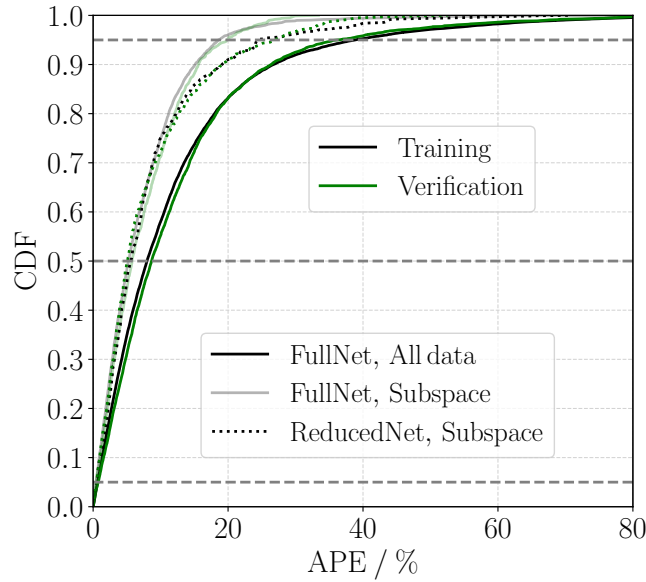


Figure 5. (a) Cumulative distribution function (CDF) of absolute percentage error (APE) for training (black color) and verification (testing and validation set together; green color) dataset. Shown are the CDFs for the FullNet evaluated with all data (solid opaque lines), for the FullNet evaluated within the subspace defined by $T_a \leq 225\text{ K}$ and $10\text{ nm} \leq \bar{r}_{d,\text{aer}} \leq 100\text{ nm}$ (transparent solid lines), and for the ReducedNet evaluated within this subspace (dotted opaque lines). Dashed horizontal lines indicate the 5th percentile, the median and the 95th percentile.

After the technical description of the neural networks in Sect. 2.2 and Sect. 3.1, we now visualize the results by comparing simulated and parameterized vertical profiles of the ice crystal number N_{ice} (Fig. 6). Ambient temperature and pressure are prescribed according to the International Standard Atmosphere (Table 3).

250 The neural network successfully reproduces the sensitivities to the various variables systematically investigated in Zink et al. (2025a). It captures the nearly linear increase of N_{ice} with aerosol number concentration n_{aer} at low n_{aer} , as well as the saturation effect at high n_{aer} (different colors in Fig. 6). It also reproduces the pronounced decrease in N_{ice} at low altitudes caused by high ambient temperatures. In the isothermal layer above 11 km, the network reasonably reflects the occasional slight decrease of N_{ice} with increasing altitude, attributable to reduced pressure. Furthermore, it accounts for the decrease in N_{ice} for
255 small aerosol sizes (second row in Fig. 6) due to the Kelvin effect, as well as the freezing point depression for well-soluble particles with a large dry radius (Fig. 6e).

The successful fit to the simulation data is achieved both for the FullNet across the entire parameter space considered and for the ReducedNet, applied to the subspace $T_a \leq 225\text{ K}$ and $10\text{ nm} \leq \bar{r}_{d,\text{aer}} \leq 100\text{ nm}$ (first row in Fig. 6).

3.3 Generalizing the parameterization

260 The neural networks were derived for a scenario with a single aerosol population and a reference engine/aircraft as characterized by the parameters listed in Table 1. The parameterization can be generalized by incorporating several scaling relations. The

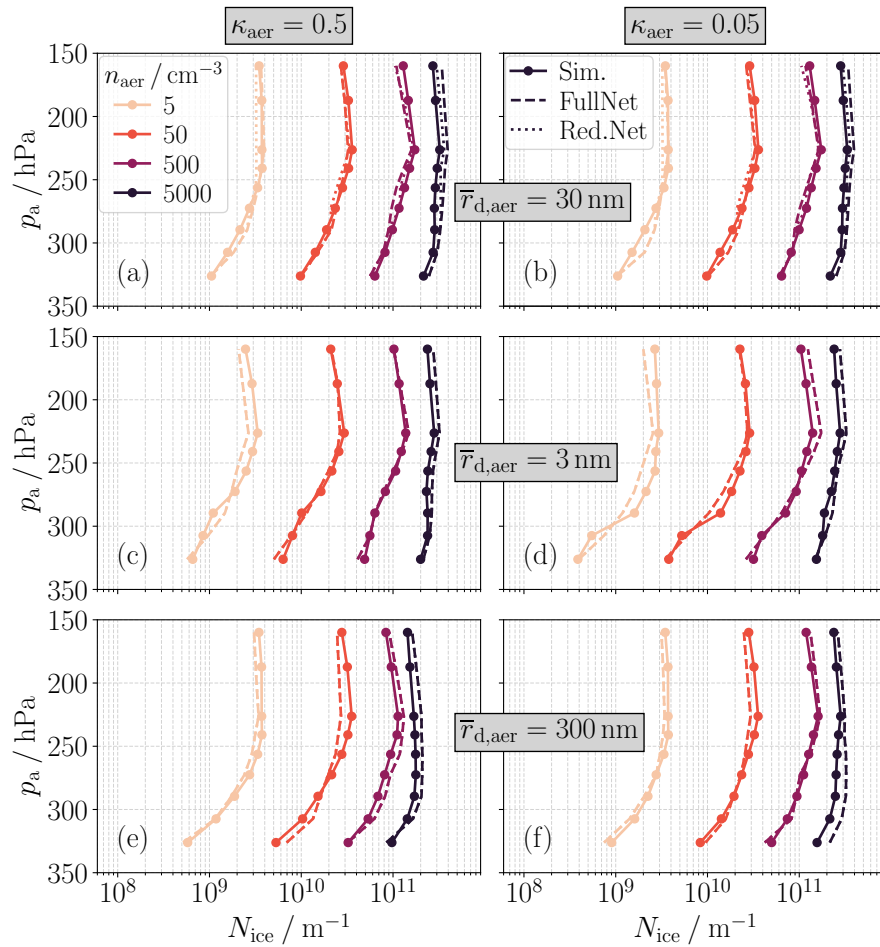


Figure 6. Simulated and parameterized ice crystal number N_{ice} as a function of different aerosol number concentrations n_{aer} (different colors), different aerosol geometric mean radii $\bar{r}_{\text{d,aer}}$ (different rows) and different hygroscopicities κ_{aer} (different columns). Ambient pressure p_a and temperature T_a values are set according to the International Standard Atmosphere (Table 3), and ambient relative humidity is fixed to $RH_{\text{ice,a}} = 120\%$. The outcome of the FullNet is shown in all panels, while the ReducedNet is additionally applied in the first row for cases with $T_a \leq 225 \text{ K}$. Results are shown for $N_{\text{ice}} > 0$.



physical basis of all proposed scaling relations has been discussed in detail in Part 1 (Zink et al., 2025a) and Part 2 (Zink and Unterstrasser, 2025) and is briefly summarized here.

In Part 1, we showed that we can mimic the effect of multiple coexisting aerosol populations by the weighted mean approach

$$N_{\text{ice,tot}} \approx \sum_i \frac{n_{\text{aer},i}}{n_{\text{aer,tot}}} N_{\text{ice},i}(n_{\text{aer,tot}}), \quad (16)$$

where $N_{\text{ice},i}(n_{\text{aer,tot}})$ is the ice crystal number obtained from a simulation that includes only population i with its hygroscopicity $\kappa_{\text{aer},i}$ and geometric mean dry radius $\bar{r}_{\text{d,aer},i}$ but with assumed total aerosol number concentration $n_{\text{aer,tot}} = \sum_i n_{\text{aer},i}$. In practice, the neural networks are separately called for each population using $\kappa_{\text{aer},i}$ and $\bar{r}_{\text{d,aer},i}$ together with $n_{\text{aer,tot}}$. The outputs are then combined through the weighted mean approach (Eq. (16)) to represent the effect of multiple co-existing aerosol populations.

The neural networks provide the ice crystal number for an engine with a reference overall propulsion efficiency of $\eta^* = 0.4$ (Table 1). In Part 2, we demonstrated that the effect of a different efficiency η on the ice crystal number can be mimicked by keeping η^* but adjusting the pressure according to

$$p_{\text{a,adj}} = p_{\text{a}} \frac{1 - \eta^*}{1 - \eta}. \quad (17)$$

We showed that this scaling works reasonably well for tested η -values in the range from 0.325 to 0.475. Consequently, to represent efficiencies different from η^* , the neural networks are called with the adjusted pressure $p_{\text{a,adj}}$.

Moreover, the neural networks return the ice crystal number for a reference engine size and jet speed (Table 1). In Part 2, we introduced scaling factors that account for differences in jet speed s_{shear} and engine size s_{E} relative to the reference values with associated change in dilution speed s_{dil} . These scaling factors are defined as

$$s_{\text{shear}} = U_{\text{jet,E}}^* / U_{\text{jet,E}} \quad (18a)$$

$$s_{\text{E}} = r_{\text{E}} / r_{\text{E}}^* \quad (18b)$$

$$s_{\text{dil}} = s_{\text{shear}} \cdot s_{\text{E}} \quad (18c)$$

$$\hat{s}_{\text{E}} = s_{\text{E}} \cdot \sqrt{U_{\text{tot,E}} U_{\infty}^* / (U_{\text{tot,E}}^* U_{\infty})} \quad (18d)$$

with $U_{\text{tot,E}} = U_{\text{jet,E}} + U_{\infty}$. The scaling factor $\hat{s}_{\text{E}}$ accounts for the fact that the number of entrained ambient aerosols scales with the effective core exit area $\hat{A}_{\text{E}} = A_{\text{E}} U_{\text{tot,E}} / U_{\infty}$ (see Eq. (12) in Zink and Unterstrasser (2025)). If only this effective core area were scaled without any change in dilution speed, then the number of ice crystals would scale simply with $\hat{s}_{\text{E}}^2$.

In Part 2 we introduced the scaling

$$\frac{N_{\text{ice}}}{\hat{s}_{\text{E}}^2 \cdot s_{\text{dil}}^a} \sim f(s_{\text{dil}}^{3/2} \cdot n_{\text{aer}}) \quad (19)$$

with

$$a = \begin{cases} -\frac{3}{2} & \text{for } T_{\text{a}} \leq 230 \text{ K} \\ \frac{1}{6} (T_{\text{a}}/\text{K} - 239) & \text{for } 230 \text{ K} < T_{\text{a}} \leq 235 \text{ K} \end{cases} \quad (20)$$



The function f depends on ambient conditions and aerosol properties but not explicitly on the engine size/dilution speed. This means that the curves for different $\hat{s}_E$ and s_{dil} values collapse when the scaling is applied. Practically, the neural networks are evaluated with the input $s_{dil}^{3/2} \cdot n_{aer}$ and the resulting ice crystal number is multiplied by $\hat{s}_E^2 \cdot s_{dil}^a$ to represent non-reference engine size and jet speed.

295 In practical applications, information about engine size and jet speed may not always be available. As a first-order approximation, the fuel consumption per meter of flight path m_C can then be used to estimate s_E . Here, m_C refers to the fuel consumption of a single engine, i.e.,

$$m_C = \frac{m_{C,tot}}{n_{engines}} , \quad (21)$$

300 where $m_{C,tot}$ is the total fuel consumption of the aircraft and $n_{engines}$ the number of engines. Since $m_C \propto s_E^2/\eta$, it follows the approximation

$$\hat{s}_E \approx s_{dil} \approx s_E \approx \sqrt{m_C \eta / (m_C^* \eta^*)} . \quad (22)$$

Clearly, this approximation implicitly assumes similar excess jet speeds and ratios of total jet speed to aircraft speed.

The weighted mean approach (Eq. (16)) and the scaling associated with jet speed and engine size (Eq. (19)) were tested independently in Parts 1 and 2. The former was applied only to the reference engine (Table 1), while the latter was tested for
305 a single aerosol population. Here, we propose combining the two scalings. The validity of using them together is exemplarily demonstrated in Fig. 7. The figure shows results from LCM box model simulations including two aerosol populations with the size s_E of the reference engine (Table 1) scaled both up and down. These simulations are compared to parameterized values obtained through the step-by-step cookbook described in Appendix A. The results are presented from three perspectives: First, scaling according to Eq. (19) shows that the simulated curves for different engine sizes almost collapse onto a single curve
310 (i.e., the scaling associated with the engine size also holds for coexisting aerosol populations). This is well approximated by the parameterized curves, which become identical under this scaling (Fig. 7a). Second, scaling only by the geometric scale $\hat{s}_E$ highlights the influence of the dilution speed s_{dil} (Fig. 7b). Third, the unscaled ice crystal numbers represent the final quantities of interest (Fig. 7c). The simulated curves are reasonably approximated by the parameterized values demonstrating that the weighted mean approach remains valid for engine sizes differing from the reference. Clearly, this is also true if the jet speed
315 had been varied.

The validity of the neural networks is guaranteed only within the variable ranges listed in Table 1. When applying the scalings, care must be taken to avoid extrapolation (for example, the aerosol number concentration supplied as input to the neural networks should not exceed 10000 cm^{-3}).

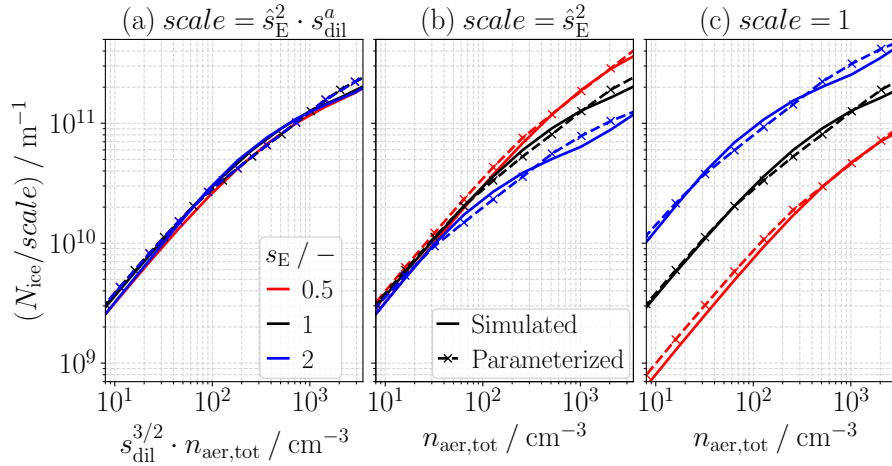


Figure 7. Number of ice crystals per meter of flight path N_{ice} as a function of (scaled) total aerosol number concentration $n_{aer,tot}$. Results from box model simulations including two aerosol populations ($\bar{r}_{d,aer,1} = 30$ nm, $\bar{r}_{d,aer,2} = 3$ nm, $\kappa_{aer,1} = 0.5$, $\kappa_{aer,2} = 0.05$, $\sigma_{aer,i} = 1.6$, $n_{aer,1} : n_{aer,2} = 1 : 1$) are compared to the parameterized values following the cookbook described in Appendix A. Different engine sizes s_E are considered (with $\hat{s}_E = s_{dil} = s_E$). Ambient temperature, ambient pressure and ambient relative humidity are set to $T_a = 225$ K, $p_a = 260$ hPa and $RH_{ice,a} = 115\%$, respectively. (a) Scaling after Eq. (19), (b) Scaling of N_{ice} by the geometric scale $\hat{s}_E^2$, (c) Unscaled data.

4 Discussion

4.1 Comparison with existing parameterization

4.1.1 The K15 model

Kärcher et al. (2015) developed a microphysical model describing contrail ice crystal formation during the jet phase, hereinafter referred to as the K15 model. The K15 parameterization was designed for conventional kerosene or alternative fuels with soot emissions within the soot-rich regime (defined as a regime where ice crystal formation on soot particles dominates) and estimates the number of ice crystals forming on soot and ambient aerosol particles. This parameterization was integrated into the GCM ECHAM-CCMod for studying the radiative forcing of contrails in soot-rich scenarios (Bier and Burkhardt, 2019, 2022). By setting the soot emission index to zero and replacing the combustion-specific parameters with hydrogen values (specific combustion heat $Q = 120$ MJ kg⁻¹ and water vapor emission index $EI_v = 8.94$ kg kg⁻¹), the model framework was adapted by Pettersson et al. (2025) to study hydrogen combustion scenarios. Using this adaptation, they employed the K15 model for contrail formation on ambient aerosol and lubrication oil particles. They integrated the outcomes of the K15 model into the Contrail Cirrus Prediction model (CoCiP) (Schumann, 2012) to assess the energy forcing of contrail cirrus from hydrogen combustion. In the following, this hydrogen-adapted model is termed K15-H2, while K15 is used when referring to the model's general framework.



Unlike our data-driven approach (of fitting box model simulation data), K15 uses an approach based on first principles. The underlying physical laws (as implemented in the box model, e.g.) are reformulated and simplified such that the reduced equations can be solved analytically. In the subsequent paragraph, we briefly summarize the key idea of the K15 model; for a more comprehensive description, the reader is referred to the original publication.

Starting point is the differential equation for the plume supersaturation $s = S - 1$, where S is the saturation ratio over water (relative humidity over water given as ratio and not in percentage). This differential equation is expressed as

$$\frac{ds}{dt} = \mathcal{P} - \mathcal{L} . \quad (23)$$

Here, $\mathcal{P}$ denotes the net production of supersaturation, consisting of a dilution term that tends to decrease the supersaturation and a cooling term that tends to increase the supersaturation (Eq. (6) in Kärcher et al. (2015)). $\mathcal{L}$ denotes the microphysical condensation sink (Eq. (45) in Kärcher et al. (2015)).

The key idea of the K15 model is to determine the point in time at which the net production of supersaturation equals the condensation sink, i.e., when $\frac{ds}{dt} = 0$. The model first checks how many droplets would be required to satisfy $\mathcal{L} = \mathcal{P}$ at a given time t . As a second criterion, it checks how many plume particles could already activate into droplets according to κ -Köhler theory (Petters and Kreidenweis, 2007). The activation-relaxation point in time $t = t_{\text{peak,K15}}$ is chosen, such that both criteria yield the same number concentration of activated particles $n_{\text{act,peak,K15}}$. Here, we introduce the notion of a peak value of supersaturation, even though the K15 model itself is not time-resolved, in order to maintain a consistent naming convention with the terminology used to describe the results of the box model simulations in Sect. 4.1.2.

For $t < t_{\text{peak,K15}}$, the K15 model assumes negligible water vapor depletion so that the supersaturation evolves as it would without microphysical sink terms. Moreover, it assumes that the number of activated aerosols is sufficient to quench supersaturation and no further droplet formation occurs beyond $t = t_{\text{peak,K15}}$. In soot-rich scenarios, this assumption of instantaneous supersaturation relaxation is justified because the largest soot particles are already activated at $t = t_{\text{peak,K15}}$ and rapidly reduce the supersaturation. As a result, the number of particles that would activate after $t = t_{\text{peak,K15}}$ becomes negligible. However, this assumption of instantaneous supersaturation relaxation becomes questionable when aerosol emissions are reduced drastically.

Finally, the K15 parameterization assumes that all aerosols that activate at $t_{\text{peak,K15}}$ subsequently freeze into ice crystals. This approximation is reasonable at the low temperatures at which kerosene contrails form, but becomes problematic at the higher temperatures at which hydrogen contrails can form as not all activated droplets may freeze.

As we report ice crystal numbers per meter of flight path in the present study, the number concentration $n_{\text{act,peak,K15}}$ is converted into the integrated number of activated particles per meter of flight path, $N_{\text{act,peak,K15}}$, by multiplying it with the plume cross-sectional area. The final number of ice crystals formed is then obtained by setting $N_{\text{ice,K15}} = N_{\text{act,peak,K15}}$.

4.1.2 Contrasting the two approaches

As the K15 parameterization was recently applied for hydrogen combustion (Pettersson et al., 2025), we compare this K15-H2 parameterization with our H2 parameterization of contrail ice crystals formed on entrained ambient aerosols. Across the

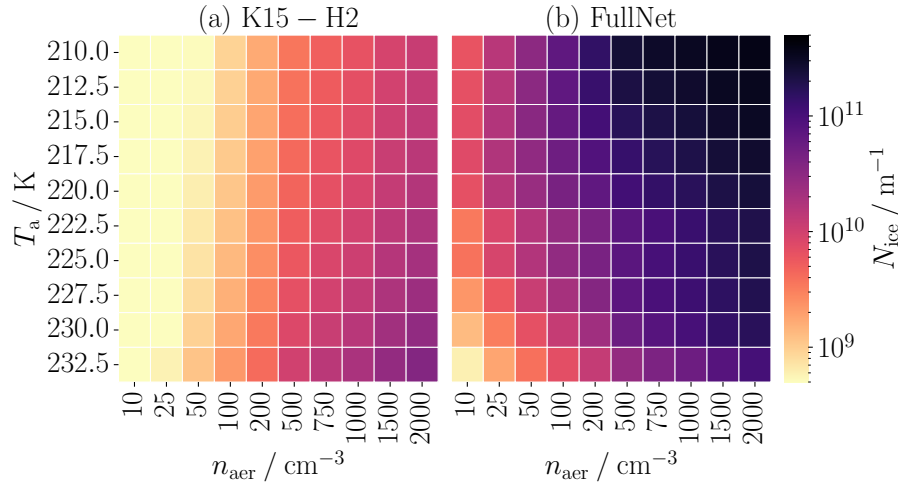


Figure 8. Number of ice crystals per meter of flight path N_{ice} for (a) the K15-H2 parameterization with $B = 0.9$ in Eq. (24) and (b) the outcome of the FullNet. Values are presented for selected combinations of ambient aerosol number concentration n_{aer} and temperature T_a .

two approaches, we consistently prescribe the parameters for aerosol geometric mean radius, geometric width, hygroscopicity, ambient pressure, and ambient relative humidity over ice. Their values are fixed at $\bar{r}_{d,aer} = 20$ nm, $\sigma_{aer} = 1.6$, $\kappa_{aer} = 0.5$, $p_a = 230$ hPa, and $RH_{ice,a} = 115\%$, respectively. Engine-related parameters are set according to the reference values listed in Table 1 for which the neural networks are valid without any scaling needed.

Fig. 8 compares the ice crystal number obtained from the K15-H2 parameterization and from the FullNet, with both approaches using the same consistent parameter set. The ice crystal number differs substantially between the two parameterizations. While the magnitudes are comparable at high ambient temperatures, the K15-H2 parameterization gives ice crystal numbers up to two orders of magnitude lower at low ambient temperatures. Moreover, the dependence on ambient temperature is reversed between the two approaches: in the K15-H2 model, the ice crystal number increases with increasing temperature, whereas in our approach, the number decreases with increasing temperature.

The trends observed in the outcome of the FullNet are confirmed by underlying LCM box model simulations. To better understand and explain the differences between K15-H2 and our parameterization, we analyze the time-resolved droplet formation and freezing processes in our box model. For consistency, we prescribe the same analytical dilution formula in the box model setup as in K15-H2. This analytical formula for the dilution factor $\mathcal{D}$ reads

$$\mathcal{D}(t > \tau_m) = \left(\frac{\tau_m}{t} \right)^B \quad (24)$$

and $\mathcal{D} = 1$ for $t \leq \tau_m$ with $\tau_m \approx 0.01$ s. The exponent B determines the dilution speed, which can be adjusted both in K15 and in the box model. In K15, the default value $B = 0.9$ was proposed in Kärcher (1999). In Part 2 (Zink and Unterstrasser, 2025), it was shown that $B = 1.15$ yields closer agreement with the FLUDILES dilution data (Vancassel et al., 2014), which were used to construct the simulation database for the training of the neural networks. Furthermore, Fig. 8b in Part 2 demonstrates that ice crystal numbers obtained with $B = 1.15$ differ only marginally from those obtained with the FLUDILES data. We



therefore prescribe each of the two values ($B = 0.9$ and $B = 1.15$) in K15-H2 and in our box model. This allows the effects of the underlying dilution data to be disentangled from those of the model physics.

Fig. 9a and 9b show selected examples of the evolution of plume relative humidity over water $RH_{\text{wat}}(t)$ with the peak values $RH_{\text{wat,peak}}$ highlighted. For the box model, two types of $RH_{\text{wat}}(t)$ evolutions are depicted: a version with microphysics switched off (transparent lines) and the standard version with microphysical water vapor depletion (opaque lines). It is apparent that both types and the K15-H2 have a basically identical $RH_{\text{wat}}(t)$ evolution up to the point in time $t = t_{\text{peak,K15}}$. Hence, the box model results support the assumption of zero water vapor depletion in K15-H2 until $t = t_{\text{peak,K15}}$. However, $RH_{\text{wat,peak,K15}}$ (marked by a blue cross) is much lower and occurs earlier than the maximum relative humidity value within the box model, $RH_{\text{wat,peak,box}}$ (marked by a magenta cross). At $t = t_{\text{peak,box}}$, microphysical water vapor depletion is already pronounced, with the amount of depleted water vapor depending on the aerosol number concentration (difference between transparent and opaque magenta lines in Fig. 9a and b, respectively).

As the K15-H2 parameterization treats $t = t_{\text{peak,K15}}$ as the point where further droplet activation ceases, $RH_{\text{wat,K15}}$ is assumed to drop abruptly to 100%. In contrast to K15-H2, the box model results show that the supersaturation is not quenched at $t = t_{\text{peak,box}}$ and supersaturation persist over an extended period.

Fig. 9c–d depicts the evolution of already activated aerosols $N_{\text{act}}(t)$ (the sum of droplets and ice crystals in the box model). Since $t_{\text{peak,K15}} < t_{\text{peak,box}}$, it follows that $N_{\text{act,peak,K15}} < N_{\text{act,peak,box}}$. At $t = t_{\text{peak,K15}}$, the number $N_{\text{act,peak,K15}}$ equals $N_{\text{act,box}}(t = t_{\text{peak,K15}})$. Thus, both approaches yield a comparable number of activated aerosols up to this point in time. Within the box model, however, the activation of continuously entrained ambient aerosols extends over a longer period, such that the final number of ice crystals formed is not only considerably higher than $N_{\text{act,peak,K15}}$ but also higher than $N_{\text{act,peak,box}}$ (marked by a magenta cross).

After the illustrative example for the ambient temperature $T_a = 220\text{ K}$, we now evaluate results across a range of T_a (Fig. 10). Fig. 10a–b shows the peak values of plume relative humidity $RH_{\text{wat,peak}}$. These values decrease with increasing ambient temperature and higher aerosol number concentration. At low T_a , the K15-H2 parameterization yields substantially lower peak values than the box model and the dependence on dilution speed is reversed: in K15-H2, slower dilution ($B = 0.9$) yields higher peak values, while in the box model faster dilution ($B = 1.15$) does. This difference arises from the assumption of zero water vapor depletion for $t < t_{\text{peak,K15}}$ in the K15-H2 model. Contrastingly, early activation in the box model already reduces water vapor until $t = t_{\text{peak,box}}$ with slower dilution resulting in lower peak values.

For all investigated scenarios, it holds $t_{\text{peak,K15}} < t_{\text{peak,box}}$ (Fig. 10c–d). In the box model, the point in time $t_{\text{supersat,end}}$ where $RH_{\text{wat,box}}$ falls below 100% is long after $t_{\text{peak,box}}$. Moreover, t_{peak} gets larger with T_a (in both modeling approaches), while $t_{\text{supersat,end}}$ generally decreases with T_a . At high T_a and slow dilution ($B = 0.9$), $t_{\text{supersat,end}}$ increases with T_a . This can be attributed to the influence of the freezing timescale at these high temperatures (Zink and Unterstrasser, 2025).

Figures 10e–f show the mean radius of activated aerosols at $t = t_{\text{peak,K15}}$. Already activated aerosols are much larger in K15-H2 than simulated by the box model at these points in time. This explains why supersaturation relaxation in the K15-H2 occurs before the relative humidity peaks in the box model: larger droplets provide enough surface area to remove supersaturation more quickly. Consequently, it holds $N_{\text{act,peak,K15}} < N_{\text{act,peak,box}}$ for all investigated scenarios (Fig. 10g–h). However, in

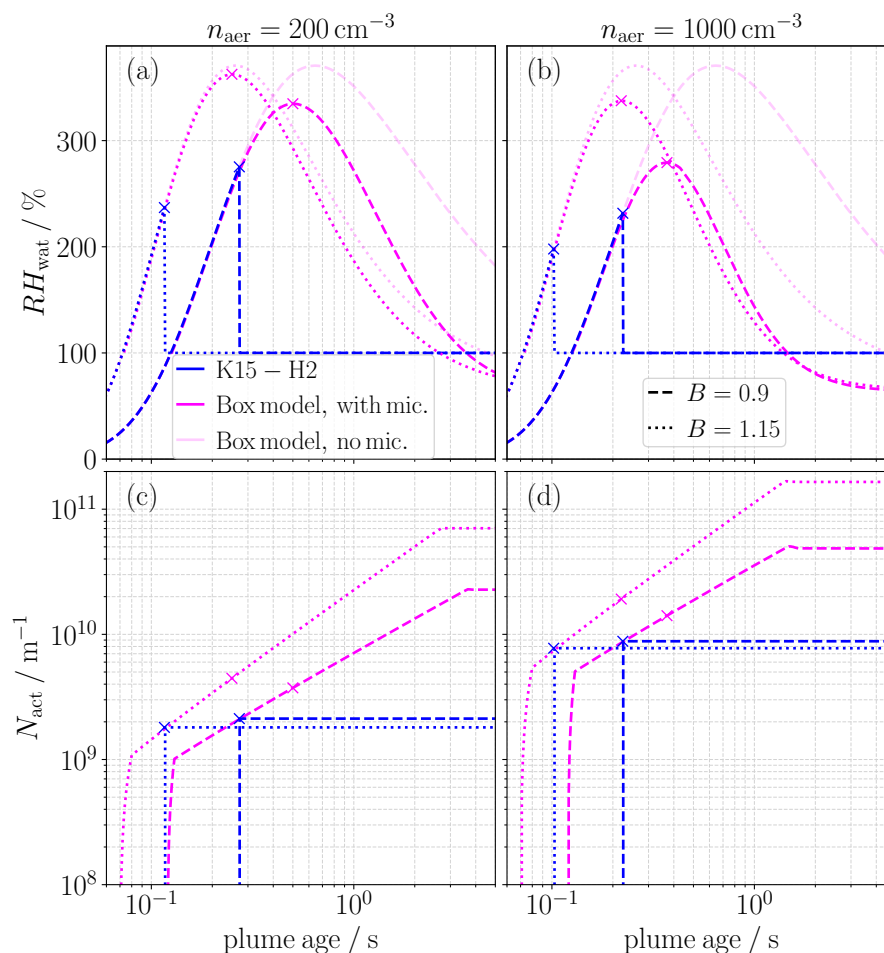


Figure 9. First row: Evolution of plume relative humidity over water RH_{wat} with peak values highlighted (crosses). Examples are shown for the ambient temperature $T_a = 220\text{ K}$ and two aerosol number concentrations n_{aer} (columns). The evolutions according to the K15-H2 parameterization (blue) are compared to LCM box model simulation results (magenta). Dashed and dotted curves correspond to exponents $B = 0.9$ and $B = 1.15$ in Eq. (24), respectively. Results are presented for cases with microphysical water vapor depletion (opaque curves) and with microphysics switched off (transparent curves). Second row: Evolution of number of already activated aerosols N_{act} (sum of droplets and ice crystals in the box model) and the nucleation pulse for the K15-H2 parameterization with the values highlighted, where the relative humidity peaks (crosses).



most cases, $N_{\text{act,peak,box}}$ remains significantly below the final number of ice crystals formed $N_{\text{ice,box}}$ due to the continuous entrainment and activation of ambient aerosols long after $t = t_{\text{peak,box}}$. The increase of $N_{\text{act,peak}}$ with increasing T_a reflects the increase of t_{peak} with T_a (in both modeling approaches). In contrast, the decrease of $N_{\text{ice,box}}$ with increasing T_a reflects the decreased duration of supersaturation and lower relative humidity peaks at higher ambient temperatures. Furthermore, the dilution-speed dependence is opposite between the two models. In line with Lewellen (2020) and Part 2 (Zink and Unterstrasser, 2025), slower dilution yields fewer ice crystals in the box model because early-activated aerosols have more time to consume the available water vapor and therefore suppress later activation more efficiently. The construction of the K15-H2 model, however, introduces a reversed dependency on dilution speed, even though the dependency is weak in our depicted examples.

The question that remains is why the droplets in the K15-H2 model are larger (Fig. 10e-f), which leads to much earlier supersaturation relaxation in K15-H2 (corresponding to $t_{\text{peak,K15}} < t_{\text{peak,box}}$). This can be explained as follows: At a given time t , the model looks backward to a past time t' when an aerosol particle would have been activated based on the aerosol dry spectrum at time t . As the K15 parameterization was originally developed for kerosene and ice crystal formation on emitted soot particles, it does not check, whether an aerosol particle present at time t was already present in the plume at t' . Thus, droplet growth is assumed to start at t' , when the critical barrier is crossed according to κ -Köhler theory, even if the particle was entrained into the plume at a later time. This leads to an overestimation of growth time in K15-H2, producing larger droplets at earlier plume ages.

In summary, contrail formation on entrained ambient aerosols cannot be resolved by a parameterization assuming a nucleation pulse as it cannot realistically represent the water vapor depletion by continuously entrained and activated ambient aerosols. This continuous process is especially critical for hydrogen combustion, where supersaturation persists longer than for kerosene due to the higher water vapor emission index (Schumann, 1996; Bier et al., 2024). The K15 contrail ice formation parameterization was developed for aviation emissions within the soot-rich regime. Our analysis demonstrates that the K15 parameterization should not be applied in regimes where droplet formation on entrained particles is dominant.

4.2 Strengths and limitations of the parameterization

The parameterization relies on the outcome of time-resolved contrail formation simulations performed with the LCM box model, which includes detailed microphysics. The neural networks are employed as fitting functions of the simulation results, so that the parameterization does not introduce any assumptions beyond those in the original box model. Together with the provided scaling relations, the neural networks yield a generalized parameterization that captures the (nonlinear) influence of many variables on the ice crystal number. Although only a few calculations are needed (Eqs. (2a)–(2d)), the neural networks are flexible enough to capture the nonlinear dependence of the ice crystal number on the input variables. The underlying physics have been discussed in detail in Parts 1 and 2 (Zink et al., 2025a; Zink and Unterstrasser, 2025).

The neural networks are trained on a systematically constructed database without weighting data points (e.g., by the joint probability density function of climatology of ambient conditions, aerosol distributions, or air traffic). This approach ensures that the parameterization is broadly applicable. This includes a wide range of potential future scenarios, reflecting uncertainties

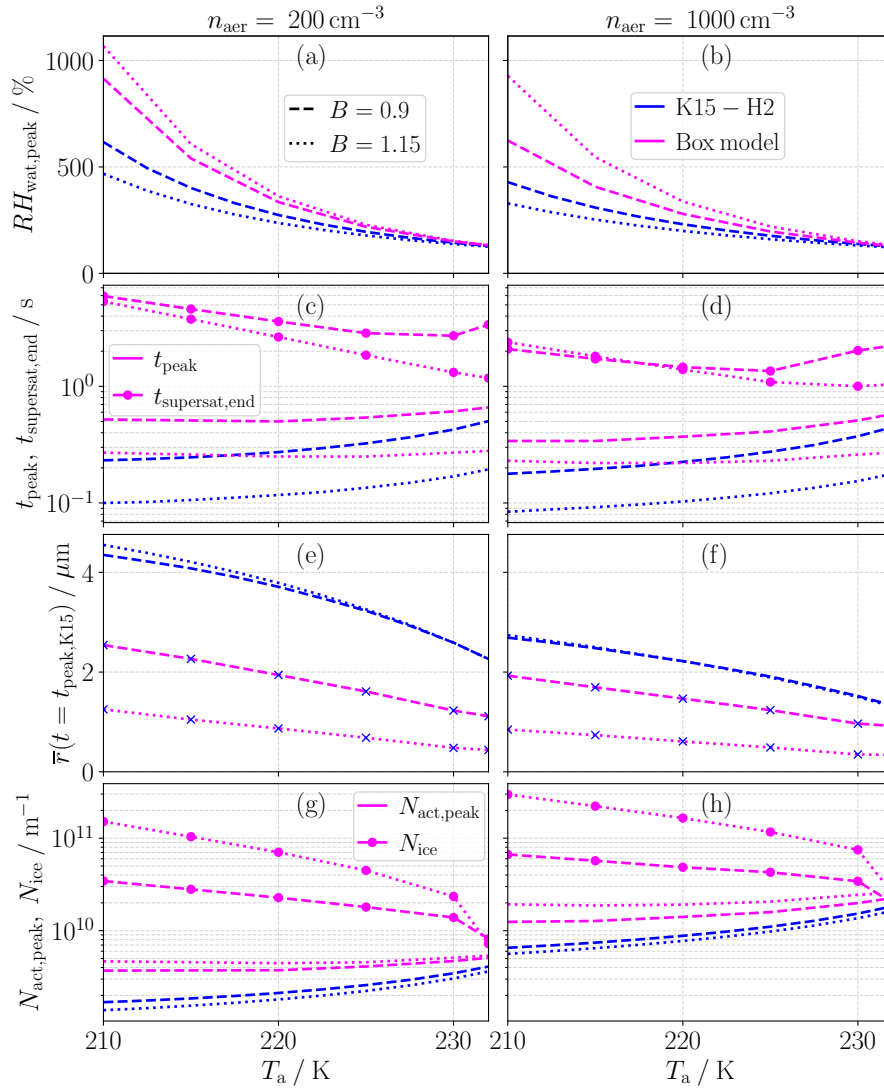


Figure 10. Comparison of the K15-H2 parameterization (blue) to LCM box model results (magenta). Dashed and dotted curves correspond to exponents $B = 0.9$ and $B = 1.15$ in Eq. (24). Results are shown as a function of ambient temperature T_a for two aerosol number concentrations n_{aer} (columns). Panels: (a)-(b) Peak value of plume relative humidity over water $RH_{wat,peak}$. (c)-(d) Point in time t_{peak} at which plume relative humidity peaks. For the box model outcome, the point in time $t_{supersat,end}$ is also depicted, where the relative humidity falls below 100 % (curves with magenta dots). (e)-(f) Mean radius of activated aerosols $\bar{r}(t = t_{peak,K15})$ at the time of activation in the K15-H2. Box model results are evaluated at the same point in time $t = t_{peak,K15}$ (magenta line with blue crosses). (g)-(h) Number of activated aerosols $N_{act,peak}$ at the relative humidity peaks. The final number of ice crystals formed N_{ice} is shown for the box model results in addition (curves with magenta dots).



455 in climate projections, ambient aerosol loading, and air traffic evolution. Due to the gridded structure of the training database, the validity is well defined by the range spanned between the lower and upper grid values (Table 1).

As the neural networks consist of only a short sequence of calculations (Eqs. (2a)–(2d)), their implementation in large-scale models is straightforward. An alternative approach based on multidimensional lookup tables would require considerably more storage than the weight matrices and necessitate interpolation between tabulated points. Neural networks therefore offer a
460 more compact and efficient way to integrate the box model simulation results into large-scale models. In addition, the proposed neural-network-based framework can be easily updated. Once a suitable training database is created, the neural networks can be retrained on a local machine within minutes. Updating the neural networks in large-scale models is equally simple, requiring only the replacement of the weights and biases.

The neural networks reproduce the box model results with the errors listed in Table 2 and any remaining limitation arises
465 from the LCM box model itself. The LCM box model has been validated against other contrail formation models for conventional kerosene combustion with ice crystal formation on soot particles (Bier et al., 2022). Parameterizations of physical processes in the box model, particularly those relevant to hydrogen combustion, introduce additional uncertainty. For example, homogeneous freezing is modeled using a combined approach (Bier et al., 2024) that accounts for both the cooling rate (i.e., the change of supersaturation) (Riechers et al., 2013) and the solution effect of aqueous droplets (O and Wood, 2016). These
470 parameterizations are based on laboratory measurements under conditions typical of natural cirrus clouds, which have lower turbulence and slower cooling rates than turbulent jets, making their applicability to contrail formation uncertain. Measurements at contrail formation conditions for which our simulations indicate a strong influence of homogeneous freezing (ambient temperatures $\gtrsim 230\text{ K}$) would be particularly valuable for validation.

A key uncertainty of the parameterization lies in the assumption that entrained ambient aerosols are the sole precursors of
475 ice crystal formation. Recently, Zink et al. (2025b) demonstrated that even a very small amount of lubrication oil released into the exhaust (on the order of a few milliliters per hour or less) can produce large numbers of particles. When the oil enters the hot sections of the exhaust, it may evaporate and re-nucleate in the subsequent cooling plume, producing a nucleation-mode particle distribution (Ungeheuer et al., 2022). As such oil particles can activate into droplets and freeze into ice crystals (Ponsonby et al., 2024), a tiny amount of lubrication oil could already lead to oil-particle-dominated ice crystal formation
480 (Zink et al., 2025b). The impact depends strongly on where the lubrication system vents. If venting occurs close to the hot core exit, entrainment into high-temperature regions promotes evaporation and re-nucleation. If the oil breather flow is released far away from the hot regions, the oil might be entrained into the plume when it has already cooled down such that it does not evaporate. These oil particles are then expected to be larger (a few hundred nanometers) and correspondingly fewer in number, thus contributing only little to ice crystal number. Thus, lubrication oil poses a potential concern for certain engine
485 configurations, though technical measures to reduce or mitigate this effect may be feasible.

Furthermore, our simulations neglected the potential impact of NO_x emissions on contrail formation. In the exhaust plume, gaseous nitric acid (HNO_3) forms through oxidation of NO_x (Kärcher, 1995). This nitric acid may influence plume chemistry and contrail microphysics in two ways. First, HNO_3 could contribute to new particle formation, on which water vapor then condenses. While electrically neutral nitric acid alone may nucleate inefficiently, the presence of ions formed during the



490 combustion process may enhance ion-induced nucleation (Yu and Turco, 1997; Kärcher et al., 2000). Clearly, the composition of ions and formation of volatile particles in the exhaust of aircraft burning hydrogen differs from that of conventional jet fuels, mainly because of the absence of sulfur and organic species in the fuel. Previous studies have additionally shown that nucleation is further facilitated in the presence of ammonia (Kirkby et al., 2023), which is not a direct emission product but is present in the ambient atmosphere. It remains an open question whether nitric acid-driven nucleation is efficient enough to
495 contribute substantially to ice crystal formation and further research is needed to clarify its significance. Second, the uptake of highly soluble nitric acid by the entrained ambient aerosols could modify their chemical properties, which in principle could be represented by a time-dependent hygroscopicity. In our simulations, however, hygroscopicity values are prescribed at the beginning and remain constant throughout the simulation runs. Simulations for a wide range of prescribed hygroscopicity values (Table 1) showed that modest variations only marginally affect the number of ice crystals (Zink et al., 2025a). We
500 therefore speculate that allowing hygroscopicity to vary slightly over time would likewise have little impact on the results, and the use of fixed hygroscopicity values is unlikely to introduce a substantial bias.

In summary, considering only entrained ambient aerosols as precursors, the presented ice crystal numbers represent an (idealized) lower limit. While other particle sources could, in principle, be reduced by technical measures, ambient aerosols cannot be removed and their abundance in the exhaust plume is constrained by their concentrations in the background atmosphere.

505 5 Conclusions

We developed a parameterization for the number of contrail ice crystals $N_{ice,f}$ formed on entrained ambient aerosols for aircraft with hydrogen combustion. This parameterization can be integrated into large-scale models with a contrail parameterization to study the climate impact of contrails from an aviation fleet powered by hydrogen combustion. The parameterization combines a neural-network-based fit to a multidimensional database of time-resolved contrail formation simulations with analytical scaling
510 relations. The comparison with a parameterization assuming a nucleation pulse and instantaneous supersaturation relaxation demonstrated that, for hydrogen combustion, a time-resolved database is essential in order to realistically capture the full contrail formation process on entrained ambient aerosols.

The provided functional relationship can be summarized as

$$\begin{aligned} N_{ice,f} &= N_{ice,f}(\mathbf{a}_{atmosphere}, \mathbf{a}_{aerosol}, \mathbf{a}_{aircraft}) \\ &= N_{ice,f}(T_a, p_a, RH_{ice,a}, \{n_{aer,i}, \bar{r}_{d,aer,i}, \kappa_{aer,i}\}_{i=1}^N, \eta, r_E, U_{jet,E}, U_\infty, n_{engines}) \\ &\approx N_{ice,f}(T_a, p_a, RH_{ice,a}, \{n_{aer,i}, \bar{r}_{d,aer,i}, \kappa_{aer,i}\}_{i=1}^N, \eta, m_{C,tot}, n_{engines}) . \end{aligned} \quad (25)$$

515 It includes input variables describing the background atmosphere $\mathbf{a}_{atmosphere}$, which are the ambient temperature T_a , ambient pressure p_a and ambient relative humidity $RH_{ice,a}$. Moreover, it contains properties $\mathbf{a}_{aerosol}$ of multiple aerosol populations i , namely the number concentration $n_{aer,i}$, geometric mean radius $\bar{r}_{d,aer,i}$ and hygroscopicity $\kappa_{aer,i}$. Finally, it incorporates aircraft-related parameters $\mathbf{a}_{aircraft}$, which are the overall propulsion efficiency η , the engine core exit radius r_E , core exit excess jet speed $U_{jet,E}$, aircraft speed U_∞ and the number of engines $n_{engines}$. If information about engine size and jet speed
520 is not available, than an approximation can be used that is based on the total fuel consumption of the aircraft $m_{C,tot}$.



Appendix A: Parameterization cookbook

1. Calculate the adjusted pressure $p_{a,adj}$ according to Eq. (17) to account for deviations of the actual overall propulsion efficiency η from the reference value η^* (Table 1).
2. Calculate the scaling factors s_{shear} , s_E , s_{dil} and $\hat{s}_E$ according to Eqs. (18a)-(18d) accounting for differences in jet speed
525 and engine size with associated change in dilution speed. If information is missing, then use the approximation after Eq. (22).
3. Determine the total aerosol number concentration $n_{aer,tot} = \sum_i n_{aer,i}$ where the index i runs over all aerosol populations.
4. For each aerosol population, determine $N_{ice,param,i}$ by following the flow chart in Fig. A1. As inputs use ambient temper-
530 ature T_a , adjusted ambient pressure $p_{a,adj}$, ambient relative humidity $RH_{ice,a}$, scaled total aerosol number concentration $s_{dil}^{3/2} n_{aer,tot}$, single aerosol population hygroscopicity $\kappa_{aer,i}$ and geometric mean dry radius $\bar{r}_{d,aer,i}$.
5. Multiply $N_{ice,param,i}$ by $\hat{s}_E^2 s_{dil}^a$ with a set according to Eq. (20).
6. Calculate the weighted mean after Eq. (16) to obtain the total ice crystal number $N_{ice,param,tot}$.
7. Multiply $N_{ice,param,tot}$ by the number of engines $n_{engines}$ to obtain the ice crystal number for the whole aircraft, assum-
535 ing that the individual plumes do not overlap during ice crystal formation.

Code and data availability. A python code following the steps described in Appendix A, along with the trained weight matrices, will be made available once the manuscript has been accepted. The LCM box model simulations used for training the neural networks are available in the Zenodo repository of Part 1 (<https://doi.org/10.5281/zenodo.17977711>).

Author contributions. JZ and SU conceptualized the study, with CWR and UB contributing in Sects 3.2 and 4.1. JZ performed the box model
540 simulations and trained the neural networks. JZ created the tables and all figures except Fig. 8, which was produced by CWR. JZ wrote the first draft of the manuscript. All authors reviewed and edited the manuscript, particularly Sect. 4.1, which was developed collaboratively by all authors. SU and UB supervised the study.

Competing interests. The contact author has declared that none of the authors has any competing interests.

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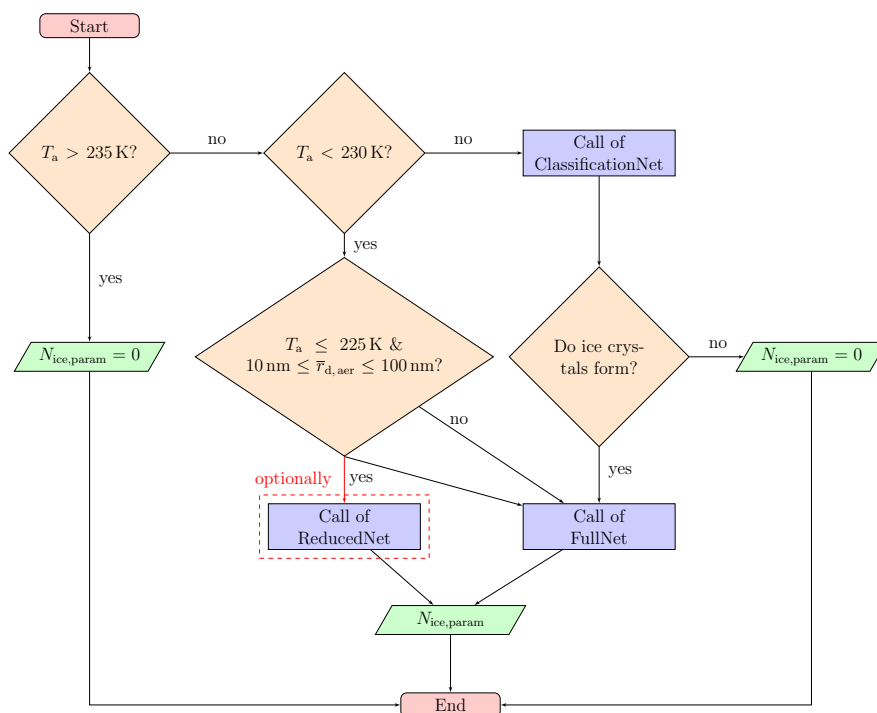


Figure A1. Flow chart for determining the parameterized ice crystal number for a single aerosol population and a single reference engine characterized by the parameter values defined in Table 1. For the subspace defined by $T_a \leq 225$ K and $10 \text{ nm} \leq \bar{r}_{d,aer} \leq 100 \text{ nm}$, either the FullNet or the ReducedNet can be used.

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P4. On the potential role of lubrication oil particles in contrail formation for kerosene and hydrogen combustion

On the Potential Role of Lubrication Oil Particles in Contrail Formation for Kerosene and Hydrogen Combustion

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Key Points:

- Particles originating from lubrication oil may serve as nuclei for the formation of contrail ice crystals
- Oil particles could be the dominant nuclei when soot particle numbers are low (soot-poor regime) or zero (e.g., for hydrogen combustion)
- Measurements are needed to constrain our hypothetical simulation scenarios

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Abstract The radiative forcing caused by contrail cirrus is nonlinearly influenced by the number of ice crystals formed in the exhaust plume behind an aircraft engine. This ice crystal number strongly depends on the properties (number, size, and solubility) of condensation nuclei in the plume available for droplet activation with subsequent freezing. In this ice crystal formation process, the relative importance of plume particles originating from lubrication oil is unclear. Therefore, we have extended the particle-based Lagrangian Cloud Module in the box model approach to simulate the formation of ice crystals on such oil particles. With this extended box model, we performed simulations for many different scenarios of emitted oil particle numbers and sizes. We examine the activation of these oil particles and investigate their competition with soot for kerosene combustion and with ambient aerosols for hydrogen combustion. Furthermore, we study the relative importance among weakly soluble/insoluble oil particles and well-soluble volatile particles from the combustion process. For present-day soot emissions, the number of ice crystals formed on oil particles may be masked by those formed on soot. However, these oil particles may be abundant enough to dominate ice crystal formation in soot-poor or hydrogen combustion scenarios. This may occur when a small amount of lubrication oil (on the order of a few milliliters per hour) evaporates in the hot exhaust plume and nucleates new particles with a size of a few nanometers during the subsequent plume cooling.

Plain Language Summary Contrail cirrus clouds contribute significantly to the overall climate impact of aviation. These cirrus clouds develop from linear contrails formed by an aircraft engine under certain atmospheric conditions. The climate impact is the stronger the more ice crystals the young contrails contain. For conventional kerosene combustion, these ice crystals primarily form on the emitted soot particles. However, when the number of soot particles is reduced or is zero (e.g., for hydrogen combustion), other particles in the exhaust plume become important. One possible source of such particles is lubrication oil. In this study, we investigate the potential role of such oil particles in the contrail formation process. We examine their activation behavior and their relative importance compared to other ice-forming particles. The results suggest that these oil particles may contribute significantly to the total ice crystal number in soot-poor or hydrogen combustion scenarios. As many different scenarios are investigated in our study, it is essential to measure their actual impact in situ flight campaigns. Nevertheless, our study clearly demonstrates that on the way to aviation technologies with reduced climate impact, every effort should be made to keep the number of oil particles in aircraft exhausts low.

1. Introduction

As part of the aviation non-CO₂ effects, contrail cirrus constitute a significant contributor to the total effective radiative forcing of aviation (Kärcher, 2018; Lee et al., 2021). The optical properties and life cycle of contrail cirrus and thus the climate impact strongly depend on the number of contrail ice crystals formed (e.g., Burkhardt et al., 2018; Unterstrasser & Gierens, 2010). These ice crystals form primarily on emitted soot particles for conventional passenger aircraft engines (e.g., Kärcher & Yu, 2009; Kleine et al., 2018). Because of the strong nonlinear relation between the global contrail cirrus radiative forcing and the number of contrail ice crystals formed (Bier & Burkhardt, 2022; Burkhardt et al., 2018), only a strong reduction in soot number and other particles is expected to have a substantial climate benefit.

Blending conventional Jet-A1 fuel with sustainable aviation fuels (SAF) reduces the soot particle number attributed to the lower aromatic content of SAF (Bräuer et al., 2021; Moore et al., 2017; Voigt et al., 2021). This can reduce young-contrail ice crystal number by up to 70% depending on the SAF proportion (Voigt et al., 2021). Moreover, using a 100% SAF fuel, Märkl et al. (2024) measured a reduction of 35% in soot number and a

reduction of 56% in ice crystal number. They attributed the stronger reduction in ice crystals compared to the soot reduction with a low sulfur content leading to a reduced ice activation of the soot particles. Similarly, hydro-processing can reduce the aromatic content of conventional kerosene (Quante et al., 2024), offering another pathway to lower soot emissions and contrail ice crystal formation.

Soot-free exhaust air is expected from hydrogen combustion due to the absence of carbon compounds in the fuel used. The usage of hydrogen in aviation, either via direct combustion or in a fuel-cell system (Richardson, 2025), is a potential pathway for the decarbonization of the aviation sector. Previous investigations on contrails from hydrogen-powered aircraft were rather academically driven (Grewe et al., 2017), whereas today, the goal of commercial hydrogen-powered aircraft is set from industry (Airbus, 2020) and politics. For thermodynamic reasons, contrails from hydrogen combustion can form at higher temperatures according to the Schmidt-Appleman threshold criterion and exhibit higher supersaturations due to a relative increase of the energy-specific water vapor emission index by a factor of around 2.6 (Bier et al., 2024; Schumann, 1996). Recently, Bier et al. (2024) studied contrail formation in such hydrogen exhaust plumes. They assumed that no exhaust particles that serve as condensation nuclei are emitted and liquid droplet activation and ice crystal formation occurs only on entrained ambient aerosols. Their simulation results suggest that the ice crystal number in the early phase is typically reduced by more than 80%–90% compared to conventional contrails.

However, Kärcher and Yu (2009) showed for kerosene combustion that nanometer sized ultrafine aqueous particles may activate at high supersaturations. Depending on the number of these volatile particles, the ice crystal number in the soot-poor regime may be similarly high at low temperatures as in a soot-rich regime. For conventional kerosene combustion, these volatile ultrafine particles form mainly on emitted charged molecular clusters (chemi-ions) which grow due to the condensation of water vapor, sulfuric acid, nitric acid, and unburned hydrocarbons (F. Yu & Turco, 1997). Because of the absence of sulfur and organic compounds in the hydrogen combustion process, nitrogen oxide species might be the only emitted source for the nucleation of ultrafine volatile particles there. Nitrate ions are potential precursors of ion clusters which may grow through condensation and recombination. However, their nucleation ability to form clusters of a significant size in the nanometer range has not yet been experimentally shown.

Yet, another potential non-combustion source for such volatile particles is lubrication oil. Lubrication oil is used to cool, seal and reduce friction of movable parts such as the drive shaft. Oil systems are generally sealed recirculation systems (Linke-Diesinger, 2010). Breather vents regulate the oil pressure system. This venting results in a controlled emission and releases a mist of oil. Next to the controlled oil emission, worn seals provide an additional uncontrolled sink of oil (Z. Yu et al., 2010). This uncontrolled loss is expected to be a few percent of the controlled oil emission and may vary over time with the degradation of seals, thus with aging of the engine. A typical engine lubrication oil consumption is on the order of a few hundreds of milliliters per hour (Decker et al., 2024; Linke-Diesinger, 2010). This oil consumption may vary among different engine types and thrust settings (Decker et al., 2024).

Several ground-based measurements behind dedicated engines as well as in the vicinity of airports have identified lubrication oil as a major component of aviation-induced ultrafine particulate matter (Fushimi et al., 2019; Ungeheuer et al., 2021; Z. Yu et al., 2019). Motivated by their findings from measurements at Frankfurt Airport (Ungeheuer et al., 2021), Ungeheuer et al. (2022) demonstrated in a laboratory experiment that heating oil particles to 300°C leads to the formation of a small-sized particle distribution. This occurs as the particles evaporate with subsequent nucleation and recondensation of low-volatility products. This experiment resembles conditions when lubrication oil is entrained into hot exhaust plumes, for example, through central venting systems. In another laboratory experiment, Ponsonby et al. (2024) generated oil particles and demonstrated their activation into water droplets and freezing into ice crystals. These particles generated in the laboratory were neither affected by any combustion process nor formed through nucleation and condensation of additional combustion products. They found that these oil particles behave such as insoluble but wettable particles. So far, in-flight emission measurements at cruise altitude have not been able to provide evidence of a dominant contribution of lubrication oil for the formation of nucleation mode ultrafine particles.

Although the experiment by Ponsonby et al. (2024) demonstrated that oil particles are capable of acting as condensation nuclei, their activation behavior under contrail formation conditions and their competition with other plume particles for the available water vapor are still unexplored. In this study, we examine these open points for a range of potential scenarios. We consider different levels of oil emissions and oil particle sizes

(Section 2). In a first step, we investigate the activation behavior of oil particles (Section 3.1). We then analyze their competition with other plume particles and investigate under which scenarios they can lead to a non-negligible or even dominant contribution to the total ice crystal number (Sections 3.2 and 3.3). The implications of the results are discussed in Section 4.

2. Methods

The following section briefly describes the model used in this study. It also outlines the initial conditions and our underlying assumptions.

2.1. Number of Oil Particles

We assume that part of the emitted oil is entrained into the hot plume, where it evaporates and re-nucleates. We assume that this nucleation is completed well before contrail formation starts so that we can prescribe a fixed number of emitted particles. This is justified by the fact that temperatures at which jet oil esters reach gas-phase supersaturation are typically well above 0°C (see, e.g., Figure 3 in Ungeheuer et al., 2022), whereas contrail formation starts well below 0°C. For simplicity and lack of density measurements, we assume that the re-nucleated oil particles have the same density as the original lubrication oil particles and are log-normally distributed with a geometric mean radius $\bar{r}_{d,oil}$ and geometric width σ_{oil} (The probability density function of a log-normal distribution reads $n(r) = \frac{N}{\sqrt{2\pi}} \frac{1}{\ln \sigma} \frac{1}{r} \exp\left[-\frac{1}{2}\left(\frac{\ln r/\bar{r}}{\ln \sigma}\right)^2\right]$ with total number N , geometric mean radius $\bar{r}$ and geometric width σ). The number of oil particles per meter of flight path can be calculated via

$$N_{oil} = \frac{\dot{V}_{oil,eff}}{\frac{4}{3}\pi\bar{r}_{d,oil}^3 \exp\left(\frac{9}{2}(\ln \sigma_{oil})^2\right)} \frac{1}{U_{\infty}}, \quad (1)$$

with the aircraft speed U_{∞} (=250 m s⁻¹ in our case) and the effective oil emission rate

$$\dot{V}_{oil,eff} = \dot{V}_{oil} \cdot \alpha_{entrain} \cdot \alpha_{evaporate} \cdot \alpha_{renucleate} \cdot \alpha_{scavenging} \cdot \beta_{condensates}. \quad (2)$$

Here, $\dot{V}_{oil}$ is the oil emission/loss (in units “volume per time”) from the venting system to the environment. The different α -values, which are supposed to range from zero to one, account for different physical effects: $\alpha_{entrain}$ represents the fraction of the emitted oil entrained into the hot exhaust plume. This value may largely depend on the position of the venting system relative to the engine. $\alpha_{evaporate}$ is the fraction of entrained oil that evaporates. We assume that the fraction $1 - \alpha_{evaporate}$ consists of larger particles originating from oil entrained when the plume is already cooled down so that the oil particles do not evaporate. We assume that the volume fraction $1 - \alpha_{evaporate}$ of the large particles does not significantly contribute to the overall number. $\alpha_{renucleate}$ is the fraction of evaporated oil that forms new particles. The fraction $1 - \alpha_{renucleate}$ remains either in the gas phase or condenses on other particles such as soot or the larger oil particles that did not evaporate. $\alpha_{scavenging}$ is the fraction of the newly formed particles that is not scavenged by other plume particles. $\beta_{condensates}$ is assumed to be larger than or equal to one and accounts for condensates of other combustion products on the re-nucleated oil particles. Equation 2 should be interpreted as conceptual framework that illustrates different physical effects that may reduce the total volume and mass of the oil particles. The values of the different efficiencies α_x are currently largely unquantified and can depend on engine and fuel characteristics (see also Section 4). Even though, the total effective volume of the lubrication oil particles serving as ice crystal precursors might be much smaller than the volume of oil lost in first place, the number of oil particles can be higher than initially due to their smaller size. Note that for a prescribed N_{oil} value, $\dot{V}_{oil,eff}$ can differ by several orders of magnitude, depending on the prescribed values of $\bar{r}_{d,oil}$ and σ_{oil} (Equation 1 and Figure 1).

2.2. Box Model Setup

We perform simulations with the Lagrangian Cloud Module (LCM), first described in Sölch and Kärcher (2010) and typically employed in a version fully coupled with the large-eddy simulation (LES) model EULAG to simulate pure ice clouds. Unlike Eulerian cloud microphysics models, LCM employs a particle-based approach and ice crystals are represented by simulation particles (SIPs). For the present study, a box model version of LCM

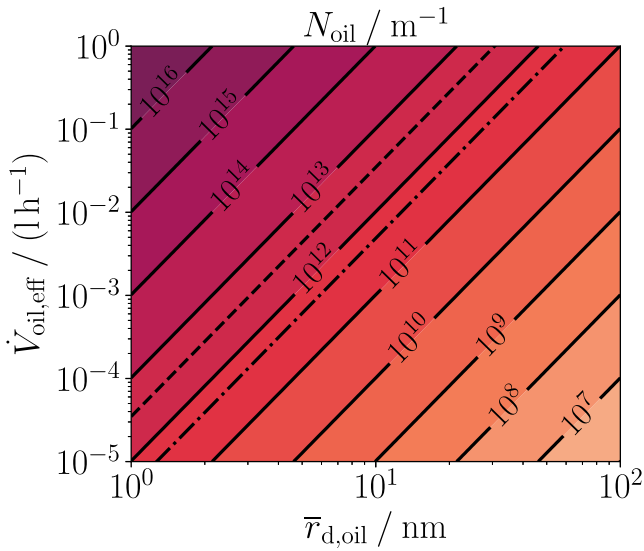


Figure 1. Number of oil particles per meter of flight path N_{oil} as a function of geometric mean radius $\bar{r}_{d,oil}$ and effective oil emission $\dot{V}_{oil,eff}$ according to Equation 1 with $\sigma_{oil} = 1.6$ (solid contour lines). The contour line of $N_{oil} = 10^{12} \text{ m}^{-1}$ is also shown for $\sigma_{oil} = 2.02$ (dashed) and $\sigma_{oil} = 1.27$ (dash-dotted). The relative distances between the solid, dashed, and dash-dotted lines would be the same for each N_{oil} value.

is employed, which is not coupled to EULAG. This LCM variant has been extended recently to capture the microphysics of contrail formation (via the liquid phase). A full description of the LCM box model is given in Bier et al. (2022, 2024), which simulate contrail formation on soot for kerosene combustion and on ambient aerosol for hydrogen combustion, respectively. As in Bier et al. (2024), we prescribe the plume dilution along an ensemble of 1,000 different trajectories to account for the plume cooling and heterogeneity. These are suitably merged trajectories from a data set of 25,000 trajectories sampling a single aircraft exhaust plume behind an engine of an A340-300 aircraft as simulated by a 3D large-eddy simulation (Vancassel et al., 2014). Each trajectory represents a fraction of plume volume and plume air mass and we apply the box model separately for each trajectory. The results from the 1,000 (sub-)simulations are then suitably combined: for extensive quantities (e.g., ice crystal number), we present the sum over all 1,000 trajectories and for intensive quantities (e.g., temperature) we present a mass-weighted average over the trajectory ensemble (see Supplement in Bier et al., 2022).

Engine and fuel properties (water vapor emission index EI_v , specific heat of combustion Q , overall propulsion efficiency η and fuel consumption m_C) and engine exit conditions (exit temperature T_E and exit area A_E) are set as in Bier et al. (2024) and summarized in Table 1. Ambient temperature T_a is a crucial parameter for contrail formation and simulations are performed and analyzed for several T_a values. Ambient pressure p_a and relative humidity over ice

Table 1
Simulation Setup

Kerosene fuel and engine properties:	$EI_v = 1.26 \text{ kg kg}^{-1}$, $Q = 43 \cdot 10^6 \text{ J kg}^{-1}$ $\eta = 0.36$, $m_C \approx 3.1 \text{ g m}^{-1a}$
Hydrogen fuel and engine properties:	$EI_v = 8.94 \text{ kg kg}^{-1}$, $Q = 120 \cdot 10^6 \text{ J kg}^{-1}$ $\eta = 0.36$, $m_C \approx 1.1 \text{ g m}^{-1a}$
Engine exit conditions:	$T_E = 580 \text{ K}$, $A_E = 0.25\pi \text{ m}^2$
Ambient conditions:	$T_a = [215, 220, 225, 232] \text{ K}$, $p_a = 260 \text{ hPa}$, $RH_{ice,a} = 120\%$
Soot properties:	$\bar{r}_{d,s} = 15 \text{ nm}$, $\sigma_s = 1.6$, $\kappa_s = 0.005$ $EI_s = [10^{12}, 10^{13}, 10^{14}, 10^{15}, 10^{16}] \text{ kg}^{-1}$ corresponds to: ^b $N_s \approx 3.1 \cdot [10^9, 10^{10}, 10^{11}, 10^{12}, 10^{13}] \text{ m}^{-1}$
Ambient aerosol properties:	$\bar{r}_{d,aer} = 15 \text{ nm}$, $\sigma_{aer} = 1.6$, $\kappa_{aer} = 0.5$ $n_{aer} = [10^0, 10^1, 10^2, 10^3, 10^4] \text{ cm}^{-3}$
Oil particle properties:	$\bar{r}_{d,oil} = [1, 5, 15, 25] \text{ nm}$, $\sigma_{oil} = [1.27, 1.6, 2.02]$, $\kappa_{oil} = 0$ $N_{oil} = [10^8, 10^9, 10^{10}, 10^{11}, 10^{12}, 10^{13}, 10^{14}, 10^{15}, 10^{16}] \text{ m}^{-1}$ Corresponds to: ^b $EI_{oil,kerosene} \approx 3.2 \cdot [10^{10}, 10^{11}, 10^{12}, 10^{13}, 10^{14}, 10^{15}, 10^{16}, 10^{17}, 10^{18}] \text{ kg}^{-1}$ $EI_{oil,hydrogen} \approx 9.0 \cdot [10^{10}, 10^{11}, 10^{12}, 10^{13}, 10^{14}, 10^{15}, 10^{16}, 10^{17}, 10^{18}] \text{ kg}^{-1}$
Volatile particle properties:	$\bar{r}_{d,vol} = 1 \text{ nm}$, $\sigma_{vol} = 1.6$, $\kappa_{vol} = 0.5$ $EI_{vol,kerosene} = [10^{12}, 10^{14}, 10^{15}, 10^{16}, 10^{17}] \text{ kg}^{-1}$ $EI_{vol,hydrogen} = 2.8 \cdot [10^{12}, 10^{14}, 10^{15}, 10^{16}, 10^{17}] \text{ kg}^{-1}$ Corresponds to: ^b $N_{vol} \approx 3.1 \cdot [10^9, 10^{11}, 10^{12}, 10^{13}, 10^{14}] \text{ m}^{-1}$

Note. See text for descriptions of parameter names. ^aCalculated with Eq. (4) and Eq. (10) in Bier et al. (2024) for $T_a = 225 \text{ K}$.
^bCalculated with $N_x = EI_x \cdot m_C$ where x denotes the emitted particle type.

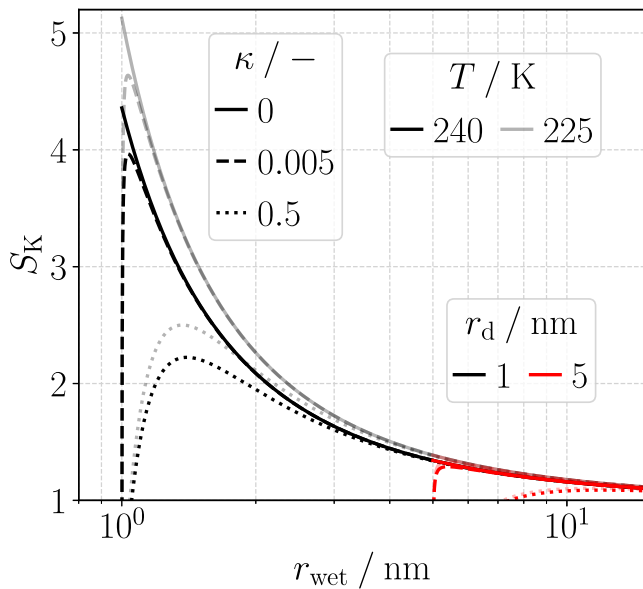


Figure 2. Equilibrium saturation ratio S_K over a droplet with wet radius r_{wet} according to κ -Köhler theory for different hygroscopicities κ (line style), two plume temperatures T (transparency), and dry radii r_d (color).

$RH_{\text{ice,a}}$, on the other hand, do not significantly affect the results and interpretations and are thus kept constant throughout the simulations shown in this study.

We consider four different particle types: soot (for kerosene combustion), ambient aerosols (for hydrogen combustion), oil particles (for both hydrogen and kerosene combustion), and volatile particles originating from the combustion products (for both hydrogen and kerosene combustion). For any particle type, we assume spherical shape and a log-normal size distribution at initialization. We use the algorithm in Unterstrasser and Sölch (2014) to generate a SIP ensemble for given size distribution properties. Typically, only a selection of particle types is switched on in a particular simulation.

For soot and ambient aerosols, we assume the baseline values for geometric mean radius $\bar{r}_d$, geometric width σ and hygroscopicity κ of Bier et al. (2022, 2024). Focusing on the oil particles, these properties are held constant throughout the simulations. The parametrizations for the activation into water droplets, their diffusional growth and freezing into ice crystals are described in detail in Bier et al. (2022) for soot and in Bier et al. (2024) for ambient aerosols. We prescribe a wide range of soot number emission indices EI_s , including present-day values as well as soot-poor scenarios accounting for technological progress in reducing the soot number. For $EI_s = 10^{15} \text{ kg}^{-1}$, the corresponding soot number per meter of flight path for the given fuel consumption is $N_s \approx 3.1 \cdot 10^{12} \text{ m}^{-1}$ (Table 1). Following Equation 1, this corresponds to a soot volume emission rate $\dot{V}_s \approx 0.1 \text{ l h}^{-1}$. In addition, a wide range of ambient aerosol concentrations n_{aer} accounts for the large variability in the atmosphere (e.g., Brock et al., 2021; Kaiser et al., 2019; Minikin et al., 2003), including also a rather extreme upper value.

Based on the findings by Ponsonby et al. (2024), we treat oil particles as insoluble ($\kappa_{\text{oil}} = 0$) but wettable particles. For $\kappa = 0$, the κ -Köhler equation for calculating the equilibrium saturation over a droplet (Petters & Kreidenweis, 2007) reduces to the Kelvin term (Figure 2). We calculate this Kelvin term for the particle dry radius and assume that the oil particle take up water vapor once the plume relative humidity exceeds this critical barrier. Assuming insolubility, we use the parametrization for pure water to determine the homogeneous freezing temperatures (Bier et al., 2022; Kärcher et al., 2015; Riechers et al., 2013). We vary the geometric mean dry radius $\bar{r}_{d,\text{oil}}$ and the geometric width σ_{oil} of the log-normal distribution. The geometric width is varied so that the width of the corresponding mass distribution is halved and doubled (assuming spherical particles). The number of emitted oil particles N_{oil} (Table 1) is varied over a very large range to account for the physical considerations presented in Section 2.1. All trajectories are initialized with the same fraction of oil particles (implying a homogeneous spatial distribution of oil particles in the initial plume). This generic treatment neglects differences that result from the specific location of the venting system.

The effect of particle dry radius, hygroscopicity, and plume temperature on the critical saturation ratio (maximum of κ – Köhler curve) is depicted in Figure 2. For a hygroscopicity $\kappa = 0$ and a dry radius $r_d = 5 \text{ nm}$ the Kelvin barrier for a given plume temperature is around 70% lower than for a dry radius $r_d = 1 \text{ nm}$. We emphasize, that the hygroscopicity of the oil particles may be larger than zero in the kerosene combustion case due to condensation of hygroscopic compounds such as sulfuric acid (Ungeheuer et al., 2022). In contrast, the composition of hydrogen combustion emission products is largely unknown. Nitric acid is formed from oxidation of nitrogen oxides in the hydrogen combustion case. Because of its hydrophilic nature after condensation, it is expected to change the hygroscopicity of the oil particles to values larger than zero, yet it is likely lower than in the kerosene case. The amount of nitric acid formed and its ability to form particles in the exhaust plume is yet still unknown. The change of critical saturation due to a higher hygroscopicity (e.g., from zero to 0.005) for a given dry radius and plume temperature, however, is less than 10%. We therefore conclude that compared to the strong increase of the Kelvin barrier with decreasing particle dry radius, hygroscopicity has a second order effect on the nucleation ability of the oil particles. As we here prescribe a lower limit of zero, the nucleation ability and thus the number of ice crystals formed on our simulated oil particles represent a lower limit.

As outlined in Section 1, some kerosene combustion products are an additional source for the formation of volatile particles. We therefore consider two types of volatile particle modes. The first mode is the already described weakly soluble/insoluble particle mode that mainly consists of lubrication oil constituents. We characterize this mode by assigning a limiting value $\kappa_{\text{oil}} = 0$, neglecting the impact of condensates from combustion products on the hygroscopicity. In addition, we consider a well-soluble mode primarily consisting of hydrophilic combustion products, which is characterized by a considerably higher hygroscopicity (here, $\kappa_{\text{vol}} = 0.5$ is assumed). This higher hygroscopicity reduces the Kelvin barrier substantially (Figure 2). Emission indices EI_{vol} of the latter mode can be on the order of 10^{16} – 10^{17} kg^{-1} (F. Yu & Turco, 1997; Haverkamp et al., 2004). We assume that the formation of the volatile particles is completed well before the onset of contrail formation. Accordingly, a fixed emission index is assumed and the volatile particles are initialized at the start of the simulation. In this study, we prescribe a range of emission indices accounting for different fuel compositions and engine settings. Since the focus is on the oil particles, we fix other properties ($\bar{r}_{\text{d,vol}}$, σ_{vol}). Although the composition of hydrogen combustion products is poorly understood, we still include an additional well-soluble volatile particle mode in our simulations. To maintain consistency, we prescribe the same number and properties of these particles as in the kerosene case, despite the likelihood of substantial differences between the two fuel types. This approach allows us to explore a range of potential scenarios under idealized conditions.

In the presentation of the results, we use different metrics for the different particle types. Following the standard of aviation community, we prescribe emission indices per kilogram of fuel burned for particles the number of which is related to the fuel consumption, such as soot and volatile particles from combustion products. In contrast, entrained ambient aerosols cannot be directly linked to the fuel consumption, so we prescribe their background number concentration. Analogously, the lubrication system is a separate system, and the emitted oil particle number is not necessarily related to the fuel consumption. Therefore, we prescribe their number per meter of flight path. Moreover, for the same total number of emitted oil particles per meter of flight path, the corresponding emission indices for hydrogen and kerosene combustion differ due to different fuel consumptions, which arise from their different combustion heats (Table 1). This complicates direct comparisons if emission indices were used. In our presentation, we consistently prescribe the total number of emitted particles per meter of flight path across the two fuel types. To help the reader and facilitate comparisons with measurements, we nevertheless provide the corresponding emission indices based on the given fuel consumptions (Table 1). While the given fuel consumptions determine the total number of emitted soot and volatile particles, the prescribed emission indices span a broad range. This variation captures a variety of engine types and operations.

3. Results

3.1. Activation of Oil Particles

First, we examine the activation of oil particles without incorporating further particle types into our simulations (Figure 3). Although these scenarios are inherently hypothetical and are unlikely to occur in reality, they are useful for understanding and interpreting the results when two or three particle types are included.

When examining the evolution of plume relative humidity in the absence of microphysics, where the evolution is solely determined by dilution, the peak supersaturations reached in the hydrogen cases are higher than those in the kerosene cases (transparent solid and dotted red curves in Figure 3a). This is because of the higher energy-specific water vapor emission index. The evolution of plume relative humidity changes substantially when microphysics is switched on and activated droplets (number N_{drop}) and ice crystals (number N_{ice}) deplete the water vapor (compare transparent and opaque red curves in Figure 3a). The activation and freezing fraction are given by

$$\phi_{\text{act}}(t) = \frac{N_{\text{drop}}(t) + N_{\text{ice}}(t)}{N_{\text{oil}}} \quad (3)$$

and

$$\phi_{\text{frz}}(t) = \frac{N_{\text{ice}}(t)}{N_{\text{oil}}} \quad (4)$$

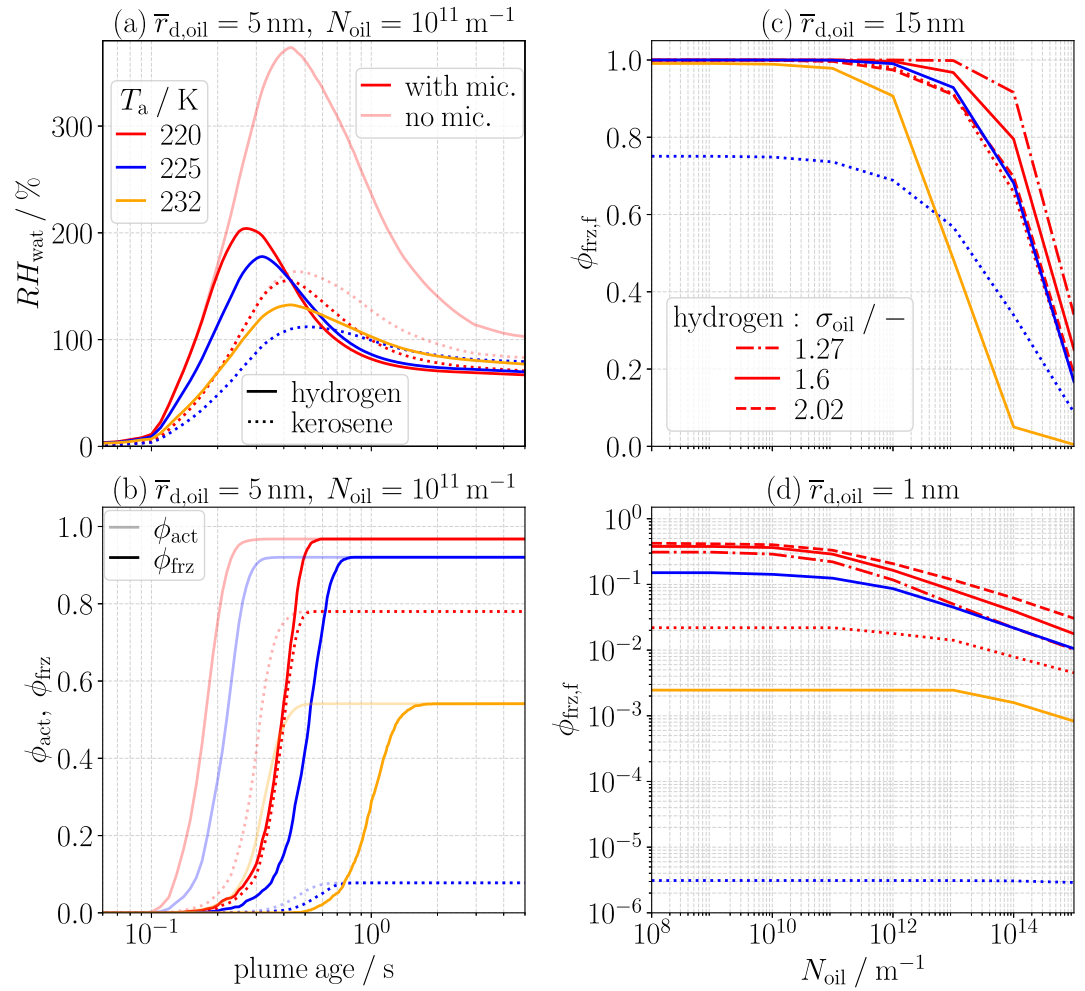


Figure 3. Activation of oil particles in kerosene and hydrogen combustion exhaust plumes without a second particle type. (a) Time evolution of plume relative humidity over water RH_{wat} for different ambient temperatures T_a (different colors) for hydrogen (solid) and kerosene (dotted) combustion. For $T_a = 220$ K the time evolution without microphysics (transparent) is shown additionally. (b) Exemplary time evolution of activation fraction ϕ_{act} (transparent) and freezing fraction ϕ_{frz} (opaque) for different T_a (different colors) for hydrogen (solid) and kerosene (dotted) combustion. (c) Final freezing fraction $\phi_{\text{frz},f}$ as a function of oil particle number N_{oil} for a geometric mean radius $\bar{r}_{d,\text{oil}} = 15$ nm. For $T_a = 220$ K and hydrogen combustion, the geometric width is varied (different line styles; the dotted line corresponds to kerosene combustion with $\sigma_{\text{oil}} = 1.6$). (d) Same as (c) but for $\bar{r}_{d,\text{oil}} = 1$ nm and a logarithmic scaling of the y-axis.

respectively. Both quantities increase over time and attain larger values for lower ambient temperature (Figure 3b) as the peak plume supersaturation is higher (Figure 3a). The simulation examples depicted in the left column of Figure 3 use $\bar{r}_{d,\text{oil}} = 5$ nm, $\sigma_{\text{oil}} = 1.6$, and $N_{\text{oil}} = 10^{11} \text{ m}^{-3}$. The higher supersaturation encountered in the hydrogen case results in an earlier activation of oil particles into water droplets. Furthermore, a larger fraction of the small particles within the size distribution are able to overcome the Kelvin barrier and activate into droplets. Consequently, the activation and freezing fraction is larger for the hydrogen case than for the kerosene case. Additionally, droplets and ice crystals can form in the hydrogen case (orange curve in Figure 3b) at temperatures where ice crystals do not form in the kerosene case in agreement with the Schmidt-Appleman criterion.

For a geometric mean radius $\bar{r}_{d,\text{oil}} = 15$ nm (almost) all emitted oil particles freeze into ice crystals for low numbers of emitted oil particles ($N_{\text{oil}} \lesssim 10^{11} \text{ m}^{-3}$) independent of combustion type and (almost) independent of ambient temperature (Figure 3c) due to the relatively small Kelvin barrier. This does not hold for the kerosene case for temperatures near the Schmidt-Appleman threshold temperature (dotted blue curve in Figure 3c). However, for a larger number of emitted oil particles ($N_{\text{oil}} > 10^{12} \text{ m}^{-3}$), the final freezing fraction $\phi_{\text{frz},f}$ (i.e., the

freezing fraction evaluated at the end of a simulation when ice formation is finished) decreases with increasing N_{oil} . This saturation effect arises from the larger particles of the log-normal size distribution with the lowest Kelvin barrier, which activate at an early stage and significantly deplete the water vapor, thereby preventing the smallest particles from overcoming the Kelvin barrier. This is more pronounced for a lower supersaturation forcing, that is, for kerosene combustion and/or increasing ambient temperature. Varying the geometric width has a small influence (red curves with different line styles for hydrogen case in Figure 3c). The broader the distribution, the lower is the activation fraction as a result of the increased number of particles on the left tail of the size distribution that experience a stronger Kelvin effect.

In contrast, looking at a geometric mean radius $\bar{r}_{\text{d,oil}} = 1 \text{ nm}$ (Figure 3d), the final freezing fraction is significantly smaller due to the strong increase of the Kelvin barrier (Figure 2). Obviously, the reduction of $\phi_{\text{frz,r}}$ at smaller particle radii is more pronounced for kerosene combustion. Moreover, the dependency on the geometric width is reversed compared to the case with $\bar{r}_{\text{d,oil}} = 15 \text{ nm}$. The broader the distribution, the more oil particles are now activated because of an increased number of particles on the right tail of the size distribution that overcome the Kelvin barrier.

3.2. Competition Between Oil Particles and Soot/Ambient Aerosols

Throughout Section 3.2, volatile particle emissions are neglected ($EI_{\text{vol}} = 0 \text{ kg}^{-1}$). Especially in soot-poor regimes of the kerosene combustion case, this may be a strong simplification. However, it allows us to isolate and better understand the competition between oil particles and a single other particle type (soot for kerosene and ambient aerosol for hydrogen combustion) before moving to more complex scenarios. Simulations with volatile particles included are presented in Section 3.3.

3.2.1. Final Ice Crystal Number as a Function of Oil Emission Rate

We investigate the total number of ice crystals formed as a function of $\dot{V}_{\text{oil,eff}}$. Figure 4 shows kerosene scenarios with $EI_s = 10^{15} \text{ kg}^{-1}$ and hydrogen scenarios with $n_{\text{aer}} = 1,000 \text{ cm}^{-3}$ for different ambient temperatures (different panels) and oil particle sizes (line style). For low ambient temperatures (Figure 4a) and small-sized oil particles with correspondingly high N_{oil} values, $\dot{V}_{\text{oil,eff}}$ values of only a few milliliters per hour lead to a significantly higher ice crystal number than a reference kerosene case with only soot particles included. At higher $\dot{V}_{\text{oil,eff}}$, also larger assumed particles ($\bar{r}_{\text{d,oil}} = 15 \text{ nm}$) are abundant in number such that the ice crystal number exceeds that of the reference kerosene case. For given $\bar{r}_{\text{d,oil}}$ and $\dot{V}_{\text{oil,eff}}$, the total ice crystal number decreases with increasing ambient temperature (Figures 4a–4c) as a consequence of the decreasing peak supersaturation and thus activation fractions. Nevertheless, for hydrogen combustion, the number of ice crystals formed on oil particles exceeds the number of ice crystals formed on ambient aerosols by up to one order of magnitude (for $\dot{V}_{\text{oil,eff}}$ of several hundred of milliliters per hour) even at high ambient temperatures (Figure 4d).

For a fixed oil emission $\dot{V}_{\text{oil,eff}}$, we observe a shift in the activation of oil particles of different radii with temperature: At low temperatures ($T_a = 215 \text{ K}$) the small oil particles ($\bar{r}_{\text{d,oil}} = 1 \text{ nm}$) can activate and freeze. Because of their abundance (for a fixed oil emission) the ice crystal number is substantially enhanced in both, the kerosene and the hydrogen combustion case. This trend shifts for higher temperatures ($T_a > 220 \text{ K}$), where in the kerosene case the particles with $\bar{r}_{\text{d,oil}} = 5 \text{ nm}$ serve as efficient precursor for the highest ice crystal number at a given $\dot{V}_{\text{oil,eff}}$. This order is a combined effect of different N_{oil} values for a fixed $\dot{V}_{\text{oil,eff}}$ value (Equation 1) and the activation suppression due to the Kelvin effect. These two effects can be separated if we plot the results as a function of N_{oil} rather than $\dot{V}_{\text{oil,eff}}$ (Figure 5). Furthermore, effects such as occasionally decreasing total ice crystal numbers with increasing $\dot{V}_{\text{oil,eff}}$ for hydrogen combustion (e.g., dashed blue curve in Figure 4a) can be better understood if we examine the contributions of the individual particle types to the total ice crystal number (Figure 5).

3.2.2. Final Ice Crystal Number as a Function of Oil Particle Number

In the case of low N_{oil} values for kerosene combustion, ice crystals predominantly originate from soot particles (the solid lines in Figures 5a–5c align with the dashed lines). As the value of N_{oil} increases, the contribution of ice crystals originating from oil particles to the total ice crystal number becomes more important. Ultimately, at high

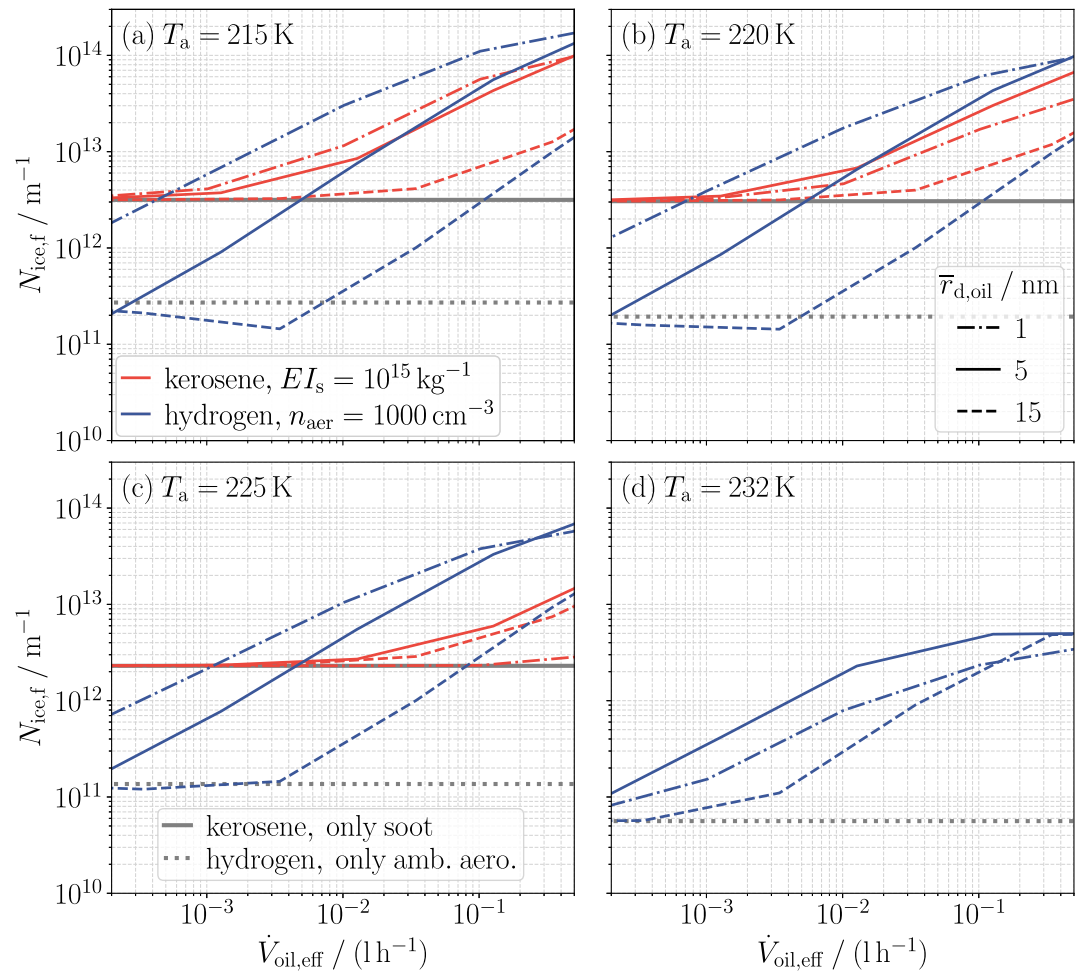


Figure 4. Total final ice crystal number $N_{ice,f}$ as a function of effective oil emission $\dot{V}_{oil,eff}$ and geometric mean radius $\bar{r}_{d,oil}$ (line style) with $\sigma_{oil} = 1.6$ for kerosene combustion with $EI_s = 10^{15} \text{ kg}^{-1}$ and for hydrogen combustion with $n_{aer} = 1,000 \text{ cm}^{-3}$. Each subplot corresponds to a different ambient temperature T_a . The solid horizontal gray lines are simulation results for kerosene combustion with only soot particles, and the dotted lines are results for hydrogen combustion with only ambient aerosols.

values of N_{oil} , oil particles become the predominant condensation nuclei (the solid lines in Figures 5a–5c start to converge toward the dotted lines). It is evident that the specific N_{oil} values at which the transition occurs are dependent upon the soot emission indices and the geometric mean radii of the oil particles. Similarly, for the hydrogen case, ice crystals predominantly originate from ambient aerosols at low N_{oil} and their formation becomes dominated by oil particles at higher N_{oil} values. This transition is contingent upon the aerosol number concentration and the geometric mean radii of the oil particles (Figures 5d–5f).

In the simulation setup of Figure 5a, soot and oil particles both feature a geometric mean radius of 15 nm. Then, the two particle types differ only in their hygroscopicity (Table 1). The activation of the oil particles is only marginally influenced by the presence of the soot particles for the high EI_s values and is essentially unaltered for the low EI_s values (the dotted lines in Figure 5a align closely with the magenta points), indicating that the different hygroscopicities play a minor role. For high N_{oil} values, we observe saturation effects (magenta points deviate from the diagonal and dashed curves bend downwards in Figure 5a). In contrast, if the initial oil particles are assumed to be smaller (in particular, $\bar{r}_{d,oil} < \bar{r}_{d,s}$), we find that the activation of the oil particles is affected by the presence of soot particles (and partly suppressed). The larger and thus earlier activated soot particles deplete the water vapor, thereby preventing the activation of some oil particles that would have activated in the absence of the soot particles (the dotted lines in Figures 5b and 5c start to deviate from the magenta points with increasing EI_s). This means, that the smaller the geometric mean radius of the oil particles the more they are hindered in their

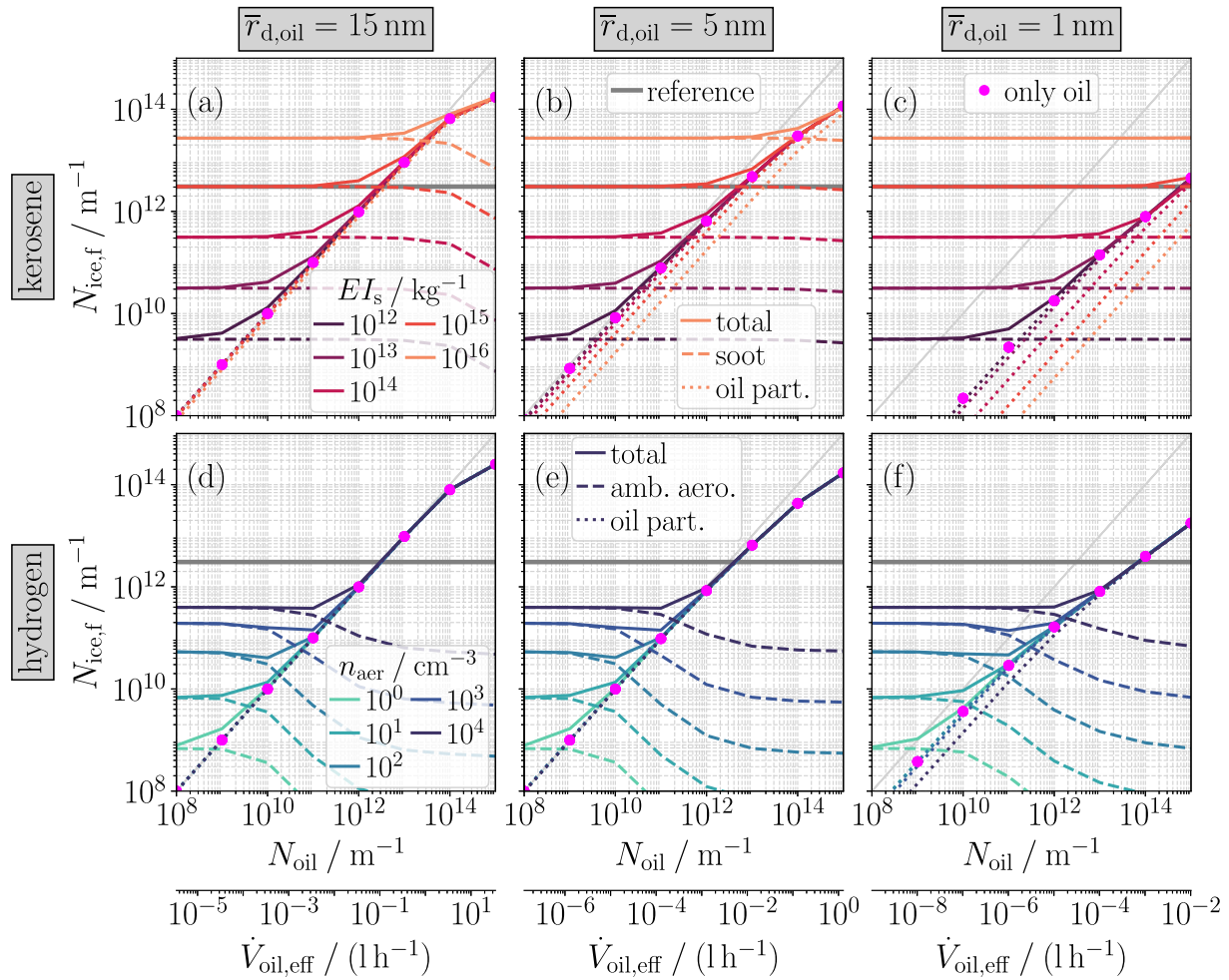


Figure 5. Final ice crystal number $N_{ice,f}$ as a function of emitted oil particle number N_{oil} and geometric mean radius $\bar{r}_{d,oil}$ (different columns) for kerosene combustion (first row) with different soot emission indices EI_s (different colors) and hydrogen combustion (second row) with different ambient aerosol number concentrations n_{aer} (different colors) for the ambient temperature $T_a = 220 \text{ K}$. Dashed and dotted line styles show the contribution of the different particle types to the total ice crystal number (solid). The magenta dots correspond to simulations including only oil particles without a second particle type. The gray horizontal lines depict a reference kerosene simulation including only soot particles with $EI_s = 10^{15} \text{ kg}^{-1}$. The light gray diagonal line indicates a final freezing fraction $\phi_{frz,f}$ of the oil particles of one. The second x-axis shows $\dot{V}_{oil,eff}$ calculated with Equation 1 with $\sigma_{oil} = 1.6$.

activation by two facts: First, the supersaturation encountered for the kerosene cases are not high enough to activate the smallest particles (Section 3.1; the magenta dots move downwards from Figures 5a–5c) and second, the larger soot particles reduce the supersaturation to further inhibit the activation of the smaller oil particles (the dotted lines significantly deviates from the magenta dots in Figure 5c for the higher EI_s values).

These two effects are less pronounced and less crucial in the hydrogen combustion scenarios where ambient aerosol particles compete with the oil particles (Figures 5d–5f). First, more oil particles can activate due to the elevated supersaturation (the magenta points are situated at higher values in Figure 5f in comparison to Figure 5c). Second, as the ambient aerosols are entrained into the plume over time, they are effectively incapable of depleting the water vapor to the extent that it can hinder the activation of the oil particles (the dotted curve only deviates notable from the magenta dots in Figure 5f for aerosol number concentrations of $n_{aer} = 10,000 \text{ cm}^{-3}$). Note, however, that the emitted oil particles partially suppress the activation of the entrained ambient aerosols for the higher N_{oil} values (down-bending dashed curves in Figures 5d–5f).

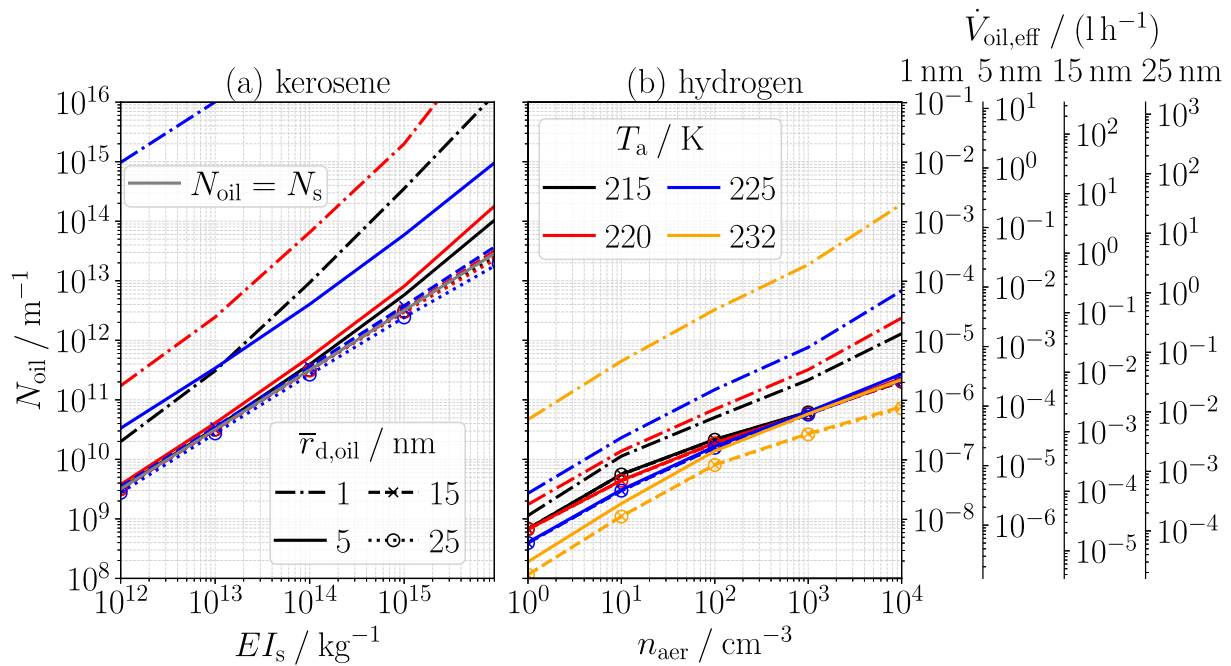


Figure 6. Transition curves where both particle types contribute equally to the number of ice crystals for (a) oil particles and soot particles for kerosene combustion and (b) oil particles and ambient aerosols for hydrogen combustion. For given temperature T_a (indicated by the color) and given geometric mean dry radius $\bar{r}_{d,oil}$ (indicated by the line style), each line separates an oil particle and a (a) soot or (b) ambient aerosol dominated regime. The gray line in (a) indicates where the emitted oil particle number equals the number of emitted soot particles. The additional y-axes show $\dot{V}_{oil,eff}$ calculated with Equation 1 for different $\bar{r}_{d,oil}$ with $\sigma_{oil} = 1.6$.

3.2.3. Regimes

Next, we investigate under which scenarios oil particles become the dominant condensation nuclei. For this, we determine the pairs of EI_s and N_{oil} values and of n_{aer} and N_{oil} values where both included particle types contribute equally to the total number of ice crystals formed. Such scenarios with equal contributions of the two involved particle types to the total ice crystal number can be evaluated in Figure 5 by determining the intersections where the dashed and dotted lines of the same colors cross. We determine these value pairs (via interpolation) for different oil particle radii $\bar{r}_{d,oil}$ and ambient temperatures T_a . The two panels of Figure 6 display the EI_s – N_{oil} values for kerosene combustion and n_{aer} – N_{oil} values for hydrogen combustion, respectively. For a given combination of $\bar{r}_{d,oil}$ and T_a , the corresponding curve in Figure 6a divides the parameter space into regimes where lubrication do or do not play a substantial role in ice crystal formation. When a specific EI_s – N_{oil} data point lies to the right of the corresponding curve, ice crystals form predominantly on soot particles. If the pair lies to the left, ice crystals form mainly on oil particles. In the same way we can read off from Figure 6b whether the ice crystals predominantly originate from ambient aerosols or oil particles for a given n_{aer} – N_{oil} pair.

The transition from a soot-dominated regime to an oil particle-dominated regime occurs at higher oil particle numbers when there is an increase in soot emission indices and/or a decrease in oil particle radii. For $\bar{r}_{d,oil} = 15$ nm, the transition curves are nearly aligned with the line where the number of emitted oil particles is equal to the number of emitted soot particles. This confirms the weak dependency on the different hygroscopicity values. For oil particle radii that are smaller than the soot radii, the transition curves shift toward higher values of N_{oil} with increasing ambient temperatures. This is attributable to the increased Kelvin barrier of the smaller particles together with the reduction in supersaturation due to an increase in ambient temperature. In contrast, if the oil particles are assumed to be larger than the soot particles, the temperature dependency is reversed and the transition curves lie slightly below the line $N_{oil} = N_s$ for the higher EI_s values caused by the slightly reduced Kelvin barrier of the larger oil particles.

In the case of hydrogen combustion, the transition curves for $\bar{r}_{d,oil} = 1$ nm shift to higher N_{oil} values with increasing temperature due to the high Kelvin barrier combined with the lower supersaturation at higher temperatures. This temperature dependency is reversed for the examined cases $\bar{r}_{d,oil} \geq 5$ nm for $n_{aer} \lesssim 1000$ cm^{-3} . This

is caused by the depletion of the water vapor by the activated emitted oil particles hindering some of the later entrained aerosols from being activated. Obviously, this depletion of water vapor by the activated oil particles has a larger influence at lower supersaturations, thus higher temperatures. Therefore, the oil particles become the dominant nuclei for already lower N_{oil} . Note that except for $T_a = 232$ K, this depends only slightly on the geometric mean radius of the oil particles. It is also noteworthy that in the case of hydrogen, in certain instances, the total number of ice crystals exhibits a slight decline with increasing N_{oil} in the vicinity of the transition region (as evidenced by the slight decline of selected solid lines in Figures 5d–5f with rising N_{oil}). This is attributed to a stronger suppression of ambient aerosol activation. However, this region is narrow, and a further increase in N_{oil} results in a higher number of ice crystals. Consequently, the oil particle-dominated region can be considered as a region where the ice crystals are present at a higher number than in the scenario with ambient aerosols only.

3.3. Competition Between Oil Particles and Other Volatile Particles

So far, we neglected the volatile particles originating from the kerosene combustion products. Especially in a soot-poor regime (here $EI_s = 10^{12} \text{ kg}^{-1}$), these particles may play an important role and compete with the oil particles for the available water vapor. If the geometric mean radii of the two volatile particle types are assumed to be the same ($\bar{r}_{\text{d,oil}} = \bar{r}_{\text{d,vol}} = 1 \text{ nm}$), the critical saturation ratios for the oil particles are significantly higher than those for the well-soluble particles (Figure 2). Thus, the oil particles are partially suppressed in their activation not only due to the high Kelvin barrier but also by the presence of the other well-soluble volatile particles (the dotted lines in Figures 7a and 7b deviate from the magenta points). In contrast, the activation of the well-soluble particles is only noticeably suppressed by the oil particles when $EI_{\text{oil}} \gg EI_{\text{vol}}$ and the ambient temperature is well below the Schmidt-Appleman threshold temperature (slightly downward bending dashed curves in Figures 7a and 7b). Moreover, because of their lower critical saturation ratios, the well-soluble volatile particles still form a considerable number of ice crystals for $EI_{\text{vol}} > 10^{12} \text{ kg}^{-1}$ at $T_a = 225$ K in contrast to the oil particles (Figure 7c). At this temperature and for $EI_{\text{vol}} = 10^{12} \text{ kg}^{-1}$ (i.e., here the same emission index as for soot), the ice crystals formed on the well-soluble but small volatile particles are entirely masked by those formed on the larger soot particles. In fact, the soot mode becomes important already at $EI_{\text{vol}} \lesssim 10^{15} \text{ kg}^{-1}$ (dashed lines are below the solid lines in Figure 7c). At lower T_a and for low EI_{oil} , the well-soluble volatile particles produce noticeable numbers of ice crystals also for $EI_{\text{vol}} = 10^{12} \text{ kg}^{-1}$ (Figures 7a and 7b). However, when the total number of emitted particles is this low, the picture may be incomplete, as ambient aerosols may also contribute non-negligibly to ice crystal formation.

If the oil particles are assumed to be larger ($\bar{r}_{\text{d,oil}} = 5 \text{ nm}$), the critical saturation ratios are lower than those of the well-soluble, but assumed small-sized particles ($\bar{r}_{\text{d,vol}} = 1 \text{ nm}$). As a consequence, the activation of the oil particles into ice crystals is only slightly affected by the second volatile particle mode (dotted lines are close to magenta points in Figures 7d–7f). Moreover, if $EI_{\text{oil}} \gtrsim EI_{\text{vol}}$, the activation of the well-soluble volatile particles is strongly suppressed by the oil particles (down bending dashed curves in Figures 7d–7f). This results in a dominant contribution of the oil particles to the total ice crystal number at significantly lower EI_{oil} values compared to the case when both modes have the same geometric mean radius. Furthermore, the oil particles contribute considerably to the ice crystal number at $T_a = 225$ K in the case of high EI_{oil} (Figure 7f).

In summary, these illustrative simulation results show that it is a complex interplay between number, size, and solubility of different volatile particle types that determine which type dominates ice crystal formation. In these illustrative examples a rather low geometric mean radius for the well-soluble mode ($\bar{r}_{\text{d,vol}} = 1 \text{ nm}$) was chosen to make the impacts of the Kelvin effect and of the solubility more discernible. Clearly in scenarios, where the well-soluble volatile particles are larger (e.g., if oil vapor mainly condenses on these particles instead of undergoing re-nucleation), their activation would be favored.

We performed analogous simulations for hydrogen combustion (Figure 8), prescribing the same number of oil particles and volatile particles as in the kerosene case (due to the lower fuel consumption in the hydrogen case, emission indices are, however, larger than in the corresponding kerosene case, see Table 1). As stated in Section 2.2, we neglect any potential differences in the properties of the volatile particles originating from hydrogen versus kerosene combustion. Moreover, we prescribe ambient aerosols with $n_{\text{aer}} = 100 \text{ cm}^{-3}$ instead of soot particles as a third particle type. Because of the higher supersaturations encountered in the hydrogen combustion case, activation fractions for both oil and volatile particles are consistently elevated compared to the kerosene scenario. This is particularly evident at $T_a = 225$ K, where oil particles can contribute significantly to the total ice

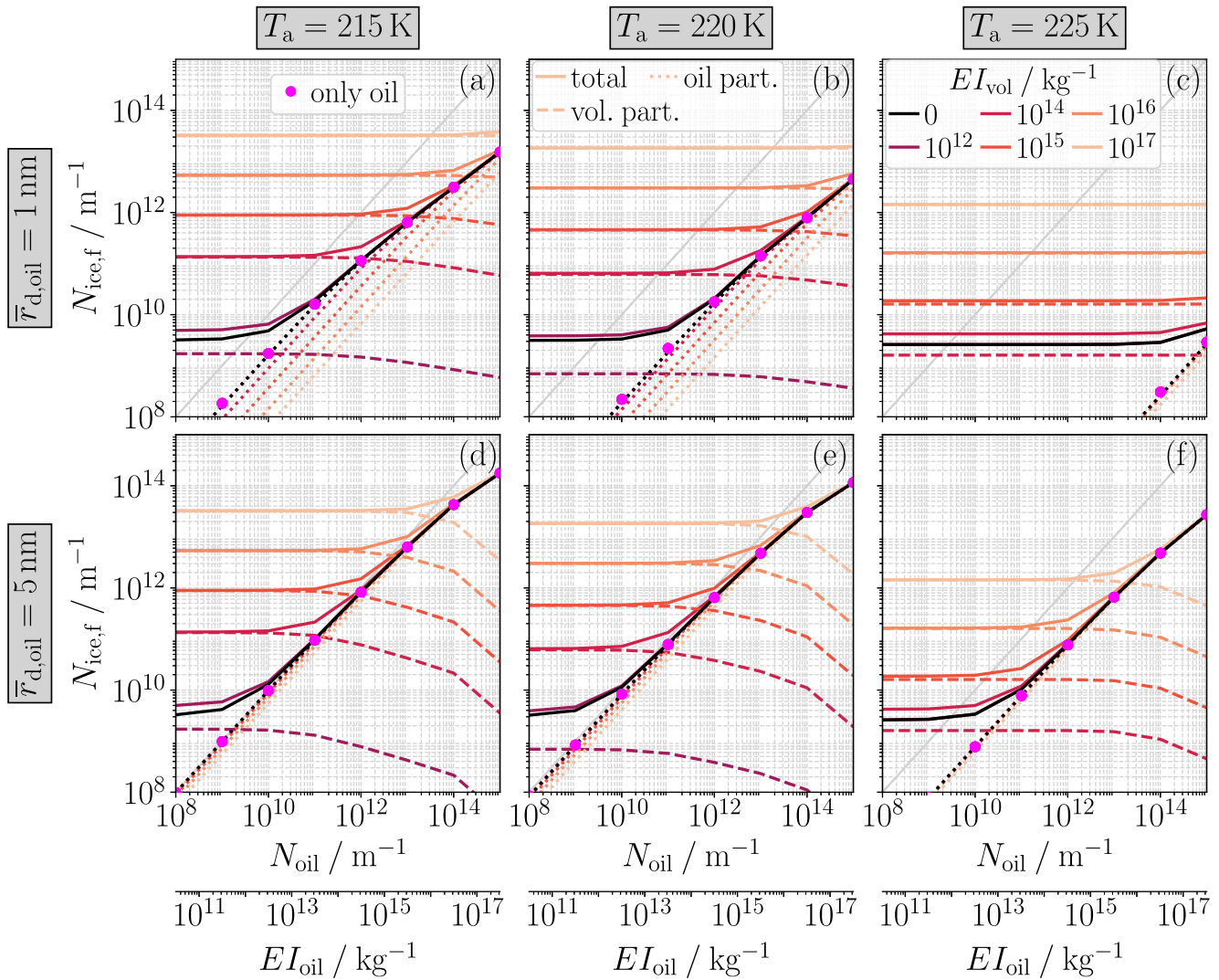


Figure 7. Final ice crystal number $N_{ice,f}$ as a function of emitted oil particle number N_{oil} (oil emission index EI_{oil}) and emission index of combustion volatile particles EI_{vol} (different colors) with $\bar{r}_{d,vol} = 1$ nm for kerosene combustion in a soot-poor regime ($EI_s = 10^{12} \text{ kg}^{-1}$). Each column corresponds to a different ambient temperature T_a and each row to a different geometric mean radius $\bar{r}_{d,oil}$. Dashed and dotted line styles show the contribution of the volatile and oil particles to the total ice crystal number (solid). The magenta dots correspond to simulations including only oil particles without other particle types. The light gray diagonal line indicates a final freezing fraction $\phi_{frz,f}$ of the oil particles of one.

crystal numbers even when their size matches that of the well-soluble volatile mode (compare Figures 7c and 8c). Moreover, for a given well-soluble volatile particle number and ambient temperature, the transition from volatile particle-dominated to oil particle-dominated ice crystal formation (intersection of dotted and dashed lines) occurs at lower N_{oil} values due to the enhanced oil particle activation under hydrogen combustion conditions. In addition, for the emission index $EI_{vol} = 2.8 \cdot 10^{12} \text{ kg}^{-1}$, the ice crystals formed on the well-soluble volatile particles are negligible (solid lines collapse with the lines for $EI_{vol} = 0 \text{ kg}^{-1}$ in Figures 8a–8f).

4. Discussion

The hot plume areas facilitate the production of vapors from (un-)controlled lubrication oil emissions that may nucleate to form small particles. This has yet not been measured in-flight as a chemical analysis of the composition of ultra-fine particles is challenging due to their low mass fraction. Furthermore, nanometer-sized particles are often depleted in the inlet lines of sampling systems, which enhances the uncertainty of the measurement (Dischl et al., 2024). In many investigated potential scenarios, oil particles play an important role in the formation of ice crystals. The question which of our investigated scenarios are actually representative for

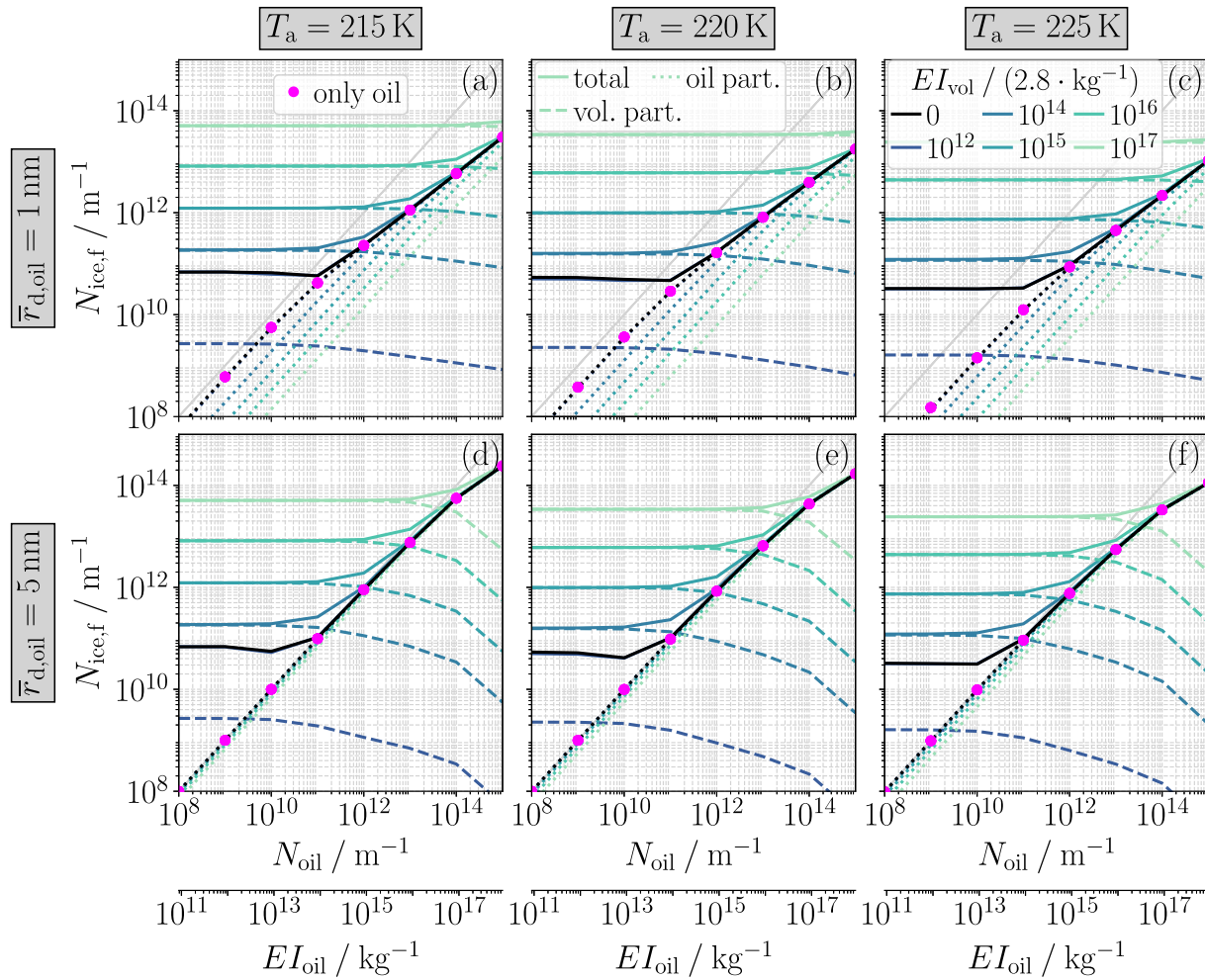


Figure 8. Final ice crystal number $N_{ice,f}$ as a function of emitted oil particle number N_{oil} (oil emission index EI_{oil}) and emission index of combustion volatile particles EI_{vol} (different colors) with $\bar{r}_{d,vol} = 1$ nm for hydrogen combustion with an ambient aerosol number concentration $n_{aer} = 100$ cm $^{-3}$. Each column corresponds to a different ambient temperature T_a and each row to a different geometric mean radius $\bar{r}_{d,oil}$. Dashed and dotted line styles show the contribution of the volatile and oil particles to the total ice crystal number (solid). The magenta dots correspond to simulations including only oil particles without other particle types. The light gray diagonal line indicates a final freezing fraction $\phi_{frz,f}$ of the oil particles of one.

conditions encountered during cruise can only be answered through in situ measurements that analyze the chemical and physical properties of the oil particles in relevant temperature and pressure conditions.

Past measurements for kerosene combustion for the present-day soot-rich regime ($EI_s \sim 10^{15}$ kg $^{-1}$) did not indicate a significant contribution of an oil particle mode to the total ice crystal number. Instead, it was experimentally shown that ice crystal formation is dominated by soot particles in the soot-rich regime (Kleine et al., 2018). A reason for this could be that oil particle numbers N_{oil} are well below the emitted soot number N_s (Figure 6a) such that the ice crystals formed on oil particles are masked by those formed on soot. Indeed, for very small oil particles ($\bar{r}_{d,oil} \sim 1$ nm) the ice crystal number is still dominated by the soot emissions even if the oil particle number is two (or more) orders of magnitude higher than the soot number corresponding to $EI_s \sim 10^{15}$ kg $^{-1}$.

The latter result, however, might be exaggerated due to the box model approach used. Compared to large-eddy simulations, Lewellen (2020) showed that for an emitted particle type with high number emission, a box model approach has the tendency to overestimate the activation fraction due to missing mixing processes between air parcels of different ages. An overestimation in total ice crystal number by a factor of ~ 3 was found in Lewellen (2020) (see his Figure 2). Moreover, the small-sized ultrafine particles were found to be relatively more important in the LES simulation than in the box model approach. Although this missing mixing process may shift

the relative importance of oil particles at high soot numbers toward lower N_{oil} values, we expect that the transition to a regime dominated by oil particles will not be significantly affected in soot-poor or hydrogen scenarios. Indeed, for low number emissions or contrail formation on ambient aerosols, results of a box model approach are comparable to those of a large-eddy simulation (Lewellen, 2020). With the development of the RadMod framework (Lottermoser & Unterstrasser, 2024), a first step has been taken to account in our models for the mixing processes between air parcels in the expanding plume. Once this new dynamical framework RadMod is fully coupled with the microphysical module LCM, the present study can be refined.

The transition into an oil particle-dominated regime at significantly lower N_{oil} for lower EI_s or for hydrogen combustion (Figure 6b), does not mean that the total ice crystal numbers are necessarily higher than in a reference kerosene case with $EI_s \sim 10^{15} \text{ kg}^{-1}$. Nevertheless, due to the nonlinear dependency of the radiative forcing on the initial number of ice crystals (Burkhardt et al., 2018), the potential increase in ice crystal number caused by the oil particles may have a significant impact on the radiative forcing, even in scenarios where the ice crystal number remains lower than in a reference kerosene case.

The transition curves for the small-sized particles ($\bar{r}_{\text{d,oil}} \sim 1 \text{ nm}$) in the soot-rich regime ($EI_s \sim 10^{15} \text{ kg}^{-1}$) occur at N_{oil} values that correspond to $\dot{V}_{\text{oil,eff}}$ values of only a few milliliters per hour—at least for temperatures well below the Schmidt-Appleman threshold temperature (Figure 6a). Given that the oil consumption $\dot{V}_{\text{oil}}$ is typically higher (on the order of several hundred milliliters per hour (Linke-Diesinger, 2010)), together with the fact that past measurements have not indicated a significant contribution of an oil mode to the total ice crystal number in the soot-rich regime, this suggests that one (or more) of the α -values introduced in Equation 2 may be low. Assuming comparable engine configurations, switching to soot-poor regimes or hydrogen combustion is not expected to substantially alter α_{entrain} (provided the relative positioning of the engine core exit and the venting system remains similar) or $\alpha_{\text{evaporate}}$ (if the exit temperatures are comparable). However, the values of $\alpha_{\text{renucleate}}$ and $\alpha_{\text{scavenging}}$ might be largely increased due to the lack of soot particles as condensation sink, potentially resulting in higher N_{oil} values. In scenarios with high oil emission number $N_{\text{oil}} \gtrsim 10^{14} \text{ m}^{-1}$, the final ice crystal number for a soot-poor and low-sulfur regime (Figure 5c) or for hydrogen combustion (Figure 5f) case might be on the same order or even higher than in a reference kerosene scenario with $EI_s \sim 10^{15} \text{ kg}^{-1}$.

The potential impact of oil vapors could be reduced by designing oil breather vents that are located far away from the hot sections (e.g., off-axis) of the engine. Thus, fewer droplets penetrate the hot sections of the exhaust. In addition, oil-air separator systems used to recover oil from the mist released from the vents should be equipped with suitable filters. These filters should, ideally, remove all the oil before the air is released into the environment. Moreover, the exchange and renewal of worn seals could reduce unintentional loss. Thus, it may be beneficial to suitably adapt the maintenance cycles of the engines. Further mitigation options could be fluid bearings that do not use oil in central regions of the engine.

In the current box model version, coagulation effects are not explicitly simulated. Yet, we indirectly accounted for these effects by varying the geometric mean radius reflecting coagulation effects among the oil particles and by introducing $\alpha_{\text{scavenging}}$ accounting for the coagulation of the oil particles with other plume particles. Furthermore, we described the activation of the oil particles using the κ -Köhler theory. An alternative approach would have been to employ Frenkel, Halsey, and Hill (FHH) adsorption theory (e.g., Kumar et al., 2009; Sorjamaa & Laaksonen, 2007). This theory accounts for the attractive forces between the insoluble material and the adsorbed water molecules. These attractive forces would reduce the Kelvin barrier, enabling the activation of oil particles at lower supersaturations. However, in the limiting case of negligible small attractive forces, which we expect for hydrophobic oil particles, the FHH equilibrium saturation curve again approaches the Kelvin curve used in this study.

Focusing on oil particles and variations of their properties, we only varied the number of the other particles but kept all other properties (geometric mean and width, hygroscopicity) constant. Clearly, there would be slight quantitative differences if their actual values deviate from the prescribed ones. However, having investigated numerous scenarios of different particle numbers, the overall picture presented in this study should be largely unaffected. Moreover, F. Yu et al. (2024) suggested to use primary soot particle sizes rather than the spherical effective sizes of soot aggregates in the κ -Köhler equation. With that hypothesis, they explained the reduced soot activation observed during the ECLIF campaigns (Märkl et al., 2024; Voigt et al., 2021). This reduced soot activation would enhance the relative importance of small-sized volatile particles. Although this suggestion seems

reasonable to us, another explanation for the measured reduced soot activation could be the mixing of plume parcels of different ages (Lewellen, 2020). This process, however, is not well represented in parcel/box models (as discussed above).

For the sake of simplicity, we neglected volatile particles from combustion products in Section 3.2. Depending on their number and size, these particles may contribute significantly to the ice crystal number (Section 3.3). Nevertheless, the results in Section 3.2 demonstrate that it is not sufficient to look only at particles resulting from combustion products. If these particles from the combustion process are managed to be low in number, the presence of oil particles could still lead to high ice crystal numbers. Furthermore, we neglected ambient aerosols in the kerosene combustion case. The activation of emitted particles, however, is only marginally influenced by ambient aerosols as they gradually get mixed into the plume over time (discussed for hydrogen combustion and oil particles in Section 3.2; but it holds also for kerosene combustion and other emitted particles (not shown)) and thus the relative importance among the emitted particles will be almost unaltered. Clearly, if all emitted particle numbers are very low, the ice crystals' formation would be dominated by ambient aerosols, similar to the hydrogen case.

5. Conclusion

The rotating parts of present-day aircraft engines require a lubrication system to cool and lubricate the bearings and other parts of the engine. (Un-)controlled emissions of lubrication oil to the environment can be a source of volatile ultrafine particles when the oil is entrained into the hot exhaust plume, where it may evaporate and nucleate new particles upon cooling of the plume. Even if only a small amount of oil (a few milliliters per hour) nucleates new particles, the number of oil particles can exceed the present-day soot levels of conventional engines, assuming the newly formed particles are small (a few nanometers in size). We incorporated such oil particles as ice forming particles into the LCM box model. Many of the investigated potential scenarios showed that particles from lubrication oil may contribute significantly to ice crystal formation in soot-poor or hydrogen combustion cases. As the investigated scenarios are rather hypothetical, in situ measurements are required to assess the actual role of oil particles in the contrail ice crystal formation. If measurements will hint at a dominant role of these particles, technical adaptations of the lubrication system may be necessary to reduce their number in aircraft exhaust plumes.

Data Availability Statement

The Lagrangian Cloud Module (LCM) in a box model approach is described in detail in Bier et al. (2022, 2024). The setup and extension of the box model to simulate contrail formation on oil particles is described in Section 2.2 of the present study. The simulation results, together with the plot script required to reproduce the figures in this study, are available on a Zenodo repository (Zink, 2025).

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