



Modeling observed aerosols and contrail ice crystals with a microphysics code

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Abstract. Contrails contribute significantly to the climate impact of aviation, however their formation depends on fuel composition, engine type and meteorological conditions and current contrail formation models may be insufficiently constrained by observations. Here we revisit the 1D microphysics code MoMiE and compare its results with recent contrails measurements from the ECLIF and NEOFUELS/VOLCAN campaigns. The sensitivity of the model to different Fuel Sulfur Contents (FSC), from 0.5 to 195 ppm, and to different engine combustion modes, i.e. lean-burn, intermediate and rich-burn, is studied, as well as to the emission index of organic compounds and ions, and to ambient temperature and relative humidity. For the first time, the recent NEOFUELS/VOLCAN data of total number of particles measured in the near-field are compared to model simulations. Adjusting the input parameters within their expected uncertainty ranges allows the model to approximate the data for different fuels and soot regimes, demonstrating a clear sensitivity to organic compounds. The model results are also compared to far-field measurements of ice crystals of ECLIF and NEOFUELS/VOLCAN. MoMiE generally captures the dependence of contrail ice crystals to non-volatile particle emissions and compares well with the measurements in the soot-rich regime. In the soot-poor regime, MoMiE results depend mainly on the ambient temperature and show little variability obtained for different FSCs. These results emphasize the need for further investigation on the role of the different parameters involved in the contrail formation, as well as the need for further measurements of the different plume components.

1 Introduction

Aviation contributes to about 3.7% of anthropogenic radiative forcing (IPCC, 2023), through CO₂ and non-CO₂ effects. The most recent study reveals that the latter may be the dominant factor (Lee et al., 2021), in particular with a significant contribution of condensation trails ("contrails"). The same study also shows that large uncertainties remain regarding the specific effect of contrails and these need to be reduced in order to properly consider the non-CO₂ effects of aviation. Contrails are ice clouds formed when aerosol particles, present in the plumes of aircraft engines, are activated under supersaturated conditions to form



water droplets, which then freeze to form ice crystals (Appleman, 1953). These exhaust aerosols can be composed of different compounds, such as soot particles formed in the combustion chamber (Kärcher et al., 1996) and volatile liquid particles, formed in the plume from sulfuric acid (Yu and Turco, 1998), organic molecules (Yu et al., 1999) or lubrication oil (Ponsonby et al., 2024), and nucleation of these volatile liquid particles is greatly facilitated by the presence of charged particles (Yu and Turco, 1997).

With the aim of achieving carbon neutrality by 2050, the aviation sector is currently focusing on sustainable aviation fuels (SAF). These new fuels differ from conventional Jet A-1 type kerosene, notably by their lower aromatics and sulfur content, as well as their higher hydrogen content (Moore et al., 2017; Voigt et al., 2021; Märkl et al., 2024; Dischl et al., 2024). Consequently, the combustion of SAF is expected to produce less soot and potentially fewer volatile particles. Several authors (e.g. Kärcher et al. (1996); Wong and Miake-Lye (2010)) have shown that for the engines operating in conventional rich burn combustion mode, i.e. high soot emission levels, ice crystals form mainly by condensation of water on the larger soot particles. Furthermore, numerous studies illustrate the influence of fuel sulfur content (FSC) on the properties of contrails (see recent overview of measurements in Dischl et al. (2025)). Sulfur is thought to play a significant role in activating soot particles as condensation nuclei (Schumann et al., 1996; Gierens and Schumann, 1996; Brown et al., 1997; Petzold et al., 1999), while also being capable of combining with water to form volatile particles that serve as additional condensation nuclei under certain conditions (Yu and Turco, 1998). Wong et al. (2014) and Wong et al. (2015) studied the role of organic matter on soot coating and volatile particles respectively, however, their model hasn't been used yet for a contrail formation study. Rojo et al. (2015) developed the code MoMiE (Modèle Microphysique pour Effluents) to explicitly solve the formation of volatile particles in the form of hydrated aggregates composed of sulfuric acid and soluble organic species in order to study ice crystal formation in the context of the use of alternative fuels and fuel blends. Recent campaigns (ECLIF, Voigt et al. (2021); Märkl et al. (2024); Dischl et al. (2024)) have been conducted to assess the impact of such fuels on contrail properties. These campaigns probe aircraft engine emissions from rich burn combustion engines with soot emissions on the order of 10^{15} per kg of fuel. Jones and Miake-Lye (2024) compare their model results to ECLIF 2 measurements data, and suggest the possible role of sulfur in activating soot surface, explaining the fewer ice crystals formed in the case of low fuel sulfur content (< 10 ppm) and high soot emission levels. On the other hand, Yu et al. (2024) studied with their ACM model the data of ECLIF1, 2 and 3 campaigns, which covered two engine types of two different generations operating in the soot-rich regime and showed the less than-unity fractions of soot particles forming contrail ice particles may be rather driven by the size of the primary soot particles than by the effective size of soot aggregates. Dischl et al. (2025) also recently emphasized the potential role of sulfur in soot-rich conditions, where volatile particles might be able to compete with the numerous non-volatile particles as ice condensation nuclei. This could explain the increased ice crystal number in comparison to the soot particle number in the case of high fuel sulfur content (500 ppm) and certain ambient conditions.

For lower soot emissions (under 10^{14} particles per kilogram of fuel), models suggested that, volatile particles could become significant cloud nuclei (see Yu and Turco (1998), Schumann et al. (1996). Indeed, modeling studies (Kärcher, 2018; Yu et al., 2024) indicated that for a soot emission index below 10^{14} particles per kilogram of fuel, the number of contrail ice crystals could exceed the initial number of soot particles by one or three orders of magnitude, reaching an apparent ice crystal emission



index of the same order of magnitude as that expected for a soot-rich emission ($\sim 10^{15}$ ice crystals per kilogram of fuel). These results were recently confirmed by Voigt et al. (2026), who finally provide first in situ measurement data behind a lean-burn engine for different fuel types. Engines with lean burn combustion chamber technology like the LEAP-1A equipping the A321neo family produce much less soot for both SAF and Jet A-1 fuel types (Voigt et al., 2026). The campaign also allowed to induce forced rich-burn combustion with the same aircraft, thereby providing data for both combustion modes. As these test data are considerably scattered in terms of number of total particles and ice crystals, microphysical models can help elucidate the physical mechanisms at play, as well as the dependence on ambient conditions and emission concentrations. Recent studies notably suggest the role of the lubrication oil as a further source of nucleation clusters, especially in the lean burn mode (Ungeheuer et al., 2022; Decker et al., 2024; Ponsonby et al., 2024). Zink et al. (2025) have conducted a sensitivity study on the potential effect of lubrication oil particles on contrail formation with a box model including a particle-based Lagrangian Cloud Module and concluded that if these oil-based particles are abundant, they may dominate ice crystal formation in soot-poor regime in hydrogen combustion scenarios. The model of Ponsonby et al. (2025) also studies the effect of lubrication oil and more generally of emitted organics on contrail formation. However, it is important to emphasize that these two models assume the initial distribution of volatile particles and do not explicitly simulate their nucleation. Although this assumption allows the authors to study the evolution of the contrail when an additional source of condensation nuclei is added, it completely neglects the competition between the different nucleation processes, which determines the type and characteristics of the volatile particles actually formed. While the ACM model explicitly resolved the formation of volatile particles in Yu et al. (2024), it only considered the sulfur-based pathway and therefore no unburnt hydrocarbons (organic matter) nor lubrication oil. In a recent update, ACM explicitly included the nucleation and condensation of unburned fuel organics and lubrication oils to explain the contrail observations in the lean burn regime from Voigt et al. (2026). The paper also shows comparisons with results from the MoMiE model, in which volatile particles can be formed based on sulfuric acid and soluble organic species, while lubrication oil may be represented within the code as insoluble organic vapors capable of coating particles, but does not create new particles.

The aim of this paper is to validate the results obtained with the 1D detailed microphysics code MoMiE developed at ONERA (Rojo et al., 2015) by providing an in-depth analysis of the recent ECLIF and VOLCAN measurement data for different types of fuels and combustion modes. Section 2 describes the model. Section 3 compares the model results with measurement data for the total number of particles measured in the near-field by the NEOFUELS/VOLCAN campaign. Section 4 compares the model results with measurement data for the number of ice crystals measured in the far-field by the ECLIF campaign. Section 5 compares the model results with measurement data for the ice crystals measured in the far-field by the NEOFUELS/VOLCAN campaign. Finally, Section 6 summarizes and concludes the study, and Section 7 presents the implications and future prospects of this work.



2 Modeling the detailed contrail microphysics with MoMiE

2.1 General

The 1D code MoMiE (Modèle Microphysique pour Effluents) developed at ONERA is a 'box model' representing detailed microphysics of contrail formation. It accounts for the different processes involved in the formation of ice particles in the case of combustion of fossil kerosene and Sustainable Aviation Fuels (SAF). In this section, a short overview of the model is given, more details can be found in Sorokin et al. (2001); Vancassel et al. (2010); Rojo et al. (2015).

The MoMiE code considers that a jet engine plume is initially composed of vapors of different species (water, sulfur oxide and organic compounds), mixed with ions (charged particles of molecular diameter) and soot particles (solid particles of a few nanometers). The plume is emitted at high temperature and mixes with the cold ambient air, which increases saturation in water vapor and leads to the formation of different particle types. Sulfur reacts with water to form sulfuric acid and the mix of water, sulfuric acid and organic vapors can condense on soot particles. Soot particles coated by a solution of different components are defined as non-volatile particles. On the other hand, sulfuric acid and soluble organics can combine with water to nucleate and form small liquid droplets, those are the so-called volatile particles. Both volatile and non-volatile particles grow by condensation and coagulation, up to reaching the freezing critical radius and becoming ice crystals. In the version of the code used in this study and described in Rojo et al. (2015), and given the difficulty of representing the wide diversity of emitted organic compounds, these are represented by two different types (Turpin et al., 2000): soluble organics (OM_{sol}) and insoluble organics (OM_{insol}). "Soluble organics" comprise organic species that are able to combine with water to form volatile particles, while "insoluble organics" account for hydrophobic organic species that can only condense on soot. The repartition between both types of organics has so far been based on measurements from (Spicer et al., 2009) and (Knighton et al., 2009) indicating higher concentrations of soluble organics than insoluble organics. However, the actual repartition may vary from one fuel composition to another, in particular from usual kerosene to alternative fuels (Knighton et al., 2009). Thermodynamical properties have also to be assumed for the two types of organic compounds and correspond to species able to condense under the encountered conditions of an aircraft plume. The following simplifications are made into the code: the saturation vapor pressure of acetaldehyde is considered for soluble compounds (D'Avila and Silva, 1970), and of pyrene (Fu et al., 2010) for insoluble organic compounds (Rojo Escude-Cofiner, 2012).

2.2 Upgrades of the code

This work presents results from a revised version of the code described in Rojo et al. (2015). The main revision regards two different aspects described in this section.

The activation of soot particles by sulfuric acid described in Rojo et al. (2015) relies on a surface coverage criterion based on previous studies such as in Wyslouzil et al. (1994); Andronache and Chameides (1997); Kärcher et al. (1998); Wong and Miake-Lye (2010), which were mainly focused on fuels with high sulfur contents. Preliminary studies have indicated that such an hypothesis becomes too restrictive in the conditions of low and very low fuel sulfur contents in the soot-rich regime. Indeed, the assumption that water can only condense on soot particles once a threshold in sulfuric acid coverage has been



120 reached, drastically slows down and reduces the rate of ice crystals formation by $\sim 60\%$ with regard to the initial amount of
soot particles in the cases of high FSC (not shown here), which is not observed in the data (see data observations in Voigt et al.
(2021); Yu et al. (2024), also plotted in Figure 8). This result aligns with Kärcher et al. (1998) conclusions that "soot triggers
freezing even for low fuel sulfur contents, suggesting a sulfur-independent water activation pathway". Therefore, the activation
of soot by sulfuric acid coverage is removed from the revised version of the code, i.e. water condensation on soot particles only
125 depends on saturation as calculated in Equation 1. This approach is consistent with the representation adopted in other existing
contrail microphysics models (Yu et al., 2024; Ponsonby et al., 2025; Zink et al., 2025). However, the subtle role of sulfuric
acid in soot surface activation would deserve further investigation, as highlighted by (Jones and Miake-Lye, 2024), as it could
account for the variability observed in ice crystal formation in the soot-rich regime.

Another modification of the code relates to the condensation of insoluble organic species. As described in Section 2.1, the
130 insoluble organic species OM_{insol} were only capable of condensing on soot particles. In the revised version of the code presented
in this paper, the condensation of OM_{insol} has been extended to all types of particles. This means insoluble organic matter
also contributes to the growth of volatile particles and modifies their composition. Depending on the engine configuration,
lubrication oil may also be released as larger droplets (diameter of around 100 nm), when vented in the cold bypass flow, or
gaseous emissions, when vented in the engine hot core (Williams et al., 2026). Oil vapor emissions present a wide range of
135 volatility and lead to either nucleating new particles or to condensing organic matter (Yu et al., 2010; Decker et al., 2024;
Ungeheuer et al., 2022). As a basic and preliminary approximation, and given their hydrophobic nature, oil vapors can be
assimilated to insoluble organics, and therefore, can be included in the family of insoluble organic compounds of the MoMiE
code described here. Therefore, in the MoMiE code, oil vapors can only contribute to the growth of already existing particles
by condensation, but not to the formation of new particles.

140 2.3 Particle types and physical processes

Table 1 lists the different particles represented in the code and their composition, while Figure 1 schematically describes the
main processes represented by MoMiE. It particularly illustrates the two pathways of ice nucleation, respectively through soot
and volatile particles. There are eleven different particle types represented in the model: dry soot particles corresponding to
soot, which have not been covered by water, sulfuric acid or collection of volatile particles ("DS"); "activated" or "mixed"
145 soot particles ("MS"), composed of a soot nucleus covered by volatile species composed of sulfuric acid, soluble and insoluble
organics and water in the liquid phase; neutral volatile clusters composed of a solution of water and sulfuric acid ("SA");
negative ions, prescribed to be clusters of negatively charged sulfur species, e.g. HSO_4^- ("I⁻"); neutral volatile clusters com-
posed of a solution of water and soluble organics ("OM"); positive ions, prescribed to be clusters of positively charged soluble
organic species ("I⁺"); neutral volatile particles composed of a mix of water, sulfuric acid and soluble organics ("V"); negative
150 volatile particles, composed of a mixed hydrated solution of sulfur and organic compounds ("V⁻"); positive volatile particles,
composed of a mixed hydrated solution of sulfur and organic compounds ("V⁺"); ice particles formed by soot nucleation path-
way, i.e. composed of a soot nucleus, water, sulfuric acid and organic compounds ("IS") and ice particles formed by volatile
nucleation pathway, i.e. essentially composed of water, sulfuric acid and organic species without soot nucleus ("IV"). The



Table 1. Particles simulated by MoMiE and their associated composition. There are eleven particle types in total, which can be distinguished into three categories: non-volatile particles, containing a soot nucleus, volatile particles, formed by nucleation of emitted gaseous species, and ice particles, which are formed by freezing of non-volatile and volatile particles. Five components can be found in the different particles : water (H_2O), sulfuric acid (H_2SO_4), soluble organic (OM_{sol}) and insoluble organic (OM_{insol}). The "+" means the particle can contain the component, the "-" means it cannot.

Particle type	Particle name	Components				
		H_2O	H_2SO_4	OM_{sol}	OM_{insol}	soot
Non-volatile particles	Dry Soot (DS)	-	-	-	-	+
	Mixed Soot (MS)	+	+	+	+	+
	Sulfuric acid clusters (SA)	+	+	-	-	-
	Organic clusters (OM)	+	-	+	-	-
Volatile particles	Positive ions (I^+)	-	-	+	-	-
	Negative ions (I^-)	-	+	-	-	-
	Positive mixed volatile (V^+)	+	+	+	+	-
	Negative mixed volatile (V^-)	+	+	+	+	-
	Neutral mixed volatile (V)	+	+	+	+	-
Ice crystals	Ice particles formed from soot nucleus (IS)	+	+	+	+	+
	Ice particles formed from volatile nucleus (IV)	+	+	+	+	-

nucleation of hydrated sulfuric acid clusters (SA, see Table 1 and scheme 1) as volatile particles is determined by the classical binary homogeneous nucleation scheme defined in Wilemski and Wyslouzil (1995). The same nucleation scheme is adopted for hydrated soluble organics (OM, see Table 1 and scheme 1) (Yu et al., 1999). Brownian coagulation of the different particle types is represented based on Jacobson (2002), including the interaction with ions (Yu and Turco, 1997). Vapors of water, sulfuric acid and organics can condense or evaporate on the non-volatile and volatile particles. Ice growth and sublimation is also represented (Pruppacher et al., 1998). Further details on the calculation of the saturation ratio are given in Section 2.4. All particle types (volatile, coated soot and ice) are distributed in size and number on a hybrid size grid of 180 bins using a volume ratio of 1.2 from the 10th bin, the first bin corresponding to the size of a single molecule of sulfuric acid as in Yu (2006). The code keeps track of the number concentration of the different particle types, as of their composition in volume fraction, per bin. The number and size distribution of dry soot particles, positive and negative ions, as well as concentrations (emission indices) of gaseous emissions of sulfuric acid, soluble and insoluble organics are prescribed. The code also includes the entrainment of ambient particles (background soot, sulfuric acid, and ice particles). The entrainment is not activated in the simulations presented here. The dilution of the plume is calculated based on the analytical law derived by Schumann et al. (1998) and is described in details in Section 2.5.

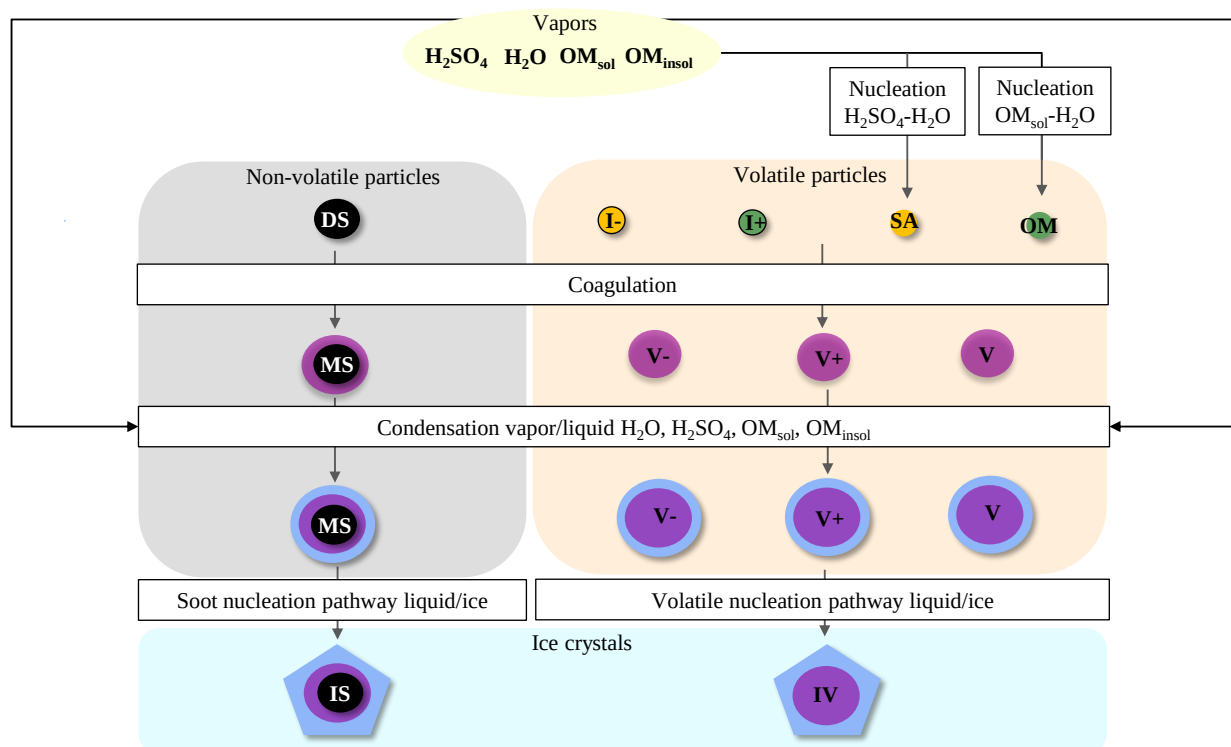


Figure 1. Scheme illustrating the main processes and the particle types modeled by the microphysics code MoMiE. The particle types are described in Table 1.

2.4 Saturation ratio

The code represents the condensation of water vapor on the different types of particles by calculating the saturation ratio above the surface of the particle, taking into account both Kelvin and Raoult effects. The saturation ratio is defined as follows (Petters and Kreidenweis, 2007):

$$S = a_{sol} \exp \left(\frac{2M_{H_2O}\sigma_{sol}}{RT\rho_{H_2O}r} \right) \quad (1)$$

The exponential term of the equation corresponds to the Kelvin effect with ρ_{H_2O} the density of water, M_{H_2O} the molecular weight of water, R the universal gas constant, T the temperature, and r the radius of the droplet. σ_{sol} is the surface tension of the solution/air interface and is calculated in the code according to the components present in the solution, i.e. sulfuric acid and organics, as follows (Poling et al., 2001):

$$\sigma_{sol} = \sum_i^n x_i \sigma_i \quad (2)$$

With x_i the molar fraction of the compound i present in the solution (water, sulfuric acid or soluble organic) and σ_i the surface tension of the pure component.



MoMiE accounts for the Raoult effect by determining the activity a_{sol} of the solution composed of water, sulfuric acid and organic species. It represents the solution effects (Petters and Kreidenweis, 2007) and is the product of the activity of water within a solution of hydrated sulfuric acid $a_{H_2SO_4}$, calculated in the code with the formula expressed in Kulmala et al. (1998), and of the activity of water within a solution of hydrated soluble organics a_{OM} (the insoluble organics are by definition not taken into account in the activity of the solution), calculated according to the work of Jun (2011).

Most microphysics codes (Zink et al., 2025; Ponsonby et al., 2024; Yu et al., 2024) represent the term of the Raoult effect using the k-Köhler theory and an hygroscopicity parameter to account for the hydrophylic or hydrophobic character of particles corresponding to the solution effects involved in the calculation of the saturation ratio (Petters and Kreidenweis, 2007). Both approaches involve uncertainties: on the species composing the solution and the calculation of their activity in the case of MoMiE, on the approximation of this term and the value of the hygroscopicity coefficient in the case of the k-Köhler theory.

2.5 Dilution

The MoMiE code can be applied to different dilution and temperature profiles, which can be defined by analytical laws based on empirical studies or by multiple trajectories extracted from a 3D simulation (Vancassel et al., 2014). In this paper, the dilution of the plume is calculated based on the analytical law derived by Schumann et al. (1998), where the dilution factor $D(t)$ is defined as:

$$D(t) = \frac{AFR}{7000(t/t_0)^{0.8}} \quad (3)$$

Where AFR is the air-to-fuel ratio in kg.kg-fuel^{-1} , t the time in seconds (with $t > 0.006$ s) and $t_0 = 1$ s.

Temperature $T(t)$ can be assimilated to a passive tracer and estimated in function of the dilution factor $D(t)$, the engine exit temperature T^e and the ambient temperature T^a as follows:

$$D(t) = \frac{T(t) - T^a}{T^e - T^a} \quad (4)$$

Considering the plume dilutes isobarically, i.e. the pressure within the plume is constant and equal to the one of ambient air, the dilution factor can also be defined as in Kärcher (1995):

$$D(t) = \frac{x_i(t) - x_i^a}{x_i^e - x_i^a} = \frac{P_i(t) - P_i^a}{P_i^e - P_i^a} = \frac{N_i(t)T(t) - N_i^aT^a}{N_i^eT^e - N_i^aT^a} \quad (5)$$

Where x is the volume ratio in mol mol^{-1} , N the concentration in number of particles in m^{-3} , P the pressure in Pa and T the temperature in K , considered respectively for the species " i ", for the ambient air " a " and at the nozzle exit " e ", and at the time " t ". k_B is the Boltzmann constant. Equation 5 leads to:

$$\frac{D(t+dt)}{D(t)} = \frac{N_i(t+dt)T(t+dt) - N_i^aT^a}{N_i(t)T(t) - N_i^aT^a} \quad (6)$$

And at every timestep dt the new concentration in number $N_i(t+dt)$ of each particle distribution can then be calculated as:

$$N_i(t+dt) = \left(N_i(t) \frac{D(t+dt)}{D(t)} + \frac{N_i^aT^a}{T(t)} \left(1 - \frac{D(t+dt)}{D(t)} \right) \right) \frac{T(t)}{T(t+dt)} \quad (7)$$



Simulations are run with a timestep of 10^{-3} s. In order to compare the results of our simulations with measurement data we define a non-volatile emission index (EI_{nvpm}) and an apparent ice emission index (AEI_{ice}) as follows:

$$EI_{nvpm}(t) = \frac{N_{nvpm}(t)(AFR + 1)}{\rho(t)D(t)} \quad (8)$$

$$AEI(t) = \frac{N_{ice}(t)(AFR + 1)}{\rho(t)D(t)} \quad (9)$$

205 With $N_{nvpm}(t)$ and $N_{ice}(t)$ being the concentrations in number per m^3 of the considered particles (non-volatile particle matter or ice) at the time t , AFR the air-to-fuel ratio and $D(t)$ the dilution ratio, defined in 2.5. $\rho(t)$ is calculated by assuming constant pressure in the plume and equal to ambient pressure.

2.6 Simulation setup and initialization

Exhaust conditions and fuel emission characteristics have to be initialized in order to run a simulation. The corresponding
 210 parameters are listed in Table 2 and are described in the two following paragraphs. Exhaust conditions include ambient air parameters, such as ambient temperature and pressure, and engine characteristics, such as engine outlet temperature and air-to-fuel ratio (AFR). The sensitivity to ambient temperature (T^a) is studied in the further sections, and ambient pressure (P^a) is imposed according to available data studied. It appears that its variation does not have much impact on the results compared to temperature (not shown here). The static temperature at the engine core nozzle exit (T^e) is typically around 580 –600K and is
 215 arbitrary fixed to 600K in our simulations. The AFR typically varies from 50 to 75 kg-air.kg-fuel $^{-1}$ (Schumann et al., 1998) and is also arbitrary set to 60 in our simulations.

Fuel emissions characteristics also have to be defined. The AFR mainly impacts on the calculation of the initial partial pressures P_x of the different gaseous components at the exhaust (H_2O , H_2SO_4 , OM_{sol} , OM_{insol} as cited before), based on their imposed emission index in kilogram per kilogram of fuel. These partial pressures are determined as follows :

$$P_x = \frac{EI_x}{(AFR + 1)} \frac{M_{air}}{M_x} P^a \quad (10)$$

220 with EI_x the emission index of the component, AFR the air-to-fuel ratio of the engine, M_{air} and M_x the molar mass of the air within the plume and of the component x respectively, and P^a the ambient pressure (the pressure is supposed to be constant within the plume and equal to ambient pressure as in Schumann et al. (1998)). The EI_{H_2O} is provided by the measurement data. In the special case of H_2SO_4 we introduce the conversion factor SC corresponding to the percentage of fuel sulfur content (FSC), which is provided by fuel data, converted to sulfuric acid in the exhaust plume, which is generally between 2 and 4%
 225 (Kärcher et al., 2000; Schumann et al., 2002; Jurkat et al., 2011) and which we assume here to be 3 % for all studied cases, as in Yu et al. (2024). The equation 10 becomes for H_2SO_4 :

$$P_{H_2SO_4} = \frac{FSC}{(AFR + 1)} \frac{M_{air}}{M_S} P^a SC \quad (11)$$



Table 2. Parameters to be initialized in MoMiE to run a simulation. T^a is the ambient temperature, P^a the ambient pressure, T^e the exit temperature at the engine core exhaust, AFR the air-to-fuel ratio, FSC the fuel sulfur content, EI_{OMsol} and $EI_{OMinsol}$ the emission indices of respectively soluble and insoluble organics, EI_{H_2O} the emission index of water vapor, EI_{ions} the emission index of ions, EI_{nvpm} the emission index of soot particles, synonymously called non-volatile particles. "data" correspond to the measurement data described in Tables 3,4 and 5. The values given for the other parameters correspond to those of a reference simulation.

Exhaust conditions					
Ambient			Engine		
T ^a (K)		P ^a (Pa)	AFR		T ^e (K)
data		data	60		600
Fuel and emission characteristics					
Vapor				Particles	
EI _{H2O} (kg kg-fuel ^{−1})	FSC (ppmm)	EI _{OMsol} (mg kg-fuel ^{−1})	EI _{OMinsol} (mg kg-fuel ^{−1})	EI _{ions} (kg-fuel ^{−1})	EI _{nvpm} (kg-fuel ^{−1})
data	data	35	110	10 ¹⁷	data

EI_{OMsol} and $EI_{OMinsol}$ are initialized based on the reference values used in Rojo et al. (2015) for the Jet A-1 case. It should be noted, however, that EI_{OM} values can vary from one engine type to another and also, within a given engine family, from one engine to another. The typical emission index of charged particles EI_{ions} used in the simulations for each ion type (positive and negative) is 2.6×10^{17} particles per kilogram of fuel, corresponding to a concentration of about 2×10^8 particles per cm³ (Arnold et al., 2000; Yu and Turco, 1997). As described in Section 2.3, the code assumes that positively charged particles are initially made of organic matter, while negatively charged particles are initially composed of sulfuric acid (Arnold et al., 2000; Yu et al., 1999). Both ion types are initialized with the recombination parameters described in Sorokin et al. (2001). In the simulations presented here soot particles are initialized by a log-normal distribution with a median diameter of 35 nm and standard deviation of 1.6, as imposed in the simulations of Yu et al. (2024).



3 Model results compared to the total number of particles measured by NEOFUELS/VOLCAN

3.1 The measurement data

This section aims at comparing MoMiE outputs to the total particle numbers measured during the NEOFUELS/VOLCAN campaign. This is the first time that results of a microphysics model are compared to the measurements of total number of
 240 particles. The number concentrations of soot and volatile particles measured shortly behind the aircraft can give insights into the potential precursors for contrail formation, such as soot hydrated particles and volatile droplets composed of different species. It is crucial for models to reproduce the formation of those precursors, since they represent the first step of contrail formation.

The VOLCAN project (VOL avec Carburants Alternatif Nouveaux) with involvement of Airbus, Safran, ONERA and Das-
 245 sault Aviation, as well as Direction Générale de l'Aviation Civile (DGAC) as funding organism, aimed at analyzing the compatibility of unblended sustainable aviation fuel (SAF) with commercial aircraft engine and fuel systems, and at determining the impact on emissions and contrails. Airbus, DLR and ONERA performed in-flight and ground measurements to analyze the impact of Jet A-1 and SAF and of rich and lean-burning engine configurations on emissions and contrails (Voigt et al., 2026). The in-flight measurements were performed with the DLR research Falcon 20E, while the NEOFUELS project funded
 250 the DLR Falcon operations. On-ground and in-flight emissions used an A320neo-family test aircraft powered by "CFM LEAP-1A engines". The LEAP-1A was operated in "normal" lean burn mode (soot-poor regime) and in forced rich burn (soot-rich regime) via FADEC (Full Authority Digital Engine Control) adjustments. The campaign results provide the first in-flight data set on engine emissions and contrail properties produced by an aircraft with lean-burn engines (Voigt et al., 2026). The measurements of emissions and contrail properties have been conducted for several fuel types: conventional petroleum-based fossil
 255 kerosene Jet A-1, 100 % bio-based hydro-processed ester and fatty acids synthetic paraffinic kerosene (HEFA-SPK) and as well as blends of the HEFA-SPK with Jet A-1 and 8 and 18% fossil mono-aromatics; and for different ambient conditions (Voigt et al., 2026). A first test campaign was conducted in 2021 with an A319neo aircraft and a second campaign in 2023 with an A321neo aircraft, both powered by the same engine model.

To explore the formation of volatile particles in both soot regimes, the concentrations of non-volatile particulate matter
 260 (nvpm) and total particulate matter (tpm) were measured in near field, i.e. about 40 to 250 m behind the aircraft (plume age of 0.2 – 1.4 s), with a constant air speed of 0.59 Mach at an altitude of 9–10 km at high ambient temperature (228 – 232 K) and low relative humidity of the ice phase (40 – 90 %) to prevent aerosols from being influenced by the formation of ice particles (see Dischl et al. (2026)).

Different datasets were selected for the comparison with MoMiE simulations in order to cover the variability of different
 265 parameters. Table 3 presents the datasets selected for the total number of particles measured in the near-field, based on the measurement data presented in Dischl et al. (2026) (see Table S1 in the cited paper). There are six different fuels studied, corresponding to two cases of conventional petroleum-based fossil kerosene Jet A-1, a case of contaminated HEFA-SPK, a case of 100 % bio-based HEFA-SPK, a case of high-aromatic HEFA-SPK blend, and a case of low-aromatic HEFA-SPK blend, also corresponding to different hydrogen, aromatic and naphthalene compositions (see Table 1 in Voigt et al. (2026)).



Table 3. NEOFUELS/VOLCAN near-field measurements of total and non-volatile particle number emission indices, obtained for the 6 different cases (labeled "VT1-6") of Jet A-1 and HEFA-SPK blends studied in this work and obtained in lean-burn, intermediate (only case 1 presents this regime) and rich-burn combustion modes (Dischl et al., 2026).

Case name	VT1	VT2	VT3	VT4	VT5	VT6
VOLCAN step	2	1	2	1	2	2
Fuel	100 % Jet A-1	100 % Jet A-1	19 % Jet A-1 + 81 % HEFA-SPK	100 % HEFA-SPK	blend HEFA-SPK+LA	blend HEFA-SPK+HA
El _{H₂O} (kg kg _{fuel} ⁻¹)	1.26	1.26	1.32	1.37	1.32	1.28
FSC (ppmm)	195	138	41	6	1.9	0.5
near-field EI _{nvp} (kg _{fuel} ⁻¹)						
lean-burn	6.1 × 10 ¹¹	2.5 × 10 ¹¹	3.6 × 10 ¹¹	1.4 × 10 ¹¹	1.2 × 10 ¹¹	4.8 × 10 ¹¹
split	1.5 × 10 ¹³	-	-	-	-	-
rich-burn	8.8 × 10 ¹⁴	7.6 × 10 ¹⁴	4.6 × 10 ¹⁴	2.6 × 10 ¹⁴	5.1 × 10 ¹⁴	8.1 × 10 ¹⁴
near-field std EI _{nvp} (kg _{fuel} ⁻¹)						
lean-burn	5.5 × 10 ¹¹	1.1 × 10 ¹¹	4.0 × 10 ¹⁰	4.0 × 10 ¹⁰	6.0 × 10 ¹⁰	4.5 × 10 ¹¹
split	0.2 × 10 ¹³	-	-	-	-	-
rich-burn	8.0 × 10 ¹³	2.5 × 10 ¹⁴	3.0 × 10 ¹³	2.0 × 10 ¹³	3.0 × 10 ¹³	1.0 × 10 ¹⁴
near-field EI _{tot} (kg _{fuel} ⁻¹)						
lean-burn	3.2 × 10 ¹⁵	1.1 × 10 ¹⁵	1.1 × 10 ¹⁵	4.0 × 10 ¹⁴	5.0 × 10 ¹⁴	7.0 × 10 ¹⁴
split	1.3 × 10 ¹³	-	-	-	-	-
rich-burn	2.4 × 10 ¹⁵	1.4 × 10 ¹⁵	1.6 × 10 ¹⁵	5.0 × 10 ¹⁴	9.0 × 10 ¹⁴	1.5 × 10 ¹⁵
near-field std EI _{tot} (kg _{fuel} ⁻¹)						
lean-burn	1.7 × 10 ¹⁵	4.0 × 10 ¹⁴	2.0 × 10 ¹⁴	1.0 × 10 ¹⁴	1.0 × 10 ¹⁴	1.0 × 10 ¹⁴
split	0.1 × 10 ¹³	-	-	-	-	-
rich-burn	8.0 × 10 ¹⁴	1.0 × 10 ¹⁴	4.0 × 10 ¹⁴	1.0 × 10 ¹⁴	1.0 × 10 ¹⁴	3.0 × 10 ¹⁴

El_{H₂O} is the emission index of water in kg per kg of fuel (kg kg_{fuel}⁻¹); FSC is the fuel sulfur content in ppmm; EI_{tot} is the emission index of the total number of particles in number per kg of fuel (kg_{fuel}⁻¹); std EI_{tot} is the standard deviation of the emission index of the total number of particles in number per kg of fuel (kg_{fuel}⁻¹); EI_{nvp} is the emission index of non-volatile particles in number per kg of fuel (kg_{fuel}⁻¹); std EI_{nvp} is the standard deviation of the emission index of non-volatile particles in number per kg of fuel (kg_{fuel}⁻¹).

270 During the campaign three different combustion modes were tested: forced rich-burn mode (soot-rich regime) for an EI_{nvp} higher than $\sim 10^{14} \text{ kg}_{\text{fuel}}^{-1}$, lean-burn mode (soot-poor regime) for this same emission index being lower than $\sim 5 \cdot 10^{12} \text{ kg}_{\text{fuel}}^{-1}$, and an intermediate split point between lean-burn and forced rich-burn combustor condition (medium regime) for the emission index comprised in-between these two values.



3.2 MoMiE reference simulations

275 Six cases of MoMiE simulations have been run and initialized with the EI_{H_2O} , FSC and EI_{nvpm} provided in Table 3. Reference values for the other initial parameters of the code are defined in Table 2. Figure 2 plots the model results for the reference case in function of the corresponding measurement data for the three combustion modes lean-burn, intermediate and rich-burn. The model results are shown at $t = 0.5$ s, with t the time of simulation equivalent to the plume age, and the error bars correspond respectively to $t = 0.2$ s and $t = 1.4$ s, which cover the min/max of the plume age indicated in the Extended Table 280 4 in (Voigt et al., 2026). In order to properly compare model outputs with the test flight results, the same lower size cut-offs as in the measurement data have been imposed on the diameters of the model outputs shown in the figures, i.e. 14 nm for the non-volatile particles and 5 nm for the total particles (Voigt et al., 2026).

Measurements reveal that the total number of particles are similar in the lean-burn and the rich-burn combustion regimes and that this total number exceeds the amount of non-volatile particles in all cases, suggesting the formation of additional 285 volatile particles in each soot regime (Voigt et al., 2026). These volatile particles are suspected to be composed of different species such as H_2SO_4 , organics or lube oil (Ungeheuer et al., 2022). Model results are very sensitive to the plume age at this early stage (in the soot-poor regime in particular, the number of particles may increase by a few orders of magnitude between $t = 0.2$ s and $t = 1.4$ s) and we observe some variability between the measurement data and the model results, as shown in Figure 2. Furthermore, we observe a difference in sensitivity to the plume age between the different soot regimes. Indeed, in 290 the soot-rich regime, the total number of particles is mainly driven by the number of soot particles, which are already present at the engine exhaust plane. These nvPM are relatively large and lead more rapidly to even larger particles. This corresponds to the soot nucleation pathway, which is triggered in the first instants and leads more rapidly to larger particles (we remind here that we apply a filter to the particle size of 5 nm to be consistent with the measurements). Conversely, in the soot-poor regime, the formation of particles relies mostly on the volatile nucleation pathway, which requires some time to make particles grow 295 above the detection limit of 5 nm.

In general, there is a good agreement between model results and measurements for the total number of particles at medium sulfur levels. However, the model seems to globally overestimate the total number of particles in these conditions for the lower FSCs at $t = 0.5$ s and with the reference values adopted for the emission index of OM_{sol} , OM_{insol} and ions, and the imposed ambient relative humidity and temperature. The next sections aim at studying the sensitivity of our model to those different 300 parameters.

3.3 Sensitivity to soluble organics

Three different initial EI_{OMsol} have been tested in the MoMiE simulations and are compared to the measurement data to study the sensitivity of the model to the presence of nucleating organic compounds in addition to the presence of sulfur.

In Rojo et al. (2015) the emission index of organic hydrocarbons from incomplete combustion is imposed between 35 – 305 45 $mg\ kg_{fuel}^{-1}$ depending on the nature of the fuel studied and based on previous measurement data. In NEOFUELS/VOLCAN, this emission index was estimated from ground to cruise projections around 50 – 66 $mg\ kg_{fuel}^{-1}$. Recent estimations of the

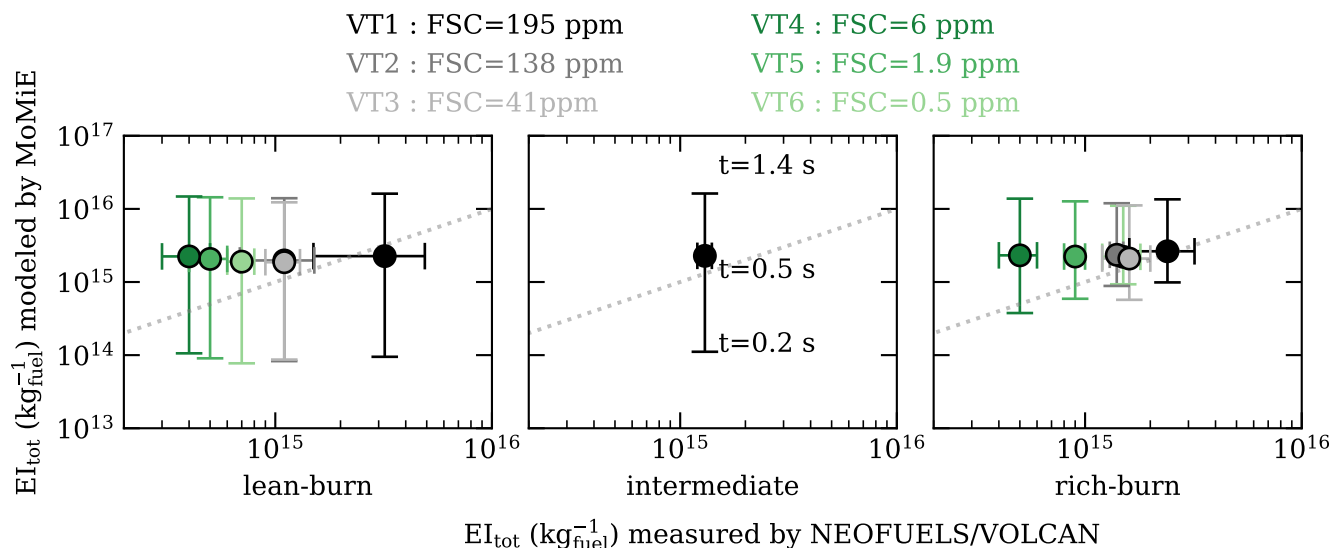


Figure 2. Reference case: sensitivity to the age of the plume. Total particle number emission index EI_{tot} in number per kilogram of fuel computed by the model in function of the corresponding NEOFUELS/VOLCAN measurements (see Table 3 for the values and error bars in x direction) obtained for the six fuel cases (gray-black: Jet A-1 fuels; light-dark green: HEFA blends) and the three soot regimes studied distributed over three different graphs (lean-burn, intermediate and rich-burn). The circles correspond to the model results obtained at $t = 0.5$ s simulation and the minimum/maximum of the bars in y direction correspond respectively to the simulation outputs obtained at $t = 0.2$ s and $t = 1.4$ s. These results are obtained for the reference case $EI_{OMsol} = 35 \text{ mg kg}_{fuel}^{-1}$, $EI_{OMinsol} = 110 \text{ mg kg}_{fuel}^{-1}$ and $EI_{ions} = 10^{17} \text{ kg}_{fuel}^{-1}$ described in Table 2. The gray dotted line represents 1:1 relationship.

volatility of diverse organic compounds suggest that only a fraction of those organic vapors may lead to particle formation (Durdina et al., 2024; Ungeheuer et al., 2022). However, the considered organics in those papers come from oil emissions, while here the supposed source of soluble organic compounds is attributed to the hydrocarbons issued from incomplete combustion.

310 The literature doesn't precisely provide an estimation of the fraction of those organics capable of nucleating under the studied conditions. Therefore, the emission index of soluble organic compounds of the reference case for MoMiE simulations is arbitrarily set to 35 mg per kg of fuel, corresponding to about 70 % to 53 % of the estimated cruise emissions. This value may also vary from one fuel type and one combustion mode to the other.

Figure 3 shows the model outputs in function of the measurement data for three different initial emission indices of soluble organics EI_{OMsol} , respectively of 25 , 35 and 50 mg kg_{fuel}^{-1} (corresponding to 38, 53 and 76% of the maximum estimated value mentioned above) for the three engine combustion modes at time $t = 0.5$ s.

On average over the six cases studied, the reduction in the initial emission index of soluble organics from 35 to 25 mg kg_{fuel}^{-1} in the model reduces the emission index by several orders of magnitude in the soot-poor regime, while it reduces it from 50 to ~75% in the soot-rich regime. The difference in sensitivity to the soluble organics in the two soot regimes can be explained

320 by the dominance of one nucleation pathway on the other. Indeed, in the soot-rich regime, the higher the non-volatile emission

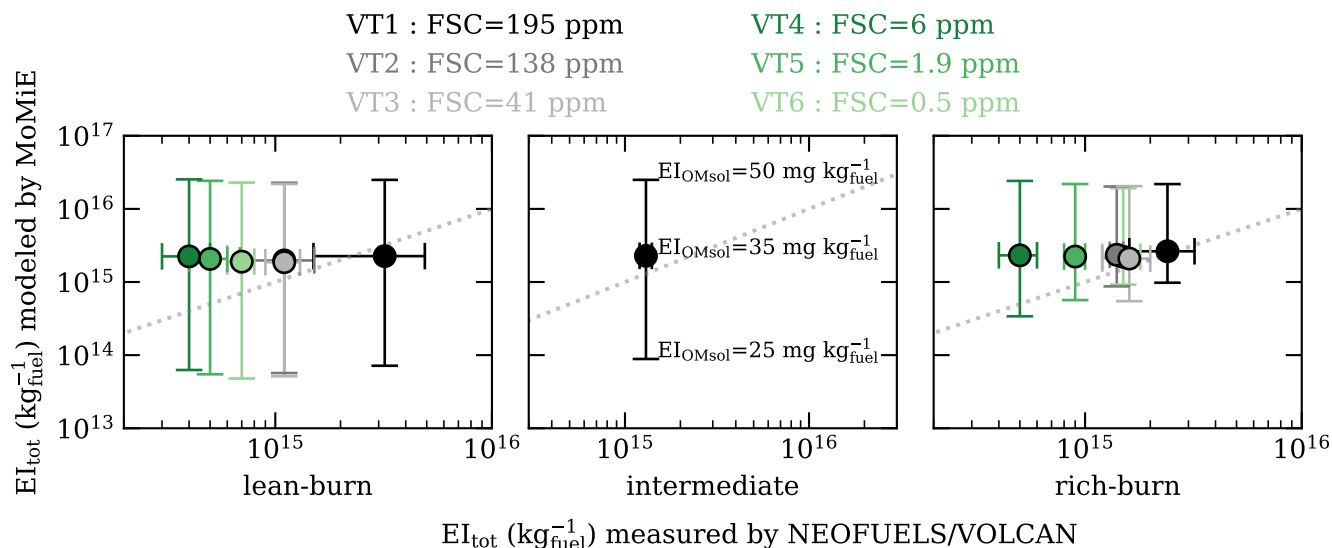


Figure 3. Sensitivity to soluble organics. Same layout as for Figure 2 : the circles correspond to model results obtained using the reference case parameters described in Table 2 at a simulation time of $t = 0.5$ s, while the minimum and maximum of the bars this time correspond to simulation results obtained respectively for $EI_{OMsol} = 25$ and 50 mg kg_{fuel}⁻¹ at $t = 0.5$ s.

index, the lower the sensitivity to soluble organics, i.e. to the formation of volatile particles. Conversely, in the soot-poor regime, the dominance of the volatile nucleation pathway leads to higher sensitivity to the soluble organics, which in this case significantly contribute to the formation of volatile particles. On the other hand increasing this emission index from 35 to 50 mg kg_{fuel}⁻¹ multiplies to total number of particles by ten in the two soot regimes. This can be simply explained by the increased formation of volatile particles when the initial quantity of species capable of nucleation—such as soluble organic compounds—is increased.

To conclude this sub-section, according to the presented results, MoMiE outputs compare well with the NEOFUELS/VOLCAN measurement data of total number of particles in all soot regimes, only when soluble organic species are considered and their initial emissions range between 30 and 35 mg kg_{fuel}⁻¹. This suggests that, according to MoMiE, other species than sulfur have to be involved in the volatile nucleating process to explain the observed number of total particles.

3.4 Sensitivity to FSC

Test flight results seem to show a dependence on the FSC, with the highest FSCs corresponding to the highest total particle numbers. However, we remark that FSC doesn't fully control the ranking in particle number. Indeed, cases VT2 and VT3, which differ in FSCs by a factor of 3, display the same amount of particles in the data measurements, while the model estimates a slightly higher proportion of particles formed in the case of the higher FSC (case VT2 with FSC= 138 ppmm in comparison to case VT3 with FSC= 41 ppmm). Case VT1, with FSC= 195 ppm, differs from the other cases with a factor of ~ 4.9 and



~ 2.4 respectively for the soot-poor and soot-rich regimes, see Table 3. The model also sees the highest gap in total number of particles between case VT1 and the other cases. However, differences between the different fuels characterized by different FSCs tend to diminish, when equally increasing the amount of El_{OMsol} for each case. Indeed, the averaged ratio between the particle number obtained for case VT1 of Jet A-1 and for the cases of HEFA-SPK blends VT3,5,6 and pure VT4 is around ~ 1.3 for both regimes in the case of $El_{OMsol} = 35 \text{ mg kg}_{fuel}^{-1}$. Note that this ratio is higher when El_{OMsol} is low, (e.g. around 2.5 in soot-poor regime and 1.7 in soot-rich regime for a case of $El_{OMsol} = 15 \text{ mg kg}_{fuel}^{-1}$, not show here). This influence of adding the nucleating organic compounds on the difference between FSCs can be explained by the direct comparison of the initial amount imposed for both species. Indeed, the emission index of H_2SO_4 is calculated into the code as follows (see Section 2.6):

$$EI_{H_2SO_4} = SC \frac{M_{H_2SO_4}}{M_S} FSC \quad (12)$$

with $SC = 3 \%$ and $M_{H_2SO_4} = 98.08 \text{ g mol}^{-1}$ the molar mass of H_2SO_4 and $M_S = 32.07 \text{ g mol}^{-1}$ the molar mass of sulfur. Consequently, the highest FSC of 195 ppm corresponds to an emission index of H_2SO_4 of around 17.8 ppm, which is the same order of magnitude as the El_{OMsol} tested in the presented MoMiE simulations. Despite the highest chemical activity of sulfur, the higher initial amount of soluble organic species makes them dominate the nucleation processes in the shown cases. This behavior is also predicted in the model of Yu et al. (1999) including the organics, where the lower limit for which FSC is dominant over organic species is around ~ 100 ppm. In our simulations, the initial amount of organics is evenly imposed in the different cases presented here, which is not representative of the reality. Indeed, the emission of organics depends on the fuel type and composition, and on the power settings of the engine, with alternative fuels a priori emitting more organic compounds than usual kerosene fuels (Knighton et al., 2009), which has to be further investigated by ground and in-flight measurements. Simulations reveal that only a few milligrams of organics can make a strong difference in the total particle amount. This emphasizes the need for further estimations of those compounds to constrain the model. The same remark can be done for the conversion factor SC of sulfur into sulfuric acid, which is imposed to be constant for all the cases studied here, although it may also be varying according to the different studied conditions and contribute to the observed variability in the measurements.

Finally, the representation of the nucleation process of both sulfur and organic species in the model can be mentioned here. Indeed, the use of the classical binary nucleation of water and sulfuric acid as defined in Wilemski and Wyslouzil (1995) is shown to potentially overestimate the number of volatile clusters in comparison to the quasi-unary nucleation scheme described in Yu (2005). The overestimation of volatile particles tends to slow down the process of condensation, as the same amount of water vapor has to condense on a larger population of particles. This could explain the difficulty of the model to reproduce the amount of total particles with a diameter larger than 5 nm, notably in the case VT1 of the higher FSC of 195 ppm.

To conclude this sub-section, although the model predicts higher amount of particles for the case of the highest FSC (VT1), as observed in the measurements, it tends to bring the number of total particles closer from one fuel case to the other, which tends to underestimate the number of particles for the highest FSC and overestimate it in the cases of the low FSCs (VT4,5,6). As discussed, the underestimation of total particles in comparison to measurements in the case of the highest FSC could be



370 explained by the representation of the nucleation process in the model. The overestimation in the cases of low FSCs could also be attributed to the sensitivity to the initial proportions of soluble organics, but also of ions, insoluble organics and ambient temperature and relative humidity. Indeed, these parameters were arbitrarily set to identical values for the six different fuel cases and the sensitivity to those latter parameters is studied in the next sub-sections.

3.5 Sensitivity to insoluble organics

375 In the simulations presented here, we consider that insoluble organics may also include oil vapors (see Section 2). While the emission index of the insoluble organics is set between 5 – 15 mg kg_{fuel}⁻¹ in (Rojo et al., 2015), it is estimated between 110 – 140 mg kg_{fuel}⁻¹ by the engine manufacturer for the tested LEAP-1A engine, also comparable to recent ground measurements for different engines (Decker et al., 2024; Durdina et al., 2024). Then, the reference value adopted in our simulations is 110 mg kg_{fuel}⁻¹.

380 In the code, insoluble organic matter plays a role in the growth of particles by condensing on both volatile and soot particles, but doesn't create new volatile nuclei. Sensitivity to the amount of vapors of insoluble organics OM_{insol} is shown in Figure 4 with three different initial emission indices EI_{OMinsol} = 5, 110, 400 mg kg_{fuel}⁻¹. Results show that in our model, the variation of the initial amount of insoluble particles has little influence on the total number of particles in the considered ambient conditions. Indeed, on average over all cases, increasing the emission index of insoluble organic matter from 110 mg kg_{fuel}⁻¹ to 400 mg kg_{fuel}⁻¹ increases the total number of particles by ~ 1.2 % in both soot regimes for the different fuel cases. Simulations reveal that, 385 in our model, insoluble organic compounds rather deposit on bigger particles, such as soot particles which correspond to 0.1 % of the total number of particles, than on small volatile droplets. Therefore, increasing insoluble organic species from 110 to 400 mg kg_{fuel}⁻¹ don't show significant impact on the total amount of particles in our simulations. However, those could be much more significant if they would be considered able to nucleate to form an additional population of volatile nuclei, as 390 it is supposed to happen with lubrication oil vapors, as shown in the sensitivity study presented by (Zink et al., 2025). The nucleation process of such oil vapors is not yet included in our model.

3.6 Sensitivity to ions and ambient conditions

Ions are initialized with the emission index of 10¹⁷ kg_{fuel}⁻¹, corresponding to the order of magnitude retained in Rojo et al. (2015), based on Yu and Turco (1997).

395 Figure 5 compares simulations run with three different initial amounts of charged particles, respectively 10¹⁶, 10¹⁷ and 10¹⁸ per kilogram of fuel. On average over all cases, going from EI_{ions} = 10¹⁷ kg_{fuel}⁻¹ to EI_{ions} = 10¹⁸ kg_{fuel}⁻¹ charged particles per kg of fuel, increases the number of particles formed by ~ 26 % in the soot-poor regime, and by ~ 16 % in the soot-rich regime. This can be merely explained by the fact that increasing the initial ions population increases the number of initial volatile particles. Those volatile charged particles easily coagulate and strongly contribute to the particle size growth. The initial amount of ions 400 is another source of uncertainty in the initialization of the studied fuel and combustion modes.

Ambient temperature and relative humidity reference values are respectively imposed to 230 K and 60%, based on the ranges of values provided in Extended Table 4 in Voigt et al. (2026).

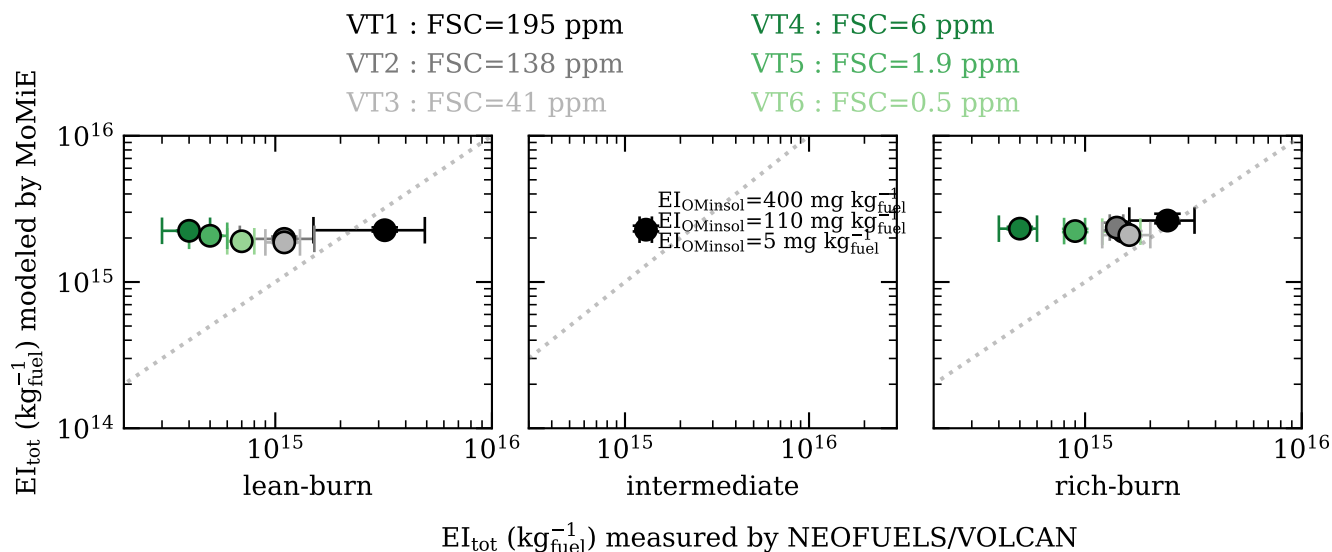


Figure 4. Sensitivity to insoluble organics. Same layout as for Figure 2 : the circles correspond to model results obtained using the reference case parameters described in Table 2 at a simulation time of $t = 0.5$ s, while the minimum and maximum of the bars this time correspond to simulation results obtained respectively for $EI_{OMinSol} = 5$ and 400 mg kg_{fuel}^{-1} at $t = 0.5$ s.

Figures 6 and 7 show the sensitivity of the model results to ambient conditions such as temperature and relative humidity according to the ice phase, in comparison to measurement data. Decreasing the ambient temperature by 2 K increases the emission index of the total number of particles by ~ 40 % in the soot-poor regime, while the impact fluctuates more in the soot-rich regime with a variation below 20 % from the reference case. On the contrary, increasing the ambient temperature by 2 K decreases the total number of particles by kg of fuel by ~ 24 % in the soot-poor regime and by ~ 15 % in the soot-rich regime. This behavior is globally expected as the ambient temperature impacts on the evolution of the relative humidity within the plume. Increasing the ambient relative humidity up to 90 % makes the total number of particles per kg of fuel increase by ~ 55 % in the soot-poor regime and by ~ 29 % in the soot-rich regime. This behavior is also expected, as higher ambient relative humidity increases the amount of water vapor available in the atmosphere to condense, in addition to that present in the jet.

To summarize, the model is quite sensitive to the initial amount of ions, which significantly impact the coagulation process, but, in the considered conditions, it is only slightly sensitive to ambient temperature, as well as to ambient relative humidity. We will see in the next sections that it is not the case when temperature is lower than 220 K.

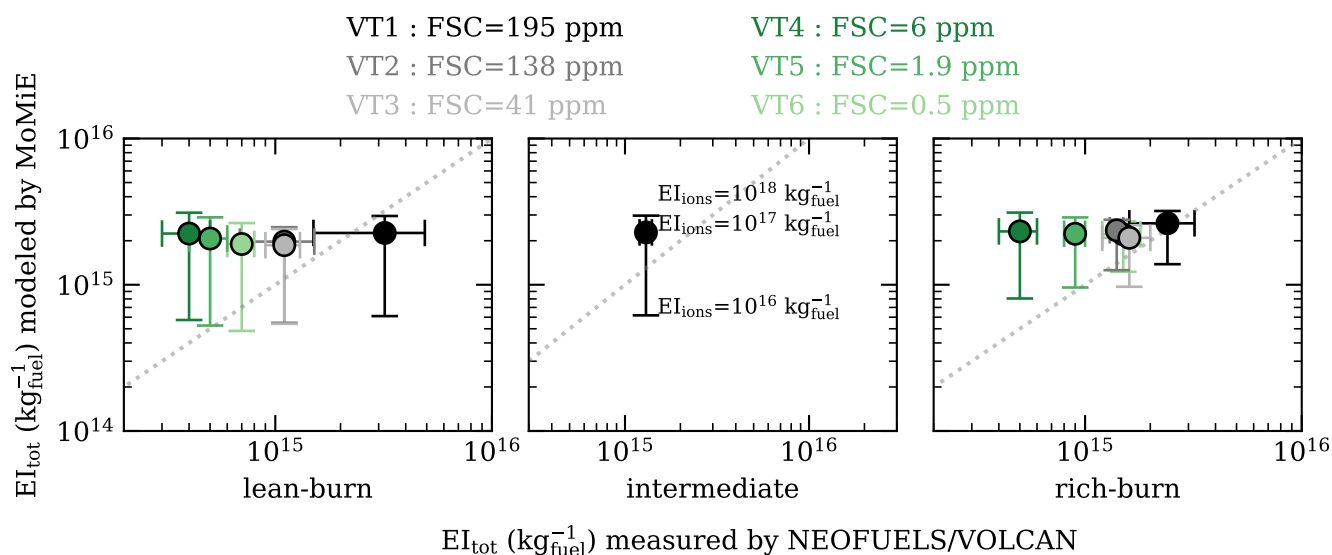


Figure 5. Sensitivity to ions. Same layout as for Figure 2 : the circles correspond to model results obtained using the reference case parameters described in Table 2 at a simulation time of $t = 0.5$ s, while the minimum and maximum of the bars this time correspond to simulation results obtained respectively for $EI_{ions} = 10^{16}$ and $10^{18} mg kg_{fuel}^{-1}$ at $t = 0.5$ s.

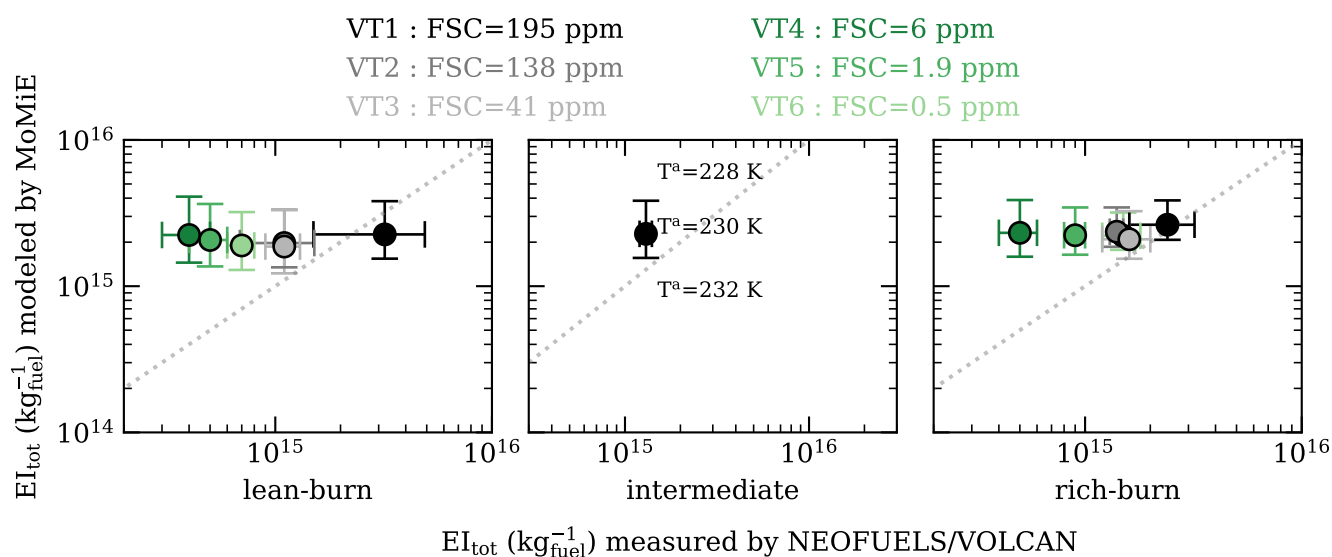


Figure 6. Sensitivity to ambient temperature. Same layout as for Figure 2 : the circles correspond to model results obtained using the reference case parameters described in Table 2 at a simulation time of $t = 0.5$ s, while the minimum and maximum of the bars this time correspond to simulation results obtained respectively for $T^a = 232$ and $228 K$ at $t = 0.5$ s.

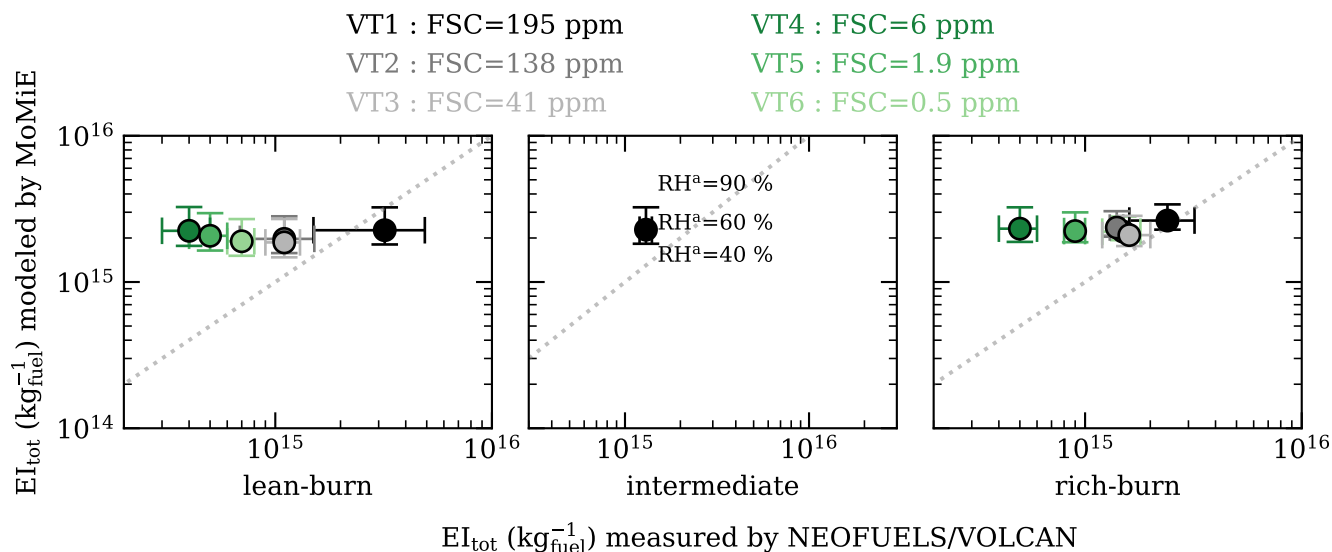


Figure 7. Sensitivity to ambient relative humidity according to the ice phase. Same layout as for Figure 2 : the circles correspond to model results obtained using the reference case parameters described in Table 2 at a simulation time of $t = 0.5$ s, while the minimum and maximum of the bars this time correspond to simulation results obtained respectively for $RH^a = 40$ and 90% at $t = 0.5$ s.

4 Model results compared to the number of ice crystals measured by ECLIF

4.1 The measurement data

Measurements cannot probe simultaneously total number of particles and ice crystals, which would reveal the fraction of nucleated particles actually transformed into ice. Therefore, models have to adapt to the available measurements and decompose the comparison. The comparison of model results to the total number of particles in the near-field is crucial to constrain models with the estimation of ice crystals potential precursors. The next sections focus on the comparison of the model results with the ice crystals measurements in the far-field.

Within the ECLIF projects a series of measurement campaigns was conducted for Rich Burn engines. ECLIF1/2 probed emissions and contrails from the DLR A320 aircraft equipped with IAE V227-A5 engines and using different fuels (Voigt et al., 2021; Bräuer et al., 2021b, a). ECLIF3 involved an A350-941 with Trent XWB engines and again different fuels including 100% HEFA-SPK as first of a kind (Märkl et al., 2024). The DLR Falcon 20-E5 research aircraft was used to probe plume composition and thermodynamic properties for the ECLIF1 and ECLIF3 campaigns, whereas NASA's DC-8 aircraft was used for ECLIF2. These measurements aimed at characterizing the properties of contrails and at estimating the impact of using sustainable alternative fuel (SAF) on their formation in comparison to usual fuels. Yu et al. (2024) have recently provided a model interpretation of contrail measurements under six conditions obtained during these campaigns, corresponding to different FSCs and ambient conditions. In particular the authors present the results of sensitivity of the ice particle formation to the initial



Table 4. ECLIF far-field measurements of non-volatile and ice particle number emission indices, obtained for the 6 different cases (labeled "EI1-6") of Jet A-1 and HEFA-SPK studied in this work in rich-burn combustion mode (Yu et al., 2024).

Case name	EI1		EI2		EI3		EI4		EI5		EI6	
ECLIF step	1		1		2		2		3		3	
Fuel	100%	Jet	59% JetA-1		51% JetA-1		70% JetA-1		100%	Jet	100%	
	A-1		+ 41% FT- SPK		+ 49% HEFA-SPK		+ 30% HEFA-SPK		A-1		HEFA-SPK	
T ^a (K)	215		220		218		216		213.3		213.8	
P ^a (Pa)	23840.6		25001.8		27570.2		27864.5		24004.8		24023.5	
RH _{ice} (%)	120		111.5		120		110		108		107.5	
EI _{H2O} (kg kg _{fuel} ^{−1})	1.227		1.283		1.287		1.297		1.258		1.35	
FSC (ppmm)	1350		570		70		4.1		211		7	
far-field EI _{nvpm} (kg _{fuel} ^{−1})												
rich-burn	4.9×10 ¹⁵		2.5×10 ¹⁵		2.7×10 ¹⁵		2.3×10 ¹⁵		0.95×10 ¹⁵		0.61×10 ¹⁵	
far-field std EI _{nvpm} (kg _{fuel} ^{−1})												
rich-burn	0.6×10 ¹⁵		0.2×10 ¹⁵		0.6×10 ¹⁵		0.6×10 ¹⁵		0.3×10 ¹⁵		0.07×10 ¹⁵	
far-field AEI _{ice} (kg _{fuel} ^{−1})												
rich-burn	4.2×10 ¹⁵		2×10 ¹⁵		2.3×10 ¹⁵		1.1×10 ¹⁵		0.78×10 ¹⁵		0.34×10 ¹⁵	
far-field std AEI _{ice} (kg _{fuel} ^{−1})												
rich-burn	0.6×10 ¹⁵		2×10 ¹⁴		0.2×10 ¹⁵		0.4×10 ¹⁵		4.0×10 ¹⁵		0.15×10 ¹⁵	

T^a is the averaged ambient temperature; P^a is the averaged ambient pressure; RH_{ice} is the averaged relative humidity with regards to ice; EI_{H_2O} is the emission index of water in kg per kg of fuel; FSC is the fuel sulfur content in ppmm; EI_{nvpm} is the emission index of non-volatile particles in number per kg of fuel measured; std EI_{nvpm} is the standard deviation of the emission index of non-volatile particles in number per kg of fuel; AEI is the apparent emission index of ice crystals in number per kg of fuel; std AEI is the standard deviation of the emission index of the ice crystals in number per kg of fuel.

soot emission index for these different cases. In the 6 cases studied the soot emission index varies over one order of magnitude between around $0.61 \cdot 10^{15}$ to $4.9 \cdot 10^{15} kg_{fuel}^{-1}$, which corresponds to a soot-rich mode of combustion of the engine. In this paper the comparison to the ECLIF measurement data is based on the same cases studied by Yu et al. (2024) and described in Table 4. It has to be noticed that the emission indices of both ice crystals and non-volatile particles displayed here and in Yu et al. (2024)'s paper correspond to the values measured in the far-field (Voigt et al., 2021; Märkl, 2024).

4.2 MoMiE reference simulations

The aim of this section is to compare MoMiE's results to the number of ice crystals measured by the ECLIF campaigns and modeled by the ACM model in Yu et al. (2024). Ten simulations per fuel case have been run with the parameters described in Table 1 of Yu et al. (2024) and recalled in Table 4 for different soot emission indices that vary between a minimum of $10^{14} kg_{fuel}^{-1}$ and $10^{16} kg_{fuel}^{-1}$ and correspond to the rich-soot regime. In this part, the organic species emission indices have been initialized



to zero to facilitate the comparison to Yu et al. (2024)' simulations, which don't include them. The simulations' duration is set to 2 s, which is much shorter than the ones studied in Yu et al. (2024), but is sufficient for our model to obtain the converged ice particle number concentration within the plume. Figure 8 shows the apparent emission index of ice particles EI_{ice} , determined by our model MoMiE, versus the emission index of non-volatile particles EI_{nvpm} for the six ECLIF cases with the same color code as in Figure 5 of Yu et al. (2024). Diamonds represent ECLIF data points, while lines are the model outputs.

4.3 Soot-rich regime

The model results reproduce the V-shaped diagram established by Yu et al. (2024) and are globally in accordance with the ECLIF measurement data, except for cases EI4 and EI6, where model outputs lie slightly outside the error bars, just as the ACM model in the same conditions and without the correction of the saturation ratio with the wet diameter of soot primary particles. The "V-shape" formed by the diagram is justified by the dominance of one ice nucleation pathway (or freezing mode as described in Section 2) over the other, according to the initial number of soot particles. In the soot-rich regime, the model predicts that the ice particle formation is completely dominated by ice nucleation on soot, while the ice nucleation on volatile particles takes the lead when the number of soot particles diminishes (see Figure 8). The location of the kink point of the V-shape depends on the FSC and the ambient temperature, just as for the ACM model and both models seem to behave similarly in rich-soot regime conditions.

4.4 Soot-poor regime

Although ECLIF observations don't cover the soot-poor regime part of the diagram, the different fuel cases considered offer the possibility to observe the behavior of our model in the soot-poor regime and to compare it with ACM. Indeed, in the results obtained by Yu et al. (2024), the differences observed between the six cases seem to mainly rely on the variability of FSC, and the cases corresponding to the lowest FSC generally lead to the lowest number of ice particles in the soot-poor regime. However, the corresponding MoMiE simulations, for which, as mentioned above, organic compounds have been deactivated for ECLIF analysis, show different results: although FSC has a significant influence, ambient temperature appears to be the main controlling parameter. The lower the ambient temperature, the higher the number of ice particles. This is well illustrated by the comparison between case EI1 with the highest FSC and case EI5 with a lower FSC by one order of magnitude. The code provides almost the same results for both cases. The lowest ice crystals emission index is obtained for case EI2 with the lowest temperature, while it is obtained for cases EI4 and EI6 in Yu et al. (2024). Also, the minimum of the plot can be located at EI_{nvpm} above $10^{15} \text{ kg}_{fuel}^{-1}$ in Yu et al. (2024)'s results, notably in the case of high FSC, which is never the case with MoMiE. The differences observed between the two models can be attributed to many sources. First, the nucleation of volatile clusters composed of sulfuric acid is based on two different approaches. The ACM model relies on the quasi-unary homogeneous nucleation (QUN) of $H_2O-H_2SO_4$ clusters described in (Yu, 2005), while MoMiE uses the approach of Wilemski and Wyslouzil (1995) based on the classical binary homogeneous nucleation (BHN) theory. As emphasized in Yu (2005), both models produce different results, with the BHN showing a tendency to overestimate the nucleation rates

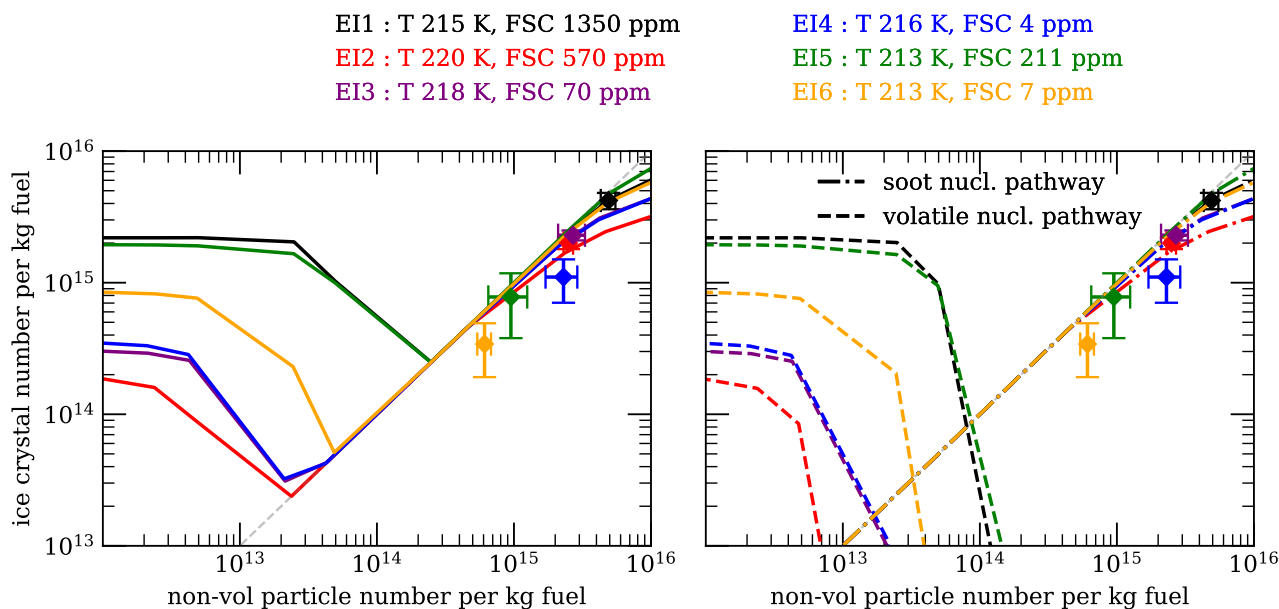


Figure 8. Apparent ice particle emission index in function of non-volatile particle emission index, both in number per kilogram of fuel. Left: Continuous lines correspond to the simulations provided by MoMiE and applied to the 6 cases studies in Yu et al. (2024) after 2 seconds simulation. Right: Dashed lines correspond to MoMiE apparent emission index of the ice particles formed by volatile-pathway freezing, while dashed-dotted lines correspond to the ice particles formed by soot-pathway freezing. The diamond points on both plots and the error bars refer to the corresponding ECLIF measurement data defined in Table 4.

475 in comparison to the QUN. However, these two approaches haven't been properly studied and compared to the most recent measurement data in different fuel and combustion mode conditions and need further investigation. Other processes may be also represented by different approaches and contribute to the observed differences. Further investigation would be needed to properly compare and account for the contribution of the different processes to the variability of the results.

5 Model results compared to the number of ice crystals measured by NEOFUELS/VOLCAN

480 5.1 The measurement data

The NEOFUELS/VOLCAN campaign described in Section 3 also measured the number of ice particles in far-field, i.e. about 6 – 29 km behind the aircraft (plume age of 24 – 122 s), at a mean typical cruise speed of 0.78 Mach and at lower ambient temperatures (210 – 223 K) and higher relative ambient humidity of the ice phase (100 – 143 %) (see Extended Table 3 in Voigt et al. (2026)). Note that near and far-field measurements are obtained at different engine power settings, which can result

485 in different emission indices of non-volatile particles in the same fuel and combustion mode conditions, as well as to different



emission indices of other species such as organics and other volatile particle precursors. However, near-field measurements of non-volatile particles are preferred for the comparison with the ice crystals measurements of the corresponding fuels and combustion modes, as discussed in Section 5. In order to allow the comparison between lean-burn and rich-burn conditions, the combustor inlet temperature T30 is fixed for the different measurement points. Table 5 presents the datasets selected for the comparison between modeled and measured number of ice crystals in the far-field. There are six different fuels studied, corresponding to one case of conventional Jet A-1 containing small amounts of HEFA fuel (5%) (Voigt et al., 2026), two cases of conventional petroleum-based fossil kerosene Jet A-1 (Märkl, 2024), a case of contaminated HEFA-SPK (Voigt et al., 2026), a case of 100 % HEFA-SPK (Märkl, 2024), and a case of low-aromatic HEFA-SPK blend (Märkl, 2024). These data were measured in selected domains with similar atmospheric conditions (relative humidity with respect to ice, ambient temperature, and pressure). They were grouped and filtered according to the methods described in (Märkl, 2024) and the raw datasets are published in the HALO database mentioned in the data availability statement. As for the measurements of tPM presented in Section 3, three different combustion modes were tested: forced rich-burn mode (soot-rich regime) for an EI_{nvpm} higher than $\sim 10^{14} \text{ kg}_{\text{fuel}}^{-1}$, lean-burn mode (soot-poor regime) for this same emission index being lower than $\sim 5 \cdot 10^{12} \text{ kg}_{\text{fuel}}^{-1}$, and an intermediate split point between lean-burn and forced rich-burn combustor condition (medium regime) for the emission index comprised in-between these two values. Note that there are uncertainties on the fuel sulfur content of the different fuels according to the different campaigns and different flight days, due to contamination in the aircraft tanks (see Dischl et al. (2026)). Therefore this value can vary from Table 3 to Table 5 for the same fuel type.

5.2 MoMiE reference simulations

The aim of this section is to compare the MoMiE model results to the ice crystals number measured during the NEOFUEL-S/VOLCAN campaigns. Six simulations corresponding to the six cases described in Table 5 have been computed and initialized with the reference parameters described in Table 2. The comparison between model simulations and NEOFUELS/VOLCAN data is displayed by Figure 9, which shows the apparent emission index of ice versus of the emission index of non-volatile particles. Cases VII, VI2 and VI3 correspond to Jet A-1 cases with an FSC of 192 – 195 ppm, while cases VI4, VI5 and VI6 correspond to the cases of HEFA-SPK, with an FSC of respectively 75, 3.2 and 1.9 ppm. The temperature ranges from 215 to 221 K, and the RH according to the ice phase (RH_i) between 110% and 130% are detailed in Table 5. The error bars correspond to the standard deviations also indicated in Table 5. Ice particles between $\sim 0.5 \mu\text{m}$ and $\sim 50 \mu\text{m}$ diameter were measured, and a cut-off of $0.5 \mu\text{m}$ has been imposed on the particles diameter for the simulations outputs. Continuous lines correspond to the model results obtained for the reference parameters described in Table 2. The minimum and maximum of the shaded envelope correspond respectively to the model results obtained for an emission index of soluble organics EI_{OMsol} of 5 and $100 \text{ mg kg}_{\text{fuel}}^{-1}$. The next sections discuss the sensitivity to FSC, organics, ions and ambient conditions on the formation of ice particles in our model.



Table 5. NEOFUELS/VOLCAN measurements of non-volatile and ice particle number emission indices, for the 6 selected cases (labeled "VII-6") of Jet A-1 and HEFA-SPK studied in this work, in lean-burn, intermediate (only case 2 presents this regime) and rich-burn combustion mode.

Case name	VII	VI2	VI3	VI4	VI5	VI6
Fuel	95 % Jet A-1 +5 % HEFA	100 % Jet A-1	100 % Jet A-1	64 % HEFA +36 % Jet A-1	100 % HEFA-SPK	blend HEFA-SPK+LA
T ^a (K)	218.0	215.5	218.9	218.3	219.0	221.4
P ^a (Pa)	30080	27450	26220	30080	26220	28760
RH _{ice} (%)	112.3	106.8	128.0	105.2	109.8	
El _{H₂O} (kg kg _{fuel} ⁻¹)	1.26	1.26	1.26	1.33	1.37	1.32
FSC (ppmm)	192	195	195	75	3.2	1.9
near-field EI _{nvpm} (kg _{fuel} ⁻¹)						
lean-burn	6.7×10 ¹¹	6.1×10 ¹¹	6.1×10 ¹¹	3.6×10 ¹¹	1.4×10 ¹¹	1.2×10 ¹¹
split	-	1.5×10 ¹³	-	-	-	-
rich-burn	8.5×10 ¹⁴	8.8×10 ¹⁴	8.8×10 ¹⁴	4.6×10 ¹⁴	2.6×10 ¹⁴	5.1×10 ¹⁴
near-field std EI _{nvpm} (kg _{fuel} ⁻¹)						
lean-burn	4.9×10 ¹¹	5.5×10 ¹¹	5.5×10 ¹¹	4.3×10 ¹⁰	4.0×10 ¹⁰	6.0×10 ¹⁰
split	-	0.2×10 ¹³	-	-	-	-
rich-burn	1.7×10 ¹⁴	8.0×10 ¹³	8.0×10 ¹³	3.2×10 ¹³	2.0×10 ¹³	3.0×10 ¹³
far-field AEI _{ice} (kg _{fuel} ⁻¹)						
lean-burn	1.6×10 ¹⁵	1.1×10 ¹⁵	1.5×10 ¹⁵	5.1×10 ¹⁴	1.3×10 ¹⁵	2.3×10 ¹⁴
split	-	9.6×10 ¹⁴	-	-	-	-
rich-burn	1.4×10 ¹⁵	9.3×10 ¹⁴	1.5×10 ¹⁵	9.1×10 ¹⁴	7.4×10 ¹⁴	2.6×10 ¹⁴
far-field std AEI _{ice} (kg _{fuel} ⁻¹)						
lean-burn	3.1×10 ¹⁴	5.3×10 ¹⁴	4.5×10 ¹⁴	2.0×10 ¹⁴	5.0×10 ¹⁴	1.4×10 ¹⁴
split	-	4.2×10 ¹⁴	-	-	-	-
rich-burn	5.1×10 ¹⁴	5.4×10 ¹⁴	6.4×10 ¹⁴	4.9×10 ¹⁴	2.9×10 ¹⁴	1.7×10 ¹⁴

T^a is the averaged ambient temperature; P^a is the averaged ambient pressure and RH_{ice} the averaged relative humidity with regards to ice; El_{H₂O} is the emission index of water in kg per kg of fuel; FSC is the fuel sulfur content in ppmm; EI_{nvpm} is the emission index of non-volatile particles in number per kg of fuel measured in the near-field (plume age of 0.2 – 1.4 s, Dischl et al. (2026) for cases VI2, VI3, VI5 and VI6, Voigt et al. (2026) for cases VII and VI4); sdt EI_{nvpm} is the standard deviation of the emission index of non-volatile particles in number per kg of fuel measured in the near-field; AEI is the apparent emission index of ice crystals in number per kg of fuel measured in the far-field (plume age of 24 – 122 s, Märkl (2024) for cases VI2, VI3, VI5 and VI6, Voigt et al. (2026) for cases VII and VI4); sdt AEI is the standard deviation of the emission index of the ice crystals in number per kg of fuel measured in the far-field. Note that, for case VI5, because of large uncertainties observed in step 2 measurement data of the non-volatile particle numbers for pure HEFA-SPK, VOLCAN step 1 data were used.



5.3 Sensitivity to FSC

Figure 9 shows that the model and measurements are in good agreement for case VI2 in soot-poor, intermediate and rich burn regimes, for Jet A-1. However, the model tends to underestimate the ice crystal number for cases VI1 and VI3 in both soot regimes. Regarding the HEFA-SPK pure and blend fuels, the model matches the observations in cases VI4 and VI6 in the soot-poor regime, while it underestimates them for case VI5. In the soot-rich regime, the model lies within the error bar for all cases but case VI5. In general, measurement data show similar orders of magnitude between the Jet A-1 and HEFA-SPK fuel types, except for the case VI6, where lower AEI by a factor of approximately 3 to 10 are observed. These tendencies are well reproduced by the model outputs, when considering the presence of organics. For similar ambient conditions, still according to the measurement data, the FSC doesn't seem to systematically control the determination of the number of ice crystals magnitude. This point is particularly illustrated by the comparison between cases VI3 and VI5, which display similar amount of ice particles in the soot-poor regime despite the FSC difference (respectively 195 ppm and 3.2 ppm).

Figure 9 also shows the ACM results (see Figure 2 in Voigt et al. (2026) corresponding to the data summarized in the Extended Data Table 2 of the same paper) added to the corresponding cases VI1, VI4 and VI5. It has to be noted, that ambient temperature used for the ACM simulation in case VI5 was 218 K, so 1 K lower than the one prescribed in MoMiE's results and indicated in the data measurements. While ACM results agree well with the measurement data for cases VI1 and VI4, it fails to reproduce the results of case VI5. Indeed, ACM results, as well as for the ECLIF measurements, show a high sensitivity of the model to the FSC, with the higher the FSC, the higher the number of ice crystals. Indeed, the model predicts much lower number of ice crystals in the case of VI5 (FSC= 3.2 ppm) than in the cases of VI1 and VI4 (see dashed lines in the figure). Although MoMiE results slightly underestimate cases VI1 and VI5, they reproduce the different observed tendencies of the data measurements for the different cases studied, in particular in the case VI5 of pure HEFA-SPK. In this particular case of low FSC, the study of further volatile species or parameters influencing the formation of particles is of most interest.

The representation of the different involved processes in the models can also be discussed here. In addition to the nucleation process, which as mentioned above, is different from one microphysics model to the other, the freezing process can also be represented by different theories. Indeed, in MoMiE, the homogeneous and heterogeneous nucleation rates of ice particles are calculated according to the theory described in Pruppacher et al. (1998), while Bier et al. (2022) and Ponsonby et al. (2024) for example use the theory described in Köhler et al. (2015) with a freezing rate coefficient computed from a parameterization based on laboratory measurements (Riechers et al., 2013).

5.4 Sensitivity to soluble/insoluble organics and ions

Sensitivity of the ice particle formation to the initial amount of soluble and insoluble organic species, as well as to ions has been investigated. Soluble organics display significant impact on the ice particle number in the lean-burn combustion mode (see Figure 9). Indeed, increasing the initial EI_{OMsol} from 35 to 100 $mg\ kg_{fuel}^{-1}$ makes the ice particle number increase by 21 to 58 % in the soot-poor regime and by around 0.68% to 4.5 % in the soot-rich regime, respectively. For the intermediate combustion mode, the minimum of the V-shaped diagram increases by around 44% to 97 %. However, sensitivity to insoluble



organics and ions is very low in comparison. Indeed, increasing the initial amount of OM_{insol} from 110 to 400 $mg\ kg_{fuel}^{-1}$ can increase the AEI by up to 12 % in the soot-poor regime. Increasing the initial amount of ions by one order of magnitude tends to either decrease the AEI by up to $\sim 6\%$ or increase it by 0.71 % in soot-poor regime. The variations in the soot-rich regime remain quite low around 1 % (see Table A1 in the Appendix for the relative difference between the reference cases and the sensitivity tests).

This can be explained similarly to the determination of the total number of particles. In our model, the nucleation of species other than sulfur into volatile clusters, such as soluble organic matter that our model takes into account, seems to be crucial to be able to reproduce the measurement data. Indeed, while cases VI2, VI4 and VI6 are well represented by the model with the reference simulation corresponding to an emission index of soluble organics of 35 $mg\ kg_{fuel}^{-1}$, the model is only able to come closer to observation data in the cases VII1, VI3 and VI5, when considering a much higher initial emission index of soluble organics. Interestingly, this is observed for the two cases VII1 and VI3 of Jet A-1, but also for the case VI5 of 100 % HEFA with a low FSC. While, in our model, soluble organics are the only species able to create a new population of volatile droplets in addition to sulfuric acid, further species could be invoked to explain the gap between the model predictions and the observed ice crystals number, such as the already mentioned lubrication oil, which is not yet included in our model.

5.5 Sensitivity to the ambient conditions

Results for cases VII1 and VI2 show that a difference of 3 Kelvins in ambient temperature, nearly all other parameters being equal, can double the number of ice particles in the model predictions. Generally, the results show that the model is mainly controlled by the ambient temperature: regardless of other parameters a reduction in ambient temperature always leads to an increase in ice crystal number. In the measured data, this strict correlation between temperature and ice particle number is not fully represented. There, the highest values of ice particle numbers in the soot-poor regime are obtained for cases VII1 and VI3, correspond respectively to ambient temperature of 218 K and 219 K.

At the timescale considered (2 seconds after exhaust), the model shows that the ambient relative humidity has little influence on the ice crystal number (see for example difference between the model lines for cases VII1 and VI3, where the higher relative humidity for case VI3 doesn't compensate the higher temperature that lowers the amount of ice crystals). This is also seen by comparing cases VI3 and VI5. Although a higher relative humidity tends to slightly increase the number of ice crystals, the model shows that emitted water vapor is the main contributor to the ice growth at this stage of the contrail formation. While the relative humidity is expected to play a significant role on the persistence of the contrail, its effective influence is hard to distinguish within the presented measurement data, which correspond to contrail ages of tens to hundreds of seconds (see Extended Data Table 3 in Voigt et al. (2026)).

5.6 Near-field versus far-field

Ice crystal measurements are conducted in the far-field, i.e. at plume ages around 30 to 120 s, corresponding to the timing of the vortex phase of the contrail life cycle. Microphysics box-models such as MoMiE do neither take into account the interaction with the aircraft aerodynamics, which drive the contrail towards lower altitudes, nor the interaction with the atmosphere

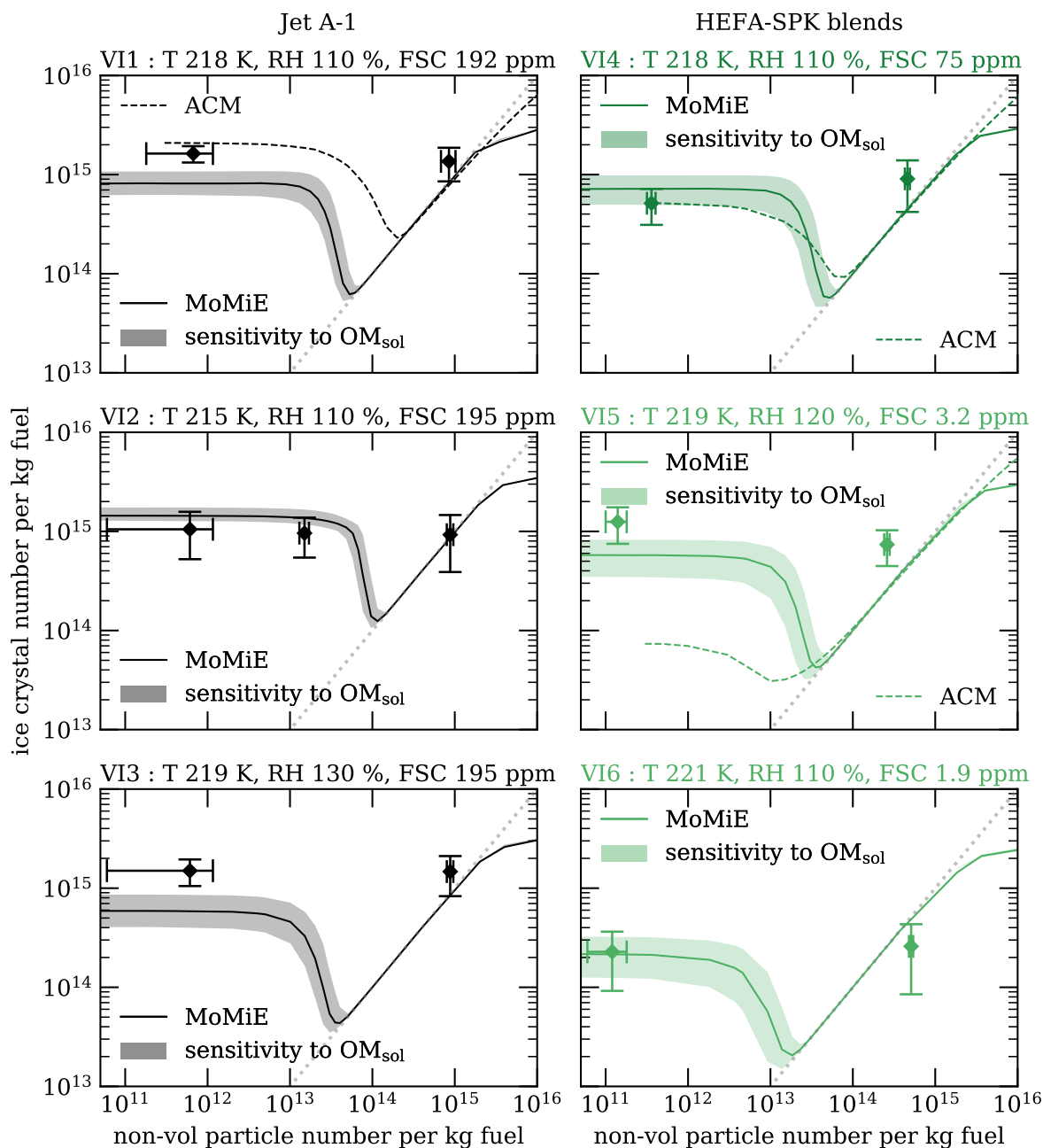


Figure 9. Apparent ice particle emission index versus the non-volatile particle emission index, both in number per kilogram of fuel, calculated by the MoMiE model for the 6 different fuel cases described in Table 5 and compared to the NEOFUELS/VOLCAN measurement data indicated by the diamond points and their standard deviation. The continuous lines correspond to the reference cases initialized with the parameters of Table 2. The minimum and the maximum of the shaded envelopes correspond to the same model simulations run with an initial amount of soluble organics of respectively $EI_{OM_{sol}} = 5 \text{ mg kg}_{fuel}^{-1}$ and $EI_{OM_{sol}} = 100 \text{ mg kg}_{fuel}^{-1}$. The dashed lines superposed in cases VI1, VI4 and VI5 correspond to the ACM results presented in Figure 2 of Voigt et al. (2026).



(wind, thermal stratification etc.) (Unterstrasser, 2014). Therefore, although the number of ice particles formed in the jet phase stabilizes within seconds in the model and already provides information on the order of magnitude of the ice crystals produced, the relevance of comparing data and simulations at these time scales can be discussed. Indeed, in the case of the NEOFUELS/VOLCAN campaigns, some ice crystal measurement sequences may have occurred in the primary wake, where the vortex could have caused losses in the ice crystals number, and affect the comparison with MOMIE, which focuses on the jet regime. Furthermore, the number of non-volatile particles compared to the number of ice crystals can also be addressed. Measurements in near and far-fields correspond to different flights with different conditions, consequently potentially leading to different emissions of non-volatile particles. This can be observed, for example, in case EI5 of the ECLIF 3-1 data, which appears below or on line 1:1 in the presented results, corresponding to the EI_{nvpm} and EI_{ice} measured in the far-field, while the same point locates above line 1:1 when using the EI_{nvpm} of the near-field, as highlighted by Dischl et al. (2025) Figure 4, and also in (Märkl, 2024). This is also the case for the rich-soot regime NEOFUELS/VOLCAN measurements, notably shown in Figure 9, which show ice crystal numbers above the 1:1 line except for case VI6, which is in lower temperature conditions. Dischl et al. (2025) notably mention the difficulty for the measuring devices to evaluate the number of non-volatile particles in the presence of contrails/ice crystals. For this reason, near-field EI_{nvpm} is preferably used. However, especially in the soot-rich regime, there can be a non-negligible difference between the EI_{nvpm} measured in near field (outside of contrail forming conditions) and the actual EI_{nvpm} in the operating conditions of the far-field contrail measurements. Consequently, these uncertainties observed in the far-field are all arguments for completing the comparison of the model results with measurements in the near-field, where the simulation conditions are closest to those of the measurements.

6 Summary and conclusions

The MoMiE code, developed at ONERA, models the key processes governing contrail microphysics. In particular, it enables the representation of both non-volatile and volatile particle nucleation—the latter playing a crucial role under the operating conditions of next-generation lean-burn engines fueled by low-sulfur fuels. The code accounts for the nucleation of sulfur and so-called soluble organic species, while also considering the condensation of insoluble organic species onto pre-existing particles. As part of this study, the code was improved and validated using three sets of measurement data covering different fuel sulfur contents, engine combustion modes, and ambient conditions.

The first datasets correspond to the NEOFUELS/VOLCAN campaign and comprise near-field total particle number measurements for rich, intermediate, and lean-burn combustion regimes, as presented in Dischl et al. (2026). This is the first comparison between simulations from a detailed microphysics model and the total number of particles measured within contrails. These results reveal that in addition to sulfur content, the total particle number predicted by the model is particularly sensitive to the initial quantity of soluble organic compounds, and simulations align with measurements for an initial emission index EI_{OMsol} comprised between 25 and 35 $mg\ kg_{fuel}^{-1}$. A sensitivity study also revealed that the chemi-ion concentration at the engine exit also influences the total particle number, resulting in a 20 to 30 % increase or decrease depending on the combustion mode, when the magnitude changes by an order of magnitude. The ambient temperature considered for near-field conditions is high



(228-230 K) and has only a slight effect on the number of volatile particles formed. The same observation applies to the effect of ambient relative humidity, ranging from 40 to 90 %. Although it accounts for the nucleation of idealized soluble organic species, the model does not specifically represent the nucleation of lubrication oil, or the variability in the properties of organic compounds present in engine exhaust. Nevertheless, for the conditions studied, the code suggests that, in addition to sulfur, other nucleation species are crucial for the formation of volatile condensation nuclei, particularly in lean-burn combustion mode.

The second dataset relates to the ECLIF test campaigns and comprises far-field ice crystal number measurements analyzed in Yu et al. (2024), focusing primarily on the rich-burn mode. Comparison with ECLIF measurements reveals that, in the soot-rich regime, the code's results agree well with the measurements as well as with those from another microphysics code (ACM, developed by the University of Albany (Yu et al., 2024)), which also models the nucleation of non-volatile and volatile sulfur-containing particles. The comparison of model results can be extended to the low-soot emission indices, where differences in parameter dependence are observed. In the MoMiE model, the number of ice crystals formed appears to be primarily controlled by the ambient temperature, whereas the ACM model seems more sensitive to FSC. However, both models do show an influence from these two parameters. The differences observed between the two codes require in-depth investigation and could be attributed to differences in the representation of certain processes (such as nucleation, condensation, etc.).

The third dataset compiles additional measurements from the NEOFUELS/VOLCAN campaign regarding far-field ice crystal counts for rich, intermediate, and lean-burn combustion regimes; these data are primarily presented in Voigt et al. (2026) and Märkl (2024). The comparison shows that the MoMiE code estimates the formation of more than 10^{15} particles per kg of fuel in lean-burn combustion mode. Under the conditions studied, sensitivity to ambient relative humidity, the initial number of ions, and the initial emission index of insoluble organic compounds remains very low compared to the influence of soluble organic compounds. However, the model results appear much more sensitive to variations in ambient temperature, which ranges between 215 and 221 K in the far-field. In the lean-burn combustion mode, the model results suggest that the ice crystal formation essentially depends on the number of volatile particles capable of nucleating. Although including organic compounds better aligns MoMiE results with measurement data, the code still tends to underestimate the number of ice particles for the high FSC / low soot cases compared to VOLCAN observations and also compared to the microphysics model ACM, which now considers nucleation of lubrication oil. However, the MoMiE code succeeds in approximating the data measurements in the case of low FSC (notably VI5), which is not the case for ACM, which seems to be more sensitive to FSC. These results indicate that further model comparisons are needed to better understand ice formation mechanisms in contrails, and that measurements of emitted organic compounds (unburned hydrocarbons, lubricating oil), ideally including their speciation, are also required, in addition to FSC, to help explain observations and constrain models.

7 Implications and Perspectives

The presented study particularly highlights the importance of considering the total number of particles, in addition to ice crystals, when comparing simulations from contrail models with measurements, especially in the case of lean-burn combustion and



low-sulfur fuels. Indeed, the formation of nucleation clusters is a crucial step in ice crystal formation and total particle numbers
650 can also be used as additional validation data for models. It also emphasizes the difficulty to compare model simulations and
measurement data in the same conditions, for example in accounting for the differences between conditions in the near-field
and the far-field. These results underline the need to conduct further measurement campaigns of total particles and ice crystals
within contrails in different conditions to constrain the model simulations. Further investigations are also needed to elucidate
and characterize uncertain parameters such as ions or organic compounds issued from different sources, which seem to impact
655 on the different nucleation pathways (e.g. in-flight but also ground measurements of size distributions, organics speciation...).
Combined with model developments, those are necessary to advance our understanding on contrail formation - in particular
in cases of low sulfur fuels. Finally, this work contributes to the collective effort to reduce uncertainties regarding the quan-
tification of the impact of aviation's non-CO₂ effects. Indeed, the development of detailed microphysics models is a crucial
step toward improving the initialization of models capable of quantifying the radiative impact of contrails, such as the CoCiP
660 (Contrail Cirrus Prediction) model (Schumann and Seifert, 2025), which is used worldwide, and currently relies on simplified
assumptions regarding ice crystal number and size distribution (Akhtar Martínez et al., 2025).

Further developments of the code will include the improvement of the organic compounds representation, in particular
with the integration of the nucleation of lubrication oil as additional condensation nuclei. Modeling parameterizations for
various microphysical processes, such as nucleation, condensation, and freezing, also require in-depth analysis, which will be
665 conducted notably within the framework of the contrail model intercomparison project Eastham et al. (2026).

Code availability. The Modèle Microphysique pour Effluents (MoMiE) model has been developed by and is the proprietary intellectual
property of ONERA, France, and is not publicly available. The use of the MoMiE code requires research collaboration within the framework
of a contractual partnership (contact margaux.vals@onera.fr or nicolas.bonne@onera.fr).

Appendix A: Sensitivity of the modeled ice crystal number to different parameters

670 Table A1 shows the difference in percentage of ice crystal numbers obtained for various model simulations relative to the
reference case displayed in Figure 9. Six different cases are shown and correspond to a sensitivity study to the emission index
of soluble organics, insoluble organics, and ions.



Table A1. Relative difference e_r between the model results obtained for the different sensitivity test simulations (AEI_{ice}^s) and the model results obtained for the reference simulations (AEI_{ice}^{ref}) shown in Figure 9. The relative difference is calculated for the apparent emission index of ice crystals number as $(AEI_{ice}^s - AEI_{ice}^{ref}) / AEI_{ice}^{ref}$ in percents and is averaged over the range of considered non-volatile emission indices corresponding to respectively lean-burn, intermediate and rich-burn combustion modes.

Case	1	2	3	4	5	6
e_r in % for $EI_{OMsol} = 5 \text{ kg}_{fuel}^{-1}$						
lean-burn	-24.	-12.	-32.	-32.	-41.	-48.
split	-29.	-26.	-33.	-35.	-39.	-13.
rich-burn	0.68	-0.5	0.24	-0.8	0.0090	0.5
e_r in % for $EI_{OMsol} = 100 \text{ kg}_{fuel}^{-1}$						
lean-burn	32.	21.	46.	37.	44.	58.
split	69.	49.	89.	76.	97.	44.
rich-burn	0.71	4.5	0.80	0.68	1.7	2.1
e_r in % for $EI_{OMinsol} = 5 \text{ kg}_{fuel}^{-1}$						
lean-burn	-2.9	-3.6	-1.6	-3.1	-3.1	-5.2
split	1.1	3.2	1.8	-1.9	1.7	-5.2
rich-burn	-4.2	-4.3	-5.1	-5.9	-5.3	-5.2
e_r in % for $EI_{OMinsol} = 400 \text{ kg}_{fuel}^{-1}$						
lean-burn	9.7	6.5	7.4	12.	9.1	9.9
split	6.6	-0.39	-0.90	3.1	2.0	6.8
rich-burn	8.3	7.5	5.8	8.0	7.8	6.6
e_r in % for $EI_{ions} = 10^{16} \text{ kg}_{fuel}^{-1}$						
lean-burn	-2.2	-0.47	-4.1	-2.6	6.4	15.
split	2.4	1.2	0.67	1.5	9.6	5.4
rich-burn	1.7	0.79	0.25	0.66	0.77	1.0
e_r in % for $EI_{ions} = 10^{18} \text{ kg}_{fuel}^{-1}$						
lean-burn	-0.6	0.71	-2.5	-0.95	-6.4	-6.6
split	-1.9	-0.78	-4.1	-3.2	-6.0	-1.7
rich-burn	1.1	-0.16	-0.034	-0.25	0.14	0.74

Author contributions. M.V. performed the model runs and wrote the paper. N.B. assisted with using the code and with analyzing and discussing the model results. I.O. provided expertise on the volatile nucleation pathway. E.T. assisted with using the MoMiE model. C.V. coordinated the ECLIF1 and 2 flight experiments. Airbus led the ECLIF3 project and CV and CR coordinated the ECLIF3 flight campaign. K.S led the VOLCAN project and C.V, K.S, S.K, C.R coordinated the NEOFUELS/VOLCAN flight experiment. R.M., D.S., R.D., S.K., A.M. and A.R. performed the in-flight measurements and analyzed the data. R.M. and R.D. provided the filtered measurement data, as well as their expertise regarding the datasets. K.S. provided fuel compositions. A.R. assisted with engine data interpretation. All authors contributed to the paper.



680 *Competing interests.* The authors declare no competing interests.

Acknowledgements. This work was supported by the French VOLCAN programme funded by the Direction Générale de l'Aviation Civile (DGAC), by the DLR Aeronautics Research Programme within the Project NEOFUELS, and by Airbus and Safran Aircraft Engines. We thank the flight crews of the DLR Falcon and the Airbus A321neo for excellent flight operations. C.V., and D.S. acknowledge funding by the European Union's Horizon Europe program under grant no 101192301 (A4CLIMATE).



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