#### **ORIGINAL PAPER**



# A contribution to mitigate NO<sub>x</sub> and H<sub>2</sub>O emissions **for a hydrogen‑powered hypersonic vehicle**

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## **Abstract**

Hypersonic transport fueled with liquid hydrogen (LH<sub>2</sub>-HST) is currently considered as long-term future technology of civil aviation to fy with speeds greater than Mach 5 at stratospheric altitudes of 25–38 km. In this paper, we present a comprehensive methodology to assess the emission mitigation potential (via  $NO<sub>x</sub>$  and  $H<sub>2</sub>O$ ) of future LH<sub>2</sub>-HST through operational measures, considering realistic constraints such as the sonic boom carpet as well as tolerable g-forces acting on the passengers while flying with hypersonic speeds. Both  $NO<sub>x</sub>$ - and  $H<sub>2</sub>O$ -optimal 4D-trajectories are identified by a brute-force algorithm that varies the initial cruise altitude from 30 to 36 km. As case study, the Mach 8 passenger aircraft STRATOFLY-MR3, which was conceptually developed in the framework of the H2020 STRATOFLY project, is operated on a single route from Brussels (BRU) to Sydney (MYA). The fndings are highlighted as relative changes regarding MR3's design fight altitude set at 32 km, respectively, 105 000 ft. As scientifc contribution, 3D emission inventories are calculated and made publicly available for a world fleet of MR3 aircraft operated along the BRU-MYA route on both  $NO<sub>x</sub>$ - and  $H<sub>2</sub>O$ -optimal mission profles in the year 2075.

**Keywords** Hypersonic transport · Emission mitigation potential · 4D-Trajectories · HTCM · Stratofy · More and Less



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## **1 Introduction**

The era of hypersonic fight began on June 23, 1963, when Robert White was the frst person to reach a hypersonic fight speed of Mach 5.24 as part of the *North American X-15* flight program  $[1]$  $[1]$ . From that day on, a significant impetus to consider commercial HST is spurring Europe to conduct a thorough assessment [\[2](#page-17-1)[–9](#page-17-2)] of the potential for civil highspeed aviation with regard to environmental, technical and economic viability, along with aspects related to human factors, social acceptance and operational measures. HST could revolutionize long-haul air travel primary through a major reduction in fight times, especially for antipodal routes, and secondary by " decarbonizing" air transport within Europe. This would be achieved through the adoption of new advanced high-speed propulsion systems such as combined-cycle turbojet/scramjet engines powered by postfossil, renewable fuels like green hydrogen, whose overall  $CO<sub>2</sub>$ -balance is considered neutral in the biogenic carbon cycle, but whose production is very energy-intensive and not yet deployed due to a lack of infrastructure. In addition, the difficulty of safely storing large quantities of liquid hydrogen on board of aircraft as well as the complexity of turbojet and scramjet engine combinations and their integration into the airframe pose signifcant hurdles, which, despite ongoing research, are still far from being ready for deployment (see e.g.  $[10-12]$  $[10-12]$ .

The pursuit of zero  $CO_2$ -emissions and the goal of reducing fight times by one order of magnitude have nevertheless led to the conceptualization of a novel aircraft named STRATOFLY-MR3, which is shown in Fig. [1](#page-1-0).

However, the realization of HST as a future concept may face considerable obstacles from an operational and climatological point of view: As per [[14\]](#page-17-5), the contribution of high-altitude (stratospheric) emissions to the effective radiative forcing primarily depends on non- $CO<sub>2</sub>$  effects such as



<span id="page-1-0"></span>**Fig. 1** Hypersonic passenger aircraft STRATOFLY-MR3 (fnal structural layout, based on [[13](#page-17-10)])

water vapour  $(H<sub>2</sub>O)$  and nitrogen oxides  $(NO<sub>x</sub>)$ , with  $H<sub>2</sub>O$ being identifed as the key climate driver due to it's large residence time of ∼ 3–4 years. Given that the time, quantity, and geographical location (longitude, latitude, altitude) of an emission contribute to climate impact in varying proportions, operational measures are needed which

- (i) reduce the total amount of emissions emitted along the aircraft's fight trajectory by optimizing its 3D fight profle through an adaption of the fight altitude *h*, respectively ICA;
- (ii) guarantee that specifc operational constraints during the fight mission are not violated.

These constraints come from (ii-1) the current regulatory framework for civil supersonic transport (SST) and HST alongside (ii-2) the passenger comfort when fying at speeds greater than Mach 5: On one hand, en-route noise emissions in the form of a sonic boom are emitted by the aircraft when it surpasses Mach 1 forming a *sonic boom carpet* [[15\]](#page-17-6) on ground that makes overland SST/HST impossible due to prevailing international noise regulations as § 91.817 in CFR Title 14 [\[16\]](#page-17-7). Hence, only water dominated routes can be considered for HST limiting the benefcial location (longitude  $\lambda$ , latitude  $\varphi$ ) of an emission with respect to climate impact. On the other hand, anthropometric passenger g-forces - that have been adjusted to tolerable loads on the passengers' musculoskeletal system - are necessary to comply with a realistic fight routing leading to large turn radii as well as long deceleration and acceleration phases. For instance, a hypersonic cruise speed of Mach 8 yields a substantial turn radius reaching up to 905 km to ensure a normal load factor of  $n<sub>z</sub> = 1.2$ . Consequently, executing even a modest course adjustment, such as  $\Delta \chi = 10^{\circ}$ , requires more than 1 min of fight time, posing considerable operational challenges for hypersonic fight missions that are addressed in this work.

#### <span id="page-1-1"></span>**1.1 The EU research project STRATOFLY**

From June 2018 to May 2021, the *Stratospheric Flying Opportunities for High-Speed Propulsion Concepts* (STRATOFLY) project has been funded by the EC, under the framework of the Horizon 2020 Program. One of the main project goals relates to the conceptual design and revision of the hypersonic passenger aircraft STRATOFLY-MR3 [\[17](#page-17-8)] (see Fig. [1](#page-1-0)), which is an enhanced waverider configuration of the design base LAPCAT-MR2.4 [[18\]](#page-17-9) being developed in previous EC funded projects LAPCAT I/II.

With a maximum take-off weight (MTOW) of 410 446 kg, the primary objective of MR3 is to convey 300 passengers (33 000 kg) over 18 520 km (10 000 nm) at a speed of Mach 8 maintaining a cruise altitude of 32 km (105 000 ft) using

181 250 kg of liquid hydrogen  $(LH<sub>2</sub>)$  as fuel. Due to the large range and high-speed requirements, the LH<sub>2</sub>-powered propulsion system is designed according to the ascent trajectory and consists of six air turbo rockets (ATR) and a dual mode ramjet (DMR) engine. The ATR/DMR engines are arranged coaxially and share the same elliptical air intake and thrust nozzle  $([13])$  $([13])$  $([13])$ .

# <span id="page-2-1"></span>**1.2 Methodology for environmental analysis of civil high‑speed aircraft**

As a corollary to the previous section, the future goal of revolutionizing long-haul air travel through  $LH<sub>2</sub>$ -HST requires a multi-disciplinary model approach that satisfes (i) and (ii) including (ii-1) and (ii-2) with a high level of detail to assess the potential of novel HST confgurations being operated at fight profles with a reduced amount of gaseous engine emissions. Such a comprehensive approach was developed by the *Institute of Air Transportation Systems* (ILT) at *Hamburg University of Technology* (TUHH) using a holistic simulation tool chain (see Fig. [2\)](#page-2-0) that incorporates:

- The *Hypersonic Trajectory Calculation Module* (HTCM) as mission simulator to calculate high-fdelity 4D-trajectories;
- A ray tracing algorithm to estimate primary sonic boom carpets along the aircraft's fight path, considering real weather data including winds;
- An emission model that determines the quantity and distribution of gaseous engine emissions;
- An algorithm that generates a noise-optimal fight path based on operational changes in route waypoints (2D trajectory optimization);
- An algorithm that produces an emission-optimal fight profle based on operational changes in cruise altitude (1D trajectory optimization);
- The *Global Air Trafc Emission Distribution Laboratory* (GRIDLAB) [[19\]](#page-17-11) that rasterizes emission profles into a 3D discrete spatial and temporal coordinate grid;
- A hypersonic airline network [[9](#page-17-2)] with respect to HST passenger demand.

These software tools and models are interconnected within MATLAB through an iterative procedure to identify the emission quantity mitigation potential (EQMP) of civil hypersonic passenger aircraft ensuring meaningful, comparable, and reliable results. For this paper, the simulation chain is applied to the MR3 vehicle to reveal the  $EQMP<sub>NO</sub>$ and  $EQMP<sub>H2O</sub>$  in relation to its design flight altitude of 32 km (105 000 ft).

## <span id="page-2-2"></span>**1.3 Outline**

The remainder of this paper is organized as follows: Sect. [2](#page-1-1) provides an overview of the HTCM along with the emission model, followed by the description of the sonic boom carpet determination algorithm in Sect. [3](#page-2-1). Section [4](#page-2-2) elaborates on



<span id="page-2-0"></span>**Fig. 2** Methodology for environmental assessment of hypersonic air transportation systems

the trajectory optimization algorithms. Section [5](#page-3-0) outlines the results of applying the methodology for environmental analysis of HST, including the 3D emission inventories. Finally, the paper concludes with a summary and highlights future research directions.

# <span id="page-3-0"></span>**2 Hypersonic trajectory calculation module (HTCM)**

To precisely determine 4D-trajectories, which represent the physical space curve (3D) along which the aircraft moves as a function of time ([1](#page-3-1)D), the software tool  $HTCM<sup>1</sup>$  is utilized. This tool simulates the aircraft's movement from lift-off to touch-down based on a nonlinear 3-degree-offreedom (3DoF) point mass model in which the diferential equations of motion are solved numerically using the *Euler method,* while including model-based fight performance data from the aerodynamic and engine characteristics. The aircraft dynamics are afected by a direct thrust force control  $F_{TW_c} \in \mathbb{R}$  as well as a virtual control input vector  $\vec{u} = [\tau_{\dot{V}}, \tau_{\dot{\gamma}}, \tau_{\dot{\gamma}}, \tau_{\dot{\mu}}] \in \mathbb{R}^4$ , which results from the linear feedback laws of the state control loops; both contributing to the nonlinear simulation of the controlled hypersonic vehicle. The computed 4D-trajetory contains the complete history of the aircraft state vector  $\vec{x} = \begin{bmatrix} V, \chi, \gamma, \mu, \lambda, \varphi, h, m \end{bmatrix}^T \in \mathbb{R}^8$ , where *V* represents the fight-path velocity,  $\chi$  the flight-path azimuth angle,  $\gamma$  the flight-path inclination angle,  $\mu$  the flight-path bank angle,  $\lambda$  the longitude,  $\varphi$  the geocentric latitude, *h* the geometric altitude, and *m* the aircraft's mass, but also all state variables that collectively describe the overall HTCM model state at any given point in time, such as e.g. the load factor  $n_z$  or the ambient temperature  $T$ .

Within the HTCM, particular emphasis was placed on a detailed modelling of the intricate mechanics of hypersonic fight on the one hand, which causes distinct phenomena that are not present in conventional aircraft such as fctitious forces due to the curvature of Earth (Term $\star$ ; Eq. [4\)](#page-4-0), and a sufficient numerical calculation accuracy on the other hand that enables a realistic implication of the quantity and distribution of high-altitude emissions for a single mission, which can subsequently be scaled to a global feet level.

## <span id="page-3-3"></span>**2.1 Nonlinear diferential equations of motion for hypersonic aircraft**

According to [[20](#page-17-12)], the movement of a hypersonic aircraft, approximated as point mass, over a spherical, rotating earth can be expressed by the following nonlinear diferential equations:

$$
\dot{V} = \frac{F_{\text{TW},c} \cdot \cos \alpha - D}{m} - g \cdot \sin \gamma
$$
  
\n
$$
- \omega_{\text{E}}^2 \cdot (r_{\text{E}} + h) \cdot \cos \varphi \cdot [\cos \gamma \cdot \cos \chi \cdot \sin \varphi - \sin \gamma \cdot \cos \varphi]
$$
  
\n
$$
\dot{\chi} = \frac{F_{\text{TW},c} \cdot \sin \alpha + L}{m \cdot V \cdot \cos \gamma} \cdot \sin \mu
$$
  
\n+  $[\tan \gamma \cdot \cos \chi \cdot \lambda \cdot \cos \varphi - \tan \gamma \cdot \sin \chi \cdot \varphi - \lambda \cdot \sin \varphi]$   
\n
$$
- 2 \cdot \omega_{\text{E}} \cdot [\tan \gamma \cdot \cos \chi \cdot \cos \varphi - \sin \varphi]
$$
  
\n
$$
+ \frac{\omega_{\text{E}}^2 \cdot (r_{\text{E}} + h)}{V \cdot \cos \gamma} \cdot [\sin \chi \cdot \sin \varphi \cdot \cos \varphi]
$$
  
\n(1)

<span id="page-3-4"></span>
$$
\dot{\gamma} = \frac{F_{\text{TW},c} \cdot \sin \alpha + L}{m \cdot V} \cdot \cos \mu + 2 \cdot \omega_{\text{E}} \cdot \sin \chi \cdot \cos \varphi
$$
  

$$
- \frac{g}{V} \cdot \cos \gamma + \left[ \sin \chi \cdot \lambda \cdot \cos \varphi + \cos \chi \cdot \dot{\varphi} \right]
$$
  

$$
+ \frac{\omega_{\text{E}}^2 \cdot (r_{\text{E}} + h)}{V} \cdot \cos \varphi \cdot \left[ \sin \gamma \cdot \cos \chi \cdot \sin \varphi \cdot + \cos \gamma \cdot \cos \varphi \right]
$$



<span id="page-3-1"></span><sup>&</sup>lt;sup>1</sup> The HTCM is a derivative of the Trajectory Calculation Module (TCM) software tool [[31](#page-18-0)], which is implemented in MATLAB $^{\circ}$  and has been developed and applied by DLR Institute of Air Transport since 2009.

<span id="page-3-2"></span>**Fig. 3** Flight dynamics modelling of the hypersonic aircraftwithout atmospheric winds



<span id="page-4-1"></span>**Fig. 4** Trim tables used for HTCM simulation of MR3: Drag coefficient  $C_D$  and aerodynamic efficiency ( $C_L/C_D$ -ratio) as function of Mach number Ma and angle of attack  $\alpha$  (data from [\[18\]](#page-17-9))

$$
\begin{aligned}\n\dot{\varphi} &= \frac{V \cdot \cos \gamma \cdot \cos \chi}{(r_{\rm E} + h)} \\
\dot{\lambda} &= \frac{V \cdot \cos \gamma \cdot \sin \chi}{(r_{\rm E} + h) \cdot \cos \varphi} \\
\dot{h} &= -V \cdot \sin \gamma \\
\dot{m} &= -\dot{m}_{\rm TW}\n\end{aligned}
$$

with

$$
g = g_0 \cdot \left(\frac{r_{\rm E}}{r_{\rm E} + h}\right)^2 \tag{2}
$$

Describing the motion of an aircraft using a geodetic system in non-rotating geocentric coordinates (an inertial frame) at the aircraft's *center of gravity* (CoG) allows for the consideration of Earth's rotational speed  $\omega_{\rm E}$ . The aircraft's CoG position is defined in spherical coordinates with geographical longitude  $\lambda$ , geocentric latitude  $\varphi$ , and distance  $r_{\rm E} + h$  from the center of Earth. Additionally, the kinematic system, also located at the CoG of the moving vehicle, results from rotating the geodetic system with  $\chi$  ( $z<sub>O</sub>$ -axis) and  $\gamma$  ( $y<sub>K</sub>$ -axis). Another consecutive rotation with  $\mu$  ( $x_K$ -axis) yields the intermediate kinematic system. Lastly, tilting this system by the angle of attack  $\alpha$  ( $y_{\overline{k}}$ -axis) results in the body-fxed frame (see Fig. [3\)](#page-3-2).

## <span id="page-4-3"></span>**2.2 External forces**

The external forces acting at the CoG of the hypersonic aircraft are depicted in Fig. [3](#page-3-2) and are generated by an aerodynamic and an engine model. Both models are fed with theoretical fight performance data published in [\[18,](#page-17-9) [21\]](#page-17-13) and [[22](#page-17-14)]. These data are frst processed into n-dimensional lookup tables, which serve as input for the HTCM software tool.

The aerodynamic model provides the lift and drag force as well as the angle of attack:

<span id="page-4-2"></span>
$$
L = \frac{1}{2} \cdot \rho \cdot V^2 \cdot S \cdot C_L
$$
  
\n
$$
D = \frac{1}{2} \cdot \rho \cdot V^2 \cdot S \cdot C_D \text{(Ma, } C_L)
$$
  
\n
$$
\alpha = \text{(Ma, } C_L)
$$
\n(3)

Here, *S* is the wing reference area of the vehicle that is given by 2517 m.<sup>2</sup>. Note that due to the absence of atmospheric wind, the fght-path velocity corresponds to the true airspeed of the vehicle. To decrease the computational time needed per simulation step, we only consider small inclination angles and small angles of attack for determining the aerodynamic lift coefficient so that  $C_L$  can be formulated as ([\[20\]](#page-17-12))

<span id="page-4-0"></span>
$$
C_L = C^* \cdot [m \cdot g + 2 \cdot m \cdot \omega_E \cdot V \cdot \sin \chi \cdot \cos \varphi] + C^* \cdot [m \cdot \omega_E^2 \cdot \cos^2 \varphi \cdot (r_E + h)] - C^* \cdot m \cdot V \cdot [\sin \chi \cdot \lambda \cdot \cos \varphi + \cos \chi \cdot \varphi],
$$
  
Term  $\star$ 

with  $C^* = 2/(\rho \cdot V^2 \cdot S \cdot \cos \mu)$ . Since the aerodynamic drag coefficient and the angle of attack depend on the Mach number Ma and lift coefficient, we use stationary trim tables as data input to interpolate for  $C_D$  and  $\alpha$ , which are shown in Fig. [4.](#page-4-1) This encompasses the contribution of the aerodynamic control surfaces involved in the longitudinal movement such as canards, elevons and bodyfaps (see Fig. [1\)](#page-1-0), to bring the pitching moment coefficient  $C_m$  to zero ensuring static stability, namely  $\delta C_m/\delta \alpha < 0$ , at every point of the trajectory. Additional contributions to the built-up approach of the stationary trim tables, as e.g. the non-negligible efect from the misalignment of the thrust vector with the vehicle's *x*-axis, can be found in [\[18\]](#page-17-9). The U.S. Standard Atmosphere 1976 [[23](#page-17-15)] serves as the foundation for modeling the static states of the atmosphere incorporated in Eq. [3](#page-4-2) and [4](#page-4-0) by establishing the correlation between locally prevailing atmospheric conditions, such as air density  $\rho$ , and the geopotential height  $H_G = (r_E \cdot h) / (r_E + h)$ , based on reference values at mean sea level.

The engine model is tailored to the STRATOFLY-MR3 powerplant, featuring a combined turbojet (ATR)- scramjet (DMR) propulsion system, with each propulsion unit represented by distinct 3D lookup tables. This mathematical model interpolates the net thrust, which inherently incorporates both the gross thrust and the internal drag contribution, as a function of altitude, Mach number and equivalence ratio  $\phi_{\text{I}}$ :

$$
F_{\rm TW} = F_{\rm TW,net}(h, \text{Ma}, \phi_{\rm L})
$$
\n(5)

The equivalence ratio for  $LH<sub>2</sub>$  in air combustion is defined as the ratio of the actual hydrogen/air mixture ratio to the stoichiometric hydrogen/air ratio and can be interpolated from the net lookup tables for the current engine operating conditions, which are described by the altitude and Mach number:

$$
\phi_{\rm L} = \frac{\left(\frac{\dot{m}_{\rm LHZ}}{\dot{m}_{\rm air}}\right)_{\text{actual}}}{\left(\frac{\dot{m}_{\rm LHZ}}{\dot{m}_{\rm air}}\right)_{\text{stoich}}} = \frac{\dot{m}_{\rm LHZ} \cdot 34.33}{\dot{m}_{\rm air}} = f(h, \text{Ma})\tag{6}
$$

Another engine characteristic provided by the model is the net fuel consumption of the ATR and DMR propulsion unit. This is obtained through linear interpolation from

the 3D lookup tables and scaled linearly using the virtual throttle ratio  $\delta_{TW}$ , as outlined in Section [2.4:](#page-6-0)

<span id="page-5-1"></span>
$$
\dot{m}_{\text{TW}} = \dot{m}_{\text{TW},\text{net}} \left( h, \text{Ma}, \phi_{\text{L}} \right) \cdot \delta_{\text{TW}} \tag{7}
$$

Figures [5](#page-5-0) and [6](#page-6-1) show the nominal operating limitations of the ATR and DMR propulsion units for a fight with stoichiometric combustion ( $\phi_{L,\text{max}} = 1$ ) and for a flight without  $LH_2$  supply ( $\phi_{L,min} = 0$ ). In terms of the ATR net lookup tables, engine properties are given along discrete interpolation points for a flight envelope of Ma  $\in$  [0.3, 4] and  $h \in [0 \text{ km}, 25 \text{ km}]$ , whereas the DMR net lookup tables provide engine characteristics for Mach numbers ranging from 4 to 8 and altitudes ranging from 24 to 25 km. To further increase the net thrust at critical points along the fight trajectory, an over-stoichiometric combustion of  $\phi_{L, \text{max}} = 1.5$  can be realized. The resulting 50% increase in  $LH<sub>2</sub>$  net consumption is depicted alongside the net thrust increase in Fig. [6](#page-6-1) (marked in red); exemplary covering a Mach number range from 4 to 5.

## **2.3 Load factors**

To uphold the concept of travel comfort while fying with hypersonic speeds, anthropometric passenger g-forces must be guaranteed over the whole fight envelope, which are understood as physical loads on the passengers' musculoskeletal system that have been adapted to tolerable levels of force magnitude. The physical unit of g-forces is meters per second squared  $(m/s<sup>2</sup>)$ , whereas an equivalent dimensionless notation is referred to as load factor. In



<span id="page-5-0"></span>Fig. 5 ATR lookup tables used for HTCM simulation of MR3: Total net thrust  $F_{TW,net}$  and total net fuel consumption  $\dot{m}_{TW,net}$  as function of Mach number Ma and height h (data from [\[21\]](#page-17-13))



<span id="page-6-1"></span>**Fig. 6** DMR lookup tables used for HTCM simulation of MR3: Total net thrust  $F_{TW,net}$  and total net fuel consumption  $m_{TW,net}$  as function of Mach number Ma and height h (data from [\[22\]](#page-17-14))

orthogonal direction to the fight path, the so-called normal load factor can be expressed by the ratio of the lift force *L* to the weight force *mg* of the aircraft, corrected by the fctitious force component resulting from the curvature of Earth:

$$
n_{z} = \frac{L}{mg} - \frac{V^{2} \cdot \cos^{2} \gamma}{\underbrace{g \cdot (r_{E} + h)}_{\text{Term} \star \star}}
$$
(8)

Note that the posterior fictitious term  $(**)$  is identical to term  $(*)$  of Eq. [4.](#page-4-0) Additionally, at a hypersonic cruise speed of Mach 8 and an altitude of up to 36 km, the normal load factor is calculated to 0.9, which corresponds to an efective (long-term) g-force of −0.1*g*, causing pas-sengers to feel as if they are lifted from their seats ([\[24\]](#page-17-16)). Flight maneuvers that generate an additional (short-term) g-force perpendicular to the fight path are coordinated (non-slip) turn fights as well as climbing or descending fights. Under these fight conditions, the normal load factor is determined as follows:

$$
n_{z} = \underbrace{\frac{1}{\cos \mu} - \frac{V^{2} \cdot \cos^{2} \gamma}{g \cdot (r_{E} + h)}}_{\text{Turn flight}} = \underbrace{\frac{V \cdot \dot{\gamma}}{g} + \cos \gamma - \frac{V^{2} \cdot \cos^{2} \gamma}{g \cdot (r_{E} + h)}}_{\text{Climb/Descend flight}}
$$
(9)

In direction of the fight path, the axial load factor is specifed as the acceleration capacity, derived from the equilibrium between thrust  $F_{TW}$  and drag *D* force, normalized by the weight force *mg* and corrected by the weight force's sine

component in the tangential plane relative to the fight-path velocity:

<span id="page-6-3"></span>
$$
n_x = \frac{F_{\text{TW}} - D}{mg} + \sin\gamma \tag{10}
$$

During HTCM simulations, the fight control system outlined in Section [2.4](#page-6-0) prevents dynamic exceedance of the load factor limits. To maintain passenger comfort over the whole flight envelope,  $n_z$  is constrained to a specific range of  $[+0.85g; +1.2g]$ , whereas  $n_x$  is limited to a specific range of  $[-0.2g; +0.3g]$ .

## <span id="page-6-0"></span>**2.4 Closed‑loop control system for nonlinear simulation**

<span id="page-6-2"></span>For a high-precision path-guidance of the hypersonic aircraft in terms of position, translation and time, the closed-loop fight control system shown in Fig. [7](#page-7-0) is used within the HTCM software. This system comprises of a nonlinear plant model (see Sect. [2.1](#page-3-3)), four linear feedback controllers, a pure feed-forward control to affect the aircraft dynamics as well as a state generator to defne the reference (commanded) aircraft states or rather the target condition vector  $\vec{w} = [V_c, \chi_c, \gamma_c, \mu_c, n_{x,c}] \in \mathbb{R}^5$  in each fight phase of the mission. This implies that the four controlled aircraft states  $V$ ,  $\chi$ ,  $\gamma$  and  $\mu$  are allocated among five pseudo controls  $\tilde{\tau}_V$ ,  $\tilde{\tau}_\chi$ ,  $\tilde{\tau}_\chi$ ,  $\tilde{\tau}_\mu$  and  $F_{TW,c}$  to bring the state control error vector  $\vec{e} = \begin{bmatrix} e_V, e_\chi, e_\gamma, e_\mu \end{bmatrix} \in \mathbb{R}^4$  to zero, utilizing both a proportional-integrating (PI) control algorithm to formalize the control laws and a thrust force mapping to

<span id="page-7-0"></span>



ensure anthropometric passenger g-forces. Additionally, limiters are included into the closed-loop system to ensure that the input vector of the plant  $\vec{u} = [\tau_{\hat{v}}, \tau_{\hat{x}}, \tau_{\hat{v}}, \tau_{\hat{\mu}}, F_{TW,c}] \in \mathbb{R}^5$  stays bounded at any time of the numerical simulation.

#### **2.5 Velocity controller**

To control the speed of the aircraft, the fight-path velocity serves as a model state, which corresponds to the true airspeed (TAS) in a windless, static atmosphere. Depending on the specifc fight phase, the guidance command can be either a target calibrated airspeed (CAS)  $V_{\text{CAS}}$  or a target Mach number Ma<sub>c</sub>, both of which are mathematically converted to the equivalent TAS. Hence, the speed control error is

$$
e_V = [V - V_{\text{TAS,c}}(\text{Ma}_c, T)]; e_V = [V - V_{\text{TAS,c}}(V_{\text{CAS,c}}, \rho, p)]
$$
\n(11)

When formalizing the control law for the velocity controller, the control error is proportionally combined and integrated over time, then negatively amplified by the constant factors  $k<sub>P</sub>$ and  $k_I$ , respectively:

$$
\widetilde{\tau}_V = -k_P \cdot e_V - k_I \cdot \int (e_V) dt \tag{12}
$$

As the pseudo-control law has the physical unit of an acceleration, it is limited to  $\tilde{\tau}_V \in [-0.2 \, g; \, 0.3 \, g]$  per numerical simulation time step.

#### **2.6 Flight‑path controller**

To compensate impermissible deviations from a desired climb or descent angle, the vertical navigation guidance command  $\gamma_c$  is subtracted from the state feedback  $\gamma$  to define the control error  $e_{\gamma} = (\gamma - \gamma_c)$ . This serves as the basis for contriving the pseudo-control law:

$$
\widetilde{\tau}_{\gamma} = -k_{\rm P} \cdot e_{\gamma} - k_{\rm I} \cdot \int \left( e_{\gamma} \right) dt \tag{13}
$$

Since Eq. [13](#page-7-1) has the inherent unit of a rational speed, it is limited to  $\tilde{\tau}_{\gamma} \in [-0.024^{\circ}/s; 0.068^{\circ}/s]$  per each time step of the numerical simulation (refer to Eq. [9](#page-6-2)).

#### **2.7 Navigation controller**

The navigation controller's objective is to control the remaining flight-path angles  $\gamma$  and  $\mu$  in such a way that the lateral navigation guidance commands, namely a target bank angle  $\mu_c$  and a target course  $\chi_c$ , are tracked while maintaining tolerable passenger load factors. The target course is associated with the desired ground track of route waypoints (WPs) specified by the user  $[\lambda_{c,1}|\varphi_{c,1} \dots \lambda_{c,n}|\varphi_{c,n}] \in \mathbb{R}^{2 \times n}$ , whereas the target fight-path bank angle results from the kinematics of stationary (non-slip) turn fights:

$$
\mu_c = \arctan\left(\frac{V^2}{g \cdot r_t} \cdot \text{sign} \,\Delta \chi\right) = \arctan\left(\sqrt{n_{z,\text{max}}^2 - 1} \cdot \text{sign} \,\Delta \chi\right) \tag{14}
$$

Here,  $r_t$  denotes the turn radius, which is inherently correlated to the maximal normal load factor  $n_{z, \text{max}}$ , and  $\Delta \chi$  is the course deviation between the respective WPs. By defning the control errors  $e_{\chi} = (\chi - \chi_c)$  and  $e_{\mu} = (\mu - \mu_c)$ , we can write the pseudo-control laws as

$$
\widetilde{\tau}_{\chi} = -k_{\rm P} \cdot e_{\chi} - k_{\rm I} \cdot \int (e_{\chi}) dt
$$
\n
$$
\widetilde{\tau}_{\mu} = -k_{\rm P} \cdot e_{\mu} - k_{\rm I} \cdot \int (e_{\mu}) dt
$$
\n(15)

As per [\[25\]](#page-17-17), civil passenger aircraft require approximately 5*s* to reach a target bank angle of 30°. Thus,  $\tilde{\tau}_{\mu}$  is preliminary constrained within the acceptable range of  $\left[-6^{\circ}/s; +6^{\circ}/s\right]$ . Similarly, for  $\tilde{\tau}_{\chi}$ , the control limitation is directly derived from Eq. [9](#page-6-2), resulting in a permissible range of [ −0.16◦∕*s*; +0.16◦∕*s* ] .

#### **2.8 Thrust force mapping**

<span id="page-7-1"></span>Based on Eq. [1](#page-3-4) and [10,](#page-6-3) we model the ATR/DMR thrust force as pure feedforward control devoid of time-varying delays:



<span id="page-8-0"></span>**Fig. 8**  $\text{EI}_{\text{NO}}$  as function of Ma, h and  $\phi_{\text{I}}$  (data from [\[26\]](#page-17-18) scaled with 0.147 according to [[27](#page-17-19)])

$$
F_{\text{TW},c} = \frac{m \cdot g \cdot n_{\text{x,c}} + D}{\cos \alpha} + \frac{\omega_{\text{E}}^2 \cdot (r_{\text{E}} + h) \cdot \cos \varphi}{\cos \alpha} \cdot [\cos \varphi \cdot \cos \varphi \cdot \cos \varphi]
$$
  
(16)

This scalar mapping guarantees that the maximal  $F_{TW,c,max}$  and minimal  $F_{TW,c,min}$  thrust force commands correspond to the maximal  $n_{x, max}$  and minimal  $n_{x, min}$  load factors based on the guidance command  $n_{x,c}$ . The operating condition of the ATR and DMR propulsion units is ascertained through the virtual throttle ratio, which is calculated as the quotient of the commanded thrust force to the interpolated thrust, given by the engine model, and used for linear scaling of the fuel consumption calculation, as indicated in Eq. [7:](#page-5-1)

$$
\delta_{\rm TW} = \frac{F_{\rm TW,c}}{F_{\rm TW}}\tag{17}
$$

## **2.9 Emission model**

Given the signifcant impact of pollutant quantity and species on climate responses in terms of changes in the chemical composition of the atmosphere, the task of the emission model is to meticulously expand the engine reactions delineated in Sect. [2.2](#page-4-3) to encompass the gaseous engine emissions of NO,  $H_2O$ , and  $H_2$  generated during hypersonic fight. For this purpose, the model extends the HTCM state variables by the emission mass flows  $\dot{m}_i$  as well as the emission quantities  $m_i$  of the individual trace substances with  $i \in \{NO, H_2O, H_2\}$ . To determine the emission characteristics of the ATR and DMR propulsion units, theoretical emission data published in [[26\]](#page-17-18) is further processed into 3D lookup tables, which serve as input for the emission model.

These tables specify the emission indices  $EI_i$  of the trace species as a function of  $h$ , Ma and  $\phi_{\text{L}}$ , indicating the quantity of the exhaust gas product g*<sup>i</sup>* generated per kilogram of fuel burned (kg<sub>LH2</sub>). By evaluating these tables (refer to Figs. [8](#page-8-0)) and  $9)^2$  $9)^2$  $9)^2$  using a linear interpolation routine for each time step *t* of the numerical simulation, the emission mass fows can be calculated using Eq. [7](#page-5-1):

<span id="page-8-2"></span>
$$
\dot{m}_i(t) = \text{EI}_i(h, \text{Ma}, \phi_L) \cdot \dot{m}_{\text{TW}} \tag{18}
$$

The partial quantities of NO,  $H_2O$ , and  $H_2$  emissions released along the fight trajectory are calculated through the multiplication of Eq. [18](#page-8-2) with the numerical integration step size  $\Delta t$ , resulting in 3D emission profiles:

$$
m_i(t) = \dot{m}_i(t) \cdot \Delta t \tag{19}
$$

To determine the total emission quantities of the hypersonic fight mission, the time integral is calculated over the emission mass flows from the start  $(t_0)$  to the end time  $(t_f)$ of the numerical simulation:

<span id="page-8-3"></span>
$$
m_i = \int_{t_0}^{t_f} \dot{m}_i(t) dt
$$
\n(20)

## **3 Sonic boom carpet computation**

When an object moves through the atmosphere at speeds faster than the speed of sound, it unavoidably emits compression waves that are sensual perceived as loud bangs by

<span id="page-8-1"></span><sup>&</sup>lt;sup>2</sup> EI<sub>H2</sub> is ranging from 12.29 g/kg to 192.24 g/kg in ATR and from 0.00022 g∕kg to 1.16 g∕kg in DMR mode ([\[26\]](#page-17-18)).



<span id="page-9-0"></span>**Fig.** 9 EI<sub>H2O</sub> as function of Ma, h and  $\phi_L$  including  $\varnothing$ EI<sub>H2O</sub> for ATR/DMR mode (data from [[26](#page-17-18)])

an observer on the ground. The wave propagation efect of these shock waves can usually be modelled with locally planar wave models, when the radial distance from the source is sufficiently large. This assumption can be summarized with the term *far-feld*, in contrast to the *nearfeld*. In other words, the far-feld can be considered as the area of the sound feld, in which the curvature of the wave front is negligible for small elements of the wave front, due to its large distance from the source. Under this assumption, planar wave propagation models can be employed to describe the motion characteristics of small pieces of the shock wave front.

With the far-field assumption, the aircraft is considered as a moving point mass source, which generates a conical shock wave front, i.e., the Mach cone. Due to the locally planar wave assumptions in the far-field, ray theory can be used to describe the propagation of the shock wave front. This theory is based on geometric acoustics to estimate the shock wave front behaviour in an inhomogeneous medium, such as the atmosphere of Earth ([\[28](#page-17-20)]).

## **3.1 Ray tracing algorithm**

We ascertain the geographic positions of the sonic boom shock waves on ground by applying ray theory equations within a ray-tracing algorithm that was previously described in [\[15\]](#page-17-6). This algorithm primarily relies on coupled diferential equations in a tensor formulation, which are solved numerically to compute the ray paths ([[29\]](#page-18-1)):

$$
\frac{d\vec{r}}{dt} = a \cdot \vec{n} + \vec{w}, \qquad \frac{d\vec{n}}{dt} = \left(I - \vec{n} \otimes \vec{n}^T\right) \nabla \left(a + \vec{w} \circ \vec{n}\right) \tag{21}
$$

Here,  $\vec{n} \in \mathbb{R}^3$  denotes the wave front normal vector, which is the vector perpendicular to the shock wave front surface,  $\vec{r} = \begin{bmatrix} x & y & z \end{bmatrix}_{N}^{T} \in \mathbb{R}^{3}$  represents the position vector of that specifc shock wave front in the navigation frame,  $\vec{w} \in \mathbb{R}^3$  denotes the wind speed vector, *t* denotes the time variable of the numerical simulation, *I* symbolizes the unit tensor and *a* is the ambient speed of sound that is given by the ideal gas law:

<span id="page-9-1"></span>
$$
a = \sqrt{\kappa \cdot R \cdot T(h)}\tag{22}
$$

In Eq.  $22$ ,  $\kappa$  denotes the adiabatic index of air, set to a value of 1.4, while *R* represents the specifc gas constant of air, with an empirical value of 287.058 J∕kg K. The ambient temperature *T* is described as a function of altitude.

To initiate the tracing procedure, we defne the initial position of a specifc ray by extracting the position states  $\lambda$ ,  $\varphi$  and *h* of the aircraft state vector  $\vec{x}$  for a valid flight condition ( $Ma > 1$ ). The initial orientation of the ray is likewise defined by using the orientation states  $\chi$ ,  $\gamma$  and  $\mu$  of the aircraft. This also includes the initialization of the Mach angle  $\sigma = \sin^{-1}(1/Ma)$ , since the rays start their propagation perpendicular to the Mach cone. The only varying parameter that distinguishes rays which are sent out perpendicularly to the Mach cone surface is the azimuthal angle *θ*. Note that this is a peculiarity of the sound feld of a supersonically moving source, as the wave front is not propagating in a spherical manner. Figure [10](#page-10-0) shows the concept of the ray tracing approach.

The rays start perpendicular to the Mach cone surface (not depicted), such that they propagate towards the front of the aircraft's initial position. Depending on the azimuth angle, the propagation begins down-wards (i.e., on-track ray at  $\theta_0 = 0^\circ$ ; highlighted in black) or with a lateral deviation



<span id="page-10-0"></span>**Fig. 10** Schematic view of tracing a sonic boom shock wave front in the supersonic fight regime for diferent atmospheric conditions (left: ISA; right: Real atmospheric data including wind)

(i.e., off-track rays with  $\theta \neq 0^{\circ}$ ; lighter colours depict a higher deviation in relation to  $\theta_0$ ). As the aircraft travels faster than the shock wave front, it should be mentioned, that the rays depicted in Fig. [10](#page-10-0) represent the progression of small parts of the shock wave front at every time step  $t_0 + \Delta t$ of the numerical simulation until they reach the ground (or bend upwards), while the aircraft is only depicted at its initial position for  $t_0$ . Due to refraction in the atmosphere (as the temperature increases towards the ground), the sonic rays tend to bend up before reaching the ground. All remaining rays that still reach the ground, defne the primary sonic boom carpet, as this is the region, where the sonic boom shock wave front emitted at that specifc location will hit the ground. The impact points of the lateral cut-off rays define the carpet width, which can be scaled up notably when comparing the tracing results for a windless standard atmosphere (ISA, left) [[23\]](#page-17-15) and a realistic atmosphere (right), derived from measured weather data including wind.

## **4 Trajectory optimization**

As 4D solution of the numerical simulation, the flight trajectory maps the fight profle (3D) of the aircraft as a function of time (1D). This profle can be enhanced using both vertical (1D) and lateral (2D) optimization algorithms, which are presented in the following sections. They yield an emission- and noise-optimal 3D fight profle based on operational changes in cruise altitude (1D) and fight path waypoints (2D).

#### **4.1 Vertical optimization (1D)**

The vertical trajectory optimization entails a numerical search algorithm designed to assess the potential for mitigating the overall emissions of NO and  $H<sub>2</sub>O$  in comparison to a reference trajectory. The relative potentials are called EQMP<sub>NO</sub>, respectively, EQMP<sub>H2O</sub>. The algorithm relies on a brute force method, which allows the HTCM to be triggered with varying operational measures that defne the trajectory simulation such as the target initial cruise altitude (ICA; user input<sup>3</sup>). To activate the iterative calculation process shown in Fig. [11,](#page-11-0) the algorithm incrementally adjusts the ICA for each HTCM simulation in small constant steps ΔICA until the search interval is completed. The total number of calculation steps  $n_{\text{ICA}}$  is referring to the search limits  $\left[\text{ICA}_{\text{min}}, \text{ICA}_{\text{max}}\right]$ and can be determined as follows:

$$
n_{\text{ICA}} = \frac{\text{ICA}_{\text{max}} - \text{ICA}_{\text{min}}}{\Delta \text{ICA}} + 1 \tag{23}
$$

The attainable set of mitigation potentials is computed by assessing each solution of the iteration based on Eq. ([20\)](#page-8-3) and comparing it as relative ratio to the reference solution (indexed as 'ref'):

<span id="page-10-1"></span><sup>&</sup>lt;sup>3</sup> The HTCM user inputs are as follows: 1) Integration step size  $\Delta t$ 2) Cruise Mach number Ma, 3) Cruise altitude ICA 4) Route waypoints  $\left[\lambda_1|\varphi_1 \dots \lambda_n|\varphi_n\right]$  5) Take-off mass  $m_0$  6) Continuous Climb Cruise (CCC; yeslno).

EQMP<sub>NO,j</sub> = 100 · 
$$
\frac{m_{NO,j}(ICA_j)}{m_{NO,ref}} - 100
$$
  
\nEQMP<sub>H2O,j</sub> = 100 ·  $\frac{m_{H2O,j}(ICA_j)}{m_{H2O,ref}} - 100$  (24)

with *j*  $\in \{1, 2 \dots n_{\text{ICA}}\}$ . Finally, the minima EQMP<sup>\*</sup><sub>NO</sub> and  $EQMP_{H2O}^*$  are determined from Eq. ([24\)](#page-11-1), which are referred to those trajectories that have the highest potential for reducing the environmental impacts in terms of total emissions. Note that the corresponding optimal ICA<sup>∗</sup> may difer for these minima.

#### <span id="page-11-3"></span>**4.2 Lateral optimization (2D)**

The lateral trajectory optimization relates to the sonic boom carpet propagation and involves an iterative route design process, as illustrated in Fig. [12](#page-12-0), to automatically modify the ground track of the trajectory based on encountered infringements of the boom carpet. These infringements occur when sonic booms (SBs) reach the ground or inhabited areas along the fight path, leading to routes that are predominantly over water. Similar to the vertical optimization, the algorithm allows the HTCM to be called with varying operational measures that predefne the trajectory simulation such as the route WPs  $\left[ \lambda_1 | \varphi_1 \dots \lambda_n | \varphi_n \right]$ .

Within each iteration step, these waypoints are modifed until the 4D-trajectory becomes noise-optimal, supposing that constraint (ii-1) is satisfed. The process comprises the following steps or software tools, whereby their contentrelated algorithmic functionality is reproduced below in simplifed form to support a compact formulation:

#### **A) Initial Waypoints**

The initial fight route for a hypersonic mission is drafted in Google Earth<sup>[4](#page-11-2)</sup> for a given city pair connection, or socalled *Stratoports* [\[9](#page-17-2)]. This initial draft incorporates a preliminary approximation of the sonic boom carpet, ensuring sufficient bufer zones on both sides of the fight path relative to the coastlines. Next, an initial set of route waypoints, exclusively positioned over water, can be manually derived and utilized as input for the trajectory simulation in step B.

#### **B) Hypersonic Trajectory Calculation Module**

The HTCM software tool (refer to Sect. [2](#page-1-1)) serves as the mission simulator, employed to compute the 4D-trajectory based on predefned user inputs, which also include the initial set of route WPs derived in step A. As input for the sonic boom carpet computation the time-history of the aircraft state vector  $\vec{x}(t)$  is transferred to step C.

#### **C) Sonic Boom Carpet Computation**

The sonic boom (SB) ray tracing algorithm (refer to Sect. [3\)](#page-2-1) is used to calculate the SB carpet for the hypersonic flight mission based on  $\vec{x}(t)$  as input. The output of step C encompasses the position vector

<span id="page-11-1"></span>

<span id="page-11-0"></span>**Fig. 11** Numerical search algorithm for EQMP approach

 $\vec{r}_{SB} = \left[ \lambda_{SB,1} | \varphi_{SB,1} \dots \lambda_{SB,n} | \varphi_{SB,n} \right]^T \in \mathbb{R}^{n \times 2}$  of all (n) sonic rays reaching the ground. These shock wave coordinate pairs defne the outermost boundary of the geometric SB carpet as polygonal chain.

#### **D) Check Sonic Boom Infringements (Constraint ii-1)**

To ensure compliance with operational constraint (ii-1), we employ the land\_or\_ocean.m [[30](#page-18-2)] MATLAB function during step D, which relies on a polygonal approximation to delineate land masses and oceans as mathematical meshes. This function takes  $\vec{r}_{SR}$  as input vector and returns a vector of binary classifers indicating whether the sonic shock wave coordinate pairs are located on land or water.

#### **E) Flight-Path Modifcation Module**

The Flight-Path Modifcation Module (FPMM) is a software tool developed to modify the initial fight path of a reference trajectory using a geometric approach aimed at minimizing the impact of noise emissions from primary sonic booms on inhabitant areas. For the sake of consistency, this approach relies on great circle formulas for determining distances and course angles between trajectory-, route- and SBrelated geodetic model states. Thus, tool inputs are not only provided from step D, but also from B and C. With regard to the binary classifers from step D, land-based SB coordinate pairs are clustered and averaged arithmetically (indexed as

<span id="page-11-2"></span><sup>4</sup> Available at [www.google.com/earth.](http://www.google.com/earth)



<span id="page-12-0"></span>Fig. 12 Iterative procedure of lateral trajectory optimization

'SB, land, i') to obtain the shortest distance to the geodetic trajectory states:

optimal  $ICA_{NO}^*$  and  $ICA_{H2O}^*$  values. By adapting the route waypoints and varying the initial cruise altitude from 30

$$
d_{min} = \min \left[ r_{\rm E} \cdot \cos^{-1} \left\{ \sin \overline{\varphi}_{\rm SB, land, i} \cdot \sin \overrightarrow{\varphi}(t) + \cos \overline{\varphi}_{\rm SB, land, i} \cdot \cos \overrightarrow{\varphi}(t) \cdot \cos \left( \overline{\lambda}_{\rm SB, land, i} - \overrightarrow{\lambda}(t) \right) \right\} \right]
$$
(25)

The corresponding magnetic heading (QDM) from the identified trajectory state (indexed as 'min') to the previously defined SB-related model state is calculated as follows:

$$
QDM = \cos^{-1}\left(\frac{\sin\overline{\varphi}_{SB,\text{land},i} - \cos\sigma \cdot \sin\varphi_{\text{min}}}{\sin\sigma \cdot \cos\varphi_{\text{min}}}\right) \tag{26}
$$

If the distance from  $\lambda_{\min}|\varphi_{\min}$ , which guarantee the shortest distance to the SB-related geodetic state, to the subsequent or previous route WP is greater than a predefined threshold  $s_{\text{req}}$ , a new route WP is set. Otherwise, the route WP is adjusted by a user-specified offset  $s_{des} = \sigma_{mod} \cdot r_E$ so that the modified route WP coordinate pairs (indexed as 'mod') are calculated and incorporated as

$$
\varphi_{\text{mod}} = \sin^{-1}\left\{\sin\varphi_{\text{min}} \cdot \cos\sigma_{\text{mod}} + \cos\varphi_{\text{min}} \cdot \sin\sigma_{\text{mod}} \cdot \cos\left(QDM + \pi\right)\right\}
$$
\n(27)

and

$$
\lambda_{\text{mod}} = \lambda_{\text{min}} - \tan 2^{-1} \left( \frac{\sin (QDM + \pi) \cdot \sin \sigma \cdot \cos \varphi_{\text{min}}}{\cos \sigma_{\text{mod}} - \sin \varphi_{\text{min}} \cdot \sin \varphi_{\text{mod}}} \right)
$$
(28)

## 5 Evaluation of methodology

The results outlined in this section are based on applying the methodology shown in Sect. 1.2 on the MR3 vehicle, aiming to identify NO- and H<sub>2</sub>O-optimal 4D-trajectories as well as their relative emission quantity mitigation potentials (EQMP<sub>NO</sub> and EQMP<sub>H2O</sub>), along with the associated to 36 km at a mission level, with a reference flight altitude set at 32 km, operational measures are applied to achieve objective (i) while simultaneously ensuring compliance with operational constraint (ii-1) and (ii-2). The resulting optimized emission profiles are then scaled to represent a world fleet of MR3 aircraft and transformed into a discrete 3D coordinate grid, forming the scientific contribution of the simulation chain for outsourced studies with 3D climate models.

#### 5.1 Setup of holistic simulation chain

The overall setup of the simulation chain comprises multidisciplinary inputs, which are partly given in Table 1. The route operated in the year 2075 by MR3 is derived from the hypersonic airline network [9] providing an initial set of route WPs between distributed city pair connections. As a case study, we evaluate the reference mission from Brussels (BRU) to Sydney (MYA) with a corresponding passenger load factor of 1 - without any fuel planning or reserves. The initial flight conditions remain consistent across all calculated trajectories. We consider a departure from Brussels airport (BRU:  $\lambda_0 = 4.49 \mid \varphi_0 = 50.9$ ) at an altitude of  $h_0 = 45.41$ m, a lift-off velocity of  $V_0 = 110$ m/s, and an initial flight-path angle  $\chi_0$  of 342.7°. The flightpath inclination  $\gamma_0$  and bank angle  $\mu_0$  are both initially set to zero, like the initialization of all other HTCM model states.

<span id="page-13-0"></span>**Table 1** Inputs for holistic simulation chain (refer to Fig. [2\)](#page-2-0)

Input	Description	Value	Unit
Ma	Cruise Mach number	8	$[\cdot]$
$ICA_{ref}$	Initial cruise altitude (ref)	32 000	$\lceil m \rceil$
$\Delta t$	Integration step size.		[s]
m <sub>0</sub>	Initial Take-Off Weight	410446	[kg]
$\triangle$ ICA	Height increment for EOMP	152.4	$\lceil m \rceil$
$r_E$	Nominal earth radius	6 356 766	$\lceil m \rceil$
$\omega_{\rm E}$	Earth rotational speed	$7.292115 \times 10^{-5}$	$\lceil \text{rad/s} \rceil$
$g_0$	Acceleration of gravity at MSL	9.80665	$[m/s^2]$
$S_{\text{des}}$	Great circle offset for FPMM	25 000	$\lceil m \rceil$



<span id="page-13-1"></span>**Fig. 13** Sonic boom carpet edges (white) and ground track of trajectory (yellow) are illustrated in Google Earth without explicit axis labels (left: North Sea; right: Bering Strait). Additionally, the load factors n<sub>n</sub> (left) and n<sub>y</sub> (right) are depicted in orange over the relative flight time t/t<sub>f</sub>

## **5.2 Optimized fight route for operational constraint (ii‑1) and (ii‑2)**

Figure [13](#page-13-1) shows the optimization results of the iterative route design process aimed at generating a noise-optimal flight path for the reference trajectory, with  $ICA_{ref}$  set at 32 km, satisfying operational constraint (ii-1). The resulting sonic boom carpet edges are depicted in white for exemplary fight segments across the optimized fight path, which is highlighted in yellow in Google Earth.<sup>[5](#page-13-2)</sup> Due to the embedment of the HTCM (see Sect. [4.2](#page-11-3); Step B) into the iterative route design process, the navigation controller ensures the adherence of acceptable passenger loads at hypersonic speeds, particularly during turn fights. This further compliance with operational constraint (ii-2) is also evident in Fig. [13](#page-13-1), with the normal load factor highlighted in orange (left y-axis<sup>[6](#page-13-3)</sup>) across the relative flight time t/t<sub>f</sub>  $\in$  [0, 1].

We calculated the sonic boom carpet by repeating the tracing approach for every valid flight condition of the 4D-trajectory and connecting the outermost impact points. For the numerical propagation of the rays, an open access set of globally discretised weather data was included into the tracing algorithm and interpolated in such a manner that the 3D atmospheric derivatives of temperature and wind speeds are continuous for a variety of exemplary days in the year 2015. This weather dataset was published by the European

<span id="page-13-2"></span><sup>5</sup> Available at [www.google.com/earth](http://www.google.com/earth).

<span id="page-13-3"></span><sup>6</sup> For the sake of consistency, the axial load factor is also shown on the right y-axis of Fig. [13](#page-13-1).



<span id="page-14-1"></span>Fig. 14 Results of numerical search algorithm (vertical trajectory optimization via NO and H<sub>2</sub>O) for reference mission. The total emission quantities and the relative EOMP are depicted over ICA, along with the residual quantity of fuel  $(LH<sub>2</sub>)$ 

Centre for Medium-Range Weather Forecasts  $(ECMWF)^{7}$  $(ECMWF)^{7}$  $(ECMWF)^{7}$ and describes the atmospheric state at a specifc point in time with a grid resolution of  $0.75^{\circ} \times 0.75^{\circ}$  (latitude  $\times$  longitude). The third spatial dimension nodes are discretized in a range from 0 to 40 km, whereby the resolution decreases at higher altitudes. Georeferencing was accomplished using the World Geodetic System 1984 (WGS84) ellipsoid, with each day partitioned into four timesteps to capture the full diurnal cycle. For the carpet simulation, we used a variation of datasets from 2015, as e.g., a 3D grid from November 5th at 06:00 AM.

Note that the iterative route design process failed to converge for the fight segment over Bering Strait, as shown on the right side of Fig. [13](#page-13-1), primarily due to the considerable width of the boom carpet at this location, ranging from 140 to 255 km. Given the prior discussions of this issue in [\[9](#page-17-2)] and the sparse population in this region, the authors decided to manually adjust the route WPs for that particular fight segment to minimize the observed sonic boom carpet infringements to the greatest extent possible.

## **5.3 Emission quantity mitigation potential (mission level)**

Figure [14](#page-14-1) illustrates the optimization results to quantify the potentials for reducing high-altitude emissions, where each marker represents a 4D-trajectory for diferent values of the

initial cruise altitude. The total quantities of NO emissions  $m_{NO}$  (left) and H<sub>2</sub>O emissions  $m_{H2O}$  (right) are shown each on the left y-axis and the corresponding relative mitigation potentials  $EQMP<sub>NO</sub>$  and  $EQMP<sub>H2O</sub>$ , which refer to the reference trajectory at ICA<sub>ref</sub> = 32km, are shown on the right y-axis. By including the residual propellant mass as metric in our analysis, we note that  $m_{LH2,f}$  (top) is insufficient to cover the entire ICA range for the BRU-MYA fight mission. As the aerodynamic drag force decreases with altitude, we observe that the mission is only feasible for ICAs ranging from 31.4 km to 36 km, precluding any additional fuel reserves. The comparison between both optimization results reveals that NO emissions notably diminish with altitude, while  $H<sub>2</sub>O$  emissions remain relatively constant. Consequently, the relative mitigation potential of NO emissions shows a higher variability of up to 19.29% within the achievable ICA range compared to the  $H<sub>2</sub>O$  emissions, which only fuctuate by 1.29%. We fnd that the NO-optimal solution is located at an altitude of  $ICA_{NO}^* = 34.75$  km with a EQMP $_{\text{NO}}^{*}$  of -18.75%, which corresponds to a minimal emission quantity of  $m_{\text{NO}}^* = 7.7675 \text{ Mg}$ . The H<sub>2</sub>O-optimal solution is located at an altitude of  $ICA_{H2O}^* = 32.77$  km with a EQMP $_{\text{H2O}}^{*}$  of -0.11% corresponding to a minimal emission quantity of  $m_{\text{H2O}}^* = 1519.4 \text{ Mg}$ . As H<sub>2</sub>O emissions are proportional to the engine's  $LH_2$ -flow, the  $H_2O$ -optimal trajectory coincides with the fuel-optimal trajectory and yields the highest mission-specifc residual propellant mass of  $m_{LH2,f} = 2.271 \text{ Mg}.$ 

Figure [15](#page-15-0) depicts the resulting 4D-optimal trajectories with respect to NO (left) and  $H<sub>2</sub>O$  (right) emissions. Both altitude and Mach profles are plotted over the relative fight

<span id="page-14-0"></span> $7$  2015 ERA-Interim data, provided by European Centre for Medium-Range Weather Forecasts [\(www.ecmwf.int](http://www.ecmwf.int)).



<span id="page-15-0"></span>Fig. 15 Altitude and Mach profile of the identified NO- and  $H_2O$ -optimal trajectories are illustrated across the relative flight time  $t/t_f$ , along with colored magnitude of emission release

time t/t<sub>f</sub> ∈ [0, 1] including the varying magnitude of emission releases denoted by color. This magnitude is defned as the ratio of local emission quantity to the maximum emission quantity within the fight envelope. The vertical fight profle is based on typical fight phases in the subsonic regime and complies with today's regulations of air traffic control (ATC) regarding speed and altitude constraints, such as maintaining a speed limit of 250 kts below FL100 (10 000 ft). As the distance from Brussels to the coast is short, there are no Mach number limitations to prevent sonic booms over land, allowing for an accelerated supersonic climb until reaching the desired ICA. The cruise phase is modelled as a continuous climb cruise (CCC) ensuring a constant Mach number and lift coefficient during cruise, which is assumed to be suitable for HST to approximate real subsonic fights with ATC-required step climbs. The descent to Sydney airport (MYA:  $\lambda_f = 150.15 \mid \varphi_f = -35.89$ ), reaching a final altitude of  $h_f$  = 5m with a final approach speed of Ma = 0.325, includes two level deceleration segments in the hypersonic and supersonic fight regime to ensure stable trim conditions before transitioning into the subsonic regime, where ATC restrictions are met again.

#### **5.4 Emission inventories (feet level)**

We compute 3D emission inventories for the Brussels to Sydney mission based on a global feet of MR3 aircraft operated in the year 2075 on the NO-optimal and  $H<sub>2</sub>O$ -optimal mission profiles (refer to Fig. [15\)](#page-15-0) by using DLR's software GRIDLAB [\[31\]](#page-18-0). In GRIDLAB, the total quantity of emitted emissions is gridded along the aircraft's fight trajectory using numerical grids with a horizontal resolution of 1° in longitude and latitude and a vertical resolution of 305 m. For simplifcation, we assume an

entry into service (EIS) of MR3 in 2050 and use a generic factor *S* published by [[32](#page-18-3)] to scale the optimized emission profles to an annual basis in 2075:

$$
S = \underbrace{4}_{\text{New MR3 per year}} \times \underbrace{25}_{\text{Projected years}} \times \underbrace{1}_{\text{Frequency}} \times \underbrace{360}_{\text{Annual basis}} = 72000 \tag{29}
$$

Figure [16](#page-16-0) shows the longitudinal and latitudinal distribution of the optimized NO (left) and  $H<sub>2</sub>O$  (right) fleet emissions being aggregated over altitude and normalized per grid cell volume. We note that the MR3 feet emits 0.55926 Tg of NO emissions and 109.398 Tg of  $H_2O$  emissions, covering a total travelled distance over ground of 1.3697 Tm.

## **6 Summary and Future Work**

This paper describes a comprehensive methodology to quantify the mitigation potential of  $NO<sub>x</sub>$  and  $H<sub>2</sub>O$  emissions for a Mach 8 passenger aircraft fuelled with liquid hydrogen. Realistic operational constraints arising from the current regulatory framework for civil HST operations due to the issue of sonic booms making landfall as well as passenger comfort when fying at hypersonic speeds are addressed in detail in this study. The investigated measures comprise operational changes in the initial cruise altitude and the lateral routing through an adaption of route waypoints. For a reference mission from Brussels (BRU) to Sydney (MYA) our analysis shows that increasing the ICA towards higher altitudes results in a reduced total discharge of both  $NO<sub>x</sub>$  and  $H<sub>2</sub>O$  emissions along the aircraft's fight trajectory. We observe that the NO-optimal ICA is located at 34.75 km with a relative mitigation potential



<span id="page-16-0"></span>**Fig. 16** Geographical distribution of emissions (left: NO; right: H2O) for reference fight mission, vertically aggregated and normalized per grid cell volume given in  $log_{10}$  kg/km<sup>3</sup>

of -18.75%, whereas the  $H_2O$ -optimal ICA is located at 32.77 km with a relative mitigation potential of -0.11%, both in comparison to the reference ICA being set at 32 km. Additionally, both relative mitigation potentials can be augmented up to -19.18% (NO) and -1.23% (H<sub>2</sub>O) by adjusting the reference ICA to 31.4 km, which corresponds to the lower boundary of the mission-specifc achievable ICA range. Certainly, these fndings provide a new foundation for the redesign of future civil hypersonic passenger aircraft with  $LH_2$ -powered scramjet combustors for operating points guaranteeing reduced emission quantities; even though their EIS is not anticipated in the near term.

Based on market forecast data, we scaled the NO- and H<sub>2</sub>O-optimal 4D-trajectories by a generic factor from the mission to a full feet level, established in the projection year 2075. This enabled us to calculate 3D emission inventories with 0.55926 Tg of nitrogen oxides and 109.398 Tg of water vapour emitted by the MR3 feet per year on the Brussels to Sydney mission.

Future work is planned to calculate 3D emission inventories as well as the emission quantity mitigation potentials for the hypersonic airline network outlined in [[9\]](#page-17-2), which is based on assumptions for a realistic market penetration of civil HST in the future. To be able to evaluate the climate impact from hypersonic aviation, climate response models must be incorporated into ILT's multi-disciplinary simulation chain to calculate adequate climate metrics, such as the radiative forcing (RF). This will not only provide a valid foundation for conducting trade-off analyses between emission- and climate-optimal fight trajectories, but will also facilitate a detailed investigation of the following scientifc research questions:

- 1. How big is the climate impact mitigation potential (CIMP) compared to the EQMP of future HST for the reference mission from Brussels to Sydney?
- 2. Will the climate-optimal ICA be higher or lower than the emission-optimal ICAs?
- 3. To what extent the analysed measures can be used to optimize 4D-trajectories of future HST regarding climate impact on a mission level while guaranteeing operational constraint (ii-1) and (ii-2)?
- 4. What is the CIMP on a feet level when using the 3D emission inventories of the hypersonic airline network [[9\]](#page-17-2) as input?

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**Data availability** The 3D emission inventories of the MR3 feet operating along the Brussels to Sydney route on the H2O and NO-optimal mission profle in the year 2075, are accessible as NetCDF fles at [www.zenodo.org](http://www.zenodo.org) with the DOI: [https://doi.org/10.5281/zenodo.10948](https://doi.org/10.5281/zenodo.10948393) [393](https://doi.org/10.5281/zenodo.10948393).

## **Declarations**

**Conflict of interest** The authors declare that they have no confict of interest.

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