

# Physical principles of contrail formation

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Wissen für Morgen



# Engine emissions and their mixing with ambient air

Aircraft engines emit under cruise conditions inter alia

- water vapour (1.23 kg per kg kerosene burnt)
- soot particles ( $O(10^{15})$  per kg kerosene)
- sulphur dioxide, that gets partly oxidized into sulphuric acid
- heat (about 26-31 MJ per kg kerosene)

These emissions **get quickly** mixed with ambient air. The mixing proceeds **isobarically**, i.e. species concentrations and enthalpy in the plume decrease in a constant proportion, until eventually plume conditions are relaxed to ambient conditions.

As we know from cloud physics, isobaric mixing of two air masses can yield supersaturated conditions. **If water (super)saturation is temporarily achieved during the mixing process, a condensation trail (contrail) will form.** This is the **Schmidt-Appleman criterion**.



## Fast mixing

- The ambient atmosphere is a huge **gas reservoir with pressure  $p$**  (at flight altitude); thus the emissions quickly assume the same pressure. The further expansion of the plume is thus **isobaric**.
- The **expansion of the plume proceeds very fast**. At engine exit the emissions contain about 1 part of combustion gases within about 60 to 70 parts of air (unburnt air from the core engine and bypass air). After just one second the dilution factor,  $N$ , has typically increased by a factor of 100 and Schumann found an empirical formula

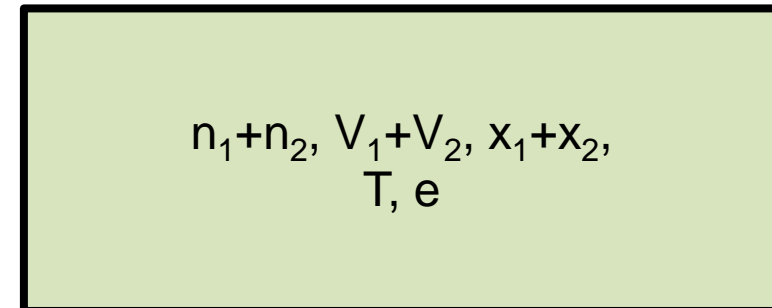
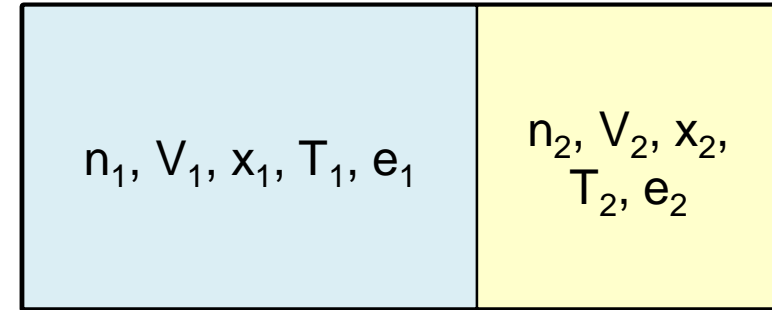
$$N(t) = N(1s) (t/1s)^{0.7} \text{ where } N(1s) \approx 7000$$

- Because this proceeds so fast, one can assume that core and bypass gases are mixed already at engine exit. It is not necessary to consider them separately.



# Isobaric mixing (1)

- Two compartments of **ideal gases** 1 and 2
- isobaric mixing **without chemical reactions and without condensation**
- $n_i$ : mole numbers
- $V_i$ : Volumes
- $x_i$ : mole numbers of water molecules
- $T_i$ : temperatures
- $T$ : temperature of the mixture
- $e_i$ : partial pressures ( $e_i/p=x_i/n_i$ )
- $e$ : partial pressure of the mixture
- $p$ : constant ambient pressure
- **Definitions:**  $\alpha=V_2/V_1$ ,  $\beta=n_2/n_1$
- Hence:  $T_2/T_1= \alpha/\beta$



## Isobaric mixing (2): conservation of heat energy

- $\frac{p}{R} = \frac{n_1}{V_1} T_1 = \frac{n_2}{V_2} T_2$  and  $\frac{p}{R} = \frac{n_1+n_2}{V_1+V_2} T = \frac{n_1(1+\beta)}{V_1(1+\alpha)} T$  where R is the universal gas constant

- with our definitions of  $\alpha$  and  $\beta$  this gives  $T = \frac{1+\alpha}{1+\beta} T_1$

- but we want to see where T lies in the range spanned by  $T_1$  and  $T_2$ . That is, we seek an expression as

$$T = T_1 + \delta(T_2 - T_1)$$

- after a little calculation we find  $\delta = \frac{\beta}{1+\beta}$  and thus  $T = T_1 + \frac{n_2}{n_1+n_2} (T_2 - T_1)$

- for the expanding plume this reads as  $T_{\text{plume}} = T_{\text{amb}} + \frac{n_{\text{exit}}}{n_{\text{amb}} + n_{\text{exit}}} (T_{\text{exit}} - T_{\text{amb}})$



## Isobaric mixing (3): conservation of mass

- $e_i = p \frac{x_i}{n_i}$ ,  $0 \leq x_i \leq n_i$  and  $e = p \frac{x_1+x_2}{n_1+n_2} = p \frac{x_1+x_2}{n_1(1+\beta)}$

- replacing p gives  $e = e_1 \frac{1}{x_1} \frac{x_1+x_2}{(1+\beta)} =: e_1 + \delta'(e_2 - e_1)$

- where again we want to know where e lies in the range between  $e_1$  and  $e_2$ . A further question is whether  $\delta'=\delta$ .
- After a little calculation we find that indeed  $\delta'=\delta$  and thus

- $e_{\text{plume}} = e_{\text{amb}} + \frac{n_{\text{exit}}}{n_{\text{amb}} + n_{\text{exit}}} (e_{\text{exit}} - e_{\text{amb}})$





## Isobaric mixing (4): phase trajectory in the (e,T) diagram

$$T_{\text{plume}} - T_{\text{amb}} = \frac{n_{\text{exit}}}{n_{\text{amb}} + n_{\text{exit}}} (T_{\text{exit}} - T_{\text{amb}})$$

$$e_{\text{plume}} - e_{\text{amb}} = \frac{n_{\text{exit}}}{n_{\text{amb}} + n_{\text{exit}}} (e_{\text{exit}} - e_{\text{amb}})$$

⇒

$$\frac{e_{\text{plume}} - e_{\text{amb}}}{T_{\text{plume}} - T_{\text{amb}}} = \frac{e_{\text{exit}} - e_{\text{amb}}}{T_{\text{exit}} - T_{\text{amb}}} \stackrel{\text{def}}{=} G$$

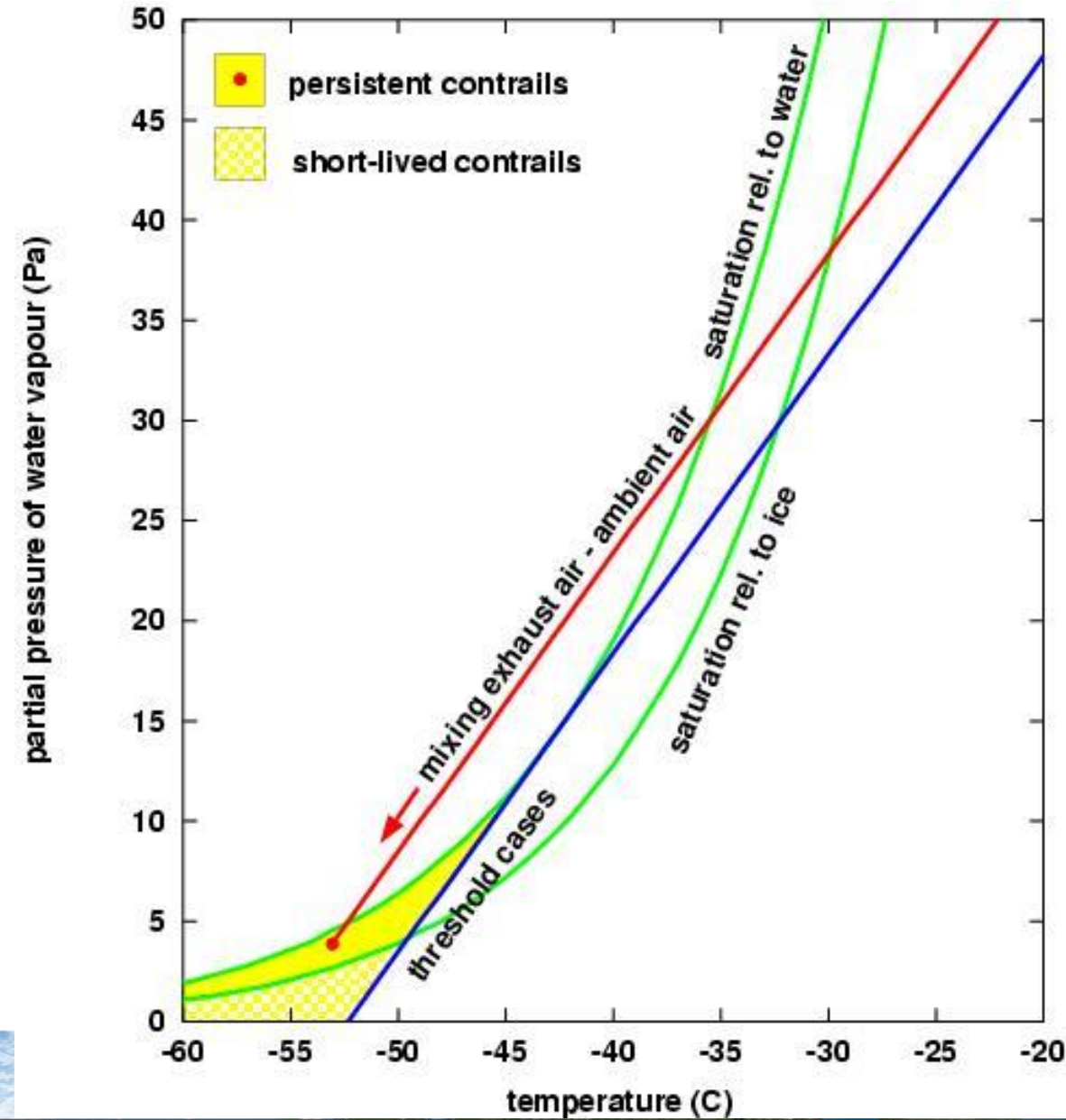
The phase trajectory in a (e,T) diagram is a straight line with constant slope G. G is known as contrail factor or G-factor.

Note the assumptions in the derivation! Is the real phase trajectory really a straight line?



## Mixing in the (e,T)-phase diagram

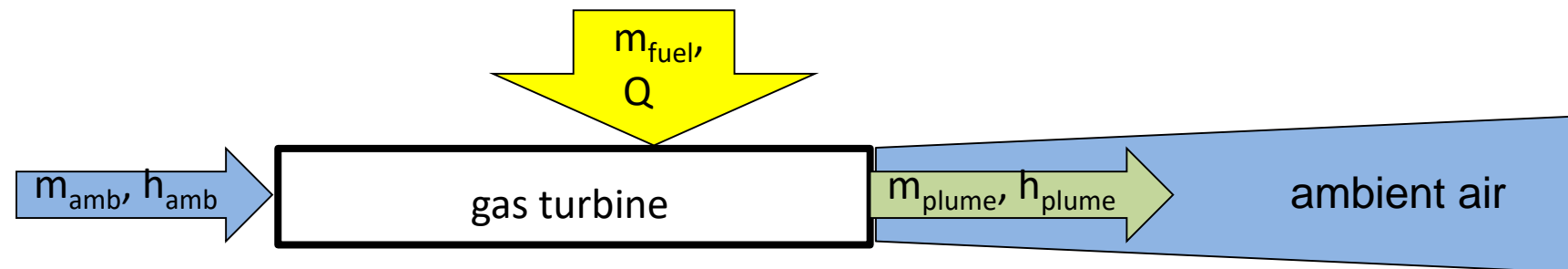
- the **saturation pressure** curves are convex (integrals of the **Clausius-Clapeyron** differential equation that give  $de/dT$ )
- the straight mixing trajectory thus cuts the saturation pressure curve (wrt liquid supercooled water)
  - twice → contrail formation
  - once → threshold case (very faint contrail)
  - never → no contrail formation
- if the trajectory ends above the saturation curve wrt to ice (**ice supersaturation**), and if the water saturation curve is cut twice, the contrail is persistent.
- The mixing trajectory is determined completely by the ambient  $e$  and  $T$  and the slope  $G$ .





# Practical determination of the contrail factor $G$ for kerosene-driven gas turbines

- Mixing the exhaust gases with the ambient air takes place isobarically and conserves
  - mass (in particular mass of water molecules)
  - energy (in form of enthalpy, since  $p=\text{const.}$ );  
 $dQ=dU+pdV$ ,  
 $dH=dU +pdV+Vdp = dQ$  (since  $dp=0$ ),  
 here  $dQ=0$  (remember: no chemical reactions, no condensation, but also no conversion of kinetic energy into heat energy)  $\rightarrow dH=0$ .
- Consider mass and enthalpy budgets of the airstream through the engine



## Derivation of the Schmidt-Appleman theory in terms of engine mass and enthalpy flows (1)

- The slope  $G$  of the mixing trajectory is simply

$$G = \frac{e_{\text{exit}} - e_{\text{amb}}}{T_{\text{exit}} - T_{\text{amb}}}$$

- $e$  and  $T$  at engine exit are engine and fuel dependent
- It is practical to use **mass mixing ratio**  $q$  instead of partial pressure

$$e = pq/\varepsilon$$

- $p$  is air pressure,  $\varepsilon=0.622$  (ratio of molar masses of water and air).



## Derivation of the Schmidt-Appleman theory (2): Water mass budget

- the water vapour mixing ratio at engine exit is determined from the mixing ratios in the air streams and the water vapour from burning the fuel. Instantaneous mixing of core and bypass streams gives

$$e_p = \frac{p}{\varepsilon} \frac{\dot{m}_{\text{amb}} q_{\text{amb}} + \dot{m}_{\text{fuel}} EI_{\text{H}_2\text{O}}}{\dot{m}_{\text{amb}} + \dot{m}_{\text{fuel}}}$$

- with  $EI_{\text{H}_2\text{O}}$ : emission index for water vapour (1.23 for kerosene, 8.98 for LH2)
- The nominator in the slope factor G is thus

$$e_p - e_E = \frac{p}{\varepsilon} \frac{\dot{m}_{\text{fuel}} (EI_{\text{H}_2\text{O}} - q_{\text{amb}})}{\dot{m}_{\text{amb}} + \dot{m}_{\text{fuel}}} \approx \frac{p}{\varepsilon} \frac{\dot{m}_{\text{fuel}} EI_{\text{H}_2\text{O}}}{\dot{m}_{\text{amb}} + \dot{m}_{\text{fuel}}}$$

since  $q_{\text{amb}} \ll EI_{\text{H}_2\text{O}}$



## Derivation of the Schmidt-Appleman theory (3): Overall propulsion efficiency

- The continuous loss of momentum due to drag and friction  $dP/dt$  has to be replaced by the thrust  $F$  of the engines:

$$F = dP/dt$$

- Thus, work has to be applied with a rate  $FV$  which has to be taken from the fuels chemical energy, that is

$$FV = \eta \dot{m}_{\text{fuel}} Q$$

- $Q$ : lower heat value of fuel,  $\eta$ : overall propulsion efficiency
- $V$ : aircraft speed



## Derivation of the Schmidt-Appleman theory (4): Conservation of energy

- Energy conservation (reference frame fixed to the ground):
- the chemical energy of the fuel is converted into work against drag, into kinetic energy and thermal energy of the exhaust

$$\dot{m}_{\text{fuel}}Q = FV + \frac{\dot{m}_{\text{amb}}}{2}(V_{\text{exit}} - V)^2 + \frac{\dot{m}_{\text{fuel}}}{2}(V_{\text{exit}}^2 - VV_{\text{exit}}) + c_p\dot{m}_{\text{amb}}(T_{\text{exit}} - T_{\text{amb}}) + c_p\dot{m}_{\text{fuel}}T_{\text{exit}}$$

- Note:  $FV = \eta\dot{m}_{\text{fuel}}Q$ , the rest is thus  $(1 - \eta)\dot{m}_{\text{fuel}}Q$ .
- Note:  $c_pT$  is the enthalpy (assumption:  $c_p$  does not vary much with  $T$ ).
- Note: kinetic energy is  $\mathcal{O}(10^{4-5} \text{ J/kg})$ , thermal energy is  $\mathcal{O}(10^7 \text{ J/kg})$ .
- Thus thermal energy  $\approx (1 - \eta)\dot{m}_{\text{fuel}}Q$ .





## Derivation of the Schmidt-Appleman theory (5): Conservation of energy

- Thus, neglecting the transformation of kinetic energy into heat (which takes time), we get

$$(1 - \eta)\dot{m}_{\text{fuel}}Q = c_p\dot{m}_{\text{amb}}(T_{\text{exit}} - T_{\text{amb}}) + c_p\dot{m}_{\text{fuel}}T_{\text{exit}} = \\ c_p\dot{m}_{\text{amb}}(T_{\text{exit}} - T_{\text{amb}}) + c_p\dot{m}_{\text{fuel}}(T_{\text{exit}} - T_{\text{amb}}) + c_p\dot{m}_{\text{fuel}}T_{\text{amb}}$$

$\Rightarrow$

$$T_{\text{exit}} - T_{\text{amb}} = \frac{\dot{m}_{\text{fuel}}}{c_p(\dot{m}_{\text{amb}} + \dot{m}_{\text{fuel}})} [(1 - \eta)\dot{m}_{\text{fuel}}Q - h_{\text{amb}}]$$

- Noting that  $(1 - \eta)\dot{m}_{\text{fuel}}Q \gg h_{\text{amb}}$ , we neglect the enthalpy of the ambient air and get instead

$$T_{\text{exit}} - T_{\text{amb}} = \frac{\dot{m}_{\text{fuel}}}{c_p(\dot{m}_{\text{amb}} + \dot{m}_{\text{fuel}})} (1 - \eta)\dot{m}_{\text{fuel}}Q$$



# Derivation of the Schmidt-Appleman theory (7)

## Slope factor

- Remember: The slope  $G$  of the mixing trajectory is simply

$$G = \frac{e_{\text{exit}} - e_{\text{amb}}}{T_{\text{exit}} - T_{\text{amb}}}$$

- nominator from water budget:

$$e_{\text{exit}} - e_{\text{amb}} = \frac{p \dot{m}_{\text{fuel}} EI_{\text{H}_2\text{O}}}{\varepsilon \dot{m}_{\text{amb}} + \dot{m}_{\text{fuel}}}$$

- denominator from enthalpy budget:

$$T_{\text{exit}} - T_{\text{amb}} = \frac{\dot{m}_{\text{fuel}}}{c_p} \frac{Q(1 - \eta)}{\dot{m}_{\text{amb}} + \dot{m}_{\text{fuel}}}$$

- Thus we finally arrive at an expression that Schumann has derived in this form in 1996:

$$G = \frac{c_p p}{\varepsilon} \frac{EI_{\text{H}_2\text{O}}}{Q(1 - \eta)}$$



# Constituents of the slope factor

$$G = \frac{c_p p}{\varepsilon} \frac{EI_{H_2O}}{Q(1-\eta)} = \left( \frac{c_p}{\varepsilon} \right) \left( p \right) \left( \frac{1}{(1-\eta)} \right) \left( \frac{EI_{H_2O}}{Q} \right)$$

Diagram illustrating the constituents of the slope factor  $G$ :

- const** (black box) points to the constant  $c_p/\varepsilon$ .
- aircraft/engine** (red box) points to the efficiency term  $1/(1-\eta)$ .
- atmosphere** (blue box) points to the pressure term  $p$ .
- energy-specific emission index** (orange box) points to the term  $EI_{H_2O}/Q$ .

fuel type	$EI_{H_2O}$ (kg/kg)	Q or $ \Delta h $ (MJ/kg)	energy specific emission index
kerosene	1.23	43.2	0.029
LH2 (liq. H <sub>2</sub> )	8.98	119.7	0.075
LNG (liq. CH <sub>4</sub> )	2.25	50.0	0.045



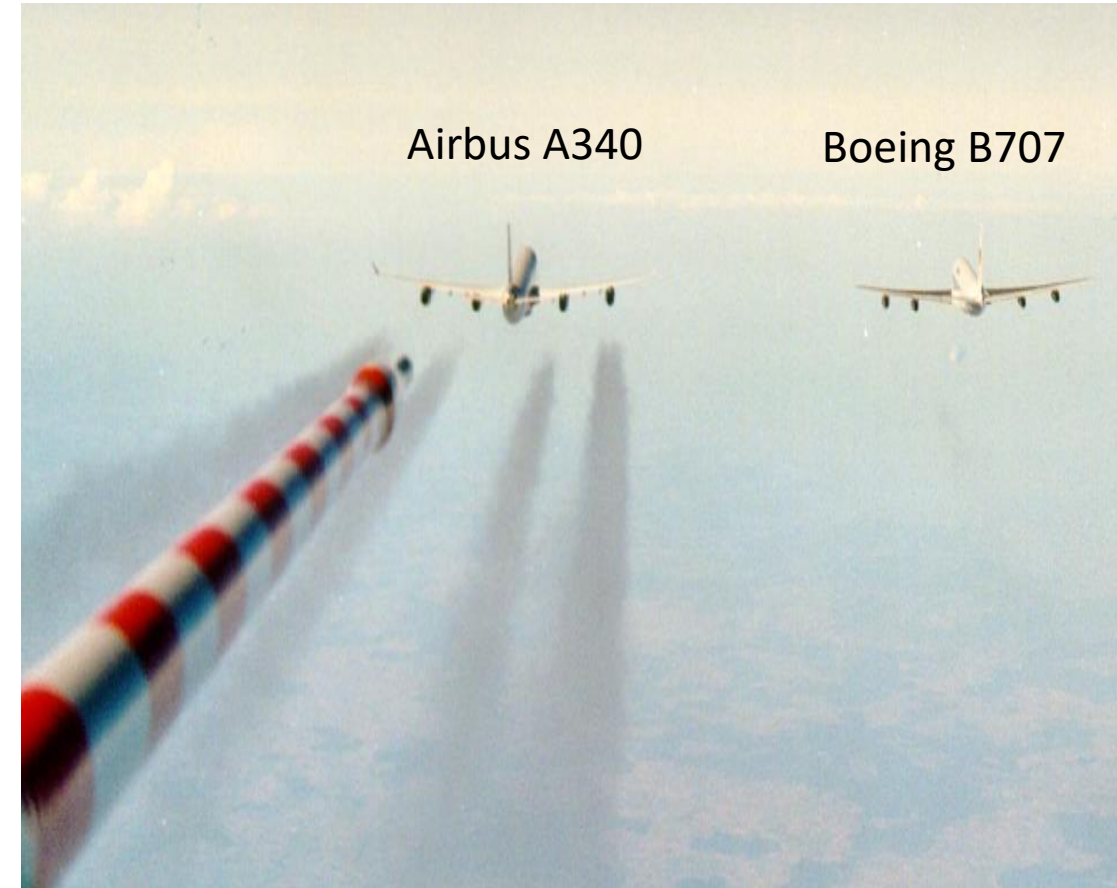
# The slope factor for various propulsion concepts

Propulsion	Mass-based G	Mole-based G
Kerosene	$G = \frac{c_p p}{\varepsilon} \frac{EI_{H_2O}}{(1 - \eta)Q}$	
Parallel hybrid battery-electric	$G = \frac{c_p p}{\varepsilon} \frac{R \cdot EI_{H_2O}}{R(1 - \eta_K)Q + (1 - R)(1 - \eta_B)Q_B}$	
H <sub>2</sub> gas turbine	$G = \frac{c_p p}{\varepsilon} \frac{EI_{H_2O}}{(1 - \eta) \Delta h }$	$G = \frac{c_p p}{(1 - \eta) \Delta h_m }$
H <sub>2</sub> fuel cell		$G = \frac{\bar{c}_p p}{(1 - \eta_E \eta_0) \Delta h_m }$

p	ambient pressure	$\eta, \eta_K$	overall propulsion efficiency
$c_p$	specific heat of dry air	$\eta_B$	similar to $\eta_K$ , for the battery part
$\bar{c}_p$	specific heat of air-vapour mixture	$\eta_E$	ratio of FC voltage to EMF value
$\varepsilon$	ratio of molar masses air to vapour	$\eta_0$	ratio $\Delta g/\Delta h$ (g: free enthalpy)
Q	lower heating value of kerosene	$\Delta h, \Delta h_m$	mass and molar based enthalpy
$Q_B$	similar to Q, but for the battery part	$EI_{H_2O}$	emission index for water vapour

## The overall propulsion efficiency $\eta$

- Definition:  $\eta = \text{rate of delivery of mechanical power (FV)} / \text{release rate of chemical energy of the fuel}$
- $\eta < 1$ , the remaining part of the chemical energy ends up eventually as waste heat.
- As contrail formation is very fast, only those parts of  $(1-\eta) m_{\text{fuel}} Q$  that are converted into heat almost immediately at engine exit are relevant for the thermodynamics of contrail formation.
- The conversion of kinetic energy of the exhaust gases into heat is probably too slow.
- For fuel cells, only the factors  $\eta_0$  and  $\eta_E$  are relevant as they determine the temperature of the exhaust gas. Other losses in the electric installation, in the electric motors and in the machinery that converts electric power into mechanical power, are not relevant to contrail formation since their waste heat comes simply too late.



Schumann et al., 2000



# Summary

- Contrails form as a result of **mixing** of two gas masses, the hot and moist exhaust gas and the cold and dry ambient air, **if the water vapour becomes supersaturated** (with respect to liquid supercooled water) during the plume expansion process.
- Contrail formation can be described by **thermodynamics alone**; it is not necessary to consider the co-emitted particles or the ambient aerosol because there is always plenty of these condensation nuclei.
- **Three quantities** determine whether a contrail can form or not: the **ambient  $e$  and  $T$  and the factor  $G$** .
- The factor  $G$  is the slope of the mixing trajectory in a  $(e,T)$  phase diagram. It can be determined for various propulsion techniques via the physical principles of **mass and energy conservation**. It depends on atmospheric pressure, and on engine and fuel characteristics.
- The highest temperature at which a contrail is possible in principle is where the water saturation curve has slope  $G$  (inversion of the Clausius-Clapeyron equation).
- **Contrails persist** for more than a couple of minutes (up to many hours) if the ambient water vapour is supersaturated with respect to ice (i.e. if the contrail is formed **in an ice supersaturated region**, ISSR).



# Questions

- Is contrail formation possible in totally dry air, i.e. where  $e_{\text{amb}}=0$ ? What would happen?
- Usually we observe contrails in the cold upper troposphere. Is it possible that contrails form at higher temperatures nearer to the ground? What would happen?
- Consider the thermodynamic derivation of the mixing line. Which assumptions have been made, what has been neglected? Is the actual mixing trajectory indeed a straight line with slope  $G$ , or is it nearly a straight line, or is it a straight line not at all?
- If it is not a straight line, why does the theory work?

