

Eulerian-Lagrangian CFD-microphysics modeling of aircraft-emitted aerosol formation at ground-level

Sébastien Cantin^a, Mohamed Chouak^a, François Garnier^a

^aDepartment of Mechanical Engineering, École de technologie supérieure, University of Quebec, Montreal, QC, H3C 1K3, Canada

CONTACT: Sébastien Cantin, sebastien.cantin.1@ens.etsmtl.ca, Department of Mechanical Engineering, École de technologie supérieure, University of Quebec, Montreal, QC, H3C 1K3, Canada.

ABSTRACT

Aviation-induced particulate matter directly affects the climate, the atmospheric composition at flight altitudes, and local air quality near airports. Meeting environmental regulations is a key challenge for the future development of air transportation. To enhance the understanding of secondary aerosol formation in aircraft plumes, an innovative methodology combining flow dynamics in aircraft engine plumes with a particle-based microphysical model is proposed. To this end, 2D axisymmetric unsteady Reynolds-Averaged Navier-Stokes simulations were conducted behind a realistic aircraft engine geometry. The CFD model was coupled with a tabulated chemistry and a detailed microphysical model accounting for soot surface activation, condensation of organic vapors and sulfur species (H_2SO_4 , SO_3), as well as scavenging of sulfuric acid-water droplets on soot surfaces. The model's predictive capacity was validated against experimental data from APEX 1-2, encompassing plume aerothermodynamics properties and the evolution of gaseous species from low-idle (4%) to take-off (100%) power settings of the CFM56-2C1 aircraft engine. The predicted size distributions of total and non-volatile particles matched reasonably well with measurements from APEX-1 within the near field (≤ 30 m). The model reveals the engine power dependency of soot and the chemical composition of volatile particles, predominantly influenced by organic compounds downstream of the engine. Adsorption of gaseous species of organic compounds and sulfuric acid were identified as the most dominant mechanism for soot particle coatings in the near field, regardless of operating conditions.

This article is deposited under the terms of the Creative Commons Attribution-NonCommercial-NoDerivatives License (<http://creativecommons.org/licenses/by-nc-nd/4.0/>), which permits non-commercial re-use, distribution, and reproduction in any medium, provided the original work is properly cited, and is not altered, transformed, or built upon in any way.

1. Introduction

Gaseous and particulate matter (PM) emissions from aircraft engines are known to have a negative impact on both the environment and human health. At ground level, PM emissions from aircraft turbine engine exhaust are mainly composed of non-volatile PM (nvPM) such as soot particles, minimal traces of metal oxides, metallic wear particles, and similar constituents. nvPM is defined as material that does not volatilize when heated to 623K (350 °C) (Saffaripour et al., 2020). The majority of nvPM produced by aircraft is carbonaceous black carbon, which is a product of incomplete combustion (Yuan et al., 2022). Aircraft-generated black carbon exists in the form of branched, fractal aggregates, which comprise many agglomerated primary particles. Volatile PM (vPM) emissions primarily comprising sulfur and organic compounds, for their part, are exclusively formed within a sufficiently diluted and cooled exhaust plume downstream of the engine. To regulate the PM emissions of aircraft turbine engines, the ICAO-CAEP (Committee on Aviation Environmental Protection) has developed a new certification method (ICAO, 2016). This method is based on continuous measurements of nvPM emissions in number and mass at the engine exit for a reference landing and take-off cycle at an altitude of less than 915 m (3000 ft), known as the Landing Take-Off (LTO) cycle. The regulatory limits for nvPM emissions apply to engine manufacturers during the certification of in-production and new commercial aircraft engines with a rated output greater than 26.7 kN. However, these regulations do not address vPM emissions because their formation and characterization require additional research (Owen et al., 2022). In this context, the study of vPM emitted by aircraft engines is gaining momentum, with several studies in the literature focusing on the characterization of aviation PM emissions both experimentally and numerically.

Experimentally, several measurement campaigns have been conducted in the past decade (Lobo et al., 2015; Yu et al., 2019; Beyersdorf et al., 2014), enabling the physical characterization of the particle size, number, shape, and composition. Regarding the composition, aviation PM emissions in the atmosphere

typically comprise both liquid-coated soot particles and liquid droplets (vPM). While nvPM particles (primarily composed of black carbon) are produced by the incomplete combustion of fuel and air in engine combustors, vPM are generated in early engine plumes through the nucleation or condensation of gaseous precursors; examples are sulfuric acid (H_2SO_4), produced by oxidation of sulfur compounds (SO_x) due to the fuel sulfur content, and volatile organic compounds (VOCs), especially polar ones such as aldehydes, whose partial vapor pressures are low enough that they condense at ambient temperature. Aircraft-engine emitted VOCs have become significant contributors to PM formation both near airports and during cruise conditions (Liang et al., 2021). The volume of aircraft-emitted VOCs is highly dependent on engine power, with the highest emissions in term of mass seen at low power settings typical of ground idle, and emissions decreasing as power increases (Beyersdorf et al., 2012). Additionally, idle emissions are combined with relatively longer periods of time spent at low power conditions. Variability in total hydrocarbons (HCs) at idle conditions has recently been reported (Kılıç et al., 2018; Kılıç et al., 2017). For instance, differences between idle (7-8%) and low-idle (3-5%) power settings have led to an average increase in VOCs EI from 2.9 to 7.8 g kg fuel⁻¹. The relative contribution of pure hydrocarbons, particularly aromatic and aliphatic compounds, in engine exhaust decreases with increasing thrust, while the fraction of oxidized compounds, such as acids and carbonyls, increases.

Considerable scientific effort has been devoted to characterizing and quantifying VOCs in engine exhausts, but the evolution of organic/sulfur PM loading in the aircraft near field remains unclear. The characterization of liquid components of these particles remains challenging due to their volatile nature, causing constant evolution in the atmosphere. Understanding the contribution of volatile components to the formation of vPM and liquid-coated soot particles is necessary to assess the environmental and health impacts of total aircraft PM emissions. Therefore, a more comprehensive approach is required to better understand the interaction between VOCs and nvPM/vPM, involving a wide range of different species and varying ambient conditions.

Even though experimental studies are highly relevant to the development of engine emission inventories and related health impact assessments, they do not provide a detailed understanding of PM formation conditions and mechanisms, particularly for vPM in engine plumes. Investigating potential mitigation strategies for aircraft PM emissions necessitates the development of advanced decision-making tools based on detailed microphysical modeling of plumes. In this regard, the review of past numerical studies can be distinguished based on cruise flight and ground level conditions.

Particle formation and evolution in early plumes have received the most interest at flight conditions in characterizing near-field contrail properties. Two different approaches are generally used in this regard. On the one hand, 3D Computational Fluid Dynamics (CFD), including Large Eddy Simulations (LES) (Lewellen, 2020; Paoli et al., 2013), or Reynolds-Averaged Navier-Stokes simulations (RANS) (Khou et al., 2016; Cantin et al., 2021) are utilized. These approaches resolve many details of the jet flow and account for spatial variation of the mixing in the plume. On the other hand, box models are employed, based on a few idealized air parcel trajectories (0D) originating from an engine (Vancassel and Mirabel and Garnier, 2014) or utilizing analytical expressions computing the entrainment rate of the plume represented by a streamline at the jet center (1D) (Kärcher et al., 2015). For ground-level aviation PM microphysics, 1D models with semi-empirical profiles are typically used (Davidson and Wang, 2002) for both jet dilution and mixing. As an example, numerical studies conducted by Wong et al. (Wong et al., 2008; Wong et al., 2014; Wong et al., 2015) focused on an idle regime and employed a 1D modeling strategy to simulate early plumes with detailed microphysics. These models accounted for complex multicomponent interactions between organic vapors and emitted soot particles. Results revealed that soot surface activation occurs immediately downstream of the engine exit plane, while condensation of volatile vapors becomes more significant further downstream. Furthermore, binary homogeneous nucleation of $\text{H}_2\text{SO}_4\text{-H}_2\text{O}$ embryos are the primary contributors to new PM formation. Organic vapors were found to not directly promote nucleation of new particles, but instead, were seen to contribute through condensation on existing homogeneous liquid droplets. However, simplified representations of plume in 1D models do not accurately capture flow field

inhomogeneities observed behind real engine-exhaust geometries (Kärcher et al., 2015). These models neglect the substantial spatial variability in jet plumes resulting from turbulent mixing of hot jet exhaust with ambient air, instead simulating only an average mixing state across the entire plume cross-sectional area (Bier and Unterstrasser and Vancassel, 2021). Spatial inhomogeneities, particularly strong radial gradients and turbulent perturbations in plume temperature and relative humidity have a strong influence on microphysical processes. When comparing a 1D dilution-based model with a 3D CFD model at cruise flight conditions, Vancassel and Mirabel and Garnier (2014) found that detailed plume dilution (using 3D CFD) with both online and offline coupling strategies predicted survival of ice particles 10 s after ejection, while the parametrized dilution model predicted the evaporation of all ice particles before this time. Regarding 3D models, only a few studies have utilized a CFD framework under idle conditions to investigate the effect of buoyancy (Synylo et al., 2020) or the dispersion of gaseous pollutants (Testa et al., 2013), but these studies did not consider the formation of liquid-coated soot particles and vPM.

In this context, the present work aims to enhance the accuracy of plume mixing and the formation/evolution of liquid-coated soot particles and vPM in aircraft plumes based on 2D axisymmetric CFD simulations, taking into account a realistic aircraft engine geometry with core and bypass flows. The CFD model is coupled with a tabulated chemistry and a detailed microphysical model that accounts for complex multicomponent interactions between organic vapors, sulfur species, and aircraft-emitted soot particles. Building upon the initial work of Wong et al. (2014) and Jun (2011), a new particle-based microphysical model PAMMAP, (PAricle-based Microphysical Model for Aircraft Plumes), is developed for online coupling.

The paper is organized as follows. Section 2 provides a model description of PM formation/evolution processes in near-field aircraft plumes. Section 3 presents the set of equations representing fluid dynamics, particle motion, gas phase chemistry, and PM microphysics. Section 4 outlines the numerical methods, including the microphysical coupling strategy and grid settings. Finally, Section 5 presents the validation

results of the model and analyzes the properties of plume gaseous and PM emissions for different engine power settings.

2. Model description of PM formation at ground level

The modeling approach followed to characterize the plume evolution of turbofan particle properties is illustrated in Figure 1. The nozzle exit flow from the turbofan engine at ground level consists of two flows: a hot core flow and a surrounding cold bypass flow. The bypass jet contains ambient moist air that is accelerated by the engine fan, while the core jet drives the fuel-combustion products composed of gaseous emissions laden with soot particles. Both jets are mixed with the freestream (ambient) moist air at rest. Freshly emitted soot particles are initially hydrophobic (non-activated). Soot surfaces can be activated by sulfuric acid or water-soluble organic species to become hydrophilic (aqueous) or by water-insoluble organic species to become hydrophobic (non-aqueous). Hence, sulfuric acid and organic liquid layers can be formed by condensation of vapor onto activated soot particles. In addition to gaseous adsorption on soot, activation by collisions of sulfuric acid droplets on soot surfaces is also considered. New particles are formed (nucleation) via binary homogeneous nucleation of small $\text{H}_2\text{SO}_4\text{-H}_2\text{O}$ molecular clusters. These clusters or droplets tend to coagulate due to their high concentration in the exhaust plume. Finally, the model takes into accounts condensation of gaseous species such as water, sulfuric acid and organic compounds onto sulfuric acid droplets.

Figure 1

3. Mathematical description

This section deals with the mathematical equation for gas flow and for the dispersed phase for particle matter (PM). Then, the chemical equations are presented. Finally, the microphysical model for PM formation is depicted.

3.1 Gas phase flow

The mean flow is assumed axisymmetric and compressible. Therefore, the unsteady Reynolds-averaged Navier-Stokes (RANS) equations expressing the conservation of the gas phase global mass, momentum, and energy were solved in cylindrical coordinates $(O, \vec{r}, \vec{y})$ (CD-Adapco, 2021). To compute the mixture composition in the gas phase ($\Phi_g = \sum_k \bar{y}_k \Phi_k$), the mass fractions of species ($\bar{y}_k$) were derived with Eq. (1) defined as follows:

$$\frac{\partial(\bar{\rho}_g \bar{y}_k)}{\partial t} + \frac{\partial(\bar{\rho}_g \bar{u}_j \bar{y}_k)}{\partial r_j} = \frac{\partial}{\partial r_j} \left(\left(\frac{\mu_g}{\sigma_g} + \frac{\mu_{t,g}}{\sigma_{t,g}} \right) \frac{\partial \bar{y}_k}{\partial r_j} \right) + \bar{w}_{chemk} + \bar{w}_{adsk} + \bar{w}_{condk} + \bar{w}_{nuclk}, \quad (1)$$

Equation (1) translates the mass conservation of species which is governed by their average mass fraction $\bar{y}_k$, their diffusion coefficient in the mixture D_k , and the average mixture gas density $\bar{\rho}_g$. The mass transfer rate $\bar{w}_{chemk}$ is a function of chemical reactions, while $\bar{w}_{adsk}$, $\bar{w}_{condk}$ and $\bar{w}_{nuclk}$ are functions of adsorption, condensation, and nucleation of gaseous species, respectively, and represent the one-way coupling with the microphysics model. A detailed description of these coupling terms will be provided later. The variables σ_g and $\sigma_{t,g}$ denote the Schmidt number and the turbulent Schmidt number, taken as being equal to 1 and 0.9, respectively.

3.2 Dispersed phase

Size binned distribution is usually employed by 1D models to predict the temporal evolution of aerosol number concentration (Jones and Miake-Lye, 2024; Yu et al., 2024). A key challenge in bin microphysics schemes is the numerical diffusion across size or mass bins that occurs during growth calculations (collision-coalescence and condensation). Such diffusion can lead to numerical artifacts, namely, unphysical broadening of particle size distributions (Morrison et al., 2020). Conversely, the Lagrangian particle-based approach avoid this numerical diffusion by individually calculating particle transport in physical space and their growth using ordinary differential equations (Unterstrasser and Hoffmann and Lerch, 2017). Consequently, a Lagrangian particles tracking method was used for the dispersed phase to

track the motion of particles. As the number density of physical particles is relatively high, number-based emission indices being around 10^{15} kg fuel⁻¹ at the exhaust nozzle plane (Wey et al., 2007), a modeling simplification is required to save simulation time. Therefore, computational particles are considered as spheres of radius r_p , with each representing N physical particles (Schröder et al., 2000). Numerically, soot particles and liquid droplets are treated as passive tracers since their size and relaxation time are relatively small compared to the characteristic scales of the gas phase flow (Garnier et al., 2014). Due to their small size, on the order of a hundred of nanometers, particles' drag and gravity forces were neglected in the model. Consequently, the particles have the same velocity as the carrier phase.

3.3 Gas phase chemistry

The major gaseous emissions from aircraft engines are carbon dioxide CO₂ and water-vapor H₂O. Minor species are nitrogen-oxides NO_x, carbon-oxide CO, hydrocarbons, and organic compounds. Sulfur oxides SO_x are also present due to the fuel sulphur content. Many chemical interactions occur between NO_x, HO_x, and SO_x in aircraft engine plumes, which need to be characterized. For instance, SO_x products are important as they act as aerosol precursors, which promote homogenous nucleation and form volatile sulfate aerosols. A kinetic reaction scheme (tabulated-chemistry) based on the works of Kärcher and Hirschberg and Fabian (1996) and Khou et al. (2016) was implemented in the CFD code Star-CCM+. However, this scheme does not include any hydrocarbon chemistry since the reactions of organic compounds occur at minute timescales, which is too long to affect conditions in our period of interest (Garmory and Britter and Mastorakos, 2008). The scheme consists of $n = 60$ reactions with 22 reactive species, including NO_x, SO_x, HO_x, and 47 non-reactive species, including organic compound chemistry. The choice of organic compound based on the previous work of Kılıç et al. (2018) and Wong et al. (2014) for the validation will be discussed later.

In Eq. (2), which gives the evolution of a mass fraction y_k of each species k , the mass reaction rate $\dot{w}_k$ is assessed with Arrhenius laws. The mass production rate $\bar{w}_{chem_k}$ of a species k can be obtained from:

$$\bar{w}_{chem_k} = M_k \sum_{r=1}^n \xi_k^r \dot{\Omega}_r, \quad (2)$$

where M_k is the species molar mass and n refers to the number of considered reactions, ξ_k^r denotes the stoichiometric coefficient of species k in a reaction, and $\dot{\Omega}_r$ the net reaction rate.

3.4 Microphysics model

This sub-section describes the particle-based microphysical model used to simulate the atmospheric evolution of aircraft-emitted particles in the plume of a turbofan. The mathematical model for computing the activation and condensation of gaseous species on particles is based on the work of Wong et al. (2014), while the All-Of-Nothing (AON) coagulation module from Unterstrasser and Hoffmann and Lerch (2017) was used. First, the models for activating soot particles through the adsorption of gaseous species and the scavenging of droplets are presented. Then, the equations of condensation growth on soot particles and sulfuric acid droplets are presented, and the coagulation of sulfuric acid-water droplets is introduced. Finally, the homogeneous binary nucleation of a sulfuric acid-water model for molecular clusters is presented. The microphysical processes implemented in the code are summarized in Figure 2.

Figure 2

3.4.1 Activation of soot surfaces

It is generally admitted that freshly emitted soot particles from gas turbine engines are bare and initially hydrophobic. The activation of soot surfaces by adsorption of vapor molecules is a prerequisite for subsequent vapor condensation on soot. Soot surfaces can be activated by sulfuric acid or water-soluble organic species to become hydrophilic (aqueous) or by water-insoluble organic species to become hydrophobic (non-aqueous). We thus track two distinct phases, aqueous (hydrophilic) and non-aqueous (hydrophobic), on a soot surface in the model. Water is not considered in this activation process because direct adsorption of water on hydrophobic soot surfaces is believed to be very unfavorable (Brown et al., 1996), especially in the presence of sulfuric acid (Kärcher, 1998). In addition to gaseous adsorption on soot,

activation by collisions of nucleated liquid droplets on soot surfaces is also considered. This process, termed scavenging, is modeled with Brownian coagulation between scavenged liquid droplets and soot particles.

In summary, the activation of a soot particle i is described in the model by:

$$\begin{aligned} \left. \frac{d\theta_i}{dt} \right|_{activation} = & \left. \frac{d\theta_i}{dt} \right|_{ads,aq} + \left. \frac{d\theta_i}{dt} \right|_{ads,non-aq} + \left. \frac{d\theta_i}{dt} \right|_{scav,aq} + \left. \frac{d\theta_i}{dt} \right|_{scav,non-aq} + \left. \frac{d\theta_i}{dt} \right|_{cond,aq} \\ & + \left. \frac{d\theta_i}{dt} \right|_{cond,non-aq}, \end{aligned} \quad (3)$$

where θ_i is the activated soot surface fraction. The adsorption of aqueous and non-aqueous vapors onto soot particle surfaces, is represented by the first two terms on the right-hand side (RHS) of Eq. (3). Similarly, the scavenging process of aqueous and non-aqueous vapor liquid droplets by soot particle surfaces is depicted by the third and fourth term on the RHS of Eq. (3). The last two terms are related to rate of change of soot surface coverage due to the condensation of vapor (Jun, 2011).

The mass of adsorption on soot particles of sulfuric acid, trioxide and organic species is calculated from:

$$\left. \frac{dm_i}{dt} \right|_{ads,aq} = 0.25 \alpha_{d,s} \bar{c}_s \mathcal{N}_A \pi d_s^2 (1 - \theta_i) (C_{H_2SO_4} M_{H_2SO_4} + C_{SO_3} M_{SO_3}), \quad (4)$$

$$\left. \frac{dm_i}{dt} \right|_{ads,HC_j} = 0.25 \alpha_{d,HC_j} \bar{c}_{HC_j} \mathcal{N}_A \pi d_s^2 (1 - \theta_i) (C_{HC_j} M_{HC_j}), \quad (5)$$

where $M_{H_2SO_4}$, M_{SO_3} , and M_{HC_j} are the molecular weights of H_2SO_4 , SO_3 , and organic species j , respectively. The mass accommodation coefficients for the adsorption of gaseous sulfuric acid and organic species j on soot (referred to as dry accommodation coefficients), respectively $\alpha_{d,s}$ and α_{d,HC_j} , describe the sticking probabilities of vapor molecules on a bare soot surface; $\bar{c}_s$ and $\bar{c}_{HC_j}$ are the mean thermal speed for the vapor phase sulfuric acid and organic species j ; $C_{H_2SO_4}$, C_{SO_3} , and C_j are the concentrations of vapor phase sulfuric acid, vapor phase SO_3 , and vapor phase organic species j , and $\mathcal{N}_A$ is the Avogadro's number.

Thus, we obtain the mass variation of each soot particle and, a fortiori, the vapor mass variation, which leads to the coupling term $\bar{w}_{adsk}$ in Eq. (1):

$$\bar{w}_{adsk} = n \left. \frac{dm_i}{dt} \right|_{ads,k} \frac{1}{\Delta V}, \quad (6)$$

where $\left. \frac{dm_i}{dt} \right|_{ads,k}$ denotes the vapor mass variation by adsorption of species k , n is the number of particles per numerical particles, and ΔV is the grid cell volume.

Beside activation by adsorption, soot particles can be activated by scavenging sulfuric acid-water droplets. In our model, it is assumed that all soot particles/droplets of a computational particle (CP) (also called SIP for SIMulation Particle (Unterstrasser and Hoffmann and Lerch, 2017)) in a cell volume are located at the same point and have the same quantities, such as the temperature. Also, the interpolated cell grid volume should be small enough for the CP to be considered well-mixed.

For the presentation of the mathematical model, we consider a case with a CP i containing more physical particles than CP j ($v_i > v_j$, where v represents the number of physical particles per CP). If CP i is a soot particle, then it will collect some mass scavenging $m_i|_{scav,aq/non-aq}$ (a droplet) from the CP j . If CP i is a droplet, then it will collect some mass scavenging $m_i|_{scav,aq/non-aq}$ (a soot particle) from the CP j . The formulation procedure is in two steps: 1) determine the probability that the CP coagulation occurs; 2) define how a pair of CP coagulate.

The probability that a collection event will happen is evaluated by the probability $p_{crit} = v_{scav}/v_{min}$, with $v_{min} = \min(v_i, v_j)$. The number of particles scavenged is calculated from:

$$\left. \frac{dv_{scav}}{dt} \right|_{scav,aq/non-aq} = K_{ij} v_i v_j \frac{1}{\Delta V} (1 - \theta_i), \quad (7)$$

where K_{ij} is the Brownian coagulation kernel between particle i (with a diameter d_i) and particle j (with a diameter d_j), and $(1 - \theta_i)$ represents the available surface on the particle. If the particle i is a soot particle

collected from a droplet j , then θ_i is the surface coverage of the soot particle. If the particle i is a droplet collecting from a soot particle j , then θ_i is 0 since droplets do not need to be activated.

Then, the probability p_{crit} is compared to the function $\text{rand}()$, which provides uniformly distributed real random numbers from 0 to 1. A total of four cases can be distinguished, depending on the comparison between p_{crit} and $\text{rand}()$. Below is the complete definition of how a pair of CP (i, j) change after they coagulate.

In the first case, the limiter mode is activated if v_{scav} is larger than both v_i and v_j . The number of droplets collected v_{scav} is artificially reduced to v_i in such a case (let us assume that $v_i > v_j$). In the second case, the multiple collection occurs if $p_{crit} > 1$, as each particle in CP i is allowed to collect more than one droplet from CP j . In the third case, if $p_{crit} > \text{rand}()$, it is a single collection. Finally, no operation on a specific CP pair is performed if $p_{crit} < \text{rand}()$.

Self-coagulation can be considered for kernels with $K_{ij} > 0$. If $2p_{crit} > \text{rand}()$, self-coagulation occurs between the soot particles/droplets in a CP. Then, every two physical particles within a CP coagulate, implying $v_i = v_i/2$ and $m_i|_{scav,aq/non-aq} = 2 m_i|_{scav,aq/non-aq}$.

3.4.2 Condensation growth of sulfuric acid, organics and water vapors on soot particles and droplets

In the model, condensation of volatile vapors can also occur on the activated parts of the soot surfaces. Our model assumes that only water, sulfuric acid, and water-soluble organics can condense on the aqueous (hydrophilic) part of the surface, and that only water-insoluble organics can condense on the non-aqueous (hydrophobic) part. The total mass of sulfuric acid, water, and organic species j on soot particles due to condensation is calculated by:

$$\left. \frac{dm_i}{dt} \right|_{cond,s} = 4\pi D_{H_2SO_4} R_p G_{H_2SO_4} \theta_{aq,i} \left(\frac{P_{H_2SO_4} - \kappa_{aq} \alpha_{H_2SO_4} P_{H_2SO_4}^{sat}}{RT} \right) M_{H_2SO_4}, \quad (8)$$

$$\left. \frac{dm_i}{dt} \right|_{cond,W} = 4\pi D_W R_p G_W \Theta_{aq,i} \left(\frac{P_W - \kappa_{aq} \alpha_W P_W^{sat}}{RT} \right) M_W, \quad (9)$$

$$\left. \frac{dm_i}{dt} \right|_{cond,HC_j} = 4\pi D_{HC_j} R_p G_{HC_j} \Theta_{aq/non-aq,i} \left(\frac{P_{HC_j} - \kappa_{aq/non-aq} \alpha_{HC_j} P_{HC_j}^{sat}}{RT} \right) M_{HC_j}, \quad (10)$$

where R_p is the radius of soot particle including liquid layers, M_W is the molecular weight of water; $D_{H_2SO_4}$, D_W , and D_{HC_j} are the diffusivities of the vapor phase sulfuric acid, water, and organic species j in air; $P_{H_2SO_4}$, P_W , and P_{HC_j} are the vapor pressure of sulfuric acid, water, and organic species j; $P_{H_2SO_4}^{sat}$, P_W^{sat} and $P_{HC_j}^{sat}$ are the saturation vapor pressure of sulfuric acid, water, and organic species j; $\kappa_{aq/non-aq}$ is the Kelvin factor of the soot particles; $\alpha_{H_2SO_4}$, α_W , and α_{HC_j} are the activity coefficients of sulfuric acid, water, and organic species j in the soot coating liquid mixtures, and $G_{H_2SO_4}$, G_W , and G_{HC_j} are the correction factors for condensation of each species on soot particles (Pruppacher and Klett, 1998).

Although organic vapors in aircraft emissions may not contribute to the nucleation process to promote new particle formation, it has been shown that only the size and the composition (not the number) of homogeneous liquid droplets is affected by condensation (Wong et al., 2015). Consequently, the condensation growth of droplets is computed. The equations are similar to the condensation growth equation for soot particles, i.e., Eqs. (8), (9), and (10). Hence, we assume that $\Theta_{aq/non-aq,i} = 1$ for droplets since droplets do not need to be activated.

Thus, we obtain the mass variation of each particle due to condensation/evaporation of a species and, a fortiori, the vapor mass variation, which leads to the coupling term $\bar{w}_{condk}$ in Eq. (1):

$$\bar{w}_{condk} = n \left. \frac{dm_i}{dt} \right|_{cond,k} \frac{1}{\Delta V}, \quad (11)$$

where $\left. \frac{dm_i}{dt} \right|_{cond,k}$ denotes the vapor mass variation by condensation/evaporation of species k.

3.4.3 Coagulation of sulfuric acid-water droplets

Our model takes into account the coagulation between $\text{H}_2\text{SO}_4\text{-H}_2\text{O}$ liquid droplets. In this scenario, we consider a CP i containing more physical particles than CP j ($v_i > v_j$, where v represents the number of physical particles per CP). Then CP i will collect some mass scavenging $m_i|_{scav,aq/non-aq}$ from the CP j that is a droplet. The formulation procedure is in two steps: 1) determine the probability that the CP coagulation occurs; 2) define how a pair of CP coagulate.

The probability that a collection event will happen is evaluated by the probability $p_{crit} = v_{scav}/v_{min}$, with $v_{min} = \min(v_i, v_j)$. The number of particles scavenged between two droplets is computed as follows:

$$\left. \frac{dv_k}{dt} \right|_{scav,aq/non-aq} = K_{ij} v_i v_j \frac{1}{\Delta V}, \quad (12)$$

where v_i and v_j are the number of droplets in a CP i and j , respectively, ΔV is the volume of a control volume, and K_{ij} is the Brownian coagulation kernel.

Then, the probability p_{crit} is compared to the function $\text{rand}()$, which provides uniformly distributed real random numbers from 0 to 1. A total of 4 cases can be distinguished, depending on the comparison between p_{crit} and $\text{rand}()$. The definition of how a pair of CP (i, j) change after they coagulate is similar to the procedure described in Sect. 3.4.1 for soot particles and sulfuric acid-water droplets scavenging.

3.4.4 Homogeneous binary nucleation of sulfuric acid-water

In addition to the growth of existing soot particles, new liquid droplets can form through binary homogeneous nucleation (BHN). The homogeneous nucleation of organic species is characterized by very slow nucleation rates, and therefore, organic gaseous precursors do not promote the formation of new particles (Wong et al., 2015). This formation is driven by the binary homogeneous nucleation of sulfuric acid and water. The clusters that are in the process of “particle formation” need to be separated from larger liquid droplets in the particle distribution. The precise threshold between clusters and particles is

ambiguous, and varies with the property of interest (Elm et al., 2020). Since the critical size for a H_2SO_4 - H_2O cluster is around 1.5-1.7 nm (Määttä et al., 2018; Du and Yu, 2006; Arnold et al., 2012), the threshold between clusters and particles was set to 1.7 nm, meaning that only computational particles with a critical radius smaller than 1.7 nm could nucleate. Given the range of ambient conditions relevant to an aircraft plume, the nucleation rate $J_{\text{H}_2\text{SO}_4-\text{H}_2\text{O}}$ (number of new embryos formed per second and per cubic meter) in the water/sulfuric acid mixture was calculated with the cluster size, composition, and nucleation rate, using the parameterization from Määttä et al. (2018).

The H_2SO_4 - H_2O nucleation rate is highly dependent on the temperature, relative humidity, and H_2SO_4 concentration. The following empirical criterion (Seinfeld and Pandis, 2016; Casati et al., 2007) is used to decide whether H_2SO_4 - H_2O nucleation commences:

$$C_{crit} = 0.16 \exp(0.1 T - 3.5 RH - 27.7), \quad (13)$$

where RH is the relative humidity on a scale ranging from 0 to 1, and T is the temperature of the gas phase. When the gas phase concentration of H_2SO_4 exceeds C_{crit} , the nucleation of H_2SO_4 - H_2O embryos starts. As in Wey and Liu (2007), the gas depletion for H_2SO_4 due to the nucleation process is calculated by:

$$\frac{dm_{\text{H}_2\text{SO}_4}}{dt} = J_{\text{H}_2\text{SO}_4-\text{H}_2\text{O}} \frac{n_{tot}^* (1 - x^*) M_{\text{H}_2\text{SO}_4} V_0}{\mathcal{N}_A}, \quad (14)$$

where $M_{\text{H}_2\text{SO}_4}$ is the molecular weight of the sulfuric acid, n_{tot}^* is the number of molecules in the critical cluster, x^* is the mole fraction of sulfuric acid in the critical cluster, V_0 is the initial volume of the cluster, and $\mathcal{N}_A$ is the Avogadro's number. The gas depletion for H_2O due to the nucleation process is calculated by:

$$\frac{dm_{\text{H}_2\text{O}}}{dt} = J_{\text{H}_2\text{SO}_4-\text{H}_2\text{O}} \frac{n_{tot}^* x^* M_{\text{H}_2\text{O}} V_0}{\mathcal{N}_A}, \quad (15)$$

where M_{H_2O} is the molecular weight of the water vapor. The nucleation rate for H_2SO_4 - H_2O liquid droplets (Kärcher, 2003) is evaluated by:

$$\frac{dn_k}{dt} = J_{H_2SO_4-H_2O}, \quad (16)$$

where n_k is the number density of liquid droplets.

Thus, we obtain the mass variation of each particle due to the nucleation of the species and, a fortiori, the vapor mass variation, which leads to the coupling term $\bar{w}_{nuclk}$ in Eq. (1):

$$\bar{w}_{nuclk} = n \frac{dm_k}{dt} \frac{1}{\Delta V}, \quad (17)$$

where $\frac{dm_k}{dt}$ denotes the vapor mass variation by nucleation of a liquid droplet of species k .

4. Methods

4.1 Characteristics of the organic gaseous species at the exhaust

The APEX campaign provides a large quantity of organic compounds from 4 to 100% engine power settings for a CFM56-2C1. Recent field measurements by Kılıç et al. (2017) characterized organic emissions at 1.5 m behind different aircraft engines to identify gaseous organic species for engine power settings ranging from 4 to 100%. In Kılıç et al. (2017), a ranking of 109 organic species by mass-based emission index (EI_m) indicates that from 34 to 22 species represent most (70%) of the emissions seen between 4 and 100% engine power settings on the basis of the (EI_m). The molar fractions of gaseous organics species were calculated from the index emission of Kılıç et al. (2018) and Wey et al. (2006).

The computation of the effective saturation concentration C^* allows to know the capacity of a volatile compound to condense at a specific temperature. The effective saturation concentration of organic species from Kılıç et al. (2017) have an effective saturation pressure that range from 10^4 to 10^{10} mg m⁻³ at room temperature (i.e. 300K) (refer to intermediate volatile and volatile organic compounds (IVOC/VOC) (Huang et al., 2021)). However, measurements showed that for a CFM56-2B1, the effective saturation

concentration of organic species in plumes can be as low as 10^{-2} mg m⁻³ for low vapor saturation pressure organic compounds (Presto et al., 2012). As our goal is to select typical organic surrogate species emitted from a large volatility range and allow interactions of volatile organics and aircraft-emitted soot particles, we had to consider volatile organics having vapor pressures low enough for them to condense onto soot particles. Consequently, we added four additional organics species, namely, C₁₄H₁₀, C₁₆H₁₀, C₂₀H₁₂ and C₂₂H₁₂ to obtain a more representative set of organic compounds in a plume. For those four species, the effective saturation pressure range from 10^{-2} to 10^3 mg m⁻³ at room temperature (i.e., 300K) (refer to low- and semi-volatile organic compounds (LVOC/SVOC) (Huang et al., 2021)). The emission indices for these species were taken from (Presto et al., 2012; Jathar et al., 2012) for a CFM56-2B1. A list of organic surrogate species selected for each regime for our modeling work is provided in Table 1.

Table 1

4.2 Microphysics implementation

4.2.1 Coagulation algorithm

The Lagrangian particle tracking microphysics module considers each computed particle one by one. Consequently, the information on computed particles (soot particles or liquid droplets) is stored in an array with up to 147 attributes (in the form of columns) characterizing the represented aerosol. Besides microphysical quantities (mass adsorbed/collected/condensed for each species), other quantities, such as the position $\mathbf{x}_p$ or the number of physical particles v_p , are also stored.

To simulate the coagulation process, the associated time step Δt_c is defined. Particles coagulate in a grid cell of a volume ΔV at the probability p_{crit} . At every time step Δt_c , a list of CP is created in the grid cell, where N_{CP} is the total number of CP in the cell. In that list, CP are permuted randomly, as per Shima et al. (2009). The coagulation algorithm simply checks each i-j combination for a possible collection event, by computing the probability p_{crit} . We ensure there is no overlapping, and therefore, that no CP could coagulate twice, in order to reduce the computation cost. As well, the linear sampling version of AON is

included in the model (Shima et al., 2009; Unterstrasser and Hoffmann and Lerch, 2020). $[N_{CP}/2]$ combinations of pairs $i-j$ are selected, with each CP appearing in exactly one pair (if N_{CP} is odd, one CP is ignored). As only a subset of all possible combinations is numerically evaluated, the extent of collisions is underestimated. To compensate for this, the probability p_{crit} is upscaled by a scaling factor γ_{corr} :

$$\gamma_{corr} = \frac{N_{CP}(N_{CP} - 1)}{2 \binom{N_{CP}}{2}}, \quad (18)$$

to guarantee an expectation value as desired. As our number of particles (around 300,000) and the storage array (147 columns for the soot particles array) are large, the linear sampling represents a good compromise providing computational cost savings.

The coagulation module was validated using the scenario set-up from Vemury and Pratsinis (1995) to evaluate the self-preserving size distributions (SPSD) in both free molecular and continuum regimes. The results showed strong agreement with the reference in the free molecular regime, with only minor discrepancies in dimensionless number concentration observed in the continuum regime. A comparison of geometric standard deviations with the theoretical SPSP values revealed discrepancies of less than 0.6%.

4.2.2 Properties of liquid organics mixture

To incorporate the organic surrogate species above in our microphysical model, certain approaches for estimating the species' physical and thermodynamic properties were implemented into the model, as in Wong et al. (2014). The boiling points and critical properties (i.e., critical temperature, pressure, volume, and compressibility factor) of the pure organic surrogate species are necessary for this estimation. The group contribution method of Nannoolal et al. (2004) and Nannoolal and Rarey and Ramjugernath (2007) was used to calculate the boiling points and critical properties. The density of a liquid mixture of sulfuric acid, water, and water-soluble organics (for the hydrophilic coverage) and of a liquid mixture of water-insoluble organics (for the hydrophobic coverage) was estimated by the Rackett equation, with the Li mixing rule (Poling and Prausnitz and O'Connell, 2001). The empirical relationship developed by Brock

and Bird was used to calculate the surface tension of a pure organic surrogate species (Poling and Prausnitz and O'Connell, 2001). The surface tension of a liquid mixture soot coating was assumed to be the molar averaged surface tension of all the species in the mixture. Activity coefficients of the components in liquid mixtures were evaluated following the principles given by Clegg and Seinfeld (2006). Since two different phases, aqueous and non-aqueous, are tracked on a soot surface, the activity coefficients of sulfuric acid, water, and the organic species were calculated separately in two phases. For the aqueous fraction, the aqueous liquid mixture was further divided into two independent components (sulfuric acid-water solution and aqueous organic solution). We assume that the interactions between the sulfuric acid-water solution and aqueous organic solution are negligible. The empirical relationship developed by Taleb and Ponche and Mirabel (1996) was used to calculate the activity coefficients of sulfuric acid and water in an aqueous sulfuric acid solution. The modified UNiVersal quasi-chemical Functional group Activity Coefficients (UNIFAC) group contribution model (Gmehling and Li and Schiller, 1993) was used to calculate the activity coefficients of the organic species in both aqueous and non-aqueous organic solutions. Finally, if available, the experimental saturation vapor pressure of an organic surrogate species expressed as the Antoine Equation was used. For heavier organic species without an experimental saturation vapor pressure, the group contribution method developed by Nannoolal and Rarey and Ramjugernath (2008) for the estimation of the vapor pressure of organic species was used for both water-soluble and water-insoluble organic species.

4.2.3 *CFD coupling with the microphysical model*

For microphysics, a fourth-order Runge-Kutta scheme was used, which is deemed less diffusive, to solve the equations governing particle activation/growth (Eqs. (4), (5), (8), (9), and (10)) and surface coverage change (Eq. (3)). Furthermore, the condensation model was tested and showed no broadening of an initial size distribution of monodisperse droplets with the simulation time. The microphysical module was implemented as a user-defined function in the commercial CFD code in STAR-CCM+ v2020.2. The methodology for coupling with the CFD solver is detailed in Figure 3. Microphysical processes and particle

storage are computationally expensive and time-consuming. To accelerate computations, we distribute mesh cells containing at least one computational particle to multiple computing cores, leveraging parallel computing techniques for more efficient simulations.

Figure 3

Three time steps, $\Delta t = 0.005 \text{ s}$ for idle (4%), taxi (7%), and approach (30%), while $\Delta t = 0.0005 \text{ s}$ and 0.0002 s for climb (85%), and take-off (100%), are respectively chosen, ensuring the Courant–Friedrichs–Lewy number does not exceed 1.0 along the plume. Convergence is determined once the average residuals of the continuity, momentum, energy, and equations decrease at least four orders of magnitude at each time step. Since the coagulation process is very sensitive to rapid humidity or temperature changes, the dynamical time step Δt may be sub-cycled (divided into smaller steps) Δt_c . The sub-step time calculation for the coagulation processes is based on the coagulation timescale (Zhao and Zheng, 2013). For condensation, the dynamical time step Δt is relatively comparable to the condensation characteristic timescale τ_c (around 0.001 s). A time step of 0.001 s is sufficiently small to account for the fast diffusional growth at high plume super-saturations (Bier and Unterstrasser and Vancassel, 2021).

4.3 CFD setup

4.3.1 Aero-thermodynamics conditions

The first task required to simulate the evolution of aero-engine emissions (gaseous and particulate) in the early plume at different Landing Take-Off (LTO) power settings is to estimate exhaust properties at the engine-exit plane. The strategy is similar to (Cantin et al., 2022). The software GASTURB (thermodynamic cycle program) (Kurzke, 2004) was used to determine the thermodynamic cycle at different LTO power settings. A generic two-spool, unmixed-flow, and turbofan engine configuration was chosen to model the CFM56-2C1 engine. The model was calibrated to simulate the conditions of APEX-1 tests Nos. 908, 914, 913, 928, and 909 for engine powers settings from 4 to 100% (Wey et al., 2006). The engine design parameters, such as the thrust settings, bypass ratio, overall pressure ratio, and mass flow rates of the core and the bypass, were gathered from Jane’s All the World’s Aircraft (Jackson and Munson, 2004) when

available. The fuel flow rates at various power settings were taken from the APEX-1 data and the International Civil Aviation Organization (ICAO) Emission Databank (ICAO, 2017). Based on these parameters, the temperature, pressure, and velocity were calculated at various engine stations, including the engine-exit plane. The latter were used as initial thermodynamics conditions for the CFD model.

Table 2 presents the engine exhaust conditions used at five different engine power settings: 4, 7, 30, 85, and 100%, as given by the gas turbine cycle program GASTURB. These conditions were set at the core and bypass duct inlets. The properties of soot particles at the exhaust nozzle from APEX-1 measurements are also presented. The soot particle size distribution follows a log-normal, meaning that all the particles have a different radius. The initial profile distribution for soot particles is computed from Jacobson (2005) as a lognormal:

$$n_i = \frac{N\Delta d_i}{d_i\sqrt{2\pi}\ln(\sigma_g)} \exp\left(\frac{-\ln^2(d_i/\bar{D}_M)}{2\ln^2(\sigma_g)}\right), \quad (19)$$

where N is the total number concentration of particles, n_i is the number concentration of the computational particle i , d_i is the diameter of the computational particle i , $\bar{D}_M$ is the geometric mean number diameter, and σ_g is the geometric standard deviation.

Freshly emitted soot particles are composed of several nanometre-sized primary spherules combined into aggregates (Wang et al., 2019). However, the soot morphology quickly evolves (few meters from the exhaust) from a linear chain-like aggregate into a more compact spherical aggregate shape, a process called soot morphology restructuring. This process is accelerated under conditions closer to supersaturation (Bessagnet and Rosset, 2001), at high engine power settings (Saffaripour et al., 2020), or when soot are liquid-coated with gaseous species such as sulfuric acid (Pagels et al., 2009) or aromatic precursors (Schnitzler et al., 2014). Hence, assuming a rapid soot morphology restructuring, a spherical shape for soot aggregates is considered. To accurately model the soot surface activation and the adsorption of gaseous species on soot aggregates, the soot distribution was initialized with the geometric mean diameter of soot

aggregates from APEX-1 measurements (Saffaripour et al., 2020; Lobo et al., 2007), rather than the GMD of primary soot spherules.

Even if soot aggregates restructure rapidly into spherical structures, they are still porous at the engine exit, having packing densities of 0.25-0.5 (Sipkens and Corbin, 2024), which underestimates the real surface area of soot aggregates. To evaluate the underestimation in terms of soot surface area related to the use of GMD of restructured soot aggregates (nonporous structure), the number of primary particles in a soot aggregate was computed according to Kelesidis et al. (2018). Using primary particle data and the GMD of soot aggregates of nvPM for a CFM56-7B26/3 (Abegglen et al., 2015; Liati et al., 2014), the calculation of the surface area of soot aggregates considering primary particle was performed using the equation by Brasil and Farias and Carvalho (1999) with an overlapping coefficient of 0.14 (Sipkens et al., 2023). Assuming spherical soot aggregates, the underestimation in terms of GMD is below 7%, which remains within the uncertainties of soot GMD measurements (Boies et al., 2015; Saffaripour et al., 2020).

For $\text{H}_2\text{SO}_4/\text{H}_2\text{O}$ molecular clusters, the mean particle radius is set to 0.277 nm according to Kärcher et al. (2007), while the initial mass fraction of H_2SO_4 is set to 0.45 (Karcher et al., 1998). The static temperature and pressure values are $T_{amb} = 293 \text{ K}$ and $P_{amb} = 930 \text{ hPa}$, respectively. The mole fraction of water vapor in ambient air is set at $X_{amb} = 4.267 \cdot 10^{-3}$ to account for a 17% relative humidity, for comparison with experimental results (Wey et al., 2006).

Table 2

4.3.2 Computational domain and grid

A 2D axisymmetric representation of the engine nozzle was considered for URANS calculations, as shown in Figure 4. The geometry of the CFM56-2C1 short-cowl nozzle is composed of a core and a bypass flow with diameters $D_c = 0.695 \text{ m}$ and $D_b = 1.508 \text{ m}$, respectively. In the engine geometry, the duct from the outlet of the exhaust nozzle plane was modeled in order to promote the development of the boundary layer on each side of the jet. The nozzle configuration is representative of a CFM56-2C1 engine, in which

a central plug is included to encourage early mixing between the core and the bypass flows (here, the inner shear layer).

As shown in Figure 4, the computational domain had a radius $R = 10 D_b$, and a length $L = 134 D_b$ to ensure ambient pressure at far-field boundaries. Three inlet sections were used upstream: a freestream pressure inlet (P_{amb}^0, T_{amb}^0), a bypass pressure inlet (P_b, T_b), and a core pressure inlet (P_c, T_c). A no-slip adiabatic condition was imposed on engine walls, while a symmetry condition was used on both lateral places. The azimuthal boundary was treated as a slip condition while the far-field axial boundary was set as a far-field condition.

A grid convergence study of the gaseous phase was performed for a high and low engine power case (7 and 100%) using three grids: coarse (53,000 cells), medium (81,000 cells), and fine (189,000 cells), respectively labelled grid 1, 2, and 3. For the gaseous phase, the mean errors computed in the inner shear layer (i.e., between the core and the bypass jets) for the static temperature, water vapor mass fraction, and axial velocity were below 2% between the medium and the fine grid. Furthermore, discretization errors estimated using the GCI method (Celik et al., 2008) at a probe point ($r = 0.7 D_c, y = 1 D_b$) were sufficiently low with the medium mesh. As such, computations were only performed on the medium grid.

The medium grid is mainly composed of hexahedral elements and boundary prismatic cells, as shown in Figure 4-c. Refinement blocks were used in the duct of the core and the bypass flow, as well as in the near field of the engine nozzle ($< 20 D_b$) to capture high gradients in the shear layer ($\Delta x = 0.03 D_b$). Then, the mesh in the far field was relatively coarser, with cells about $\Delta x = 0.15 D_b$. Typically, the cell anisotropic size in the duct is $\Delta x = 0.02 D_b$. The near-wall refinement ensured a maximum $y^+ < 5$, allowing to resolve the boundary layer with a wall law function.

Figure 4

5. Model validation – results analysis

In this section, the results regarding plume dynamics, along with a validation of the plume with the APEX-1 and -2 campaigns in the exhaust jet of a CFM56-2C1 aircraft engine, are introduced. Then, the validation about the emission index of main species and minor species is presented. Finally, the results for the microphysical model are presented in terms of the validation of the size particle distribution, the emission index in terms of both number and mass, and the composition of soot particles and liquid droplets.

5.1 Model validation

5.1.1 Plume dynamics

Figure 5 shows a comparison of the predicted and measured properties, such as the velocity (Figure 5-a), temperature (Figure 5-b), and exhaust gas fraction (Figure 5-c), in the near field of a CFM56-2C1 at 30 m downstream. These conditions were chosen to approximate APEX-1 conditions, where the ambient temperature ranged from 290 to 310K, and the ambient relative humidity ranged from 7 to 17%. Our results are compared with APEX-1 measurements across engine power settings ranging from 4 to 100%. We observe good agreement between our predictions and the measurements for all quantities. The results show that the predicted properties (velocity, temperature, and exhaust gas fraction) increase monotonically with increasing engine power. At 100% engine power, the plume contains a higher exhaust gas fraction than at lower power settings, indicating that the fraction of exhaust species at the centerline of the jet decreases more slowly.

Figure 5

Figure 6 illustrates the stream-wise (xy-plane) contours of the exhaust plume temperature at the idle and take-off regimes. The mixing of the two streams (core and bypass flow) with ambient air downstream cools the plume and decreases the temperature. Between the two streams, the shear layer is clearly more spread out for take-off as compared to the idle regime after $x/D_b = 3$. The difference of the mixing between the idle ($u_{core} = 41.8 \text{ m.s}^{-1}$) and take-off ($u_{core} = 208.3 \text{ m.s}^{-1}$) regimes is attributed to the disparity in jet speed with a lower ambient air speed ($u_{amb} = 1 \text{ m.s}^{-1}$). This difference increases the thickness of the

shear layer extending radially. Moreover, since the exhaust gas temperature at the nozzle throat is lower in the idle regime, the jet plume in take-off conditions exhibits a relatively higher temperature ($\sim 830\text{K}$) as compared to the idle plume ($\sim 700\text{K}$) on the jet centerline up to $x/D_b \approx 2$.

Figure 6

5.1.2 Gas phase emissions

Figure 7 compares the CFD-predicted emission indices (EI) (kg.kg fuel^{-1}) with APEX measurements for major (1st row) and minor (2nd and 3rd rows) species at probes located at a distance 1, 10, and 30 m behind the aircraft. Although chemical reactions are computed for only major gaseous species in the jet plume, the model's EI predictions showed a good agreement with APEX measurements, with discrepancies being below one order of magnitude. These results demonstrate the model's capacity to predict reasonably well the plume chemistry of both major (NO , SO_x , NO_x) and minor (HCs) species over the full range of LTO engine power settings. For instance, the EI of CO decreased as the power increased from 4 to 85%, and then increased slightly from 85 to 100% power. The model also accurately captures the plume mixing, as evidenced by the decrease in EI from 1 to 30 m for all species. The greatest difference in EI between 1 and 30 m is observed for lower engine power settings (4 and 7%), where the predicted exhaust gas fraction is lower at 30 m, as shown in Figure 5-c.

Figure 7

5.1.3 Particulate emissions

Figure 8 compares the CFD-predicted EI_n (kg fuel^{-1}) and particle diameter (nm) of both non-volatile PM (1st row) and total PM (2nd row) with APEX-1 measurements at distances of 1, 10, and 30 m downstream from the engine exhaust. At 1 and 10 m, the EI_n values of nvPM align well with the measurements. At 30 m, small discrepancies emerge for engine power settings below 30%, with the predicted values being about two orders of magnitude lower than the measurements. From 10 m to 30 m, the results show a constant value of the EI_n for all engine power settings.

Total PM El_n measurements show an increase between 10 and 30 m that is primarily attributed to the homogeneous nucleation of new vPM. However, the numerical results suggest that the variation in El_n for total PM and nvPM is not significant for all locations and engine power settings, indicating that new vPM are not formed in the plume, at least within the first 30 m. Indeed, new vPM could have been formed in the sampling system, as shown by (Wong et al., 2008; Onasch et al., 2009). Also, the relatively high temperature in the plume ($>297.5\text{K}$) may prevent the homogeneous nucleation of particles according to Wong et al. (2008).

Overall, the geometric mean diameter (GMD) of nvPM falls within the uncertainty range of APEX measurements, as shown in Figure 8. Non-volatile PM diameter results exhibit an increase in the plume distance for low power settings ($\leq 7\%$), while decreasing for higher power settings ranging from 1 to 30 m. Experimental observations reveal a linear increase in diameter as a function of power settings, and yet the diameters are consistently lower at 30 m as compared to at 1 m, consistent with the power thrust numerical results above 30%. The total PM results show an increase in particle diameter with increasing power until 85%, followed by a slight decrease. Our findings indicate good agreement in total particle diameter at 30 m for engine power thrust below 30%, but a slight overestimation is observed for higher power regimes. As already mentioned, this suggests that freshly nucleated vPM were detected in the sampling system, exhibiting a mean size diameter of 12 nm (smaller than that of nvPM) and consequently decrease the mean particle size at 30 m (Wey et al., 2007). At high engine power thrust, a large dispersion of the GMD measured is observed in the data 30 m downstream, depending on the ambient temperature (Lobo et al., 2007). For runs with higher ambient temperature, the GMD was larger ($\sim 35\text{ nm}$), while the reported GMD was smaller ($\sim 20\text{ nm}$) for runs with lower ambient temperature. Higher ambient air temperature suppresses nucleation in the plume, reducing the population of small nucleation-mode particles and increasing the GMD.

Figure 8

The particle number ratio of nvPM to total PM EI_n provides an effective means of assessing the EI_n of vPM. To evaluate the presence of volatile PM, the evolution of the particle number ratio up to 80 m downstream of the engine is illustrated in Figure 9. At a thrust of 30%, the PM number ratio begins to decrease at around 20 m, while for lower power regimes (4 and 7%), this decline becomes more pronounced at distances between 60 and 70 m. Remarkably, the PM number ratio remains constant at a unity value for 85%. These results suggest that volatile PM of sulfuric acid are minimally formed at 30 m, specifically under atmospheric conditions characterized by an ambient temperature of 293 K and an ambient relative humidity of 17%.

Binary homogeneous nucleation of H_2SO_4 - H_2O is mainly dependent on ambient conditions, but is also influenced by H_2SO_4 concentration (Määttä et al., 2018). Sulfuric acid is emitted in significantly higher quantities at the exhaust plane nozzle ($X_{H_2SO_4} = 2.17 \cdot 10^{-9}$), specifically at 30% engine power, as compared to other regimes ($X_{H_2SO_4} \approx 10^{-10}$), with a magnitude difference of one order of magnitude (Bisson et al., 2016). Furthermore, the static plume temperature at 30 m for 30% engine power ($\sim 309K$), is lower compared to the higher regime ($\sim 322-328K$), as illustrated in Fig. 5-b. This temperature difference suggests that the formation of volatile particulate matter (vPM) through binary homogeneous nucleation of H_2SO_4 - H_2O might be more favorable at mid-thrust conditions, of approximately 30%.

Figure 9

The soot mode calculation evaluates the performance of the microphysical model in terms of adding mass through adsorption, condensation and scavenging to soot particles. The sulfate and organic mass-based emission indices (EI_m) as a function of engine power at the 30 m location behind the engine is depicted in Figure 10. Experimental data were averaged from Aerosol Mass Spectrometer (AMS) measurements during the APEX-1 campaign (Wey et al., 2006), where the ambient temperature ranged from 290 to 310 K and the ambient relative humidity varied from 7 to 17%.

The model captured reasonably well the global trend of PM microphysics in a near-field aircraft plume at ground level, showing a decrease in EI_m soot mode for organic compounds and sulfate from low power to 30%, then an increase for higher engine power settings. The sulfate and organic mass-based emission indices increase as a function of engine power, indicating a significant increase in the surface area of the soot mode, with more gas phase components condensing on the pre-existing surface area.

For organic mass loading on soot particles, the model results agree very well with experimental data for high power settings ($\geq 85\%$) but over-predict the EI_m of organic compounds by about one order of magnitude for other engine power settings. One potential explanation for this difference is that the numerical model does not incorporate contributions from organic-enhanced nucleation processes, potentially leading to an overestimation of mass loading on soot particles at low engine power settings. Numerical results regarding sulfate mass loading across all engine power settings show good agreement, especially for engine thrusts $\leq 85\%$, where discrepancies are below one order of magnitude.

Figure 10

Figure 11 presents the particle size distribution (PSD) of nvPM as a function of the particle diameter at 7, 30, 85, and 100% engine power at 30 m. Results are compared with experimental measurements from APEX-1. Initially, nvPM emissions exhibit a log-normal distribution in a single mode. Plume mixing primarily affects the particle number density as the coagulation of soot particles is not considered in this paper. The activation process increases the surface coverage of soot particles with adsorption of gaseous species and scavenging of H_2SO_4/H_2O droplets. At high power levels, a significantly greater portion of condensed material appears as coatings as compared to low thrust levels, as evidenced by the mean particle radii reaching 18 nm and 22 nm for 7 and 100% engine power. Larger particles with a higher particle number are observed for 100% as compared to at 7%. As an example, the emission index of nvPM with a mean diameter of 100 nm is 100 times bigger at 100% than at 7%. At lower power settings, the mean particle radius shifts towards smaller radii (leftward), while higher PSDs at higher power settings exhibit

larger particle radii. The model accurately predicts the PSD. Particle number raw data were fitted using a single-mode log-normal function (Moore et al., 2017) of the form:

$$\frac{d(EI_{n,i})}{d(\log(D_p))} = \frac{N}{\sqrt{2\pi}\log(\sigma_{g,i})} \exp\left(-\frac{(\log(D_p) - \log(D_{g,i}))^2}{2(\log(\sigma_{g,i}))^2}\right), \quad (20)$$

where N is the total particle number, $EI_{n,i}$ is the corresponding number emissions index, D_p is the dry particle diameter, $D_{g,i}$ is the geometric mean diameter, and $\sigma_{g,i}$ is the geometric standard deviation.

Figure 11

To conclude on the validation results, the model is able to predict the evolution of nvPM in terms of their particle number, size and chemical composition within the first 30 m at 4, 7, 30, 85, and 100% thrust engine power levels. The next sub-section analyzes PM composition results.

5.2 Effect of engine power setting on PM composition

Results indicate that volatile particles are not formed within the first 30 m. This section provides more in-depth insights into the chemical composition of soot and volatile particles up to 50 m downstream of the engine, as volatile particles are formed at that distance. Figure 12-a presents the predicted mass fraction of soot coatings as a function of engine power settings at 50 m downstream, for organics compounds and sulfuric acid. As expected, organic compounds dominate the composition of soot coatings for all engine power settings as compared to sulphuric acid. Indeed, Onasch et al. (2009) found that organic mass loading on soot particles is higher than for sulfates in the near field (30 m) for all regimes. This aligns with Figure 10, confirming that the coatings are dominated by organic species. The contribution of organic compounds, as compared to sulfuric acid, to soot composition is high at low regimes, decreases around mid-thrust ($\approx 30\%$), and then increases at high power, which is well captured.

At low regimes ($\leq 7\%$), around 99.5% and 98.2% of the total mass fraction consists of organic compounds, that is consistent with measurements for a CFM56-2C1 by Yu et al. (2019) when comparing

the mass partitions between organic and sulfate compounds for the soot mode at low thrust ($\leq 7\%$). These authors reported mass partitions of $97 \pm 9\%$ and $79 \pm 8\%$ for organic compounds at 4 and 7% thrust, respectively. At 30% thrust, the contribution of organic compounds reaches 85%, which is higher than the $42 \pm 15\%$ mass partition measurement results found by Onasch et al. (2009). Their contribution increases for higher engine power settings to reach 93-95%. Given that our value of El_m for organic compounds closely matches the measurements in Figure 10, we believe that the over-prediction of mass emissions indices of organic compounds is due to the fact that our model does not incorporate contributions from organic-enhanced nucleation processes.

Figure 12

The results confirm that the adsorption of gaseous species is the most dominant microphysical process for all regimes. This is evident from the mass fraction of soot coatings, where it can be seen that the adsorption of organic compounds dominates at 50 m, as shown in Figure 12-b. During idling (thrust $\leq 7\%$), less sulphuric acid is adsorbed as compared to in higher regimes. Also, at lower engine power, more organic species condense onto soot particles since the temperature is relatively low as compared to higher engine power settings. However, the temperature is too high to allow the condensation of sulfuric acid and water vapor on soot particles in the near field. Additionally, activation by scavenging of droplets remains insignificant for all engine power settings at that distance.

The detailed composition of soot coatings and different compound classes of soot mode particles and homogeneous nucleation mode particles at 50 m in terms of mass fraction for all engine power settings is illustrated in Figure 12-c and -b, respectively. The results illustrate that engine power settings do have an impact on soot coatings. Acid class compounds increase with increasing power, while carbonyls and aromatics decrease. Carbonyls dominate with 56-49% at low-medium thrust ($\leq 30\%$), while acid class compounds account for 52% among other species at 100% engine thrust. At 4% thrust settings, the most abundant compound classes at the engine exit plane are carbonyls, aromatics, and non-aromatics, with mass

fractions of 50, 22, and 15% of the total organic species, respectively. Interestingly, these families contribute the most to soot coatings in terms of mass fraction in the near field. The organic species of these families were initialized with the highest initial molar fraction, as compared to the species of other families, making them major components. Wong et al. (2014) suggest that the activation of soot surfaces is driven more by the adsorption of volatile vapors than by condensation in the first 10 m downstream since at that point, the temperature of the exhaust plume is still too high for most species to condense. As activation is mainly driven by the concentration of species, this means that the most abundant species at the exhaust contribute the most to soot mass loading. This is also confirmed for 100% power settings, where carbonyls, acids, and non-aromatics contribute the most, with mass fractions of 26, 52, and 12% of the total organic species, respectively. The contribution of sulfuric acid to soot coating becomes relevant for thrust settings above 30%, as its mass fraction reaches 15% of the total species and decreases with increasing power.

Regarding the composition of volatile PM in Figure 12-d, low regimes ($\leq 7\%$) favor organic condensed material, as compared to higher regimes. The carbonyls and aromatics families account for 31% of the total mass fraction composition on volatile PM at 4%, whereas alcohols contribute to 18% of the mass fraction at 7%. For the other regimes, the composition is nearly the same as the initial one, with a distribution of 55 and 45% for water vapor and sulfuric acid, respectively.

Figure 13

Figure 13 displays the predicted hydrophilic and hydrophobic soot surface coverages at 50 m downstream of the engine exit plane as a function of engine power settings. The figure indicates that soot particles are more covered with liquid layers at low regimes (thrust $\leq 7\%$) than at higher regimes. Surface coverage decreases from almost 100% to 15% with increasing power, indicating that particles get drier with increasing thrust. One explanation may be that the surface area (i.e., the increasing number of liquid-coated soot particles) of the soot mode dramatically increases with engine power, with decreasing organic gaseous emissions, causing sulfuric acid and organic compounds to be taken up by more available soot surface. This

leads to a lower quantity of adsorbed material with increasing power. Additionally, more particles are activated at low regimes, as the residence time is higher at low regimes than at high regimes for particles at 30 m, allowing more materials to condense. This is consistent with the findings by (Wong et al., 2008). The mass fraction of water-insoluble species drops from 31% to 2% with increasing engine power settings, indicating that more water-insoluble organic species are taken up by soot particles at low regimes. For water-soluble species, our results showed that the proportion of water-soluble species is higher at low regimes, around 67%, and decreases to 13% at 100% power settings.

6. Conclusions

This study presents a CFD-microphysics coupling approach for accurately predicting the evolution and formation of liquid-coated soot particles) and volatile particulate matter (vPM) in near-field aircraft-emitted plumes at ground level. The approach employs a Eulerian-Lagrangian online coupling, based on a 2D axisymmetric Computational Fluid Dynamics (CFD) framework for engine plume dynamics coupled with a tabulated chemistry (60 reactions with 22 reactive species and 47 non-reactive species) and a detailed microphysical model. This model considers intricate multicomponent interactions involving organic vapors, sulfur species, and soot particles emitted by the aircraft.

Model validation against APEX measurements demonstrated the model's predictive capabilities in capturing jet plume aero-thermodynamics at a distance of 30 m. Gaseous chemistry evolutions, including emission indices of major pollutants such as NO_x , CO, SO_2 , and other condensable organic species were validated against experimental data from APEX-1. The proposed model's predictions exhibit a reasonable agreement with measurements for emission indices and a particle diameter of nvPM and total particles within the 1 to 30 m downstream range.

The results confirm that organic species dominate over sulfuric acid and water vapor soot coatings in the near field for all power settings. Organic compounds such as acids increase and carbonyls/aromatics decrease with increasing engine power. Microphysical processes affecting soot particles, such as

condensation, scavenging, and adsorption, were also examined. Soot surface activation was primarily driven by the adsorption of volatile vapors, particularly within the initial 50 m downstream. Notably, the adsorption of organic compounds emerged as the dominant process for all engine power settings, with lower power regimes promoting the condensation of organic gaseous species due to lower plume temperatures. The study underscores the significance of volatile particulate matter, highlighting limited droplet formation at 30 m for engine power at 30%, whereas no liquid droplet formed for other engine power settings. A composition analysis of volatile PM reveals distinct variations, with carbonyls and aromatics dominating at lower power regimes, while alcohol contributes significantly at 7% at 50 m.

This study found similar trends with 1D plume modeling regarding droplet formation at 30 meters for engine power at 7%. The activation of soot surfaces is driven more by the adsorption of volatile vapors rather than by condensation in the first 10 meters downstream. As such, simpler dilution models are capable of modeling aerosol formation as well as complex calculations that include CFD-microphysics coupling with chemistry in the near-field. However, these models might yield different results regarding aerosol properties at larger plume scales and cruise flight conditions. In such cases, when mixing is strong and the wake vortex plays an important role in the plume dynamics, plume microphysics might need to be coupled with detailed flow modeling.

In conclusion, our findings provide valuable insights into the intricate dynamics of particle formation in aircraft engine plumes, elucidating the interplay between engine power settings, particle composition, and microphysical processes. These results enhance our understanding of aviation-related particulate emissions. Furthermore, the developed modeling tool can be instrumental in studying the influence of ambient atmospheric conditions or engine parameters on PM evolution and can be upgraded to incorporate ice-microphysics for contrail formation.

Acknowledgments

CFD computations were carried out on the supercomputer Narval at École de technologie supérieure. This research was enabled in part by support provided by Calcul Québec (calculquebec.ca) and the Digital Research Alliance of Canada (alliancecan.ca).

Funding

This study was supported by Safran Aircraft Engines (SAE).

Disclosure statement

The authors report there are no competing interests to declare.

ORCID

Sébastien Cantin <https://orcid.org/0000-0002-9502-3162>

Mohamed Chouak <https://orcid.org/0000-0001-9924-0765>

References

- Abegglen, M., Durdina, L., Brem, B. T., Wang, J., Rindlisbacher, T., Corbin, J. C., Lohmann, U., and Sierau, B. 2015. Effective density and mass–mobility exponents of particulate matter in aircraft turbine exhaust: Dependence on engine thrust and particle size. *J. Aerosol Sci.* (88):135-147. doi:10.1016/j.jaerosci.2015.06.003.
- Arnold, F., Pirjola, L., Rönkkö, T., Reichl, U., Schlager, H., Lähde, T., Heikkilä, J., and Keskinen, J. 2012. First Online Measurements of Sulfuric Acid Gas in Modern Heavy-Duty Diesel Engine Exhaust: Implications for Nanoparticle Formation. *Environ. Sci. Technol.* 20 (46):11227-11234. doi:10.1021/es302432s.
- Bessagnet, B. and Rosset, R. 2001. Fractal modelling of carbonaceous aerosols—application to car exhaust plumes. *Atmos. Environ.* 28 (35):4751-4762. doi:10.1016/S1352-2310(01)00279-5.
- Beyersdorf, A. J., Thornhill, K. L., Winstead, E. L., Ziemba, L. D., Blake, D. R., Timko, M. T., and Anderson, B. E. 2012. Power-dependent speciation of volatile organic compounds in aircraft exhaust. *Atmos. Environ.* (61):275-282. doi:10.1016/j.atmosenv.2012.07.027.
- Beyersdorf, A. J., Timko, M. T., Ziemba, L. D., Bulzan, D., Corporan, E., Herndon, S. C., Howard, R., Miake-Lye, R., Thornhill, K. L., Winstead, E., Wey, C., Yu, Z., and Anderson, B. E. 2014. Reductions in aircraft particulate emissions due to the use of Fischer-Tropsch fuels. *Atmos. Chem. Phys.* 1 (14):11-23. doi:10.5194/acp-14-11-2014.
- Bier, A., Unterstrasser, S., and Vancassel, X. 2021. Box model trajectory studies of contrail formation using a particle-based cloud microphysics scheme. *Atmos. Chem. Phys.* 2 (22):823-845. doi:10.5194/acp-2021-361.

- Bisson, J., Seers, P., Huegel, M., and Garnier, F. 2016. Numerical Prediction of Gaseous Aerosol Precursors and Particles in an Aircraft Engine. *J. Propul. Power* 4 (32):918-928. doi:10.2514/1.B35943.
- Boies, A. M., Stettler, M. E., Swanson, J. J., Johnson, T. J., Olfert, J. S., Johnson, M., Eggersdorfer, M. L., Rindlisbacher, T., Wang, J., and Thomson, K. 2015. Particle emission characteristics of a gas turbine with a double annular combustor. *Aerosol Sci. Tech.* 9 (49):842-855. doi:10.1080/02786826.2015.1078452.
- Brasil, A. M., Farias, T. L., and Carvalho, M. G. 1999. A recipe for image characterization of fractal-like aggregates. *J. Aerosol Sci.* 10 (30):1379-1389. doi:10.1016/S0021-8502(99)00026-9.
- Brown, R. C., Miake-Lye, R. C., Anderson, M. R., and Kolb, C. E. 1996. Aerosol dynamics in near-field aircraft plumes. *J. Geophys. Res.-Atmos.* D17 (101):22939-22953. doi:10.1029/96JD01918.
- Cantin, S., Chouak, M., Morency, F., and Garnier, F. 2021. Eulerian-Lagrangian CFD-microphysics modeling of a near-field contrail from a realistic turbofan. *Int. J. Engine Res.* 4 (23):661-677. doi:10.1177/1468087421993961.
- Cantin, S., Chouak, M., Morency, F., and Garnier, F. 2022. Eulerian-Lagrangian CFD-microphysics modeling of Aircraft-Emitted Aerosol Formation at Ground Level, in: *AIAA SCITECH 2022 Forum*, doi:10.2514/6.2022-1823.
- Casati, R., Scheer, V., Vogt, R., and Benter, T. 2007. Measurement of nucleation and soot mode particle emission from a diesel passenger car in real world and laboratory in situ dilution. *Atmos. Environ.* 10 (41):2125-2135. doi:10.1016/j.atmosenv.2006.10.078.
- CD-Adapco. 2021. STAR-CCM+ Documentation Version 16.06.008.
- Celik, I. B., Ghia, U., Roache, P. J., and Freitas, C. J. 2008. Procedure for Estimation and Reporting of Uncertainty Due to Discretization in CFD Applications. *J. Fluid. Eng.* 7 (130):078001-078001-078004. doi:10.1115/1.2960953.
- Clegg, S. L. and Seinfeld, J. H. 2006. Thermodynamic Models of Aqueous Solutions Containing Inorganic Electrolytes and Dicarboxylic Acids at 298.15 K. 1. The Acids as Nondissociating Components. *J. Phys. Chem. A* 17 (110):5692-5717. doi:10.1021/jp056149k.
- Davidson, M. J. and Wang, H. J. 2002. Strongly Advected Jet in a Coflow. *J. Hydraul. Eng.* 8 (128):742-752. doi:10.1061/(ASCE)0733-9429(2002)128:8(742).
- Du, H. and Yu, F. 2006. Role of the binary H₂SO₄-H₂O homogeneous nucleation in the formation of volatile nanoparticles in the vehicular exhaust. *Atmos. Environ.* 39 (40):7579-7588. doi:10.1016/j.atmosenv.2006.07.012.
- Elm, J., Kubečka, J., Besel, V., Jääskeläinen, M. J., Halonen, R., Kurtén, T., and Vehkamäki, H. 2020. Modeling the formation and growth of atmospheric molecular clusters: A review. *J. Aerosol Sci.* (149):105621. doi:10.1016/j.jaerosci.2020.105621.
- Garmory, A., Britter, R. E., and Mastorakos, E. 2008. Simulation of the evolution of aircraft exhaust plumes including detailed chemistry and segregation. *J. Geophys. Res.-Atmos.* D8 (113):n/a-n/a. doi:10.1029/2007JD009104.
- Garnier, F., Maglaras, E., Morency, F., and Vancassel, X. 2014. Effect of Compressibility on Contrail Ice Particle Growth in an Engine Jet. *Int. J. Turbo Jet Eng* 2 (31):131. doi:10.1515/tjj-2013-0039.
- Gmehling, J., Li, J., and Schiller, M. 1993. A modified UNIFAC model. 2. Present parameter matrix and results for different thermodynamic properties. *Ind. Eng. Chem. Res.* 1 (32):178-193. doi:10.1021/ie00013a024.
- Huang, W., Li, H., Sarnela, N., Heikkinen, L., Tham, Y. J., Mikkilä, J., Thomas, S. J., Donahue, N. M., Kulmala, M., and Bianchi, F. 2021. Measurement report: Molecular composition and volatility of gaseous organic compounds in a boreal forest – from volatile organic compounds to highly oxygenated organic molecules. *Atmos. Chem. Phys.* 11 (21):8961-8977. doi:10.5194/acp-21-8961-2021.
- ICAO. 2016. ICAO Environmental Report 2016. International Civil Aviation Organization.
- Jackson, P. and Munson, K. 2004. *Jane's All the World's Aircraft*. 95th ed. Jane's Information Group.

- Jacobson, M. Z. 2005. *Fundamentals of Atmospheric Modeling*. 2nd ed. Cambridge University Press. Cambridge. doi:10.1017/CBO9781139165389.
- Jathar, S. H., Miracolo, M. A., Presto, A. A., Donahue, N. M., Adams, P. J., and Robinson, A. L. 2012. Modeling the formation and properties of traditional and non-traditional secondary organic aerosol: problem formulation and application to aircraft exhaust. *Atmos. Chem. Phys.* 19 (12):9025-9040. doi:10.5194/acp-12-9025-2012.
- Jones, S. H. and Miake-Lye, R. C. 2024. Parameterization of H₂SO₄ and organic contributions to volatile PM in aircraft plumes at ground idle. *J. Air Waste Manag.* 7 (74):490-510. doi:10.1080/10962247.2024.2354820.
- Jun, M. 2011. Microphysical Modeling of Ultrafine Hydrocarbon Containing Aerosols in Aircraft Emissions. PhD diss. Department of Aeronautics and Astronautics. Massachusetts Institute of Technology. Cambridge, MA.
- Karcher, B., Yu, F., Schroder, F. P., and Turco, R. P. 1998. Ultrafine aerosol particles in aircraft plumes: Analysis of growth mechanisms. *Geophys. Res. Lett.* 15 (25):2793-2796. doi:10.1029/98GL02114.
- Kärcher, B. 1998. Physicochemistry of aircraft-generated liquid aerosols, soot, and ice particles: 1. Model description. *J. Geophys. Res.-Atmos.* D14 (103):17111-17128. doi:10.1029/98JD01044.
- Kärcher, B. 2003. Simulating gas-aerosol-cirrus interactions: Process-oriented microphysical model and applications. *Atmos. Chem. Phys.* 5 (3):1645-1664. doi:10.5194/acp-3-1645-2003.
- Kärcher, B., Hirschberg, M. M., and Fabian, P. 1996. Small-scale chemical evolution of aircraft exhaust species at cruising altitudes. *J. Geophys. Res.-Atmos.* D10 (101):15169-15190. doi:10.1029/96JD01059.
- Kärcher, B., Burkhardt, U., Bier, A., Bock, L., and Ford, I. J. 2015. The microphysical pathway to contrail formation. *J. Geophys. Res.-Atmos.* 15 (120):7893-7927. doi:10.1002/2015JD023491.
- Kärcher, B., Möhler, O., DeMott, P. J., Pechtl, S., and Yu, F. 2007. Insights into the role of soot aerosols in cirrus cloud formation. *Atmos. Chem. Phys.* 16 (7):4203-4227. doi:10.5194/acp-7-4203-2007.
- Kelesidis, G. A., Furrer, F. M., Wegner, K., and Pratsinis, S. E. 2018. Impact of Humidity on Silica Nanoparticle Agglomerate Morphology and Size Distribution. *Langmuir* 29 (34):8532-8541. doi:10.1021/acs.langmuir.8b00576.
- Khou, J. C., Ghedhaifi, W., Vancassel, X., Montreuil, E., and Garnier, F. 2016. CFD simulation of contrail formation in the near field of a commercial aircraft: effect of fuel sulfur content. *Meteorol. Z.* 6 (26). doi:10.1127/metz/2016/0761.
- Kılıç, D., Brem, B. T., Klein, F., El-Haddad, I., Durdina, L., Rindlisbacher, T., Setyan, A., Huang, R., Wang, J., Slowik, J. G., Baltensperger, U., and Prevot, A. S. H. 2017. Characterization of Gas-Phase Organics Using Proton Transfer Reaction Time-of-Flight Mass Spectrometry: Aircraft Turbine Engines. *Environ. Sci. Technol.* 7 (51):3621-3629. doi:10.1021/acs.est.6b04077.
- Kılıç, D., El Haddad, I., Brem, B. T., Bruns, E., Bozetti, C., Corbin, J., Durdina, L., Huang, R. J., Jiang, J., Klein, F., Lavi, A., Pieber, S. M., Rindlisbacher, T., Rudich, Y., Slowik, J. G., Wang, J., Baltensperger, U., and Prévôt, A. S. H. 2018. Identification of secondary aerosol precursors emitted by an aircraft turbofan. *Atmos. Chem. Phys.* 10 (18):7379-7391. doi:10.5194/acp-18-7379-2018.
- Kurzke, J. 2004. GasTurb 10: A Program for Gas-Turbine Performance Calculations. Dachau, Germany.
- Lewellen, D. C. 2020. A Large-Eddy Simulation Study of Contrail Ice Number Formation. *J. Atmos. Sci.* 7 (77):2585-2604. doi:10.1175/jas-d-19-0322.1.
- Liang, Z., Yu, Z., Zhang, C., and Chen, L. 2021. IVOC/SVOC and size distribution characteristics of particulate matter emissions from a modern aero-engine combustor in different operational modes. *Fuel*:122781. doi:10.1016/j.fuel.2021.122781.
- Liat, A., Brem, B. T., Durdina, L., Vögtli, M., Arroyo Rojas Dasilva, Y., Dimopoulos Eggenschwiler, P., and Wang, J. 2014. Electron Microscopic Study of Soot Particulate Matter Emissions from Aircraft Turbine Engines. *Environ. Sci. Technol.* 18 (48):10975-10983. doi:10.1021/es501809b.

- Lobo, P., Hagen, D. E., Whitefield, P. D., and Alofs, D. J. 2007. Physical Characterization of Aerosol Emissions from a Commercial Gas Turbine Engine. *J. Propul. Power* 5 (23):919-929. doi:10.2514/1.26772.
- Lobo, P., Durdina, L., Smallwood, G. J., Rindlisbacher, T., Siegerist, F., Black, E. A., Yu, Z., Mensah, A. A., Hagen, D. E., Miake-Lye, R. C., Thomson, K. A., Brem, B. T., Corbin, J. C., Abegglen, M., Sierau, B., Whitefield, P. D., and Wang, J. 2015. Measurement of Aircraft Engine Non-Volatile PM Emissions: Results of the Aviation-Particle Regulatory Instrumentation Demonstration Experiment (A-PRIDE) 4 Campaign. *Aerosol Sci. Tech.* 7 (49):472-484. doi:10.1080/02786826.2015.1047012.
- Määttänen, A., Merikanto, J., Henschel, H., Duplissy, J., Makkonen, R., Ortega, I. K., and Vehkamäki, H. 2018. New Parameterizations for Neutral and Ion-Induced Sulfuric Acid-Water Particle Formation in Nucleation and Kinetic Regimes. *J. Geophys. Res.-Atmos.* 2 (123):1269-1296. doi:10.1002/2017JD027429.
- Moore, R. H., Thornhill, K. L., Weinzierl, B., Sauer, D., D'Ascoli, E., Jin, K., Lichtenstern, M., Scheibe, M., Beaton, B., Beyersdorf, A. J., Barrick, J., Bulzan, D., Corr, C. A., Crosbie, E., Jurkat, T., Martin, R., Riddick, D., Shook, M., Slover, G., Voigt, C., White, R., Winstead, E., Yasky, R., Ziemba, L. D., Brown, A., Schlager, H., and Anderson, B. E. 2017. Biofuel blending reduces particle emissions from aircraft engines at cruise conditions. *Nature* 7645 (543):411-415. doi:10.1038/nature21420.
- Morrison, H., van Lier-Walqui, M., Fridlind, A. M., Grabowski, W. W., Harrington, J. Y., Hoose, C., Korolev, A., Kumjian, M. R., Milbrandt, J. A., Pawlowska, H., Posselt, D. J., Prat, O. P., Reimel, K. J., Shima, S. I., van Diedenhoven, B., and Xue, L. 2020. Confronting the Challenge of Modeling Cloud and Precipitation Microphysics. *J. Adv. Model. Earth Sy.* 8 (12):e2019MS001689. doi:10.1029/2019MS001689.
- Nannoolal, Y., Rarey, J., and Ramjugernath, D. 2007. Estimation of pure component properties: Part 2. Estimation of critical property data by group contribution. *Fluid Phase Equilibr.* 1 (252):1-27. doi:10.1016/j.fluid.2006.11.014.
- Nannoolal, Y., Rarey, J., and Ramjugernath, D. 2008. Estimation of pure component properties: Part 3. Estimation of the vapor pressure of non-electrolyte organic compounds via group contributions and group interactions. *Fluid Phase Equilibr.* 1 (269):117-133. doi:10.1016/j.fluid.2008.04.020.
- Nannoolal, Y., Rarey, J., Ramjugernath, D., and Cordes, W. 2004. Estimation of pure component properties: Part 1. Estimation of the normal boiling point of non-electrolyte organic compounds via group contributions and group interactions. *Fluid Phase Equilibr.* (226):45-63. doi:10.1016/j.fluid.2004.09.001.
- Onasch, T. B., Jayne, J. T., Herndon, S., Worsnop, D. R., Miake-Lye, R. C., Mortimer, I. P., and Anderson, B. E. 2009. Chemical Properties of Aircraft Engine Particulate Exhaust Emissions. *J. Propul. Power* 5 (25):1121-1137. doi:10.2514/1.36371.
- Owen, B., Anet, J. G., Bertier, N., Christie, S., Cremaschi, M., Dellaert, S., Edebeli, J., Janicke, U., Kuenen, J., Lim, L., and Terrenoire, E. 2022. Review: Particulate Matter Emissions from Aircraft. *Atmos.* 8 (13):1230.
- Pagels, J., Khalizov, A. F., McMurtry, P. H., and Zhang, R. Y. 2009. Processing of Soot by Controlled Sulphuric Acid and Water Condensation—Mass and Mobility Relationship. *Aerosol Sci. Tech.* 7 (43):629-640. doi:10.1080/02786820902810685.
- Paoli, R., Nybelen, L., Picot, J., and Cariolle, D. 2013. Effects of jet/vortex interaction on contrail formation in supersaturated conditions. *Phys. Fluids* 5 (25):053305. doi:10.1063/1.4807063.
- Poling, B. E., Prausnitz, J. M., and O'Connell, J. P. 2001. *The properties of gases and liquids*. 5th ed. McGraw-hill New York. doi:10.1036/0070116822.
- Presto, A. A., Hennigan, C. J., Nguyen, N. T., and Robinson, A. L. 2012. Determination of Volatility Distributions of Primary Organic Aerosol Emissions from Internal Combustion Engines Using Thermal Desorption Gas Chromatography Mass Spectrometry. *Aerosol Sci. Tech.* 10 (46):1129-1139. doi:10.1080/02786826.2012.700430.
- Pruppacher, H. R. and Klett, J. D. 1998. *Microphysics of Clouds and Precipitation*. Atmos. Ocean Sci. Lib. Springer Netherlands, Dordrecht. XXII, 954 pp., doi:10.1007/978-0-306-48100-0.

- Saffaripour, M., Thomson, K. A., Smallwood, G. J., and Lobo, P. 2020. A review on the morphological properties of non-volatile particulate matter emissions from aircraft turbine engines. *J. Aerosol Sci.* (139):105467. doi:10.1016/j.jaerosci.2019.105467.
- Schnitzler, E. G., Dutt, A., Charbonneau, A. M., Olfert, J. S., and Jäger, W. 2014. Soot Aggregate Restructuring Due to Coatings of Secondary Organic Aerosol Derived from Aromatic Precursors. *Environ. Sci. Technol.* 24 (48):14309-14316. doi:10.1021/es503699b.
- Schröder, F., Karcher, B., Duroure, C., Strom, J., Petzold, A., Gayet, J. F., Strauss, B., Wendling, P., and Borrmann, S. 2000. On the transition of contrails into cirrus clouds. *J. Atmos. Sci.* 4 (57):464-480. doi:10.1175/1520-0469(2000)057<0464:OTTOCI>2.0.CO;2.
- Seinfeld, J. H. and Pandis, S. N. 2016. *Atmospheric chemistry and physics: from air pollution to climate change*. 2nd ed. John Wiley & Sons.
- Shima, S., Kusano, K., Kawano, A., Sugiyama, T., and Kawahara, S. 2009. The super-droplet method for the numerical simulation of clouds and precipitation: a particle-based and probabilistic microphysics model coupled with a non-hydrostatic model. *A. J. Roy. Meteor. Soc.* 642 (135):1307-1320. doi:10.1002/qj.441.
- Sipkens, T. A. and Corbin, J. C. 2024. Effective density and packing of compacted soot aggregates. *Carbon* (226):119197. doi:10.1016/j.carbon.2024.119197.
- Sipkens, T. A., Boies, A., Corbin, J. C., Chakrabarty, R. K., Olfert, J., and Rogak, S. N. 2023. Overview of methods to characterize the mass, size, and morphology of soot. *J. Aerosol Sci.* (173):106211. doi:10.1016/j.jaerosci.2023.106211.
- Synylo, K., Krupko, A., Zaporozhets, O., and Makarenko, R. 2020. CFD simulation of exhaust gases jet from aircraft engine. *Energy* (213):118610. doi:10.1016/j.energy.2020.118610.
- Taleb, D.-E., Ponche, J.-L., and Mirabel, P. 1996. Vapor pressures in the ternary system water-nitric acid-sulfuric acid at low temperature: A reexamination. *J. Geophys. Res.-Atmos.* D20 (101):25967-25977. doi:10.1029/96jd02330.
- Testa, E., Giammusso, C., Bruno, M., and Maggiore, P. 2013. Fluid dynamic analysis of pollutants' dispersion behind an aircraft engine during idling. *Air Qual. Atmos. Hlth.* 2 (6):367-383. doi:10.1007/s11869-012-0188-1.
- Unterstrasser, S., Hoffmann, F., and Lerch, M. 2017. Collection/aggregation algorithms in Lagrangian cloud microphysical models: rigorous evaluation in box model simulations. *Geosci. Model Dev.* 4 (10):1521-1548. doi:10.5194/gmd-10-1521-2017.
- Unterstrasser, S., Hoffmann, F., and Lerch, M. 2020. Collisional growth in a particle-based cloud microphysical model: insights from column model simulations using LCM1D (v1.0). *Geosci. Model Dev.* 11 (13):5119-5145. doi:10.5194/gmd-13-5119-2020.
- Vancassel, X., Mirabel, P., and Garnier, F. 2014. Numerical simulation of aerosols in an aircraft wake using a 3D LES solver and a detailed microphysical model. *Int. J. Sust. Aviat.* 2 (1):139-159. doi:10.1504/ijsa.2014.065480.
- Vemury, S. and Pratsinis, S. E. 1995. Self-preserving size distributions of agglomerates. *J. Aerosol Sci.* 2 (26):175-185. doi:10.1016/0021-8502(94)00103-6.
- Wang, Y., Liu, H., Li, T., Jiang, H., He, P., Liu, D., Zhang, J., Xiong, Q., and Liu, L. 2019. Characterization of the Morphology and Nanostructure of the Soot Particles Produced within Transient Diesel Reacting Jet Flame by Using Thermophoretic Sampling Technique. *Energy. Fuel* 9 (33):9124-9137. doi:10.1021/acs.energyfuels.9b00810.
- Wey, C. C., Anderson, B. A., Wey, C., Miake-Lye, R. C., Whitefield, P., and Howard, R. 2007. Overview on the Aircraft Particle Emissions Experiment (APEX). *J. Propul. Power* 5 (23):898-905. doi:10.2514/1.26406.
- Wey, C. C., Anderson, B. E., Hudgins, C., Wey, C., Li-Jones, X., Winstead, E., Thornhill, L. K., Lobo, P., Hagen, D., Whitefield, P. D., Knighton, W. B., Howard, R., Bryant, D., Corporan, E., Moses, C., Holve, D., and Dodds, W. 2006. Aircraft Particle Emissions Experiment (APEX). NASA/TM-2006-214382, also U.S. Army Research Lab. Rept. TR-3903, 2006.

- Wey, T. and Liu, N.-S. 2007. Modeling Jet Engine Aerosols in the Postcombustor Flow Path and Sampling System. *J. Propul. Power* 5 (23):930-941. doi:10.2514/1.24274.
- Wong, H.-W., Jun, M., Peck, J., Waitz, I. A., and Miake-Lye, R. C. 2014. Detailed Microphysical Modeling of the Formation of Organic and Sulfuric Acid Coatings on Aircraft Emitted Soot Particles in the Near Field. *Aerosol Sci. Tech.* 9 (48):981-995. doi:10.1080/02786826.2014.953243.
- Wong, H.-W., Jun, M., Peck, J., Waitz, I. A., and Miake-Lye, R. C. 2015. Roles of Organic Emissions in the Formation of Near Field Aircraft-Emitted Volatile Particulate Matter: A Kinetic Microphysical Modeling Study. *J. Eng. Gas Turb. Power* 7 (137. doi:10.1115/1.4029366.
- Wong, H.-W., Yelvington, P. E., Timko, M. T., Onasch, T. B., Miake-Lye, R. C., Zhang, J., and Waitz, I. A. 2008. Microphysical Modeling of Ground-Level Aircraft-Emitted Aerosol Formation: Roles of Sulfur-Containing Species. *J. Propul. Power* 3 (24):590-602. doi:10.2514/1.32293.
- Yu, F., Anderson, B. E., Pierce, J. R., Wong, A., Nair, A., Luo, G., and Herb, J. 2024. On Nucleation Pathways and Particle Size Distribution Evolutions in Stratospheric Aircraft Exhaust Plumes with H₂SO₄ Enhancement. *Environ. Sci. Technol.* doi:10.1021/acs.est.3c08408.
- Yu, Z., Timko, M. T., Herndon, S. C., Miake-Lye, R. C., Beyersdorf, A. J., Ziemba, L. D., Winstead, E. L., and Anderson, B. E. 2019. Mode-specific, semi-volatile chemical composition of particulate matter emissions from a commercial gas turbine aircraft engine. *Atmos. Environ.* (218. doi:10.1016/j.atmosenv.2019.116974.
- Yuan, R., Lobo, P., Smallwood, G. J., Johnson, M. P., Parker, M. C., Butcher, D., and Spencer, A. 2022. Measurement of black carbon emissions from multiple engine and source types using laser-induced incandescence: sensitivity to laser fluence. *Atmos. Meas. Tech.* 2 (15):241-259. doi:10.5194/amt-15-241-2022.
- Zhao, H. and Zheng, C. 2013. A population balance-Monte Carlo method for particle coagulation in spatially inhomogeneous systems. *Comput. Fluid.* (71):196-207. doi:10.1016/j.compfluid.2012.09.025.

Figure captions

Figure 1. 2D scheme of plume from a turbofan engine with gaseous and particulate matter emissions

Figure 2. Simplified pathways for aerosol formation in aircraft plume at ground level

Figure 3. Schematic of CFD-microphysics coupling and the main modules in PAMMAP

Figure 4. Computational domain and grid for CFM56-2C1, short-cowl nozzle: (a) 2D-view, (b) nozzle geometry, and (c) nozzle mesh

Figure 5. Comparison of (a) plume velocity, (b) static plume temperature (K), and (c) exhaust gas fraction predicted and measured in near-field aircraft plume at 30 m downstream

Figure 6. Stream-wise (xy-plane) contours of exhaust plume temperature at idle (7%) (top) and take-off regime (100%) (bottom)

Figure 7. Comparison emission indices of major (1st row) and minor (2nd and 3rd rows) species with experimental results from APEX-1 at 1, 10, and 30 m downstream

Figure 8. Comparison of EI_n (kg fuel⁻¹) and particle diameter (nm) of non-volatile PM (1st row) and total PM (2nd row) between APEX-1 measurement campaign and CFD results at 1, 10, and 30 m downstream of the engine. Error bars indicate the experimental uncertainties.

Figure 9. Evolution of nvPM / total PM number ratio in the plume

Figure 10. Comparison of sulfate and organic EI_m (mg kg fuel⁻¹) condensed on the soot mode between APEX-1 measurements and CFD results as a function of LTO power settings at 30 m downstream the engine exhaust

Figure 11. Particle size distribution of nvPM for 7, 30, 85, 100% engine power settings at 30 m

Figure 12. Mass fraction composition regarding sulfate and organic components of soot mode particles (a) microphysical processes of soot mode particles (b) different compound classes of soot mode particles (c) and homogeneous nucleation mode particles (d) as a function of engine power at 50 m downstream of the engine

Figure 13. Mass fraction in soot coatings regarding surface coverage as a function of engine power at 50 m

downstream of the engine

Table captions

Table 1. Exhaust properties of the CFM56-2C1 engine at LTO power settings based on GASTURB thermodynamic cycle modeling (Kurzke, 2004) and APEX measurements (Wey et al., 2006)

Table 2. List of organic surrogate species

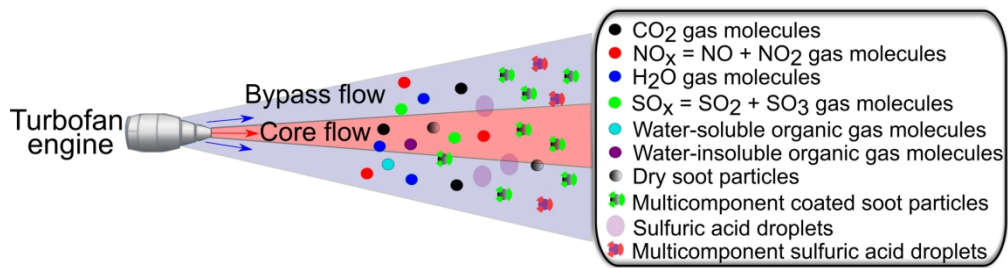
Table captions

Table 1. Exhaust properties of the CFM56-2C1 engine at LTO power settings based on GASTURB thermodynamic cycle modeling (Kurzke, 2004) and APEX measurements (Wey et al., 2006)

Power Settings (%)		4	7	30	85	100
Test point no.		908	914	913	928	909
Core flow	Velocity, U_c (m s ⁻¹)	34.5	41.8	91.1	183.2	208.3
	Static Temperature, T_c (K)	640.8	665.0	685.0	771.5	824.5
	EI_n (kg fuel ⁻¹)	4.05×10^{14}	8.51×10^{13}	9.88×10^{13}	4.83×10^{14}	1.73×10^{15}
	$\bar{D}_M$ (nm)/ σ_g	16.3/1.56	17.6/1.63	26.2/1.73	39.3/2.05	34.7/1.84
Bypass Flow	Velocity, U_b (m s ⁻¹)	44.8	59.5	117.1	168.1	174.5
	Static Temperature, T_b (K)	295.8	296.9	304.8	323.9	331.3

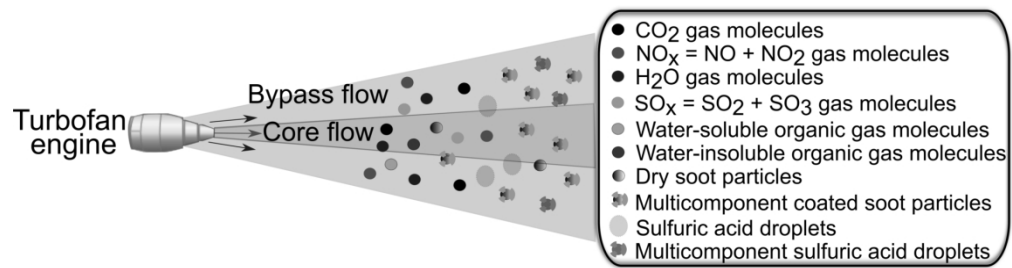
Table 2. List of organic surrogate species

		Families of HC species									
Power Settings (%)	Number of HC species	Acids	Alcohols	Aliphatic	Aromatics		Carbonyls		O-containing	Non aromatics HC	
4	38	C ₂ H ₄ O ₂ CH ₂ O ₂	C ₆ H ₆ O	C ₅ H ₁₀ C ₈ H ₁₄ C ₃ H ₄	C ₉ H ₁₂	C ₁₀ H ₁₂	C ₂ H ₄ O				C ₄ H ₈
					C ₆ H ₆	C ₈ H ₈	C ₃ H ₄ O	C ₄ H ₆ O ₂		C ₃ H ₆	
					C ₁₀ H ₁₄	C ₁₄ H ₁₀	CH ₂ O	C ₉ H ₁₀ O		C ₄ H ₆	
					C ₈ H ₁₀	C ₁₆ H ₁₀	C ₃ H ₆ O	C ₅ H ₆ O	C ₂ H ₂ O	C ₆ H ₁₀	
					C ₇ H ₈	C ₂₀ H ₁₂	C ₄ H ₆ O	C ₅ H ₈ O		C ₇ H ₁₂	
					C ₁₁ H ₁₆	C ₂₂ H ₁₂	C ₃ H ₄ O ₂	C ₈ H ₈ O		C ₃ H ₈	
					C ₉ H ₁₀					C ₆ H ₈	
7	31	C ₂ H ₄ O ₂ CH ₂ O ₂	CH ₄ O	C ₃ H ₄	C ₁₄ H ₁₀	C ₁₀ H ₁₄	C ₄ H ₈ O	C ₃ H ₆ O			C ₆ H ₁₀
					C ₁₆ H ₁₀	C ₈ H ₁₀	C ₄ H ₄ O ₃	C ₃ H ₄ O ₂		C ₇ H ₁₂	
					C ₂₀ H ₁₂	C ₉ H ₁₂	C ₂ H ₄ O	C ₄ H ₂ O ₃	C ₃ H ₄ O ₂	C ₅ H ₈	
					C ₂₂ H ₁₂	C ₆ H ₆	CH ₂ O	C ₄ H ₆ O	C ₂ H ₂ O	C ₄ H ₈	
					C ₇ H ₈	C ₃ H ₄ O	C ₄ H ₆ O ₂			C ₃ H ₆	
										C ₄ H ₆	
30	27	C ₂ H ₄ O ₂ CH ₂ O ₂		C ₃ H ₄ C ₈ H ₁₄	C ₁₄ H ₁₀	C ₇ H ₈	C ₃ H ₆ O	C ₄ H ₈ O			C ₄ H ₈
					C ₁₆ H ₁₀	C ₉ H ₁₂	C ₂ H ₄ O	C ₄ H ₄ O ₃		C ₆ H ₁₀	
					C ₂₀ H ₁₂	C ₁₀ H ₁₄	CH ₂ O	C ₄ H ₆ O ₂	C ₂ H ₂ O	C ₇ H ₁₂	
					C ₂₂ H ₁₂	C ₈ H ₁₀	C ₃ H ₄ O ₂	C ₆ H ₁₀ O		C ₄ H ₆	
							C ₄ H ₂ O ₃			C ₃ H ₆	
85	27	C ₂ H ₄ O ₂ CH ₂ O ₂		C ₃ H ₄	C ₁₄ H ₁₀		C ₃ H ₆ O	C ₄ H ₄ O ₃			C ₄ H ₈
					C ₁₆ H ₁₀		C ₃ H ₆ O ₂	C ₄ H ₆ O ₂		C ₄ H ₆	
					C ₂₀ H ₁₂		C ₂ H ₄ O	CH ₂ O	C ₂ H ₂ O	C ₆ H ₁₀	
					C ₂₂ H ₁₂		C ₃ H ₄ O ₂	C ₆ H ₁₀ O	C ₈ H ₄ O ₃	C ₅ H ₈	
					C ₇ H ₈		C ₄ H ₂ O ₃	C ₅ H ₈ O ₂		C ₇ H ₁₂	
							C ₄ H ₈ O			C ₃ H ₆	
100	26	C ₂ H ₄ O ₂ CH ₂ O ₂		C ₃ H ₄	C ₁₄ H ₁₀		C ₃ H ₆ O	C ₄ H ₄ O ₃			C ₄ H ₈
					C ₁₆ H ₁₀		C ₃ H ₆ O ₂	C ₄ H ₆ O ₂		C ₄ H ₆	
					C ₂₀ H ₁₂		C ₂ H ₄ O	CH ₂ O	C ₂ H ₂ O	C ₆ H ₁₀	
					C ₂₂ H ₁₂		C ₃ H ₄ O ₂	C ₆ H ₁₀ O	C ₈ H ₄ O ₃	C ₅ H ₈	
					C ₇ H ₈		C ₄ H ₂ O ₃	C ₅ H ₈ O ₂		C ₃ H ₆	
							C ₄ H ₈ O				



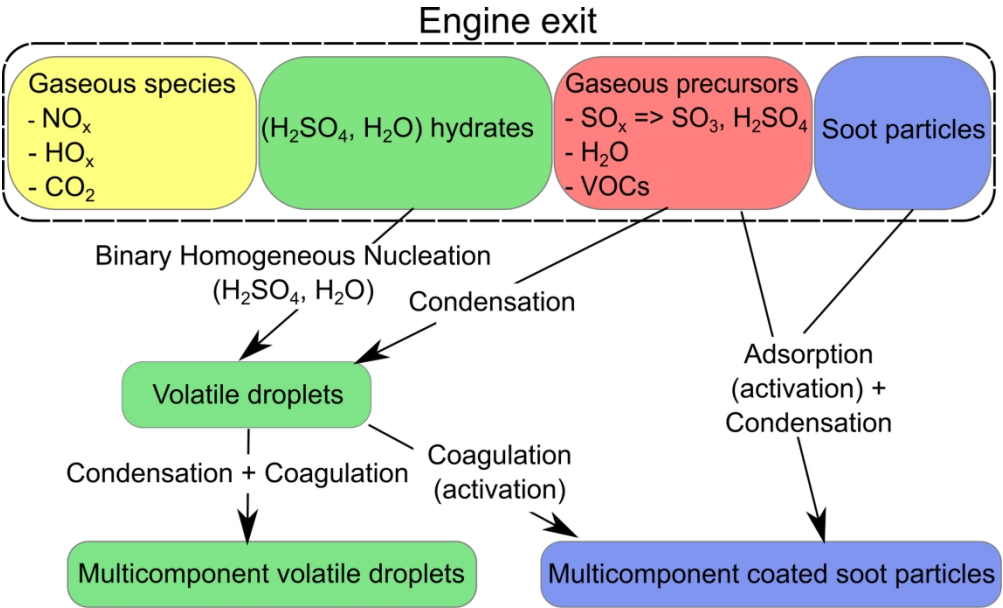
2D scheme of plume from a turbofan engine with gaseous and particulate matter emissions

182x48mm (300 x 300 DPI)



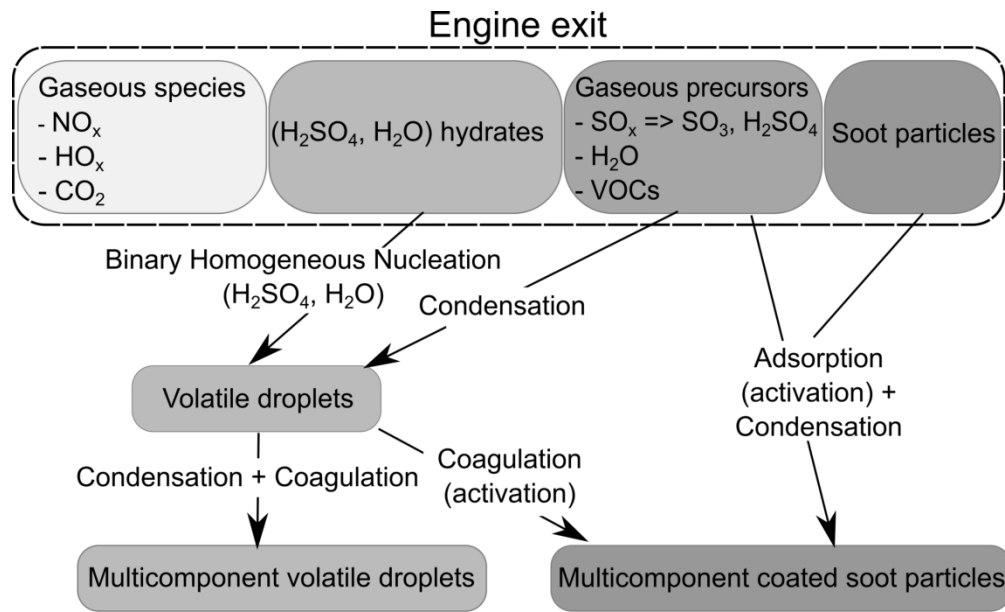
2D scheme of plume from a turbofan engine with gaseous and particulate matter emissions

182x48mm (300 x 300 DPI)



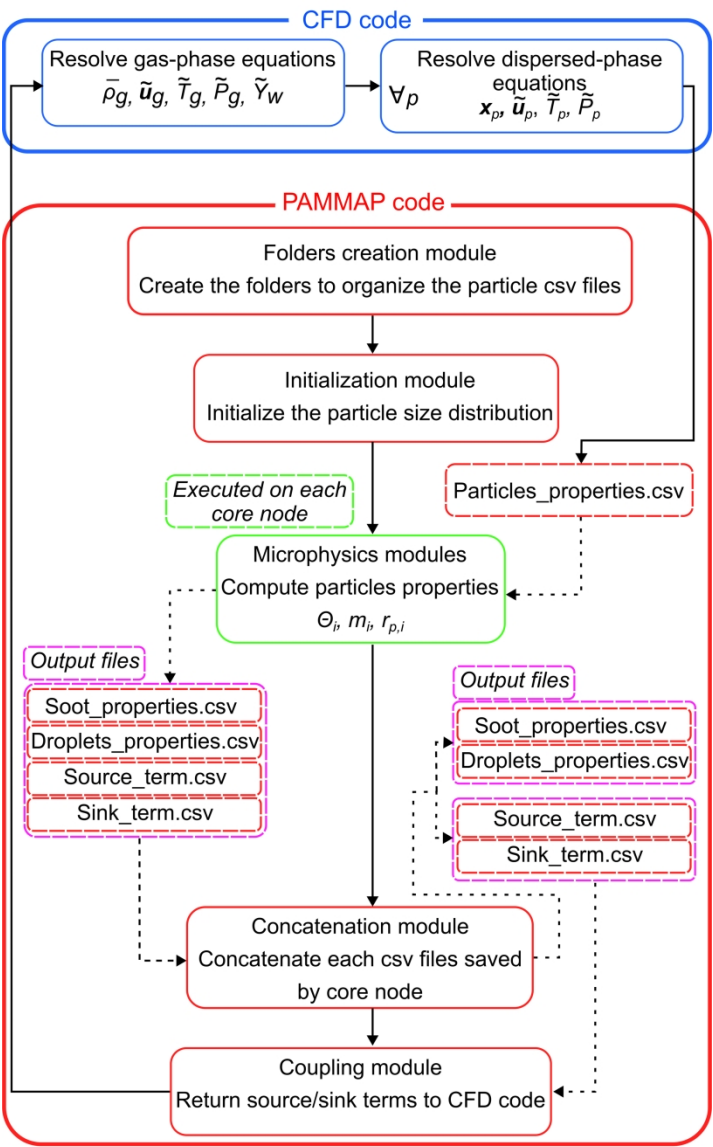
Simplified pathways for aerosol formation in aircraft plume at ground level

175x105mm (300 x 300 DPI)

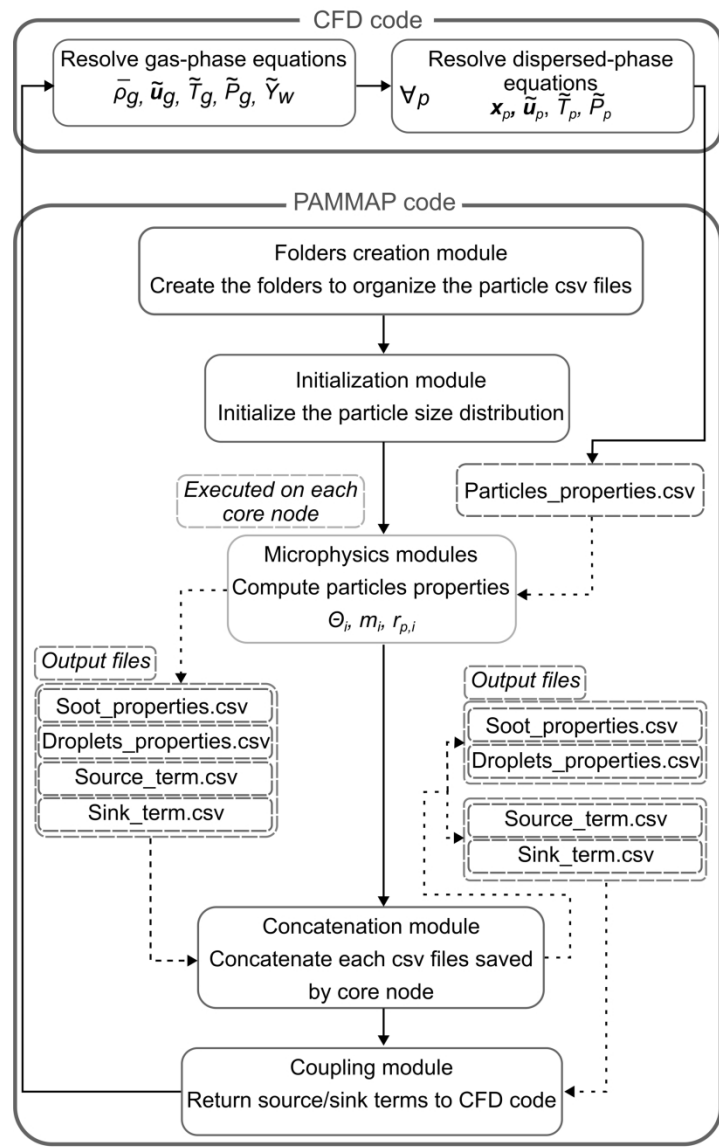


Simplified pathways for aerosol formation in aircraft plume at ground level

175x105mm (300 x 300 DPI)

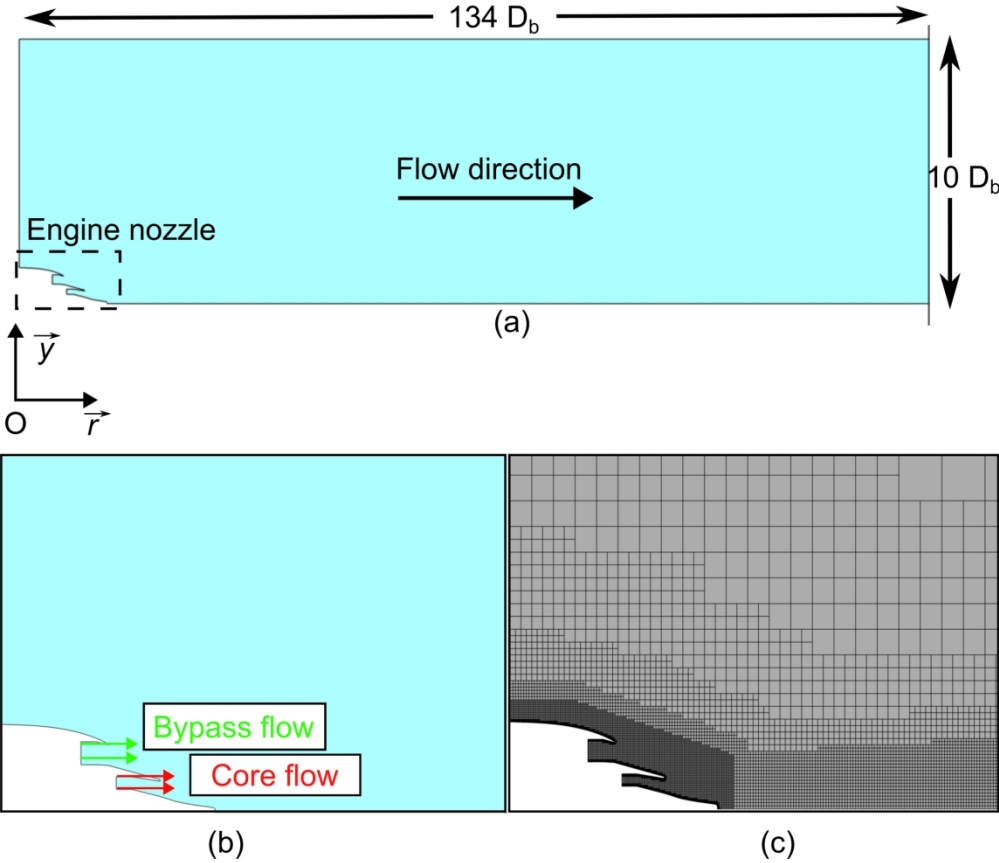


Schematic of CFD-microphysics coupling and the main modules in PAMMAP
184x311mm (300 x 300 DPI)



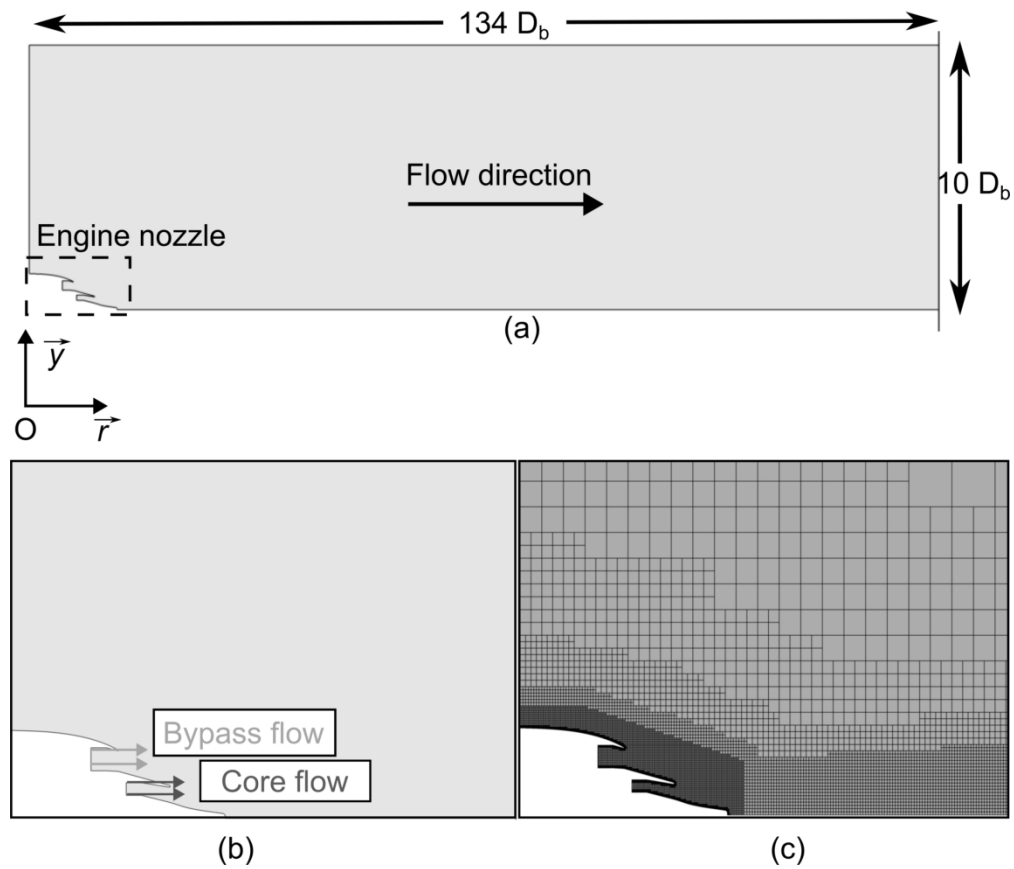
Schematic of CFD-microphysics coupling and the main modules in PAMMAP

184x311mm (300 x 300 DPI)



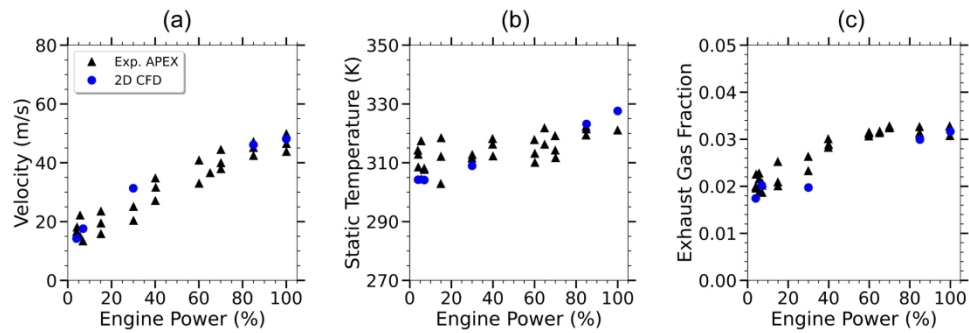
Computational domain and grid for CFM56-2C1, short-cowl nozzle: (a) 2D-view, (b) nozzle geometry, and (c) nozzle mesh

182x157mm (300 x 300 DPI)



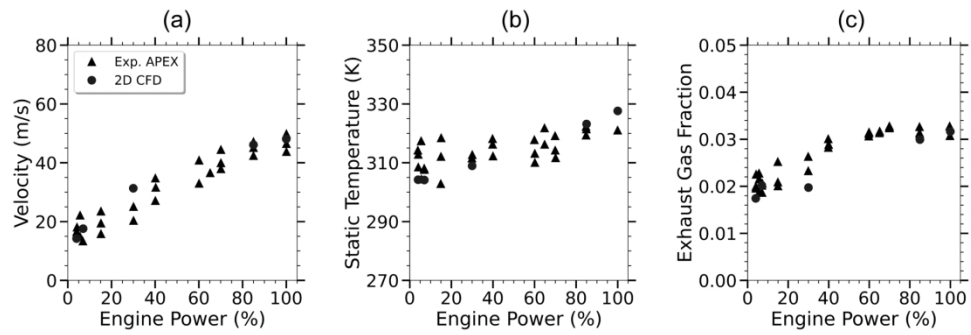
Computational domain and grid for CFM56-2C1, short-cowl nozzle: (a) 2D-view, (b) nozzle geometry, and (c) nozzle mesh

182x157mm (300 x 300 DPI)



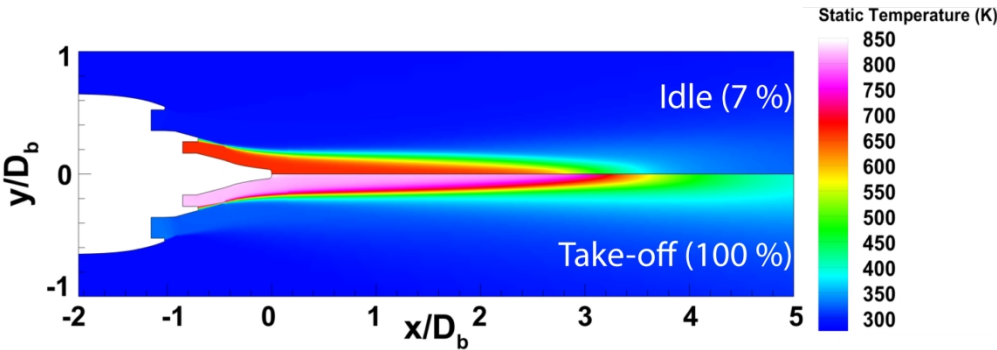
Comparison of (a) plume velocity, (b) static plume temperature (K), and (c) exhaust gas fraction predicted and measured in near-field aircraft plume at 30 m downstream

181x62mm (300 x 300 DPI)



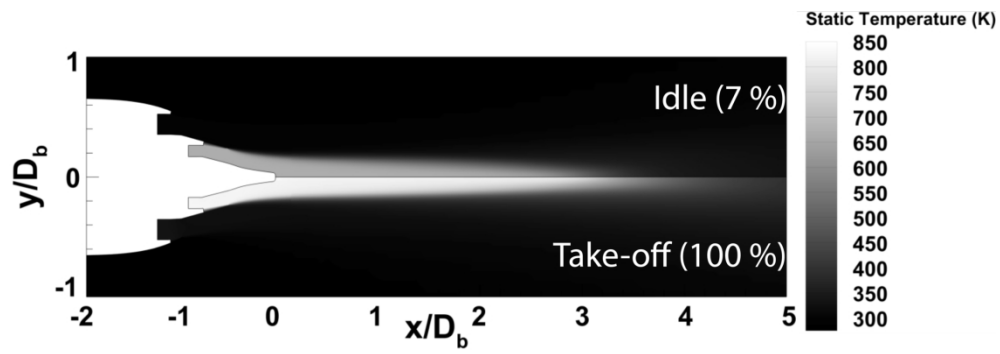
Comparison of (a) plume velocity, (b) static plume temperature (K), and (c) exhaust gas fraction predicted and measured in near-field aircraft plume at 30 m downstream

181x62mm (300 x 300 DPI)



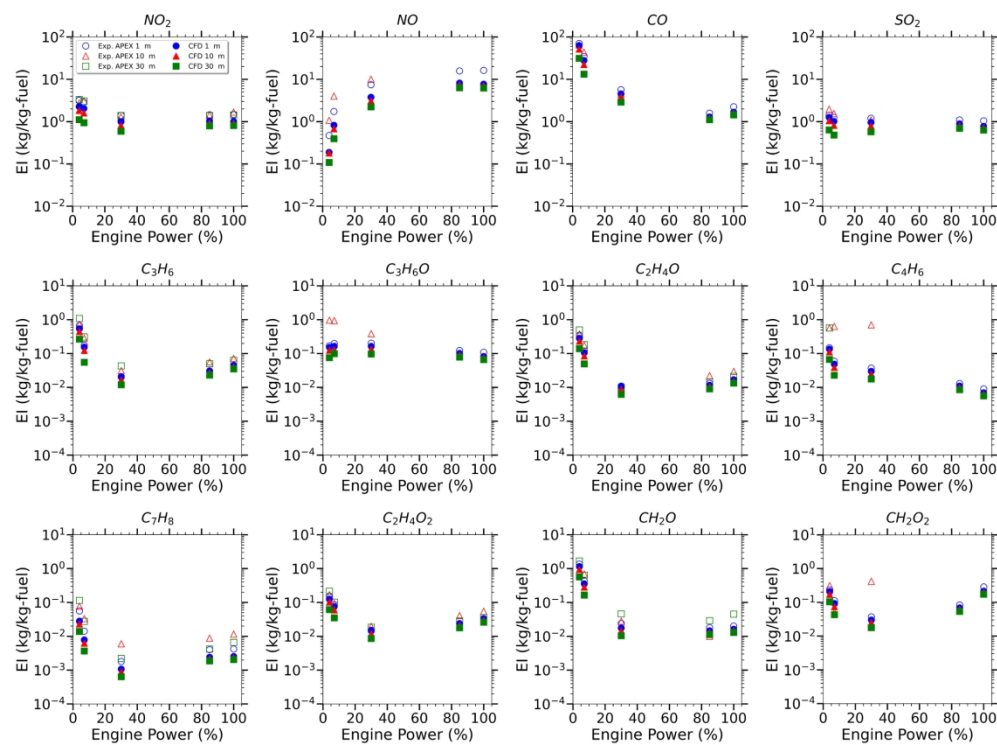
Stream-wise (xy-plane) contours of exhaust plume temperature at idle (7%) (top) and take-off regime (100%) (bottom)

181x62mm (300 x 300 DPI)



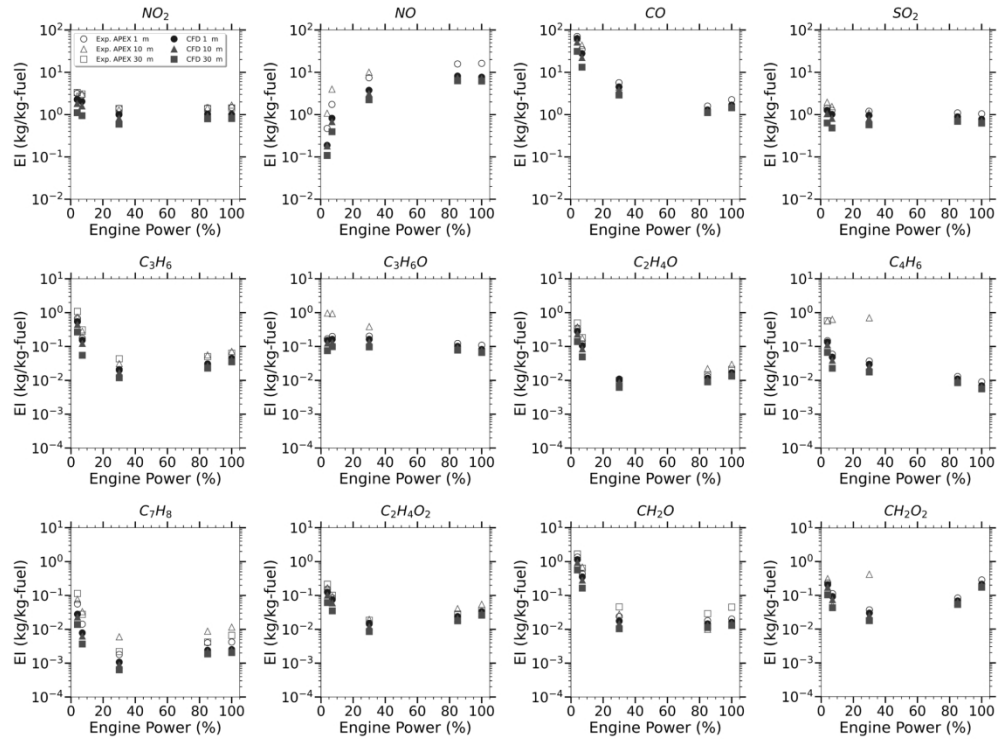
Stream-wise (xy-plane) contours of exhaust plume temperature at idle (7%) (top) and take-off regime (100%) (bottom)

181x61mm (300 x 300 DPI)



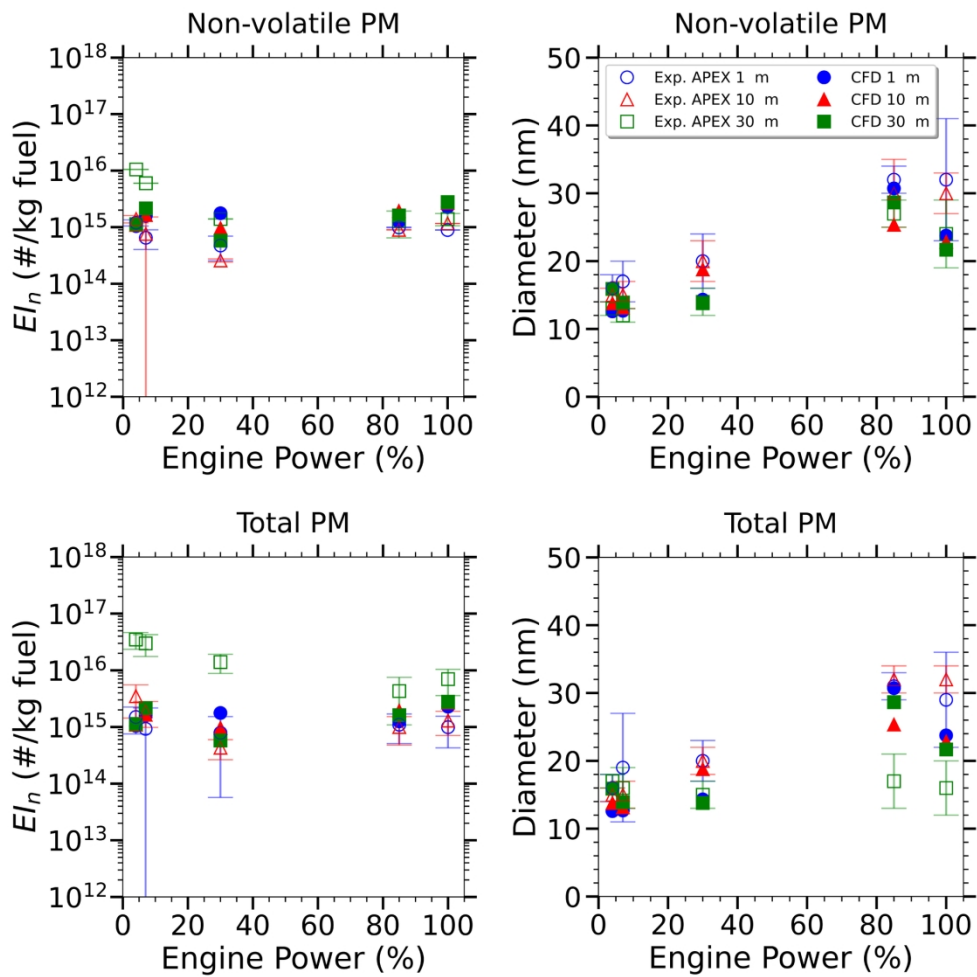
Comparison emission indices of major (1st row) and minor (2nd and 3rd rows) species with experimental results from APEX-1 at 1, 10, and 30 m downstream

184x137mm (300 x 300 DPI)



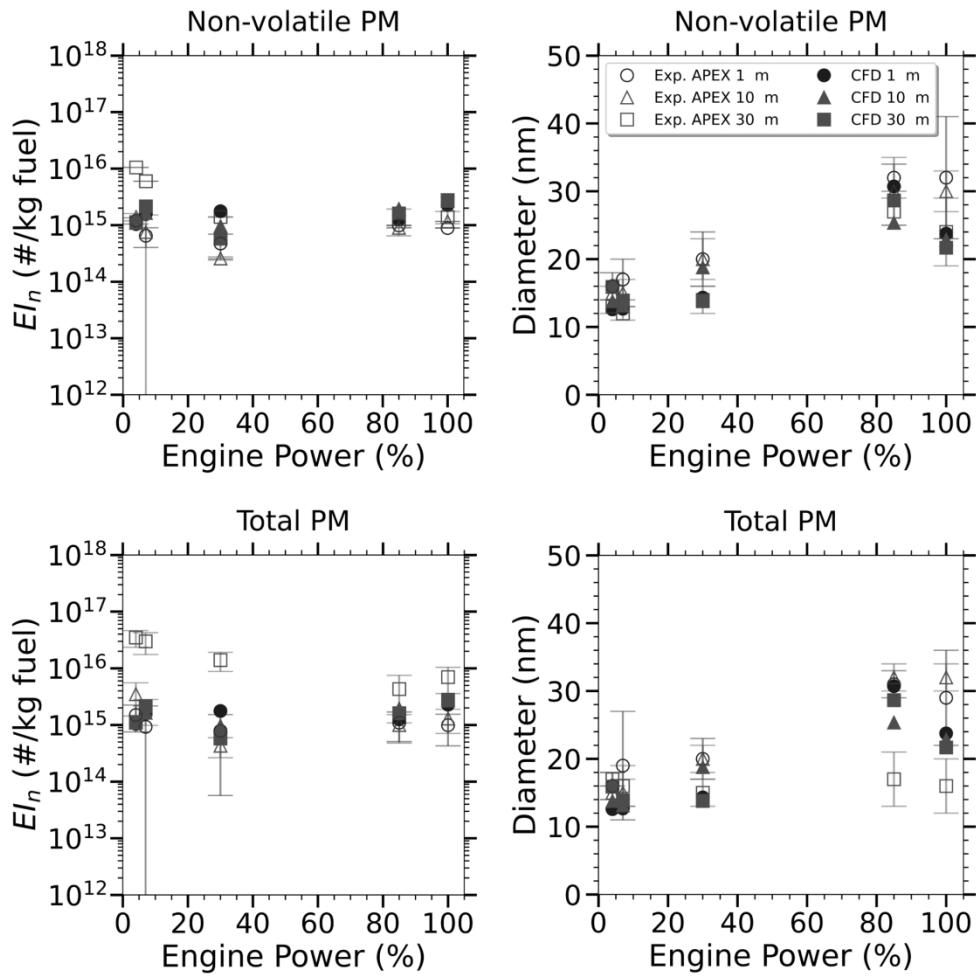
Comparison emission indices of major (1st row) and minor (2nd and 3rd rows) species with experimental results from APEX-1 at 1, 10, and 30 m downstream

184x137mm (300 x 300 DPI)



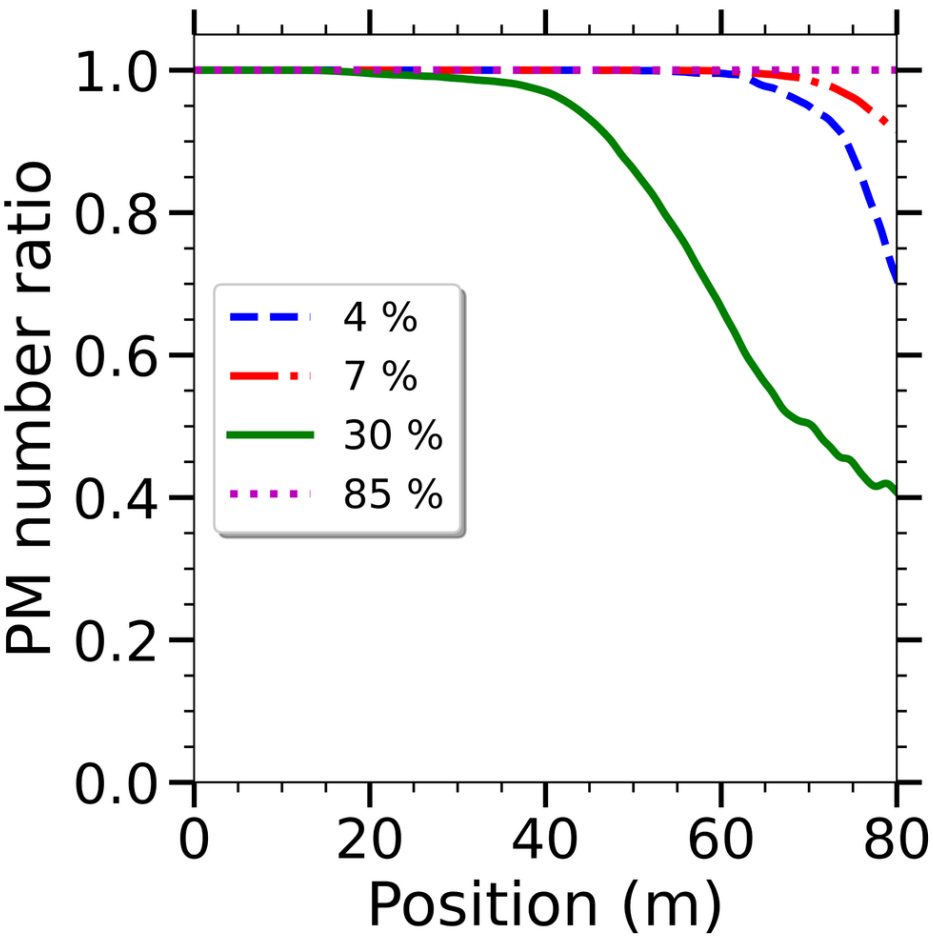
Comparison of EI_n (#/kg fuel) and particle diameter (nm) of non-volatile PM (1st row) and total PM (2nd row) between APEX-1 measurement campaign and CFD results at 1, 10, and 30 m downstream of the engine. Error bars indicate the experimental uncertainties.

184x183mm (300 x 300 DPI)



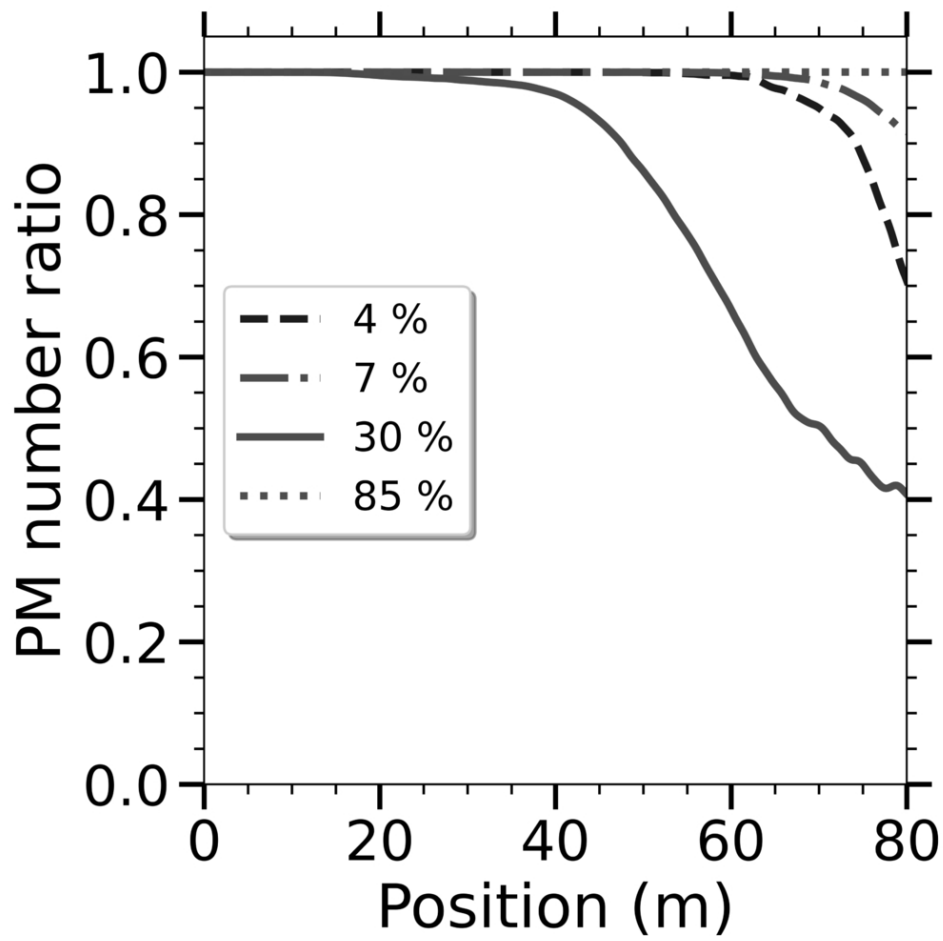
Comparison of EI_n (#/kg fuel) and particle diameter (nm) of non-volatile PM (1st row) and total PM (2nd row) between APEX-1 measurement campaign and CFD results at 1, 10, and 30 m downstream of the engine. Error bars indicate the experimental uncertainties.

184x183mm (300 x 300 DPI)



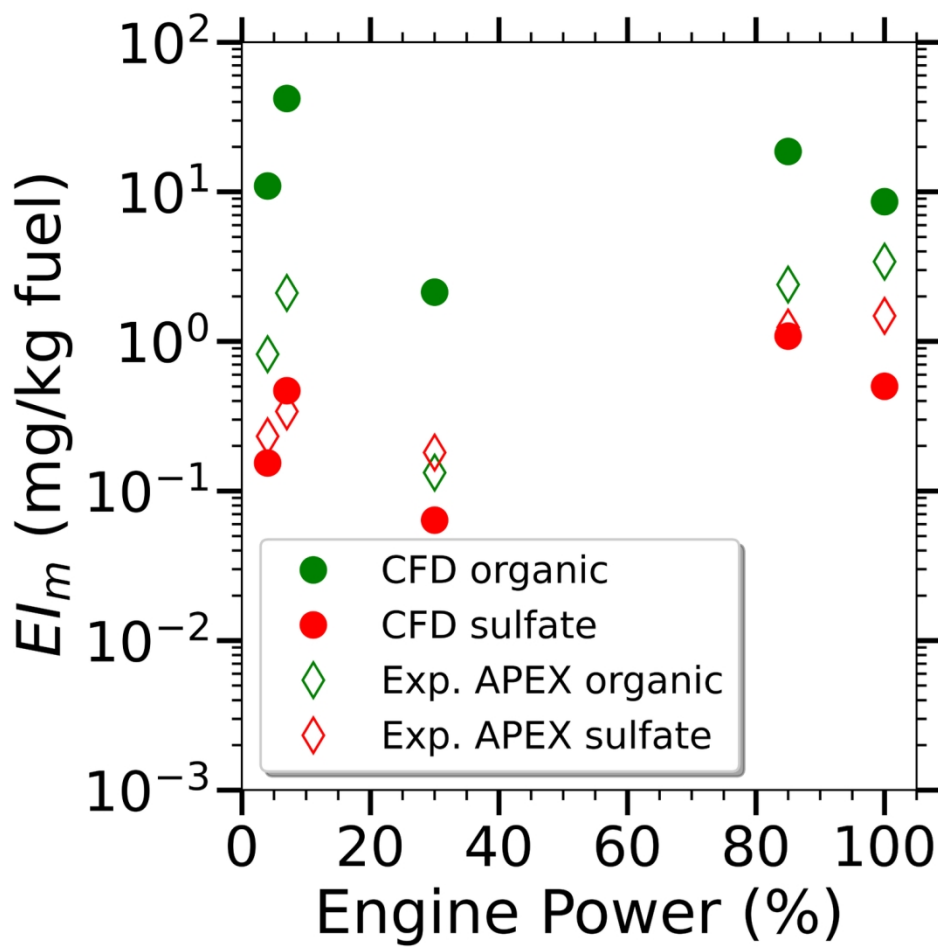
Evolution of nvPM / total PM number ratio in the plume

88x88mm (300 x 300 DPI)



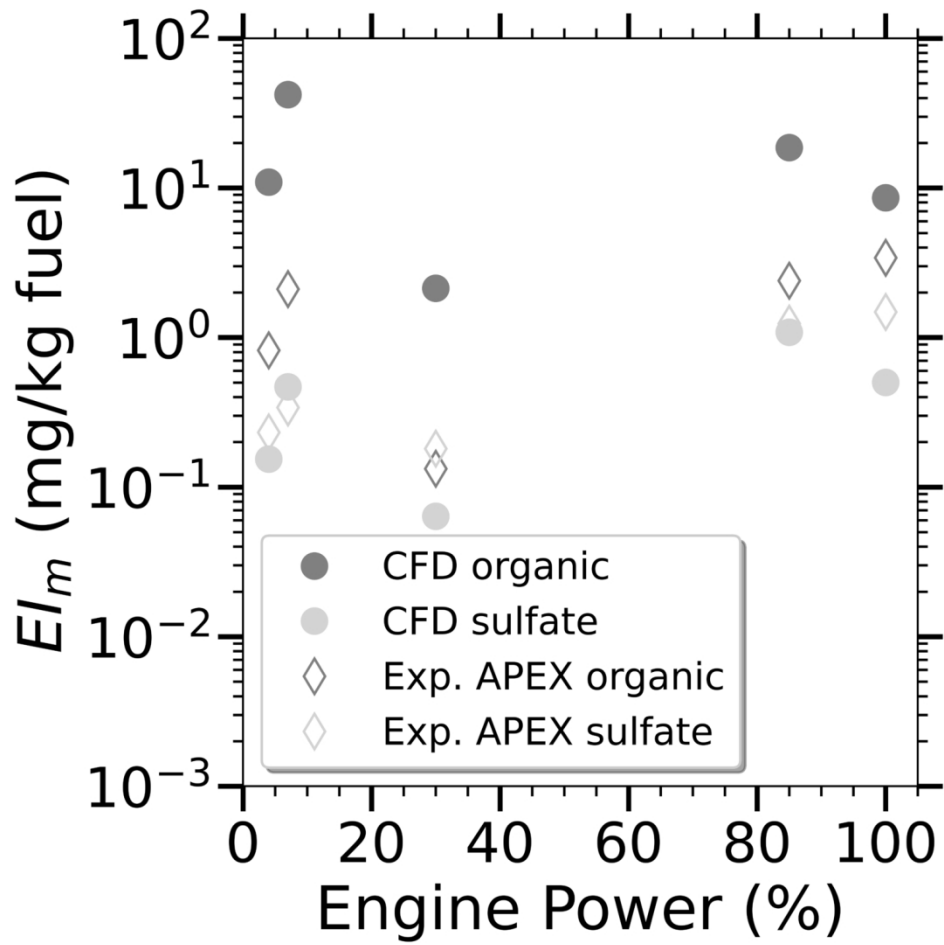
Evolution of nvPM / total PM number ratio in the plume

88x88mm (300 x 300 DPI)



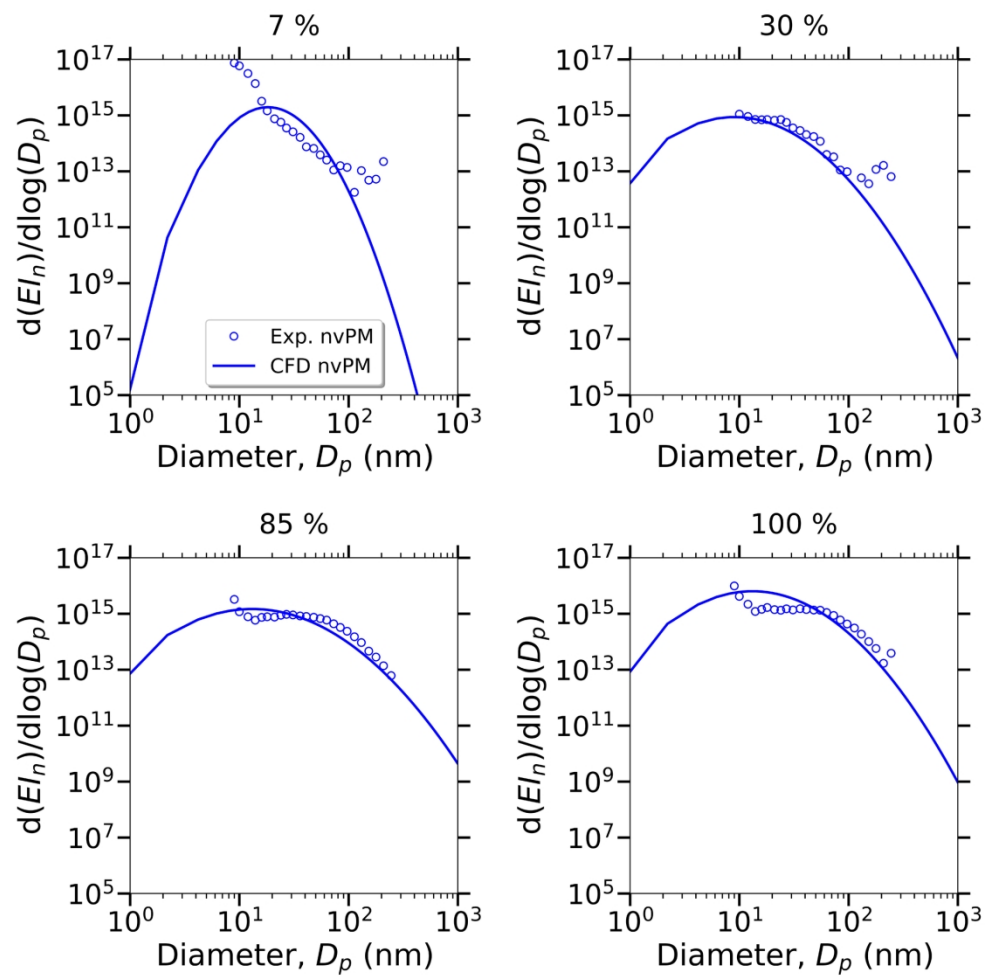
Comparison of sulfate and organic EI_m (mg kg fuel⁻¹) condensed on the soot mode between APEX-1 measurements and CFD results as a function of LTO power settings at 30 m downstream the engine exhaust

140x140mm (300 x 300 DPI)

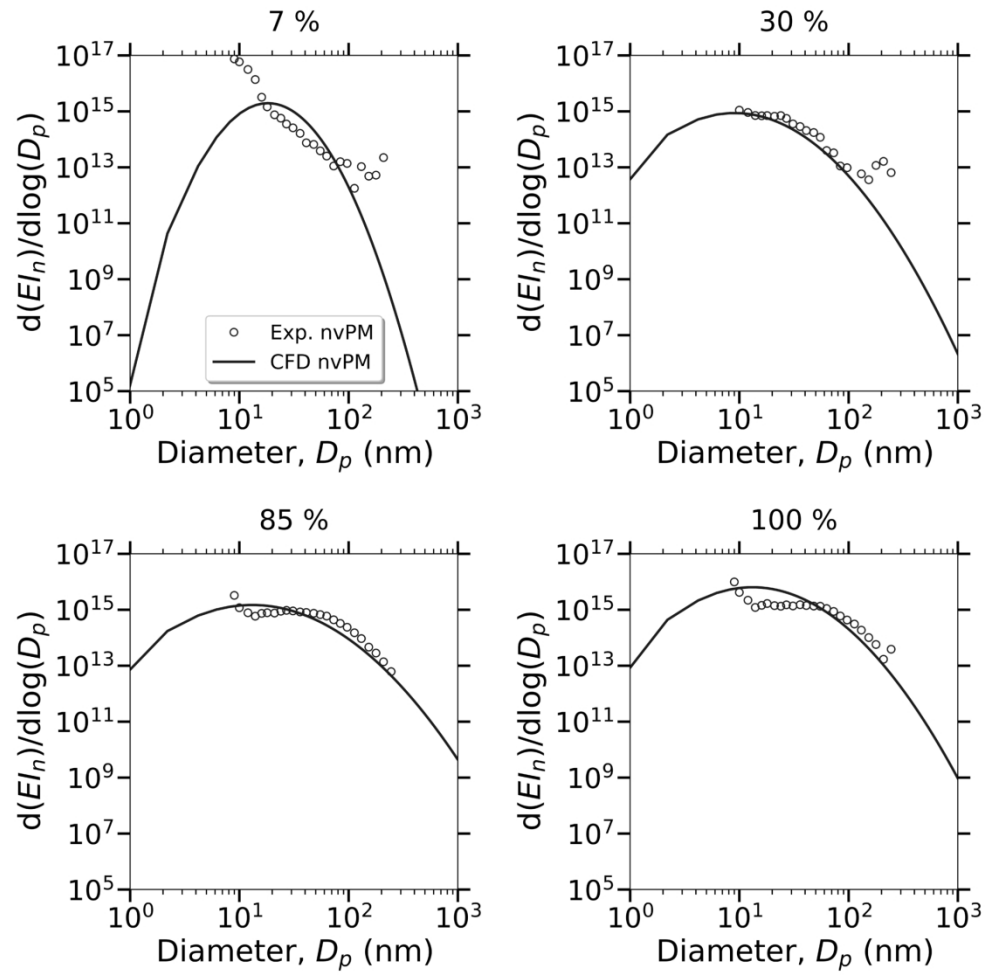


Comparison of sulfate and organic EI_m (mg kg fuel⁻¹) condensed on the soot mode between APEX-1 measurements and CFD results as a function of LTO power settings at 30 m downstream the engine exhaust

140x140mm (300 x 300 DPI)

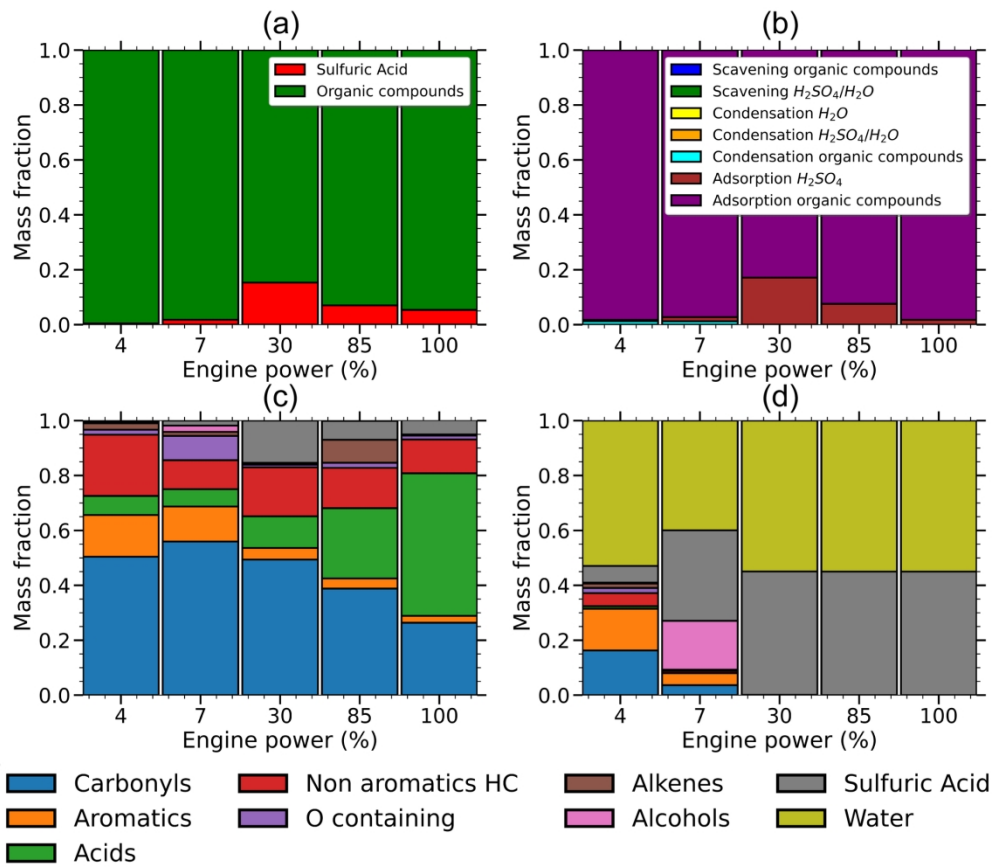


Particle size distribution of nvPM for 7, 30, 85, 100% engine power settings at 30 m
184x183mm (300 x 300 DPI)



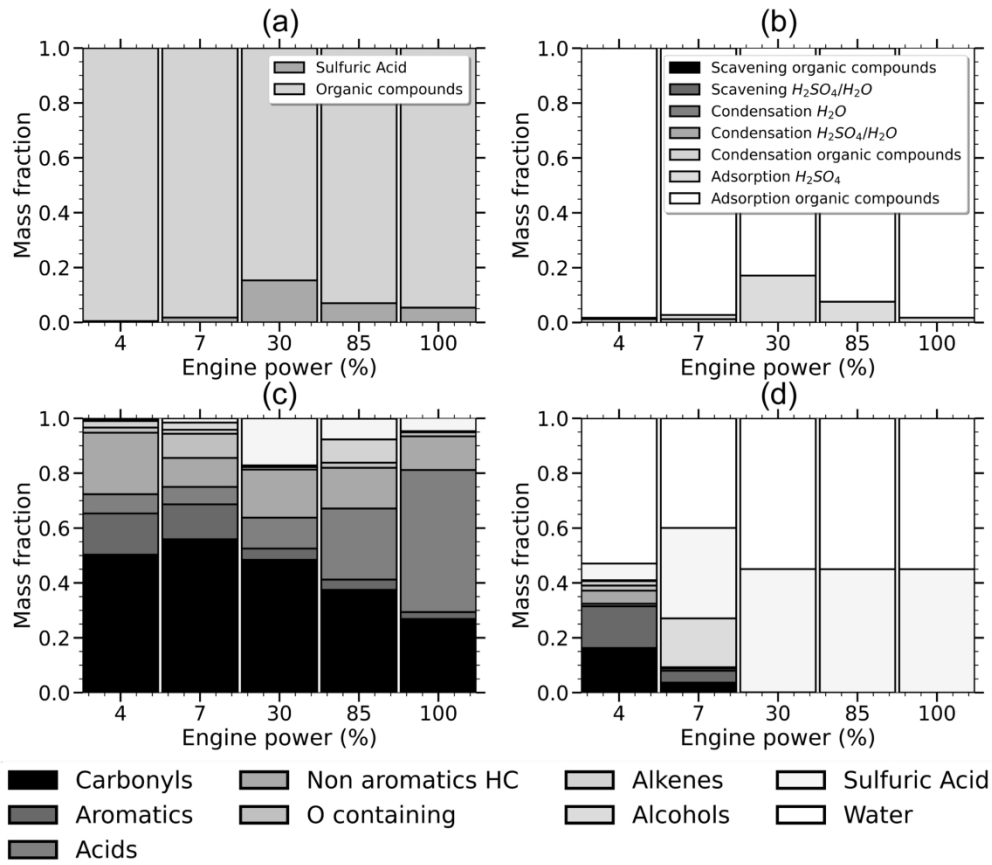
Particle size distribution of nvPM for 7, 30, 85, 100% engine power settings at 30 m

184x183mm (300 x 300 DPI)



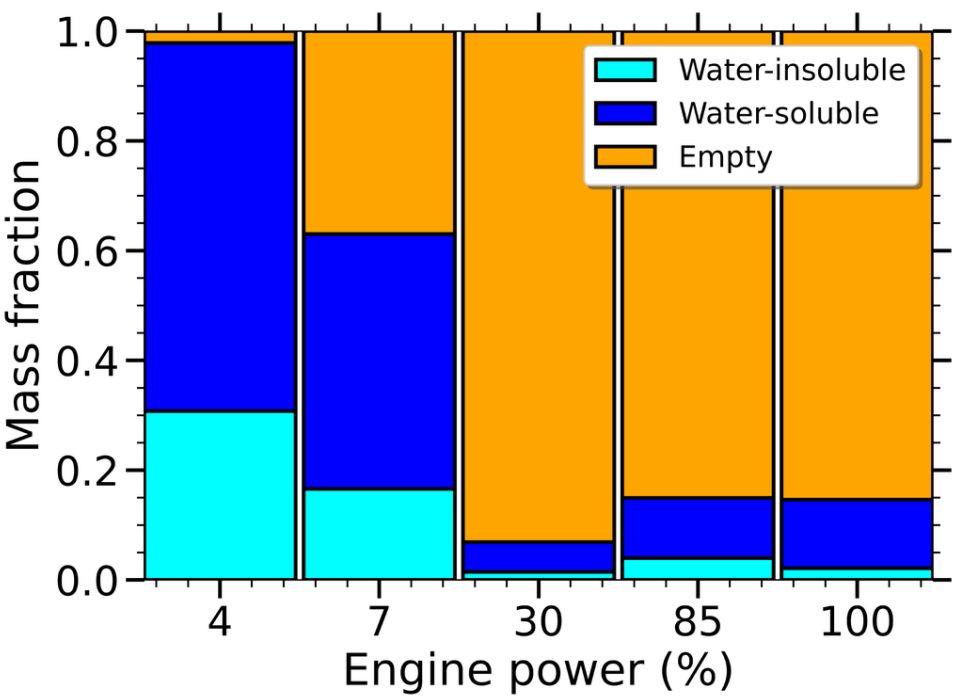
Mass fraction composition regarding sulfate and organic components of soot mode particles (a) microphysical processes of soot mode particles (b) different compound classes of soot mode particles (c) and homogeneous nucleation mode particles (d) as a function of engine power at 50 m downstream of the engine

184x159mm (300 x 300 DPI)



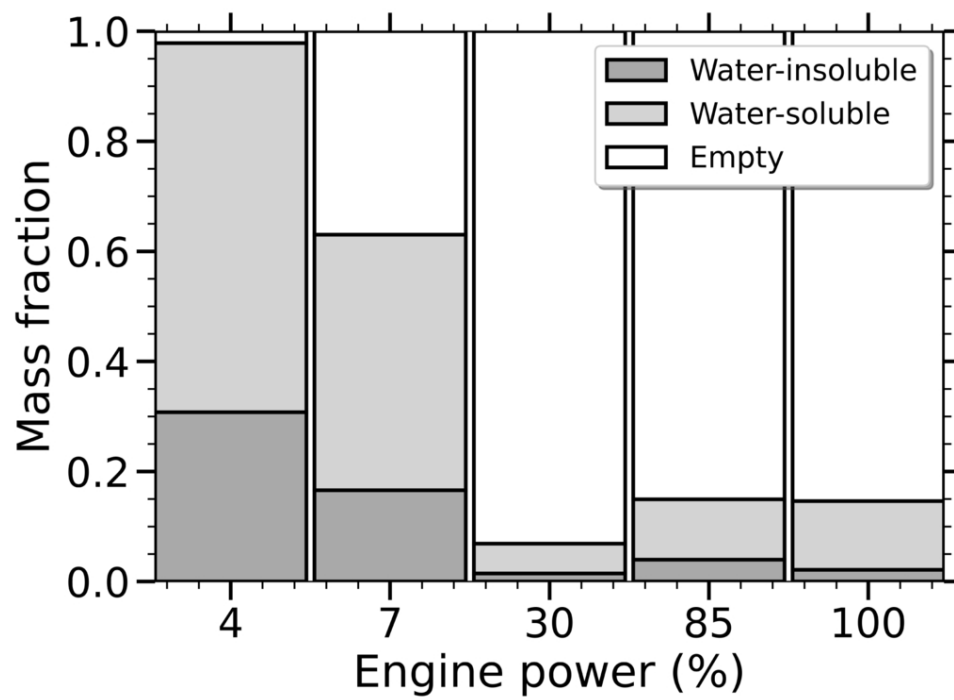
Mass fraction composition regarding sulfate and organic components of soot mode particles (a) microphysical processes of soot mode particles (b) different compound classes of soot mode particles (c) and homogeneous nucleation mode particles (d) as a function of engine power at 50 m downstream of the engine

184x159mm (300 x 300 DPI)



Mass fraction in soot coatings regarding surface coverage as a function of engine power at 50 m downstream of the engine

90x66mm (300 x 300 DPI)



Mass fraction in soot coatings regarding surface coverage as a function of engine power at 50 m downstream of the engine

89x66mm (300 x 300 DPI)