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Modelling Strategies for chemical emissions estimation: kerosene vs sustainable aviation fuels

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Abstract

Over the past decades, the aviation sector has experienced significant growth, driven by route expansion and the spread of low-cost carriers. Alongside performance and reliability requirements, the aeronautical community is now facing a challenge concerning the environmental sustainability of the sector. Promoting sustainable development of aviation without reducing operations requires effective strategies and tools to minimize its environmental impact. In this context, optimizing aircraft propulsion systems at the earliest design stages is a key pathway to meeting national and international green targets. Therefore, early-stage estimation of chemical emissions plays a crucial role in supporting the sector's sustainable transition. This thesis focuses on the development and assessment of modelling strategies for the preliminary estimation of chemical emissions from aircraft propulsion systems operating with both conventional liquid fuels and Sustainable Aviation Fuels (SAFs). In particular, the work addresses the complex phase-change phenomena that govern liquid-fuel spray combustion in aero-engine combustors, such as atomization and evaporation, and proposes a simplified modelling approach suitable for the estimation of combustion-derived chemical emissions from the outset of the design process. Atomization is modelled using semi-empirical correlations for droplet size distribution and the Sauter Mean Diameter (SMD), while evaporation is investigated under both subcritical and supercritical/transcritical conditions. For subcritical regimes, the Abramzon-Sirignano model is adopted to account for coupled heat and mass transfer effects, including Stefan flow. For high-pressure and transcritical conditions, the Peng-Robinson equation of state is used to describe phase equilibrium in mixtures via fugacity equilibrium. All physical models are implemented in dedicated Python numerical codes to allow rapid parametric studies. Mixing and combustion, which lead to pollutant formation, are simulated using chemical-kinetics mechanisms implemented in the Cantera environment. Conventional fuels are represented by physico-chemical surrogates for Jet-A, while SAFs are represented by an Alcohol-to-Jet (AtJ) surrogate for comparative analyses. The combustion model allows estimation of the thermodynamic state of the exhaust gases, useful for propulsion performance analysis, and their chemical composition, from which emission indices for pollutants and greenhouse gases (e.g., CO_2 , H_2O , CO , unburned hydrocarbons and NO_x) can be determined. To demonstrate the broad applicability of the proposed strategy, the developed methodology is applied to a Concorde-like supersonic case-study aircraft equipped with mixed-flow turbofan engines. For the turbofan engines considered in this study, developed within the H2020 European MORE&LESS project, a pre-compiled propulsion database was used as input for the analyses and modelling presented here. The emission results obtained across

the flight envelope analysed for the selected case study demonstrate the capability of the adopted modelling framework to assess the influence of fuel properties and propulsion conditions on emission trends. Comparative analyses between conventional and alternative fuels not only confirm the wide applicability of the proposed modelling approach but also highlight the potential of alternative fuels to reduce specific emissions, providing a consistent preliminary tool to support the design of more sustainable propulsion systems.

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Nomenclature

Abbreviations

AFQRJOS Aviation Fuel Quality Requirements for Jointly Operated Systems

ALR Air-to-Liquid Ratio

ASM Abramzon-Sirignano Model

ASTM American Society for Testing and Materials

AtJ Alcohol-to-Jet

BPR Bypass Ratio

CAD Computer-Aided Design

CAGR Compound Annual Growth Rate

CDF Cumulative Distribution Function

CEM Classical Evaporation Model

CFD Computational Fluid Dynamics

CO Carbon Monoxide

CO₂ Carbon Dioxide

CORSIA Carbon Offsetting and Reduction Scheme for International Aviation

EI Emission Index

EICO Emission Index of Carbon Monoxide

EICO₂ Emission Index of Carbon Dioxide

EIH₂O Emission Index of Water Vapour

EIHC Emission Index of Unburned Hydrocarbons

EINO_x Emission Index of Nitrogen Oxides

EOS Equation Of State

EoV Enthalpy of Vaporization

FT	Fischer-Tropsch
GHG	Greenhouse Gas
H ₂ O	Water Vapour (molecular formula)
H _v	Enthalpy of Evaporation
HC	Hydrocarbons
HCN	Hydrogen Cyanide
HEFA	Hydroprocessed Esters and Fatty Acids
IATA	International Air Transport Association
ICAO	International Civil Aviation Organization
IPCC	Intergovernmental Panel on Climate Change
LHV	Lower Heating Value
LLNL	Lawrence Livermore National Laboratory
MFTF	Mixed-Flow Turbofan
MORE&LESS	MDO and REgulations for Low-boom and Environmentally Sustainable Supersonic aviation (EU project)
MW	Molecular Weight
N ₂ O	Nitrous Oxide
NJFCP	National Jet Fuels Combustion Program
NO	Nitric Oxide
NO ₂	Nitrogen Dioxide
NO _x	Nitrogen Oxides
ODE	Ordinary Differential Equation
PDF	Probability Distribution Function
PM	Particulate Matter
PR-EoS	Peng-Robinson Equation of State
PtL	Power-to-Liquid
SAF	Sustainable Aviation Fuel
SMD	Sauter Mean Diameter

SN	Smoke Number
SO _x	Sulfur Oxides
SPK	Synthetic Paraffinic Kerosenes
UHC	Unburned Hydrocarbons
VKI	von Karman Institute for Fluid Dynamics
VLE	Vapour-Liquid Equilibrium

Greek letters

$\chi_{v,s}$	Vapour mole fraction
γ	Specific heat ratio
μ	Dynamic viscosity
ω	Acentric factor
ϕ	Fugacity coefficient
ϕ_d	Arbitrary variable
ρ	Density
σ	Surface tension
τ_V	Momentum response time

Nomenclature

$\dot{m}_d$	Droplet evaporation rate
A	Droplet section
B_M	Spalding mass transfer number
B_T	Spalding thermal energy transfer number
C_D	Drag coefficient
c_p	Specific heat capacity at constant pressure
D	Diameter, diffusion coefficient
d_o	Nozzle diameter
f	Fugacity
F_M	Correction factor for diffusional film thickness
F_T	Correction factor for thermal film thickness

G	Correction factor for energy transfer reduction due to evaporation
g	Gravitational acceleration
h	Enthalpy
K	Evaporation constant
k	Thermal conductivity
L_c	Characteristic dimension
L_K	Knudsen layer thickness
L_v	Enthalpy of vaporization
Le	Lewis number
m_d	Droplet mass
N_s	Number of species
Nu	Nusselt number
p	Pressure
Pr	Prandtl number
Q	Quality
q	Distribution parameter
Q_d	Energy effectively received at the droplet surface
Q_L	Latent heat of evaporation
Q_S	Sensible heat
Q_{g-d}	Total energy transferred from the gas to the droplet
Q_{g-v}	Energy carried away from droplet by diffusing vapour
R	Specific gas constant
R_u	Universal gas constant
Re_d	Droplet Reynolds number
Sc	Schmidt number
Sh	Sherwood number
T_b	Boiling temperature
T_d	Droplet temperature

T_{wb}	Wet-bulb temperature
U, u	Velocity
v_d	Atomic diffusion volume
W	Molecular weight
Y_v, Y_{fuel}^*	Vapour mass fraction
y_{fuel}^*	Vapour mole fraction
Z	Compressibility factor

Subscripts

0	Initial
A	Air
atm	Atmospheric
c	Critic
d	Droplet
eq	Equilibrium
ev	Evaporation
f	Fuel
g	Gas
h	Heat-up
i	Air/gas
$inlet, CC$	Combustion chamber inlet
j	Fuel
L	Liquid
lag	Lagrangian
m	Gas-vapour mixture, mean
p	Pre-filmer lip
r	Reduced
rel	Relative
s	Properties at the droplet surface

sat Saturation

V, v Vapour

Superscripts

eq Equilibrium

L Liquid phase

n Time step

V Vapour phase

Chapter 1

Introduction

1.1 Research Context

Over the past decades, civil aviation has experienced sustained and rapid growth due to globalization, increased mobility demand, expansion of international trade, and the proliferation of low-cost carriers. Long-term forecasts consistently indicate a steady increase in air traffic demand. The expected growth is illustrated in Fig. 1.1, which shows the projected increase in passenger numbers across all major world regions. According to the International Civil Aviation Organization (ICAO), global passenger traffic has historically doubled approximately every 15 years under stable economic conditions [1]. This expansion, while representing a remarkable technological and socio-economic achievement, has intensified concerns regarding aviation's environmental footprint. The aviation sector currently contributes approximately 2-3% of global anthropogenic CO₂ emissions. However, its total climate impact extends beyond carbon dioxide. Nitrogen oxides (NO_x), water vapour, soot particles, contrail formation, and induced cirrus clouds contribute to additional radiative forcing effects. The Intergovernmental Panel on Climate Change (IPCC) emphasizes that non-CO₂ effects significantly amplify aviation's overall climate impact [2].

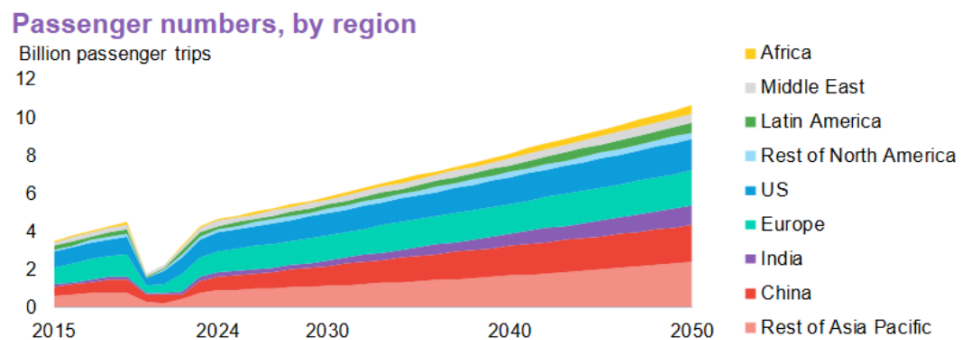


Figure 1.1: Projected passenger numbers by region (billion passenger trips), showing the expected long-term growth in global air traffic demand [3].

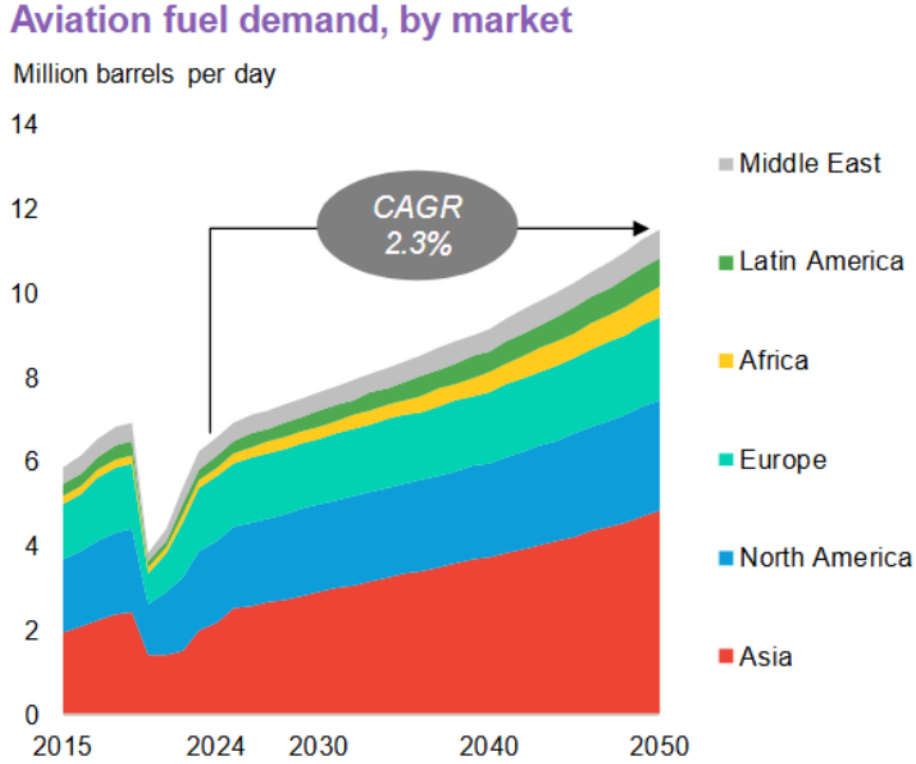


Figure 1.2: Projected aviation fuel demand by market (million barrels per day), with a compound annual growth rate (CAGR) of approximately 2.3% towards 2050 [3].

For this reason, international institutions and regulatory bodies have established ambitious decarbonization targets. ICAO introduced the Carbon Offsetting and Reduction Scheme for International Aviation (CORSIA) to stabilize net CO₂ emissions from international aviation [1]. The International Air Transport Association (IATA) committed to achieving net-zero carbon emissions by 2050 under the *Fly Net Zero* initiative [4]. At the European level the *ReFuelEU Aviation Regulation* aims to accelerate the deployment of sustainable aviation fuels (SAFs) and reduce lifecycle emissions [5]. These policy frameworks highlight a fundamental shift in perspective: environmental impact assessment must be integrated from the earliest stages of aircraft and propulsion system design. Traditionally, emission prediction methodologies have been applied during detailed design or certification phases. However, these approaches present limitations when applied to preliminary phases. At the conceptual design stage, engineers require simplified yet physically consistent tools capable of estimating emissions trends without resorting to high-fidelity computational fluid dynamics simulations or expensive experimental testing.

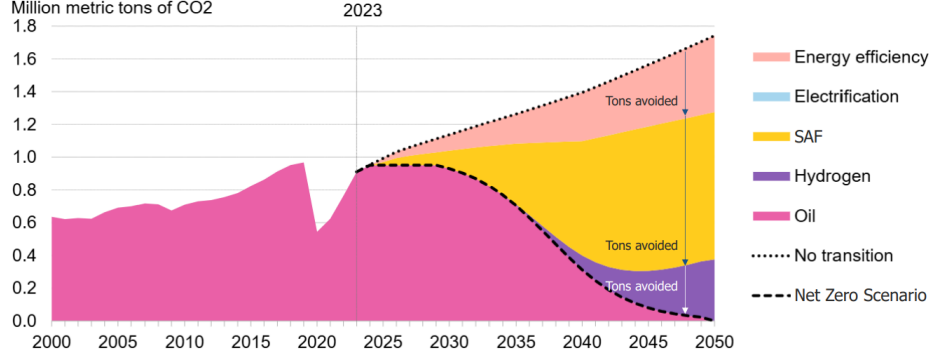


Figure 1.3: Projected aviation CO₂ emissions under a No-Transition scenario and a Net Zero Scenario [3].

Modern aircraft propulsion systems operate almost exclusively with liquid hydrocarbon fuels. Even Sustainable Aviation Fuels, although produced from alternative feedstocks, are designed as liquid drop-in fuels compatible with existing fuel systems and combustors. However, many preliminary emission estimation approaches implicitly assume homogeneous gaseous combustion, neglecting the liquid-phase processes that govern spray combustion in aero-engine combustors, such as atomization and evaporation. Atomization determines the initial droplet size distribution and strongly influences evaporation rates. Evaporation governs flame temperature, reaction rates, and ultimately pollutant formation mechanisms. Under modern combustor conditions, pressures may approach or exceed the critical pressure of surrogate fuel components, making transcritical and supercritical thermodynamic effects relevant. Neglecting these physical phenomena may compromise the robustness of emission predictions. Sustainable Aviation Fuels represent one of the most promising short- and medium-term strategies for aviation decarbonization. According to ICAO and IATA analyses, SAFs can achieve lifecycle CO₂ emission reductions between 50% and 80% compared to conventional Jet-A fuel, depending on feedstock and production pathway [1], [4]. The main certified production pathways include:

- Hydroprocessed Esters and Fatty Acids (HEFA);
- Fischer–Tropsch (FT) synthetic fuels;
- Alcohol-to-Jet (AtJ);
- Power-to-Liquid (PtL) synthetic fuels.

The ASTM D4054 qualification process guarantees that alternative fuels satisfy stringent physicochemical requirements for drop-in compatibility [6]. Nevertheless, even when chemically compatible, SAFs may exhibit differences in aromatic content, density, viscosity, and volatility distribution compared to conventional kerosene. These differences may affect spray dynamics and emission formation pathways and therefore, evaluating SAF emission trends is very important.

The renewed interest in commercial supersonic transport has emerged in recent years as a consequence of the increasing demand for reduced intercontinental travel times

and the development of more advanced propulsion and aerodynamic technologies. New research efforts were made in order to design environmentally compatible supersonic transport systems [7]. Within this context, the European research project MORE&LESS (MDO and REgulations for Low-boom and Environmentally Sustainable Supersonic Aviation), funded under the Horizon 2020 programme, was established to address the environmental challenges associated with future civil supersonic aviation. The project aims to contribute to the definition of high environmental standards for supersonic aircraft in alignment with international regulatory frameworks, including ICAO Assembly Resolution A39-1 [8]. Through a comprehensive and multidisciplinary approach, MORE&LESS investigates the environmental impact of supersonic flight by integrating research activities in aerodynamics, propulsion, jet noise, sonic boom mitigation, pollutant emissions, and overall environmental performance [9]. The project combines both low- and high-fidelity modelling tools with experimental test campaigns to improve existing simulation approaches and extend them to the supersonic regime. The resulting methodologies are integrated into a holistic multidisciplinary framework intended to support the development of future regulations and operational procedures for environmentally sustainable supersonic aviation. By applying this framework to dedicated case studies, the project evaluates whether enabling technologies and operational strategies for supersonic aircraft can meet the environmental requirements expected for future commercial deployment [9].



Figure 1.4: MORE&LESS research project [9].

1.2 Objectives of the Work

The primary objective of this thesis is to develop and assess a physics-based modelling strategy for the preliminary estimation of chemical emissions from aircraft propulsion systems operating with both conventional kerosene and Sustainable Aviation Fuels. The first step is to evaluate the differences between simplified conceptual emission models, which do not consider phase change phenomena, and those that include physical processes governing liquid-fuel combustion. The proposed modelling framework consists of the following steps:

- Atomization modelling through semi-empirical correlations for droplet size distribution and Sauter Mean Diameter (SMD);
- Evaporation modelling under subcritical conditions using the Abramzon-Sirignano formulation;
- Thermodynamic modelling under high-pressure conditions using the Peng-Robinson Equation of State.

These models are implemented in dedicated Python numerical codes in order to make parametric analyses that maintain the level of computational simplicity typically required during the conceptual design phase.

The second step is to couple the physical modelling of spray atomization and evaporation with chemical kinetic simulations performed in a zero-dimensional framework. Using reduced reaction mechanisms implemented in the Cantera environment, the combustion process is simulated to estimate the Emission Indices (EIs) for CO_2 , H_2O , CO , unburned hydrocarbons (UHC), and NO_x . Conventional fuels are represented through a physicochemical surrogate for Jet-A, while Sustainable Aviation Fuels are represented using an Alcohol-to-Jet surrogate for comparative analyses. This approach ensures physical adaptability to alternative fuel formulations and a global applicability to all liquid fuels.

Another goal of this thesis is the application of the proposed modelling strategy to the CS-1A supersonic aircraft configuration developed within the MORE&LESS framework. Using a precompiled propulsion database for the mixed-flow turbofan engines, the methodology is applied across representative operating conditions along the mission profile. This case study enables:

- Evaluation of spray behaviour under varying Mach numbers and altitudes;
- Assessment of evaporation trends under different combustor inlet pressures;
- Comparative analysis of emission indices across the flight envelope;
- Direct comparison between conventional kerosene and SAF scenarios.

Through this application, the thesis demonstrates the capability of the proposed framework to take the influence of fuel properties and propulsion conditions on

emission trends into account, especially in supersonic flight regimes.

This thesis highlights the importance of considering environmental impacts from the very beginning of the design process; rather than leaving environmental assessment to the final certification phase, it should be integrated into the conceptual design stage from the earliest phases. The integration of atomization modelling, advanced evaporation thermodynamics, and chemical kinetics simulations can be useful to support the sustainable design of future aircraft propulsion systems.

Chapter 2

Phase changes modelling strategies - Understanding physical phenomena

2.1 Atomization

Atomization is the process of generating drops. The process begins when a liquid is pushed through a nozzle. The energy stored in the liquid, expressed as liquid pressure in hydraulic nozzles or as a combination of liquid and air pressure in two-fluid nozzles, along with the nozzle's design causes the liquid to exit as thin streams or ligaments, which then disintegrate into much smaller fragments, commonly known as drops, droplets, or liquid particles. Every spray produces droplets of various sizes, known collectively as the drop size distribution. In simple terms, atomization can be described as the breaking apart of a liquid as it flows out of an opening. Different nozzle designs have differently shaped orifices and generate distinct spray patterns, such as hollow cone, full cone, or flat spray. As a result, each nozzle type produces a characteristic drop size distribution, which can differ greatly between designs. In addition, factors like liquid properties, nozzle flow rate, operating pressure, and spray angle also influence the resulting droplet size [10]. The most practical way to atomize a liquid is through pressure atomization, where the pressure droplet in a nozzle is converted into kinetic energy of emanating liquid jet or sheet. Atomization is affected by the influence of surface tension and disruptive influence of internal and external forces. When surface tension dominates it pulls a liquid into the shape of sphere because it has the minimum surface energy. Liquid viscosity causes binding influence resisting any changes in system geometry. Oppositely, aerodynamic forces acting on the liquid surface cause disturbances and contribute to disintegration of the bulk liquid. Thus, breakup occurs when disruptive aerodynamic forces prevail consolidating surface tension forces [11]. Atomization is considered to consist of two stages, first *primary atomization*, in which a bulk liquid disintegrates in ligaments, second *secondary atomization*, in which ligaments further break up into smaller droplets. Processes occurring at both stages govern the shape, structure

and penetration of the resulting spray along with characteristics of the droplet size and velocity distribution. Practically, these characteristics are affected by internal geometry and size of a nozzle, characteristics of surrounding medium in which the liquid is injected and the physical properties of the liquid itself [12].

2.1.1 Atomizers

An atomizer is a device typically used to produce a spray. Spray formation requires a sufficiently high relative velocity between the liquid being atomized and the surrounding air or gas. This condition can be achieved in different ways. In some atomizers, the liquid is expelled at high speed into an air or gas stream that is moving relatively slowly. Common examples of this approach are pressure atomizers and rotary atomizers, where the liquid is thrown outward at high velocity from the edge of a rotating cup or disk. Alternatively, atomization can be accomplished by subjecting a slowly moving liquid to a high-speed airflow. This technique is commonly referred to as twin-fluid, air-assisted, or airblast atomization [11].

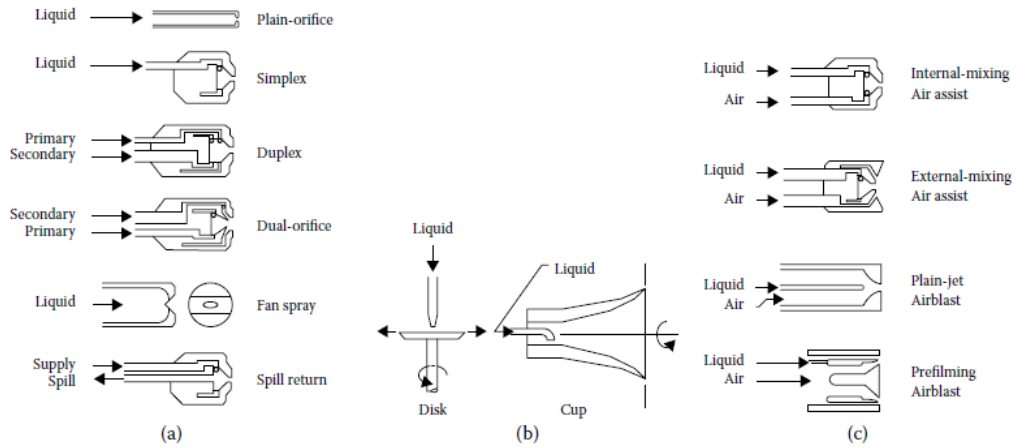


Figure 2.1: (a) Pressure atomizers, (b) Rotary atomizers, and (c) Twin-fluid atomizers [11].

Pressure Atomizers

When a liquid passes through a small opening under high pressure, its pressure energy is transformed into kinetic energy, resulting in a high exit velocity. As injection pressure increases, the liquid velocity rises with the square root of the pressure differential. Higher velocities promote liquid breakup and atomization. Pressure nozzles can operate in several configurations [11]:

- Plain-orifice: a round liquid jet is injected through a simple circular orifice. Smaller orifices improve atomization, but practical limits are imposed by clogging. These nozzles are commonly used in combustion systems such as diesel engines, gas turbines and rocket engines.

- Pressure-swirl (simplex): a swirl chamber is used upstream of the orifice, where tangential inlets impart angular momentum to the liquid. The liquid exits as a thin annular sheet that expands into a hollow-cone spray, offering good atomization, especially at high pressures and wide spray angles.
- Square-spray: this type of nozzles distorts a solid-cone spray into a square shape, providing uniform area coverage at the expense of atomization quality.
- Duplex: two sets of tangential slots (primary and secondary) are used to extend the operating flow range, which is limited by the injection pressure differential. Although these nozzles allow good atomization over a wide turndown ratio, spray quality temporarily degrades during the transition when the secondary flow is introduced.
- Dual-orifice: two concentric swirl chambers are used, effectively forming a nozzle within a nozzle. These nozzles offer greater flexibility in flow rate and spray angle control but also experience reduced atomization quality during transition between stages.
- Spill-return: these nozzles maintain high supply pressure while excess liquid is returned to the supply line, enabling very large turndown ratios with consistently good atomization and a hollow-cone spray.
- Fan-spray: these nozzles generate flat sprays using shaped orifices, deflector plates or impinging jets. While deflector and impinging-jet designs allow wide spray angles and high flow rates, their atomization quality is generally poorer. Impinging jets are particularly useful when separate liquids must remain isolated until collision, such as in hypergolic propellant systems, in which an oxidizer and fuel component will react upon contact.

Rotary Atomizers

A common type of rotary atomizer uses a disk that rotates at high speed, with the liquid introduced at its centre. As the disk spins, the liquid spreads outward due to centrifugal forces and is ejected from the edge at high velocity, forming a spray. The disk surface may be smooth or equipped with vanes or slots to help direct the liquid toward the rim. In many applications, the atomizer is housed in a cylindrical or conical chamber, where downward airflow shapes the spray into an umbrella-like pattern. In some designs, a rotating cup replaces the disk. These cups are typically smaller and bowl-shaped, and their edges may be serrated to promote a more uniform droplet size distribution. Unlike pressure nozzles, rotary atomizers allow the liquid flow rate and rotational speed to be adjusted independently, offering greater operational flexibility. At low flow rates, droplets form mainly near the disk edge, while at higher flow rates, liquid sheets or ligaments develop and subsequently break up into droplets. When operated at high rotational speeds with low flow rates,

small disks can produce sprays with relatively uniform droplet sizes and a full 360° spray pattern [11].

Air-Assist Atomizers

In this nozzle design the liquid is atomized by interaction with a high-velocity stream of air or steam. In internal-mixing designs, the gas and liquid are combined inside the nozzle before exiting the orifice, sometimes using tangential inlets to form a conical spray with a maximum angle of about 60° . Although this configuration is relatively energy-inefficient, it produces finer droplets than simple pressure nozzles. In external-mixing nozzles, the high-speed gas impacts the liquid at or just outside the discharge orifice, avoiding internal back-pressure problems. However, this arrangement requires higher gas flow rates and is less efficient than internal mixing for the same atomization quality. Both nozzle types are effective for atomizing high-viscosity liquids [11].

Airblast Atomizers

Airblast atomizers operate in much the same way as air-assist nozzles, and both are classified as twin-fluid atomizers. The key distinction between them lies in the airflow conditions: air-assist atomizers rely on relatively small amounts of air or steam moving at very high, often sonic, velocities, whereas airblast atomizers use much larger air flow rates at considerably lower velocities, typically below 100 m/s [11]. The merits of the airblast atomizer have led to its installation in a wide range of industrial and aircraft gas turbines and cover both pre-filming and plain-jet concepts. Most of the systems now in service are of the pre-filming type, in which the fuel is first spread out into a thin, continuous sheet and then subjected to the atomizing action of high velocity air. In other designs the fuel is injected into the high velocity airstream in the form of one or more discrete jets. A drawback to the thin-sheet airblast atomizer is that it is fully effective only when both sides of the liquid sheet are exposed to the air. This requirement introduces a complication in design, since it usually means arranging for two separate air flows through the atomizer. For this reason the plain-jet type of airblast atomizer is sometimes preferred, in which the fuel is not transformed into a thin sheet, but instead is injected into the high velocity airstream in the form of discrete jets [13].

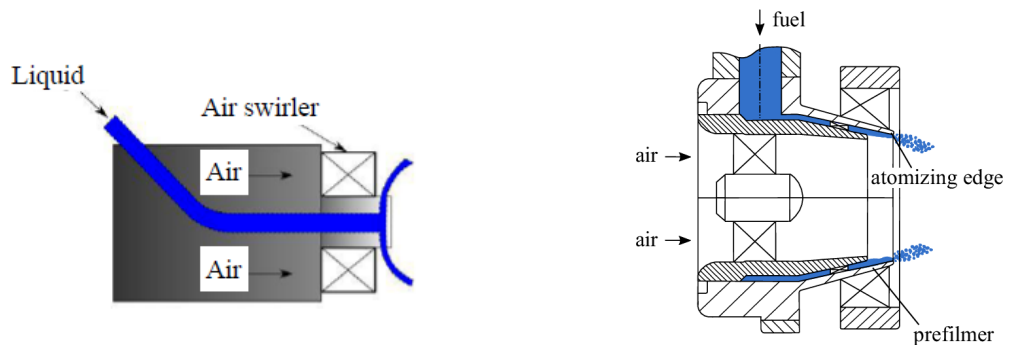


Figure 2.2: Airblast atomizers: a) Plain-jet airblast, b) Pre-filmer airblast [18].

2.1.2 Drop Size Distribution

A general definition of a spray is "a system of drops immersed in a gaseous continuous phase" [11]. Usually, atomizers produce sprays consisting of droplets whose diameters span a wide range, typically from a few micrometers up to about μm , as a consequence of different breakup mechanisms. One of the most fundamental and significant characteristics of a liquid spray is the frequency of occurrence of the various sizes of droplets, commonly referred to as the drop size distribution. It is also the property that is most difficult to predict theoretically and to determine experimentally. For this reason, a complete description of a spray cannot rely solely on a single mean droplet diameter but must also take into account the entire distribution of droplet sizes. This distribution is often represented graphically using a histogram, where the horizontal axis shows the diameter ranges and the vertical axis indicates the normalized fraction, corresponding to the percentage of the total number of droplets in the spray that are smaller than a given diameter. To describe drop size distributions mathematically, various functions have been proposed, derived either from probability theory or from empirical observations. Among the most commonly used models are the normal and log-normal distributions, as well as the Nukiyama-Tanasawa, Rosin-Rammler and upper-limit distributions [14]. The Rosin-Rammler expression is perhaps the most widely used. Although originally developed for powders, it has been applied with success to liquid drops. It can be expressed in the form:

$$F(d) = 1 - \exp \left[- \left(\frac{d}{D_m} \right)^q \right] \quad (2.1)$$

where $F(d)$ is the volume fraction of the spray occurring in drops of diameter less than d , d is a size parameter, D_m is the mean diameter (D_{32}) and q is a distribution parameter. The higher the value of q , the more uniform is the spray (if q is equal to infinite the spray has all the droplets of the same size). A typical value for q in aviation sprays is in the range between 2 and 6 but some rotary atomizers can reach a value of 7 [11].

2.1.3 Sauter Mean Diameter (SMD)

In some fields of application, it is more convenient to deal only with mean or average diameters instead of the whole droplet size distribution in order to characterize the spray. Different mean diameters have been defined and each of them is suitable for a specific purpose, as reported in the following table.

Symbol	Name of Mean Diameter	Application
D_{10}	Length	Comparisons
D_{20}	Surface area	Surface area controlling
D_{30}	Volume	Volume controlling, hydrology
D_{21}	Surface-area-length	Absorption
D_{31}	Volume-length	Evaporation, molecular, diffusion
D_{32}	Sauter mean diameter (SMD)	Mass transfer, reaction, combustion

Figure 2.3: Mean diameters and their applications [14].

Sauter Mean Diameter (also known as D_{32}) is a means of expressing the fineness of a spray in terms of the surface area produced by the spray. SMD is the diameter of a drop having the same volume to surface area ratio as the total volume of all the drops to the total surface area of all the drops. This diameter is best suited to calculate the efficiency and mass transfer rates in chemical reactions. SMD increases with increase in liquid viscosity and/or atomizer size, and decreases with increase in air/liquid ratio. SMD diminishes rapidly with increase in air velocity, according to the relationship $SMD \propto U_R^{-0.8}$. The influence of air pressure on SMD is less marked, in fact, $SMD \propto P_A^{-0.4}$ [13]. The basic drop-size equation for airblast atomizers is [15]:

$$\frac{SMD}{L_c} = A \left(\frac{\sigma}{\rho_A U_A^2 L} \right)^{0.5} \left(1 + \frac{1}{ALR} \right) + B \left(\frac{\mu_L^2}{\sigma \rho_L L} \right)^{0.5} \left(1 + \frac{1}{ALR} \right) \quad (2.2)$$

where A and B are constants whose values depend on the specific design characteristics of the atomizer and therefore must be obtained from experimental data. L_c is a characteristic dimension that represents the scale of the atomizer. The term L represents the atomizer dimension at the point or surface where the liquid first contacts the air stream. In the case of pre-filming airblast atomizers $L = D_p$, the pre-filmer lip diameter. For plain-jet atomizers $L = d_o$, the nozzle diameter [13]. Some considerations (e.g. secondary factors, such as liquid-stream Reynolds number and airstream Mach number) lead to the following modified form of equation [13]:

$$\frac{SMD}{d_o} = 0.48 \left(\frac{\sigma}{\rho_A U_{rel}^2 d_o} \right)^{0.4} \left(1 + \frac{1}{ALR} \right)^{0.4} + 0.15 \left(\frac{\mu_L^2}{\sigma \rho_L d_o} \right)^{0.5} \left(1 + \frac{1}{ALR} \right) \quad (2.3)$$

2.1.4 Post-Atomization Relaxation

After primary fragmentation, the droplets generated by the atomizer undergo a phase of adaptation to the surrounding gas flow, commonly referred to as post-atomization relaxation. This phase includes kinematic, thermal, and compositional relaxation, governed by the balance equations of motion, energy, and mass of the individual droplet [11]. Schiller-Naumann model is used for modelling the drag between fluid phases in multiphase flow. The drag coefficient C_D is given as [16]:

$$\begin{cases} C_D = \frac{24}{Re_d} (1 + 0.15 Re_d^{0.687}) & Re \leq 1000 \\ C_D = 0.44 & Re \geq 1000 \end{cases} \quad (2.4)$$

We define the dispersed phase Reynolds number (relative Reynolds number) as:

$$Re_d = \frac{\rho_g U_{rel} D}{\mu_m} \quad (2.5)$$

to measure the motion regime surrounding the droplet. The response time of a particle or droplet to changes in flow velocity or temperature plays a key role in defining non-dimensional parameters used to describe the flow behaviour. The momentum

response time represents the characteristic time needed for a particle or droplet to adapt to changes in its velocity. The equation of motion for a spherical particle in a gas is given by [17]:

$$m_d \frac{dU_d}{dt} = -\frac{1}{2} C_D \rho_g A U_{rel}^2 \quad (2.6)$$

with

$$m_d = \rho_l \frac{\pi D_d^3}{6}, \quad A = \frac{\pi D_d^2}{4}$$

If low Reynolds numbers are considered (Stokes flow), the momentum (velocity) response time is defined as:

$$\tau_V = \frac{\rho_d D^2}{18\mu_g}$$

2.2 Evaporation

2.2.1 Subcritical conditions: Abramzon-Sirignano Model (ASM)

Spray evaporation has been studied over recent decades using theoretical, experimental, and numerical approaches. Nevertheless, due to the inherent complexity of the problem, the evaporation of a single droplet suspended in a gaseous environment, often regarded as an idealized representation of the physical processes occurring in diluted spray regions, provides a fundamental starting point for understanding evaporation mechanisms. It is considered an isolated, single-component, spherical liquid droplet immersed in an infinite gaseous medium at uniform temperature and pressure. Owing to the spherical symmetry of the system, and because the liquid density is significantly higher than that of the surrounding gas under subcritical conditions, heat and mass transfer in the gas phase can be treated as quasi-steady. Heat exchange between the liquid and gas phases is assumed to occur solely through convection, while radiative effects and internal liquid circulation are neglected. Under these assumptions, the droplet temperature gradually approaches a steady or equilibrium value corresponding to the wet-bulb temperature, which depends on the ambient conditions. Once this temperature is reached, all the heat transferred from the surrounding gas is consumed by evaporation and transported away by the diffusing vapour. Consequently, the net heat flux at the droplet surface becomes zero, and the droplet temperature remains constant during the evaporation process [18]. The Abramzon-Sirignano Model (ASM) represents one of the most widely adopted formulations for predicting single droplet evaporation in spray combustion simulations. Developed in 1989, it refines the classical diffusion-controlled evaporation theory by incorporating a more realistic treatment of advective transport, specifically the Stefan flow, and its impact on the thickness of thermal and mass-diffusion boundary layers. By providing a more physically consistent description of these transport processes, the ASM is especially well suited for conditions involving moderate to high evaporation rates. Under such conditions, traditional evaporation models tend to overestimate the evaporation rate, whereas the Abramzon-Sirignano formulation

yields more accurate predictions [18]. This model assumes:

- Isolated, spherical, single-component droplet;
- Quasi-steady mass and heat transfer in the surrounding gas;
- Infinite liquid thermal conductivity (uniform droplet temperature);
- Gas ideality (infinite, hot, constant-pressure ambient gas) and energy transfer between liquid and gaseous phases is assumed to occur only through convection, neglecting radiation;
- No internal droplet liquid circulation;
- Steady vapour-gas film around the droplet: here all Nusselt/Sherwood correlations are valid.

During the initial stage of the droplet lifetime, a transient heat-up period, the energy received by the droplet is utilized to heat-up the liquid to its equilibrium temperature. Once this temperature is achieved, all the energy transferred into the droplet is exclusively employed to gasify the liquid. In other words, the net energy flux penetrating the droplet surface is zero, so the droplet temperature, T_d , remains constant. Due to the balance between heating and cooling, liquid droplets usually do not reach the boiling point, T_b , when they are heated. Instead, in absence of radiation, the temperature evolves towards the wet-bulb temperature, T_{wb} , approaching it asymptotically, as shown in Fig. 2.4.

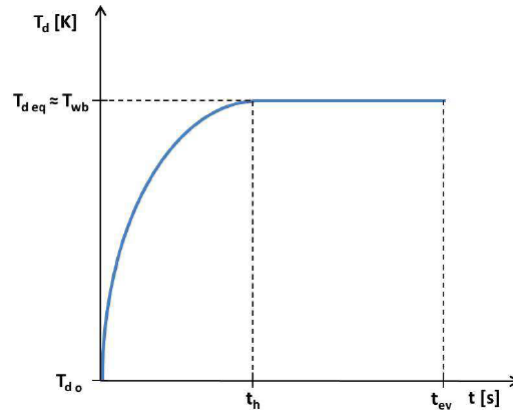


Figure 2.4: Droplet temperature evolution with time [19].

After the initial heat-up period, the D^2 -law (Eq. 2.7) is obeyed, which states that the square of the droplet diameter, D_d , decreases linearly with time. This behaviour occurs because energy and mass diffusion in the surrounding gaseous film are the rate-controlling processes. Therefore, an evaporation constant, K , can be estimated as the negative slope of the variation of the squared droplet diameter in the steady-state evaporation period, as represented in Fig 2.5 [19].

$$\frac{d(D^2)}{dt} = -K \Rightarrow D^2(t) = D_0^2 - Kt \quad (2.7)$$

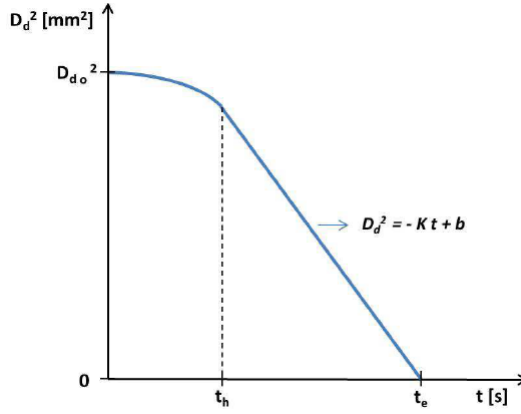


Figure 2.5: Squared droplet diameter evolution with time.

The physical improvement of ASM is its film-theory-based correction for the blowing effect induced by Stefan flow, which thickens the mass and heat boundary layers and thus reduces transfer rates. The two fundamental ODEs are:

1. Droplet diameter evolution:

$$\frac{dD_d}{dt} = -\frac{2\dot{m}_d}{\pi\rho_l D_d^2} dt \quad (2.8)$$

where $\dot{m}_d$ is the evaporation rate and ρ_l the liquid density.

2. Droplet temperature evolution:

$$m_d c_{p,l} \frac{dT_d}{dt} = Q_S \quad (2.9)$$

where $m_d = \rho_l \frac{\pi}{6} D_d^3$ is the droplet mass and Q_S is the "useful" heat that remains in the drop to heat it (i.e. the incoming convective part minus the one used for latent evaporation).

Mass Transfer

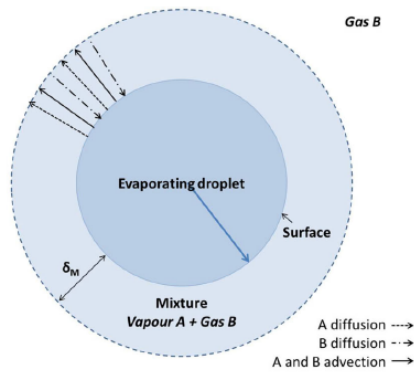


Figure 2.6: Schematic representation of mass transfer in the evaporation of a single droplet.

Using the mass transfer relation, the mass evaporation rate is:

$$\dot{m}_d = \pi D_d \rho_m D_{v,m} Sh_m \ln(1 + B_M) \quad (2.10)$$

where:

- ρ_m is the density of the gas-vapor mixture in the film around the droplet;
- $D_{v,m}$ is the fuel diffusivity in the gas;
- Sh_m is the Sherwood number at the gas-vapour mixture conditions in the film around the droplet;
- B_M is the Spalding number for mass transfer:

$$B_M = \frac{Y_{v,s} - Y_{v,\infty}}{1 - Y_{v,s}}$$

where $Y_{v,s}$ and $Y_{v,\infty}$ are the vapour mass fraction at the droplet surface and far away (in this case = 0), respectively.

The vapour mass fraction at the droplet surface can be calculated from Raoult's law. According to this relation, the molar fraction of vapour at the droplet surface, $\chi_{v,s}$, is given by the ratio between the vapour partial pressure, $p_{v,s}$, and the total pressure of the ambient gas, p_g , as shown by:

$$\chi_{v,s} = \frac{p_{v,s}}{p_g} \quad (2.11)$$

Once the molar fraction $\chi_{v,s}$ has been obtained, the vapour mass fraction $Y_{v,s}$ can be calculated by using the definition of the mean molecular weight of the mixture together with the ideal gas law:

$$Y_{v,s} = \frac{\chi_{v,s} W_v}{\chi_{v,s} W_v + (1 - \chi_{v,s}) W_g} \quad (2.12)$$

When thermodynamic equilibrium between the liquid and vapour phases is assumed at the droplet surface, the vapour concentration is considered to remain at saturation conditions. Under this assumption, and by adopting the ideal gas hypothesis, the molar fraction of vapour at the droplet surface can be determined through the Clausius-Clapeyron relation:

$$\chi_{v,s}^{eq} = \frac{p_{\text{sat}}}{p_g} = \frac{p_{\text{atm}}}{p_g} \exp \left[\frac{L_v W_v}{R_u} \left(\frac{1}{T_b} - \frac{1}{T_d} \right) \right] \quad (2.13)$$

where:

- L_v is the vapour enthalpy of vaporization (J/kg), which is a function of droplet temperature;
- W_v is the fuel vapour molecular weight [kg/mol];

- T_b is the liquid phase boiling temperature, which is calculated at p_{atm} (for n-dodecane $T_b \approx 489$ K);
- R_u is the universal gas constant;
- p_{atm} is the atmospheric pressure.

Heat Transfer

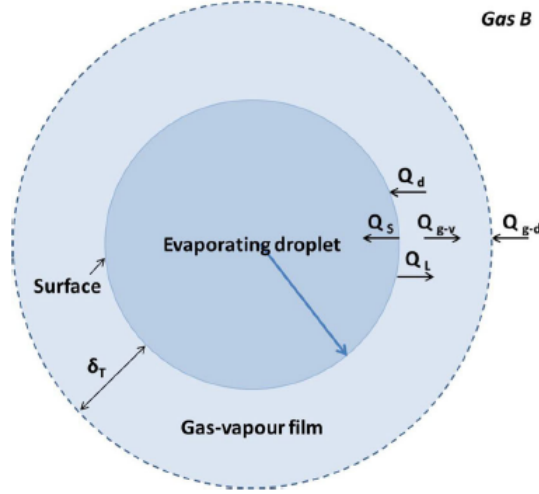


Figure 2.7: Schematic representation of thermal energy transfer in the evaporation of a single droplet.

From Fig. 2.7 it can be seen that the thermal energy reaching the droplet surface, Q_d , can be interpreted in two equivalent ways. On one hand, it corresponds to the sum of the latent heat required for phase change, Q_L , and the sensible heat used to increase the droplet temperature, Q_s . On the other hand, it can be expressed as the difference between the total energy transferred from the surrounding gas to the droplet, Q_{g-d} , and the energy transferred from the gas to the vapour, Q_{g-v} [19]. The Sherwood number used for mass transfer estimation is evaluated through the Ranz-Marshall empirical correlation:

$$Sh_m = 2 + 0.6Re_d^{1/2} Sc_m^{1/3} \quad (2.14)$$

where Sc_m is the Schmidt number given by:

$$Sc_m = \frac{\mu_m}{\rho_m D_{v,m}}$$

and the droplet Reynolds number, is defined as:

$$Re_d = \frac{\rho_g U_{rel} D}{\mu_m}$$

A correction factor, G , is introduced to account for the reduction in heat transfer caused by the evaporation process. This factor arises from the boundary conditions

applied at the droplet surface and reflects the partition of the incoming energy. Only a portion of the total energy received by the droplet, Q_d , is used to supply the latent heat necessary for vaporization, Q_L , while the remaining part contributes to increasing the droplet temperature, Q_S , during the initial heating phase. Considering the energy balance between the surrounding gas and the droplet surface, the thermal energy effectively entering the liquid phase can therefore be written as:

$$Q_S = G \pi D_d Nu_m k_m (T_g - T_d) - \dot{m}_d L_v \quad (2.15)$$

where k is the thermal conductivity and Nu is the Nusselt number, which is calculated by:

$$Nu_m = 2 + 0.6 Re_d^{1/2} Pr_m^{1/3} \quad (2.16)$$

with Pr_m being the Prandtl number, expressed as:

$$Pr_m = \frac{\mu_m c_{p,m}}{k_m}$$

The ASM is an improvement of the CEM (Classical Evaporation Model). The ASM takes the vapour flux leaving the droplet surface (Stefan flow) into account. This outward vapour motion increases the thickness of the thermal and diffusion boundary layers, reducing the efficiency of mass and heat transfer from the surrounding gas to the droplet surface. To include this effect, Abramzon and Sirignano introduced two correction factors, F_M and F_T , associated with the mass and thermal diffusion layers, respectively. These factors are used to define *modified* Nusselt/Sherwood numbers:

$$F_M = \frac{(1 + B_M)^{0.7} \ln(1 + B_M)}{B_M}, \quad F_T = \frac{(1 + B_T)^{0.7} \ln(1 + B_T)}{B_T} \quad (2.17)$$

$$Sh^* = 2 + \frac{Sh_0 - 2}{F_M}, \quad Nu^* = 2 + \frac{Nu_0 - 2}{F_T}$$

The Spalding number for heat transfer is [20]:

$$B_T = (1 + B_M^{\phi_m}) - 1$$

with:

$$\phi_m = \left(\frac{c_{pvap,m}}{c_{p,m}} \right) \left(\frac{1}{Le_m} \right) \left(\frac{Sh_m^0}{Nu_m^0} \right)$$

$$Le_m = \frac{\lambda_m}{\rho_m c_{p,m} D_m}$$

In the expressions above, $c_{pvap,m}$ represents the isobaric specific heat of the droplet species, while $c_{p,m}$ is the isobaric specific heat of the surrounding mixture composed of fuel vapour and ambient gas, evaluated under the reference thermodynamic conditions. The term Le_m corresponds to the Lewis number of the mixture [20].

When F_M and F_T approach unity, the modified Sherwood and Nusselt numbers tend to their classical values Sh_0 and Nu_0 . Since these correction factors physically

represent the increase in boundary-layer thickness caused by Stefan flow, their values are always higher than one. Consequently, the effective rates of mass and heat transfer are reduced compared with the predictions obtained using the classical evaporation model [18]. The correction factor in ASM is defined as:

$$G = \frac{\ln(1 + B_T)}{B_T}$$

2.2.2 Supercritical conditions: Peng-Robinson EOS

Droplet gasification under high-pressure conditions, in which the thermodynamic state of the liquid fuel approaches or exceeds its critical point, plays a key role in several propulsion systems. The modelling of droplet evaporation in such regimes becomes challenging, since classical low-pressure evaporation models are no longer strictly valid. At elevated pressures, gas phase non-idealities and the dissolution of ambient gas into the liquid phase become increasingly important, invalidating assumptions commonly adopted in conventional droplet models, such as the ASM one. As the droplet surface approaches transcritical conditions, the latent heat of vaporization progressively decreases and tends toward zero, while the density difference between the liquid and the surrounding gas diminishes. Consequently, the sharp liquid-gas interface characteristic of subcritical evaporation becomes less well defined and the relative importance of transient transport processes in the gas phase increases, as the characteristic time scales of heat and mass transfer in the two phases become comparable. In addition, thermophysical properties of both phases exhibit a strong dependence on pressure and temperature in the transcritical regime. Under convective flow conditions typical of gas turbine combustors, these effects are further coupled with hydrodynamic phenomena. As the surface tension decreases with increasing pressure and vanishes near the critical point, droplet deformation and breakup mechanisms may be significantly altered, potentially affecting the initial stages of atomization and subsequent vaporization [21]. In the present study, the air ambient conditions exceed the critical pressure of the fuel at relatively low altitudes and low Mach numbers. Consequently, fuel droplets injected into the combustor are rapidly exposed to transcritical or supercritical environments, requiring an evaporation model that remains valid across both regimes. Among cubic EOS formulations, the Peng-Robinson equation of state provides excellent agreement with experimental data over a wide range of pressures and temperatures compared to simpler models such as the Redlich-Kwong EOS, especially near the critical region [21].

Fugacity-based equilibrium condition

At elevated pressures, vapour-liquid equilibrium cannot be described using saturation pressure alone. Instead, equilibrium must be enforced through the equality of fugacities of each species at the interface, which describe the "escaping tendency".

For a given species i , the general equilibrium condition is written as:

$$\bar{f}_i^V = \bar{f}_i^L \quad (2.18)$$

If we introduce the fugacity coefficient:

$$\phi_i^V = \frac{\bar{f}_i^V}{P}, \quad \phi_i^L = \frac{\bar{f}_i^L}{P} \quad (2.19)$$

then Eq. 2.18 can be rewritten as:

$$\phi_i^V y_i = \phi_i^L y_i \quad (2.20)$$

where y_i is the mole fraction of species i at the droplet's surface [22].

The fugacity coefficient ϕ_i for both vapour and liquid phases is:

$$\ln \phi_i = \frac{1}{RT} \int_V^\infty \left[\left(\frac{\partial P}{\partial n_{i,T,V,n_j}} - \frac{RT}{V} \right) \right] dV - \ln Z \quad (2.21)$$

For the Peng-Robinson EOS and the van der Waals mixing rule the formulation becomes:

$$\ln \phi_i = \frac{b_i}{b} (Z-1) - \ln(Z-B) - \frac{A}{2\sqrt{2}B} \cdot \left[\frac{2}{a} \sum_j y_j a_{ij} - \frac{b_i}{b} \right] \ln \left[\frac{Z + (1 + \sqrt{2})B}{Z + (1 - \sqrt{2})B} \right] \quad (2.22)$$

In high-pressure evaporation, the fuel vapour mixes with ambient gases, forming a multicomponent mixture. In order to compute mixture parameters classical quadratic mixing rules are employed [22]:

$$a = \sum \sum y_i y_j a_{ij} \quad (2.23)$$

$$b = \sum y_j b_j \quad (2.24)$$

$$a_{ij} = (1 - k_{ij}) \sqrt{(a_i a_j)} \quad (2.25)$$

$$a_i = 0.4572 \alpha P_{ri} / T_{ri}^2 \quad (2.26)$$

$$b_i = 0.0778 P_{ri} / T_{ri} \quad (2.27)$$

$$A = \frac{aP}{(RT)^2} \quad (2.28)$$

$$B = \frac{bP}{RT} \quad (2.29)$$

$$(2.30)$$

where T_{ri} and P_{ri} are the reduced temperature and pressure of species i , respectively. The correction factor k_{ij} is derived experimentally, but in this work it is put equal to zero since there are no experimental data available for this work's ambient/fuel mixture.

The temperature-dependent parameter $\alpha(T)$ is defined as:

$$\alpha(T) = \left[1 + k \left(1 - \sqrt{T_{ri}}\right)\right]^2 \quad (2.31)$$

with:

$$k = 0.3796 + 1.485\omega - 0.1644\omega^2 + 0.01667\omega^3 \quad (2.32)$$

where ω_i is the acentric factor for a pure component.

The compressibility factor Z is obtained by solving the cubic form of the PR-EOS:

$$Z^3 - (1 - B)Z^2 + (A - 2B - 3B^2)Z - (AB - B^2 - B^3) = 0 \quad (2.33)$$

When a binary system is considered, the composition at the droplet surface can be determined by combining the phase-equilibrium condition with the mole fraction constraints for each phase. In particular, the mole fractions in the liquid and vapour phases must satisfy:

$$\sum y_i^V = \sum y_i^L = 1 \quad (2.34)$$

For a two-component mixture, the equality of fugacities at the interface leads to a direct relationship between the vapour phase and liquid-phase mole fractions of each species. For component 1, the vapour phase mole fraction at the droplet surface is expressed as:

$$y_1^V = y_1^L \frac{\phi_1^L}{\phi_1^V} \quad (2.35)$$

where ϕ_1^L and ϕ_1^V are the fugacity coefficients of component 1 in the liquid and vapour phases, respectively. The liquid-phase mole fraction of component 1 can be obtained as:

$$y_1^L = \frac{\phi_2^V - \phi_2^L}{\frac{\phi_1^L}{\phi_1^V} \phi_2^V - \phi_2^L} \quad (2.36)$$

Once the vapour phase mole fraction at the droplet surface is known, the corresponding mass fraction of fuel vapour can be evaluated and subsequently used in the evaporation model.

2.2.3 Enthalpy of vaporization

The enthalpy of vaporization represents the amount of energy required to transform a unit amount of liquid into vapour at thermodynamic equilibrium, without temperature variation. Physically, it represents the energy necessary to overcome the intermolecular attractive forces that maintain the liquid phase structure. It plays a fundamental role during evaporation, since it directly affects evaporation rates and heat transfer processes: the lower the enthalpy of vaporization, the higher the time required for the phase change to end. As temperature increases and approaches the critical point, the enthalpy of vaporization decreases progressively and ultimately vanishes at the critical state, where the distinction between liquid and vapour phases disappears [23]. There are several approaches for estimating the temperature dependence of

the enthalpy of vaporization. In this work, the Pitzer correlation is adopted, which incorporates the acentric factor to account for deviations from molecular sphericity:

$$\frac{L_v}{RT_c} = 7.08(1 - T_r)^{0.354} + 10.95\omega(1 - T_r)^{0.456} \quad (2.37)$$

where:

- R is the universal gas constant,
- T_c is the critical temperature,
- $T_r = \frac{T}{T_c}$ is the reduced temperature,
- ω is the acentric factor

This formulation is valid in the reduced temperature range $0.6 < T_r < 1$ [23].

In the present thesis, the enthalpy of vaporization is evaluated using two independent approaches:

1. Thermodynamic database approach, using the CoolProp library in Python, which retrieves thermodynamic properties from high-accuracy reference equations of state.
2. Analytical correlation approach, using the Pitzer correlation reported above, allowing for a direct and explicit evaluation.

2.3 Combustion

2.3.1 Conventional fuels combustion

For decades, fossil fuels have dominated the global energy landscape, accounting for more than 80% of total energy consumption, with oil remaining the primary contributor. Despite growing interest in alternative energy sources, petroleum-based fuels are expected to be the main source for at least the next two to three decades. The transportation sector, including the aviation one, represents the largest share of oil-derived fuel consumption and has experienced rapid and continuous growth throughout the last century. Increasing concerns related to global energy demand and environmental impact brought massive changes in the operating requirements of aircraft engines. Current research efforts are therefore focused on improving energy efficiency while simultaneously limiting environmental harm, especially through the reduction of pollutant and greenhouse gas emissions and the reformulation of conventional fuels. In this context, numerical modelling of jet fuel combustion has become an essential tool for combustion control and emission mitigation. However, accurately modelling jet fuel combustion is a big challenge due to the complex nature of real aviation fuels, which consist of hundreds of hydrocarbons such as alkanes, cycloalkanes, aromatics, and polycyclic species. For this reason, simplified fuel mixtures with controlled and well-defined compositions, commonly referred to as surrogates,

are used. These surrogates are designed to reproduce the combustion behaviour of commercial fuels while containing a limited number of representative components, and so they are used to study the influence of fuel chemistry and properties on combustion processes [24]. At present, commercial aviation relies almost exclusively on conventional kerosene-based jet fuels, with Jet A and Jet A-1 being the dominant choices for civil turbofan-powered aircraft. Although military fuels such as JP-8 are chemically similar to Jet A-1, they include specific additives and are outside the scope of civil turbofan applications. Modern turbofan engines operate under increasingly demanding conditions, characterized by high overall pressure ratios, elevated combustor inlet temperatures, and lean combustion regimes. For this reason, aviation fuels are required to satisfy strict specifications defined by international standards, such as ASTM D1655 and the Aviation Fuel Quality Requirements for Jointly Operated Systems (AFQRJOS), which establish limits on key physical and chemical properties. Among the fuel characteristics, most relevant to combustion performance in turbofan engines are volatility, viscosity, density, heating value, freezing point, aromatic content, smoke point, and thermal stability. These parameters directly influence atomization, evaporation, flame stability, and pollutant formation within the combustor. In particular, the formation of soot remains a major concern, as it can contribute to carbon deposition, increased radiative heat transfer to combustor walls, and higher particulate emissions at cruise altitude. Since aromatic and polyaromatic hydrocarbons are known to enhance soot formation, their concentration in Jet A-1 is strictly limited by specification, typically resulting in an average aromatic content of approximately 15-20% by volume. From a chemical standpoint, aviation kerosene average molecular formula is only an approximation, commonly reported in the range of $C_{10.9}H_{20.9}$ to $C_{12}H_{23}$, depending on the source and refining process [24]. This intrinsic complexity motivates the use of simplified surrogate fuels in combustion studies, enabling a controlled and reproducible description of fuel oxidation, pollutant formation, and emission indices under representative turbofan operating conditions. Depending on the objective of the study, surrogates can be classified according to whether they match the physical properties of the real fuel, its chemical composition, or both. Fuels designed to reproduce physical behaviour only are commonly referred to as physical surrogates, whereas those that replicate chemical reactivity and oxidation pathways are known as chemical surrogates. When both physical and chemical characteristics are simultaneously matched, the surrogate is described as a comprehensive surrogate [24]. Extensive reviews of surrogate fuel formulations have shown that the appropriate level of surrogate complexity depends on the physical and chemical phenomena of interest. For studies limited to non-reactive processes, such as single-phase heat transfer, a single-component surrogate with representative thermophysical properties may be sufficient. In contrast, processes involving fuel evaporation, injection, or mixing generally require multi-component surrogates capable of reproducing the distillation behaviour of real fuels. For investigations focused on ignition, combustion chemistry, and pollutant formation, chemically representative surrogates that include the main hydrocarbon classes of aviation kerosene are

necessary to capture the relevant oxidation and emission mechanisms.

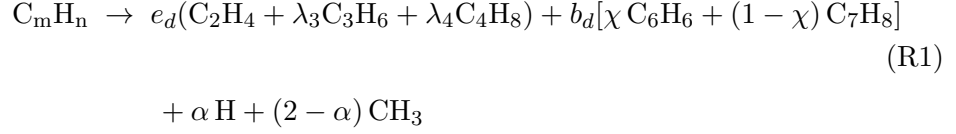
Property	Jet A-1	Jet A	Kerosene
Molecular weight [g/mol]	~160	~158	–
Approximate formula	C ₁₁ H ₂₁ -C ₁₂ H ₂₃	C _{11.6} H ₂₂	–
Liquid phase density at 15°C [kg/m ³]	804	788.1	780-810
Number of C atoms in fuel	~11	~11.6	9-13
H/C ratio [-]	1.9-1.92	~1.9	1.9–2.1
Boiling range [°C]	140-300	150-280	140-280
Freezing point [°C]	-47	-40	–
Specific gravity at 15°C [-]	~0.81	~0.81	0.77–0.83
Average composition [vol%]			
Aromatics	15-20	15-20	10-20
Cycloalkanes	~20	~20	20-30
Paraffins	55-65	55-65	50-65
Olefins	≤2	≤2	~0

Table 2.1: Properties of the conventional fuels investigated in this study [24].

Combustion is a complex physico-chemical process governed by a large number of elementary chemical reactions occurring over a wide range of temporal and spatial scales. From a chemical standpoint, the combustion of hydrocarbon fuels consists of a sequence of fuel decomposition (pyrolysis), radical formation, and oxidation reactions that ultimately lead to the formation of stable products such as CO₂ and H₂O, accompanied by heat release. At the high temperatures typical of aero-engine combustors, large hydrocarbon molecules do not oxidize directly. Instead, they undergo rapid thermal or oxidative pyrolysis, fragmenting into a limited set of smaller intermediate species (e.g. C₂H₄, CH₄, H₂, C₃H₆), which subsequently oxidize through well established radical pathways. Experimental and numerical studies have shown that this two-step behaviour is a general feature of hydrocarbon combustion and is largely independent of the detailed molecular structure of the parent fuel at sufficiently high temperatures [25].

A conventional hydrocarbon fuel can be represented by the generic formula C_mH_n. Accordingly, the generic HyChem fuel-consumption scheme may be written as the

following reactions:



with:

$$\begin{aligned} \Sigma_p = & \gamma \text{CH}_4 + e_a(\text{C}_2\text{H}_4 + \lambda_3\text{C}_3\text{H}_6 + \lambda_4\text{C}_4\text{H}_8) \\ & + b_a[\chi \text{C}_6\text{H}_6 + (1 - \chi) \text{C}_7\text{H}_8] + \beta \text{H} + (1 - \beta) \text{CH}_3 \end{aligned} \quad (2.20)$$

where:

- (R1) represents the primary decomposition of C_mH_n into light fragments and radicals;
- (R2-R7) represent abstraction/attack reactions by radical species leading to a common pool of products Σ_p ;
- The term Σ_p collects the effective products of fuel consumption (including CH_4 , light olefins, aromatics and radical fragments);
- The coefficient α represents the number of H atoms produced in the C-C fission reaction (R1) per C_mH_n ;
- The coefficient β represents the number of H atoms produced in the H-abstraction reactions (R2-R7) per C_mH_n ;
- The coefficient γ accounts for the additional production of methane per fuel molecule, beyond that arising from hydrogen abstraction by the methyl radical;
- λ_3 is the ratio $[\text{C}_3\text{H}_6]/[\text{C}_2\text{H}_4]$;
- λ_4 is the ratio $[\text{C}_4\text{H}_8]/[\text{C}_2\text{H}_4]$;
- χ is the ratio $[\text{C}_6\text{H}_6]/([\text{C}_6\text{H}_6] + [\text{C}_6\text{H}_5\text{CH}_3])$ [26].

Fuel surrogates

Real aviation fuels such as Jet-A are composed of thousands of hydrocarbon components, spanning several chemical classes (n-paraffins, iso-paraffins, cycloparaffins, aromatics). This compositional complexity makes it impractical to model combustion

using the exact molecular composition of the fuel. To overcome this limitation, the surrogate fuel approach is commonly adopted. In this framework, a real fuel is represented by one or more well-defined surrogate mixtures chosen to reproduce selected physical and chemical properties of the target fuel (e.g. H/C ratio, molecular weight, lower heating value, ignition behaviour).

In the present work, fuel chemistry is modelled using the Hybrid Chemistry (HyChem) framework. HyChem is a physics-based modelling strategy that combines:

- a lumped, experimentally constrained model for the thermal and oxidative pyrolysis of the parent fuel,
- a detailed reaction mechanism describing the oxidation of the resulting small hydrocarbon fragments.

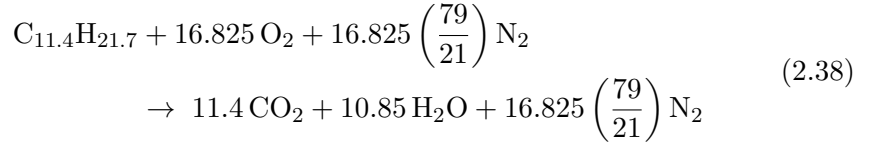
The key assumption in HyChem is that, at high temperatures, the detailed molecular structure of the parent fuel rapidly "collapses" into a small and nearly invariant set of pyrolysis products. As a result, the combustion behaviour of complex and multi-component fuels can be captured without explicitly modelling thousands of elementary fuel-specific reactions [26].

In this study, Jet-A is represented using two different surrogates depending on the physical state of the fuel. When the fuel is treated as a liquid phase, thermophysical properties such as density, viscosity, surface tension and latent heat are evaluated using n-dodecane. This choice is motivated by the availability of accurate and validated liquid-phase property models in CoolProp, which relies on n-alkanes as reference fluids for hydrocarbon fuels [27]. Conversely, when the fuel is treated as a vapour or gas phase, particularly for combustion and chemical kinetics calculations, Jet-A is represented using the A2 surrogate, identified as POSF10325 in the National Jet Fuels Combustion Program. In addition, the C1 surrogate, which is a Alcohol-to-Jet (AtJ) synthetic fuel developed by Gevo, is also considered in the present work when modelling Sustainable Aviation Fuels (SAFs) in the gas phase. The C1 surrogate is employed using its corresponding chemical kinetic description and is introduced to make a comparison between conventional Jet-A and SAF combustion behaviours in a dedicated chapter later in this thesis. These surrogates' properties are shown in Tab. 2.2.

Property	A2 (POSF10325)	n-Dodecane	C1 (POSF11498)
Average formula	$C_{11.4}H_{21.7}$	$C_{12}H_{26}$	$C_{12.5}H_{27.1}$
H/C ratio [-]	1.90	2.167	2.16
MW [g/mol]	158.6	170.3	178.0
Density [kg/m ³]	803	749	760
Kinematic viscosity at 20°C [m ² /s]	$4.5 \cdot 10^{-6}$	$1.34 \cdot 10^{-6}$	$4.9 \cdot 10^{-6}$
Surface tension [mN/m]	25.8	22.1	22.4
LHV [MJ/kg]	43.1	44.5	43.9
H_v [MJ/kg]	0.36	0.256	–
H content [wt.%]	14.0	15.2	15.3
Cetane number [-]	48.3	74.7	17.1
Fuel composition [mass%]			
n-paraffin	20.0	100.0	0.0
iso-paraffin	29.4	0.0	99.6
cycloparaffin	31.9	0.0	0.0
aromatics	18.7	0.0	0.4

Table 2.2: Properties of the surrogates considered in this work [28] [26] [29] [30].

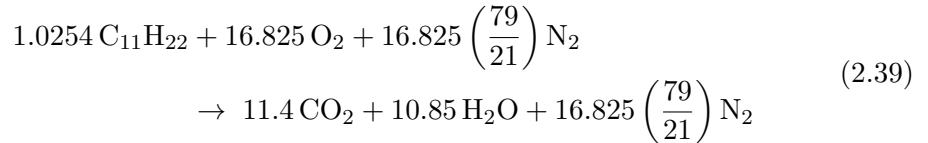
- A2: The corresponding stoichiometric reaction with air is:



which can be written in an equivalent form by expressing the fuel as a scaled amount of a nearby integer formula, here $C_{11}H_{22}$ [26]. Since the molecular weight of A2 is $MW = 158.6 \text{ g/mol}$ while $MW(C_{11}H_{22}) = 154.68 \text{ g/mol}$, the scaling factor is:

$$k = \frac{MW(A_2)}{MW(C_{11}H_{22})} = 1.0254$$

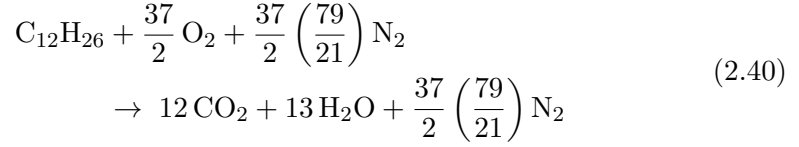
Therefore, the A2 global oxidation may equivalently be represented as:



When including air explicitly, nitrogen is introduced as an inert diluent through the standard molar ratio $N_2/O_2 = 79/21$.

- n-Dodecane: it is a linear n-alkane and is widely used as a reference fuel and surrogate in combustion studies due to its extensively documented thermochemical properties. From a chemical-kinetics perspective, the combustion of n-dodecane follows the same pathways observed for other long-chain hydrocarbons: initial

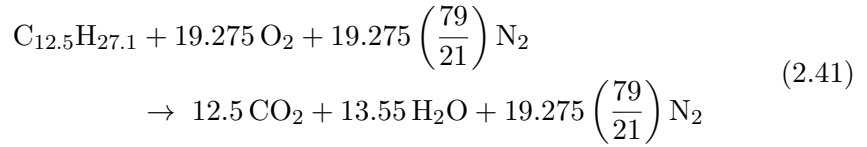
fuel pyrolysis and H-abstraction reactions generate alkyl radicals, which undergo β -scission to form smaller olefins and radicals. These intermediates are subsequently oxidized through established radical chain mechanisms involving H, O and OH radicals, ultimately producing CO_2 and H_2O as the main stable products. The global stoichiometric combustion reaction with air is:



The detailed n-dodecane combustion mechanism is obtained from the LLNL kinetic database [31].

- C1: it is a alcohol-to-jet (ATJ) synthetic fuel developed by Gevo [32] and one of the SAFs surrogates selected within the National Jet Fuels Combustion Program (NJFCP) to represent an "extreme" fuel chemistry compared to conventional Jet-A. It is described as a blend dominated by heavily branched isoalkanes, which has only two carbon numbers (C_{12} and C_{16}), and it is characterized by an extremely low derived cetane number (i.e., very low autoignition quality) [6].

The global stoichiometric combustion reaction with air is:



Introduction to Cantera software

The numerical modelling of combustion processes in aerospace propulsion systems requires tools capable of accurately describing the strong coupling between chemical kinetics, thermodynamics, and transport phenomena. In the case of aviation fuels such as Jet-A, combustion involves complex reaction networks, a large number of chemical species, and operating conditions characterized by high pressures and temperatures and non-equilibrium effects. Simplified equilibrium-based approaches are often insufficient to capture pollutant formation mechanisms and transient combustion behaviour, motivating the adoption of detailed kinetic-chemical modelling frameworks. In this context, Cantera represents a widely adopted open-source software specifically designed for the simulation of reacting flows. Cantera provides a flexible and robust environment for modelling chemically reacting systems by solving the governing equations of mass, species, and energy conservation in combination with detailed chemical kinetics. One of the key strengths of Cantera lies in its ability to decouple the definition of chemical mechanisms from the numerical solution strategy. Chemical kinetics are defined through external mechanism files, which may include hundreds or thousands of reactions and species, while the solver handles

the integration of the corresponding ordinary differential equations. This modular methodology facilitates the use of detailed or reduced mechanisms depending on the objectives of the analysis and the available computational resources. Another important feature of Cantera is its versatility in representing different physical configurations relevant to combustion modelling. The software includes a wide range of idealized reactor models, such as constant-volume or constant-pressure reactors, that can be combined to reproduce mixing, ignition, and combustion processes under controlled conditions. This adaptability lets the user construct simplified yet physically accurate representations of real combustion systems, without the need for CFD simulations [33].

2.3.2 Chemical emissions of pollutants and GHGs

The quantification of gaseous exhaust species emitted by aircraft engines is essential to provide accurate and consistent emission data for global modelling frameworks, which are required to predict the environmental impact of current and future air traffic [34]. Concentrations of emissions may be strongly dependent on specific combustion parameters such as temperature, pressure and residence time. Aircraft engines release gaseous species and particulate matter directly into the upper troposphere and lower stratosphere, where they influence atmospheric composition. The combustion of hydrocarbon-based aviation fuels in aircraft engines primarily results in the formation of carbon dioxide (CO_2) and water vapour (H_2O), which represent the dominant stable products of fuel oxidation. Since these species are directly linked to the carbon and hydrogen content of the fuel, their emissions can be reasonably assumed to scale linearly with fuel consumption. As a consequence, their emission indices are commonly treated as constant, with typical values of approximately 3155 g/kg of fuel burned for CO_2 and 1237 g/kg for H_2O . In contrast, the formation of other combustion-related species, such as nitrogen oxides (NO_x), carbon monoxide (CO), unburned hydrocarbons (UHC) and soot, depends strongly on engine operating conditions and combustion characteristics. The corresponding emission indices exhibit significant variability as a function of engine type, power setting, flight speed, altitude, and ambient atmospheric conditions [35].

Water vapour

While the direct contribution of aircraft-emitted water vapour to the greenhouse effect is generally considered negligible, its indirect radiative impact through the formation of contrails may be non-negligible, although it remains subject to considerable uncertainty. Thin contrails are the cause of a net warming effect, whereas thicker contrails may induce cooling. In addition, water vapour can promote the formation of polar stratospheric clouds, which provide surfaces for heterogeneous chemical reactions. These processes facilitate nitrogen oxide conversion and chlorine activation, ultimately contributing to ozone depletion in polar regions [36].

Carbon dioxide

This species contributes to the absorption of terrestrial infrared radiation, thereby reinforcing the greenhouse effect.

Carbon monoxide

Carbon monoxide (CO) is mainly associated with incomplete combustion processes. Under fuel-rich conditions, insufficient oxygen availability prevents the full oxidation of carbon to CO₂, leading to high CO concentrations. However, significant CO emissions are also observed under stoichiometric or lean conditions due to chemical dissociation and finite-rate kinetics. CO emissions are typically higher than equilibrium predictions, especially at low engine power settings where flame temperatures and residence times are reduced. Once formed, carbon monoxide oxidation proceeds relatively slowly and often controls the overall combustion efficiency. At high temperatures, the dominant oxidation pathway is:



whereas at lower temperatures, oxidation occurs mainly through:



The main parameters influencing CO emissions include combustor inlet temperature and pressure, equivalence ratio in the primary zone, residence time, and, for liquid fuels, spray atomization quality [8].

Unburned Hydrocarbons

Unburned hydrocarbons (UHC) are primarily formed from localized flame extinction phenomena. Two main mechanisms are responsible: extinction caused by excessive strain rates in the reacting flow, and extinction due to interaction of the flame with combustor walls or narrow geometrical features. High strain rates can locally quench the flame, preventing complete oxidation of the fuel, particularly under very lean or rich conditions where reaction rates are reduced. Similarly, wall quenching results from heat losses and radical recombination at solid surfaces, leading to incomplete combustion near liner walls and cooling flows [8].

Nitrogen oxides

Nitrogen oxides (NO_x) formed during hydrocarbon combustion originate from different chemical pathways, whose relative importance depends on temperature, pressure, equivalence ratio, and residence time. In gas turbine combustors operating under lean conditions, the dominant mechanisms are the thermal NO, prompt NO, and the N₂O pathway, while the contribution of fuel-bound nitrogen is generally negligible for aviation kerosene.

- Thermal NO: The dominant NO_x formation pathway is thermal-NO_x, also referred to Zeldovich NO_x, according to:

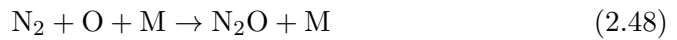


Due to the high activation energy reflecting the strong triple bond within the nitrogen molecule, the thermal NO_x pathway starts to open at high temperatures, $T > 1800\text{K}$, and becomes dominant at even higher temperatures. Hence, concentrations of NO_x emissions follow the adiabatic flame temperature of a specific fuel-air mixture and influence the concentration of ozone and other reactive intermediates in both the troposphere and lower stratosphere, influencing radiative forcing. In the middle stratosphere, nitrogen oxides participate in established catalytic cycles that lead to ozone destruction and interact with other reactive chemical families, including hydrogen, chlorine, and bromine species. Conversely, in the troposphere and lower stratosphere, the combined presence of nitrogen oxides and hydrocarbons promotes ozone formation [36].

- Prompt NO: this mechanism, also known as Fenimore NO, is formed directly in the flame front through reactions involving hydrocarbon radicals, particularly CH. Unlike thermal NO, this mechanism is active even at relatively lower temperatures and is associated with fuel-rich regions near the flame zone. The key step involves the formation of intermediate species such as Hydrogen Cyanide (HCN), which are subsequently oxidized to NO [8]:



- NO Formation via the Nitrous Oxide (N₂O) pathway: this mechanism represents an alternative route for NO formation, particularly under lean and high-pressure conditions. In this pathway, atomic oxygen reacts with molecular nitrogen in the presence of a third molecule M to form nitrous oxide:



Nitrous oxide can then decompose through reactions with oxygen atoms, yielding NO:



Although often a minor contributor under conventional conditions, the N₂O pathway can become relevant when both thermal and prompt NO formation are suppressed, such as in lean, high-pressure combustors [8].

Chapter 3

Case study

3.1 Concorde-like supersonic aircraft

The aircraft considered in this study is the CS-1A, a civil supersonic aircraft designed for commercial operations within the MORE&LESS project and based on the Concorde-NEO concept. The MORE&LESS program aims to achieve low-boom and environmentally sustainable solutions for future supersonic aviation [37]. The CS-1A configuration is inspired by a Concorde-like layout, characterized by a separation between fuselage and wing, following a tube-and-wing architecture adapted to supersonic flight through the adoption of a delta wing planform. Within the MORE&LESS framework, the CS-1 family includes multiple variants, among which the CS-1A represents the *drop-in* configuration, operating with conventional aviation fuel. Unlike hydrogen-powered alternatives investigated in parallel within the project (CS-1B), the CS-1A directly resembles the original Concorde layout and was therefore defined without a full iterative conceptual design process [37]. It is designed to operate at a cruise Mach number of 2 and is intended to operate as a commercial supersonic transport [38]. Its main geometric and mass characteristics are derived from a reference CAD model, shown in Fig. 3.1, inspired by the real Concorde aircraft in order to ensure coherence with payload capability and mission requirements.

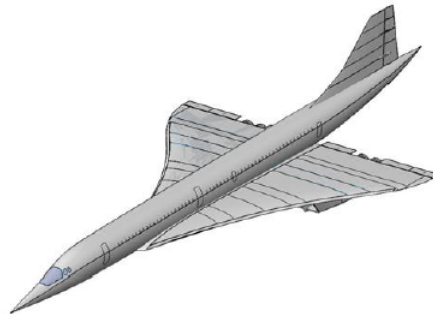


Figure 3.1: CS-1A CAD model.

From a propulsion standpoint, the CS-1A has been investigated using both turbojet and mixed-flow turbofan architectures. In particular, the mixed-flow turbofan option

was introduced to improve fuel consumption while maintaining the thrust levels required for sustained supersonic cruise. The corresponding propulsive databases were generated using engine performance simulations over a wide range of Mach numbers and altitudes, and subsequently employed in mission analyses [37].

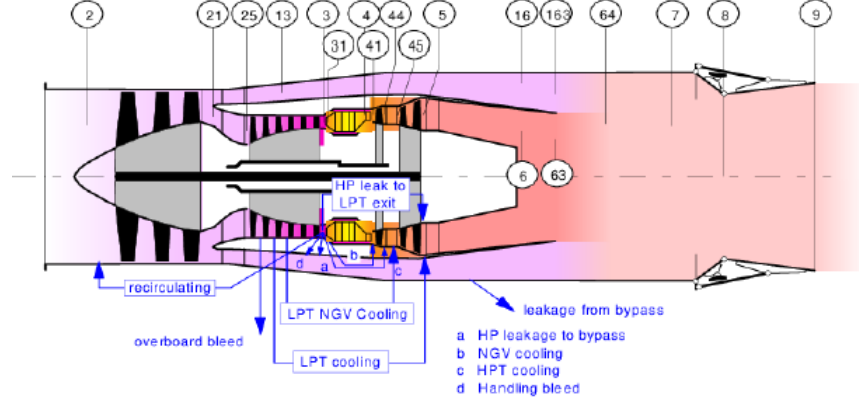


Figure 3.2: Mixed-flow turbofan scheme.

3.2 Mission profile and engine operating conditions

The mission profile adopted in this work is the same as the one defined within the MORE&LESS project, in particular with the aircraft equipped with a mixed-flow turbofan propulsion system. The trajectory spans a wide flight envelope, covering altitudes from sea level up to approximately 18 km and Mach numbers ranging from 0 to 2 during cruise conditions, as shown in Fig. 3.3.

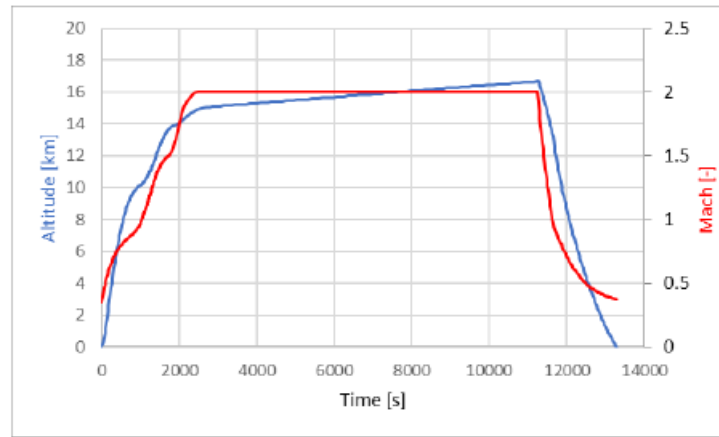


Figure 3.3: CS-1A mission profile.

In the present analysis, engine performance maps are evaluated at $NH100$, which corresponds to full throttle operation. Here, NH is the rotational speed of the high-pressure shaft, normalized with respect to its maximum design value, and therefore $NH100$ represents 100% of the high-pressure spool speed.

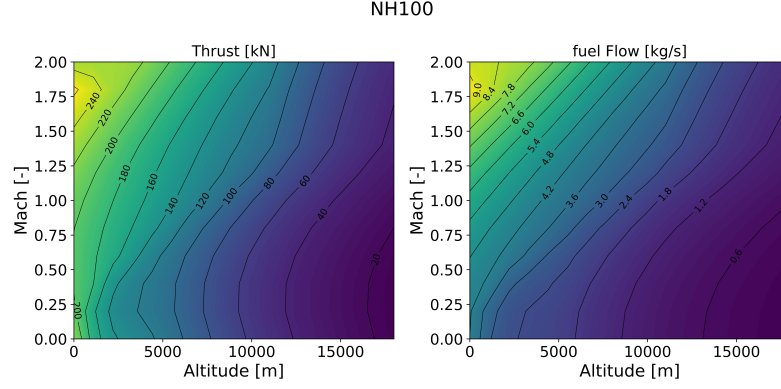


Figure 3.4: Thrust and fuel flow outputs in NH100 conditions for the MFTF engine database.

The propulsive data used in this study originate from engine performance decks provided by the von Karman Institute for Fluid Dynamics (VKI). The main dataset contains engine performance parameters evaluated over a wide flight envelope, covering a broad range of altitude and Mach number combinations representative of the reference mission profile. In order to reduce the computational effort while retaining a physically meaningful representation of the mission, a reduced set of ten representative altitude-Mach pairs was extracted from the main database. These points form an approximate discretized trajectory spanning the most relevant phases of the mission, from low-altitude subsonic conditions to high-altitude supersonic cruise. All subsequent analyses of atomization and evaporation processes were therefore performed at these ten operating points, shown in Tab. 3.1, which are assumed to be representative of the overall mission envelope.

Altitude [m]	Mach Number [-]
0	0.2
1100	0.4
3300	0.6
7700	0.8
9900	1
11000	1.2
13000	1.4
14000	1.6
15000	1.8
18000	2

Table 3.1: Altitude-Mach pairs for the discretized trajectory.

The VKI propulsive database provides a comprehensive set of parameters that are directly relevant for spray and combustion modelling. In particular, it includes the total temperature and pressure of the air at the combustor inlet, as well as the air and fuel mass flow rates, all evaluated consistently for each altitude-Mach operating

condition. These quantities are some of the inputs for liquid fuel atomization, droplet heating, and evaporation processes, as they define the thermodynamic and flow environment experienced by the spray downstream of the injector.

While ambient air conditions are directly taken from the propulsive database, the fuel thermodynamic state at the combustor inlet is prescribed independently in the present work. Specifically, the fuel temperature and pressure at injector entry are imposed as 300 K and 3 bar (2.96 atm), respectively. These values are representative of typical Jet-A fuel conditions at the exit of the atomizer injector in aero-engine combustors, as commonly assumed in spray combustion studies and injector-scale modelling [21]. Under these conditions, the fuel can be reasonably treated as a subcooled liquid prior to atomization, allowing the evaporation process to be driven primarily by the surrounding hot compressed air rather than by fuel preheating effects. To further analyse the operating conditions relevant to spray atomization and evaporation, two scatter plots were generated in MATLAB. The first plot reports the air temperature and pressure at the combustor inlet as a function of Mach number, while the second plot shows the air and fuel mass flow rates as a function of the flight Mach number.

In the plot shown in Fig. 3.5, the fuel mass flow rate (WF) remains small (of the order of a few kg/s) and generally decreases with increasing Mach number. This behaviour is consistent with the reduction in required net thrust at high-altitude, high-Mach cruise conditions. The total air mass flow rate (WA) also exhibits a decreasing trend with Mach number, reflecting the combined effects of reduced air density at altitude and engine operating characteristics at constant NH100. In the case of the turbofan configuration considered, only a fraction of the total air flow effectively enters the combustion chamber, while the remaining part is bypassed. The air mass flow rate at the combustor inlet was therefore computed as:

$$W_{\text{air,inletCC}} = \frac{W_{\text{air}}}{1 + BPR}$$

where BPR is the bypass ratio. As expected, $W12$ is significantly lower than WA and follows a similar decreasing trend with Mach number.

The second scatter plot shows the evolution of air temperature and pressure at the combustor inlet along the mission. The combustor inlet pressure shows a clear decreasing trend with Mach number, primarily due to the progressive increase in flight altitude and the associated reduction in ambient pressure, combined with intake and compression system behaviour. Conversely, the increase in combustor inlet total temperature observed at the highest Mach numbers can also be attributed to the transition from the troposphere to the lower stratosphere. Above approximately 11 km altitude, the ambient temperature no longer decreases with altitude and may even slightly increase which, combined with enhanced ram compression at supersonic speeds, leads to higher inlet total temperatures despite the low ambient pressure. The decrease in combustor inlet pressure with Mach number tends to reduce the gas density, which can slow down droplet evaporation, whereas the increase in air

temperature at high Mach numbers strongly enhances heat transfer to the droplets, promoting faster evaporation.

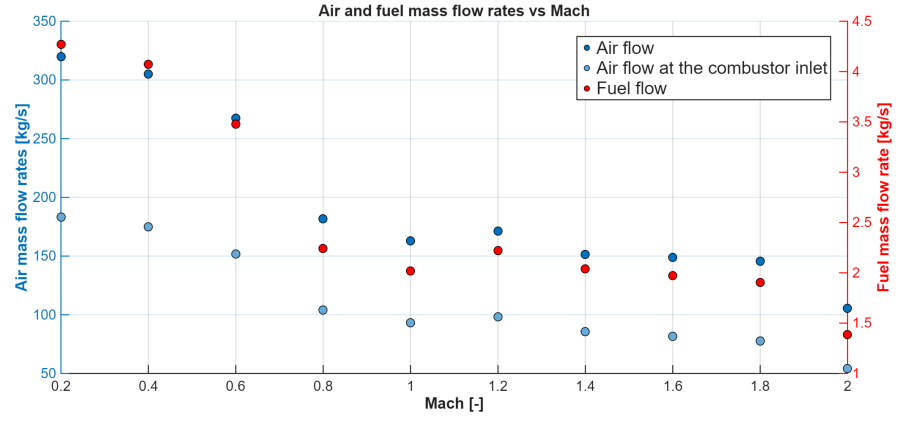


Figure 3.5: Air and fuel mass flow rates vs Mach.

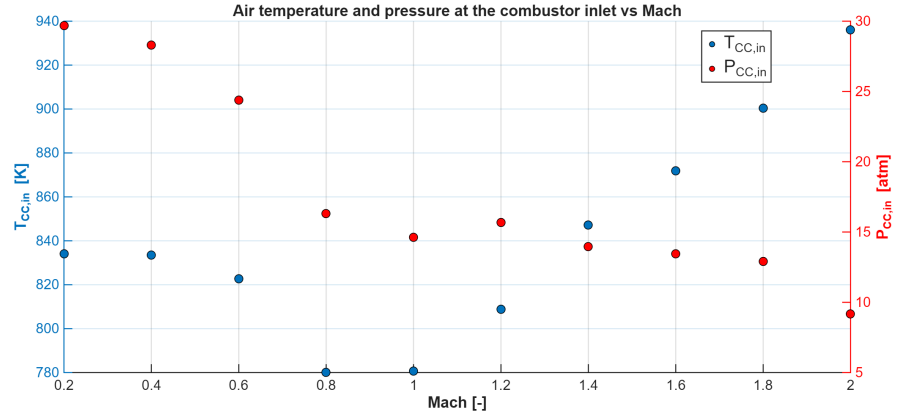


Figure 3.6: Air temperature and pressure at the combustor inlet vs Mach.

Chapter 4

Modelling methodology

The modelling methodology adopted in this work is based on a modular and sequential approach, where each physical process involved in fuel preparation, combustion, and emission formation is represented by a dedicated numerical model. The overall framework is organized as a chain of interconnected computational blocks, each corresponding to a specific stage of the physical process and implemented through an independent Python code. Starting from the reference operating conditions extracted from the Propulsive Database, the methodology progressively accounts for fuel atomization, evaporation, mixing, and combustion. Each block receives input parameters and generates intermediate outputs that are transferred to the subsequent stage. The numerical implementation relies on Python scripts coupled with structured input and output files, written in Excel format. Intermediate results, such as droplet size distributions, evaporation time histories and thermodynamic states are stored and post-processed before being used as inputs for the next modelling layer. The final stage of the methodology focuses on the kinetic-chemical modelling of combustion using the Cantera software framework. The exhaust gas composition predicted by the combustion model is then employed to compute emission indices, which constitute the Emissive Database of the CS-1A aircraft. The block diagram, shown in Fig. 4.1, summarizes the applied methodology and highlights the logical connection between all the physical processes.

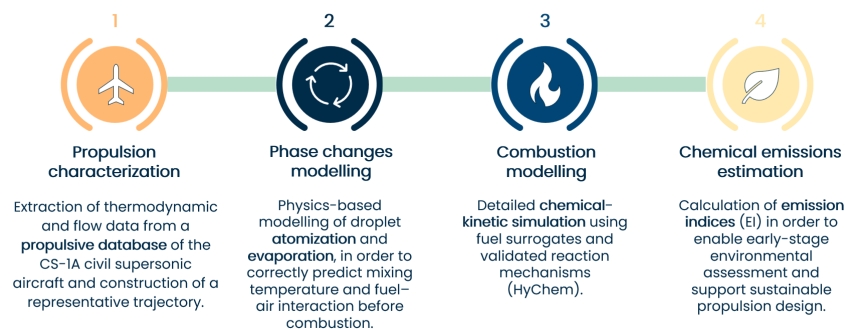


Figure 4.1: Modelling methodology.

4.1 Atomization

Within the sequential framework adopted in this work, atomization represents the first computational block. Starting from the engine/combustor reference operating conditions extracted from the Propulsive Database and the derived trajectory, such as air pressure and temperature at the combustor inlet, this block provides:

- an estimate of the Sauter Mean Diameter (D_{32}),
- a droplet size distribution, using the Rosin-Rammler correlation.

The diameter is then passed to the subsequent blocks (post-atomization relaxation and evaporation) as initial condition.

The injector is modelled as a plain-jet airblast atomizer, for which the droplet mean size is evaluated using an empirical correlation commonly attributed to Rizk & Lefebvre. In this approach, the SMD depends on:

- Liquid properties: dynamic viscosity μ_L and surface tension σ ;
- Gas property: ambient air density ρ_A ;
- Relative velocity: $U_{\text{rel}} = |U_{\text{air}} - U_{\text{fuel}}|$
- Injector geometry: fixed orifice diameter $d_o = 0.66 \text{ mm}$;
- Air-to-liquid ratio: $ALR = \dot{m}_{\text{air}}/\dot{m}_{\text{fuel}}$.

A key methodological point is the consistent sourcing of atomization inputs by combining two libraries:

1. **CoolProp** for liquid-fuel properties (surrogate fluid),
2. **Cantera** for gas-phase properties (air and, in the broader workflow, gas mixtures).

For the atomization stage, the liquid fuel is represented by n-dodecane, selected because it is directly available in the CoolProp library and ensures consistent thermo-physical property models over the relevant range. In the present work, this surrogate is adopted both for the conventional and SAF cases in the liquid-property evaluation step of atomization; the differentiation between fuels is then handled in the subsequent gas-phase/combustion modelling, where chemical surrogates and reaction mechanisms are considered.

The SMD correlation requires, at minimum, μ_L and σ . In the implementation, these are obtained as:

```

1  import CoolProp.CoolProp as CP
2
3  def kerosene_liquid_props(T, P, fluid="n-Dodecane"):
4  return {

```

```

5      "rho":    CP.PropsSI("Dmass", "T", T, "P", P, fluid),
6      "cp":    CP.PropsSI("Cpmass", "T", T, "P", P, fluid),
7      "mu":    CP.PropsSI("VISCOSITY", "T", T, "P", P, fluid),
8      "sigma": CP.PropsSI("SURFACE_TENSION", "T", T, "Q", 0, fluid),
9  }

```

Here, μ_L is evaluated at $(T_{\text{fuel}}, P_{\text{fuel}})$, while σ is obtained from the saturated-liquid state (quality $Q = 0$) at the specified temperature.

The gas density ρ_A in the atomization correlation is computed using Cantera by imposing temperature, pressure and composition at the combustor inlet. The air composition is modelled as a binary mixture of oxygen and nitrogen.

```

1  import cantera as ct
2  gas = ct.Solution(MECH_YAML_PATH)
3  AIR_COMP = "O2:0.21, N2:0.79"
4
5  def set_air_state(T, P):
6      gas.TPX = T, P, AIR_COMP
7
8  def rho_gas(T, P):
9      set_air_state(T, P)
10     return gas.density

```

The air velocity entering the combustor, U_{air} , is not directly taken from the database but is reconstructed from the local thermodynamic state by imposing a fixed combustor inlet Mach number:

$$M_{\text{inlet,CC}} = 0.286$$

This value corresponds to the combustor inlet Mach number of the Concorde engine at cruise Mach 2 [39], and is assumed constant for all operating points in the present atomization analysis. The air velocity is computed from the definition:

$$U_{\text{air}} = M_{\text{inlet,CC}} \cdot a \quad (4.1)$$

where a is the local speed of sound:

$$a = \sqrt{\gamma R T_{\text{static}}} \quad (4.2)$$

The specific heat ratio γ and the specific gas constant R are evaluated consistently using Cantera at the local air state.

For each selected altitude-Mach operating point, the atomization block proceeds as follows:

1. Read combustor inlet conditions $(T_{\text{air,in}}, P_{\text{air,in}}, \dot{m}_{\text{air}}, \dot{m}_{\text{fuel}})$ from the propulsive database;
2. Compute air density with Cantera, which is an open-source suite of software tools for problems involving chemical kinetics, thermodynamics and transport

processes, and it can be used from Python and Matlab, or in applications written in C/C++ and Fortran 90 [33]. Currently, this tool is widely used for evaporation and combustion applications. In the present work, the Cantera library is used to compute the physical properties of the gaseous substances, given their temperature, pressure and chemical composition;

3. Compute liquid properties with CoolProp;
4. Build flow parameters: $ALR = \dot{m}_{\text{air}}/\dot{m}_{\text{fuel}}$ and $U_{\text{rel}} = |U_{\text{air}} - U_{\text{fuel}}|$, knowing that $U_{\text{fuel}} = 5 \text{ m/s}$;
5. Evaluate SMD D_{32} using the airblast correlation;
6. Generate Rosin-Rammler distribution and compute percentile diameters (D_{10} , D_{30} , D_{50} , D_{90}), which represent volume-based percentile diameters of the droplet population, in order to describe the polydispersity of the spray.

4.2 Evaporation

Droplet evaporation and heating are modelled through a coupled set of ordinary differential equations (ODEs) describing the temporal evolution of droplet diameter (Eq. 2.8) and droplet temperature (Eq. 2.9). Using numerical integration schemes, this set of equations is transformed into algebraic equations, which are solved by an iterative process. In the present work, two numerical methods are employed to perform this task: the first-order Euler method and the 4th-order Runge-Kutta method. The general form of a first-order ordinary differential equation is:

$$\frac{d\phi_d}{dt} = f(\phi_d, t) \quad (4.3)$$

where ϕ_d is an arbitrary variable that is transported by a Lagrangian droplet, as U_d , D_d or T_d , and $f(\phi_d, t)$ is a given function [40].

1. For the parametric study, the explicit Euler method is adopted because of its minimal computational cost per time step, which is advantageous when evaluating multiple operating points across the mission envelope. Applying the first-order Euler method explicitly to Eq. 4.3, the value ϕ_d at the new time step $n + 1$ reads:

$$\phi_d^{n+1} = \phi_d^n + f(\phi_d, t)|^n \Delta t_{\text{lag}} \quad (4.4)$$

where n is a given time step and Δt_{lag} is the Lagrangian time step. Since the above time integration is a first-order method, its global error, at a given time, is proportional to the step size. Therefore, this method should be used with care in order to ensure that the Lagrangian time step is always low.

2. For the validation with documented model in the literature and for the CS-1A supersonic case study (the main case analysed in this thesis), the fourth-order

Runge-Kutta scheme is selected to improve numerical accuracy and robustness. Applying this method, also explicitly, to Eq. 4.3 results in [41]:

$$\phi_d^{n+1} = \phi_d^n + \frac{1}{6}(k_0 + 2k_1 + 2k_2 + k_3)|^n \Delta t_{lag} \quad (4.5)$$

with

$$k_0 = f(\phi_d, t), \quad k_1 = f(\phi_d + k_0/2, t), \quad k_2 = f(\phi_d + k_1/2, t), \quad k_3 = f(\phi_d + k_2, t)$$

In this work, the droplet dynamics are represented by the Abramzon-Sirignano Model (ASM) under subcritical assumptions, which improves classical evaporation theory by accounting for Stefan-flow-induced film thickening through correction factors applied to Sherwood and Nusselt numbers.

Thermophysical properties are evaluated as follows:

- Gas/vapour mixture properties (ρ_m , μ_m , k_m , $c_{p,m}$, $D_{v,m}$) are computed with Cantera.
- Liquid fuel properties are obtained using CoolProp.
- Properties are assumed constant within each time step, but they vary from one time step to another due to the corresponding changes in droplet temperature.

For each operating point, the evaporation solver advances the droplet state according to the following sequence:

1. **Interfacial equilibrium:** compute using either PR-EOS or Raoult (depending on the selected main model for that case), then convert to
2. **Film properties:** evaluate gas/vapour mixture properties at (T_m, P) with Cantera.
3. **Dimensionless numbers:** compute the Reynolds, Prandtl and Schmidt numbers (Re_d , Pr_m , Sc_m)
4. **ASM corrections:** compute B_M , solve for the coupled heat-transfer correction through B_T and obtain corrected Sherwood and Nusselt numbers (Sh^* , Nu^*), together with the evaporation correction factor G in the convective term.
5. **Mass and heat rates:** compute the mass evaporation rate $\dot{m}_d$, obtaining the latent energy of evaporation $\dot{m}_d L_v$.
6. **ODEs update:** advance the droplet Lagrangian variables (D_d , T_d , U_d) using explicit Euler or 4th-order Runge-Kutta methods.

The evaporation modelling outputs are then saved in a structured Excel file for post-processing and plotting purposes. In particular, a summary sheet contains all the thermodynamic and propulsive parameters for each operating point and a time-history sheet contains the full temporal evolution of the main variables. The

end-state conditions (e.g., fuel and air temperatures and pressures at the end of the phenomenon) are then passed to the subsequent mixing/combustion modelling stage.

4.2.1 Thermodynamic model at the droplet surface: PR-EOS vs Raoult

A key element of the ASM formulation is the surface fuel vapour mass fraction Y_{fuel}^* , which governs the Spalding mass transfer number B_M and therefore the evaporation rate. In this work, Y_{fuel}^* is obtained from the surface fuel mole fraction y_{fuel}^* and converted to mass fraction using molecular weights. Two alternative approaches are implemented to calculate the molar fraction:

1. **High-pressure/real-gas equilibrium (PR-EOS, fugacity-based):** the surface composition is computed by applying fugacity equilibrium between liquid and vapour phases using a Peng-Robinson equation of state. This method is required when the pressure approaches the critical pressure of the surrogate fuel and non-idealities become relevant.
2. **Low-pressure equilibrium (Raoult's law):** at lower pressures, the interfacial fuel mole fraction is approximated as:

$$y_{\text{fuel}}^* = \frac{p_{\text{sat}}(T_d)}{P} \quad (4.6)$$

where p_{sat} is the saturation pressure at the droplet temperature T_d .

To reflect the fact that real-gas effects become practically relevant only for the highest-pressure operating points, a hybrid strategy is adopted in the analysed trajectory:

- PR-EOS is used as surface model for the first three Altitude-Mach trajectory points, where the ambient pressure is higher than the n-Dodecane critical pressure ($P_c = 18.2 \text{ bar}$);
- Raoult's law is used as surface model for the remaining operating points.

4.2.2 Enthalpy of vaporization L_V : CoolProp vs Pitzer

The droplet energy balance requires the enthalpy of vaporization, which is a function of the droplet temperature. Two formulations are implemented:

1. **CoolProp:** L_v is evaluated as the enthalpy difference between saturated vapour and saturated liquid at the droplet temperature:

$$L_v = h_v - h_l \quad (4.7)$$

When $T_d \geq T_c$, the enthalpy of vaporization tends to zero, as shown in Fig. 4.2, consistent with the disappearance of a distinct phase change above the critical point.

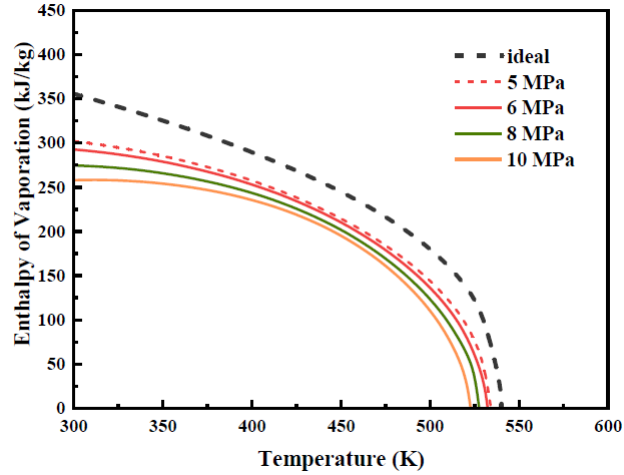


Figure 4.2: Enthalpy of vaporization of n-heptane in nitrogen environment under various ambient conditions [42].

2. **Pitzer correlation:** A semi-empirical correlation is implemented to provide an independent estimate of L_v in the subcritical range, useful for comparison plots.

4.3 Chemical kinetic simulation for emission estimation

Prior to the combustion analysis, a dedicated Propulsive Database was established to describe the reference operating conditions of the CS-1A aircraft at design point. Subsequently, the Propulsive Database was updated by incorporating new parameters derived from fuel atomization and evaporation modelling, in order to have a more realistic representation of the fuel state at the combustor inlet. The data extracted from the updated Propulsive Database are employed as input conditions for the kinetic-chemical modelling of the CS-1A turbofan engine and, consequently, for the construction of the Emissive Database. The propulsion system of the CS-1A features a conventional single-stage combustor operating with Jet-A fuel. Therefore, the thermodynamic state of the flow entering the main combustion chamber, defined by pressure, temperature and mass flow rate, is obtained directly from the propulsion and performance analysis of the engine. These inlet conditions are used as boundary conditions for the chemical kinetics simulations aimed at predicting the composition of the exhaust gases. The mass fractions of the major combustion products and pollutant species at the combustor outlet are evaluated through detailed chemical modelling. In this work, the Cantera software is adopted due to its proven capability and robustness in solving coupled problems involving chemical kinetics, thermodynamics, and reacting flow processes. This open-source framework is particularly suitable for evaluating the thermodynamic properties of reacting gas mixtures and for computing the mass fractions of combustion products under representative engine operating conditions [33]. The species mass fractions obtained at the exit of the main combustion chamber are subsequently used to calculate emission indices, which constitute the

core of the Emissive Database and provide a consistent link between propulsion performance, combustion modelling and environmental assessment.

4.3.1 Cantera software

The combustion process is modelled through a zero-dimensional kinetic-chemical approach. The methodology is based on a sequential modelling strategy that decouples mixing, combustion and emission post-processing, allowing a clear interpretation of the role of chemical kinetics and thermodynamic effects. The combustion model is implemented using Cantera, which enables the simulation of chemically reacting systems through detailed reaction mechanisms. The adopted approach consists of two conceptual layers.

In the first layer, the thermodynamic state of the reacting mixture is established assuming idealized conditions representative of adiabatic flame behaviour, which provides an upper bound for flame temperature and allows a preliminary assessment of combustion completeness. Under adiabatic conditions, no heat transfer to the surroundings is considered, and the energy released by chemical reactions is fully retained within the reacting mixture. This assumption is commonly adopted in combustion studies to isolate the influence of chemical kinetics from heat losses and to establish reference thermodynamic conditions for subsequent reactor-based simulations. Although real gas turbine combustors are not adiabatic, this idealized framework offers valuable insight into fuel oxidation behaviour.

In the second layer, the combustion process is modelled through a reactor-based formulation, accounting for finite-rate chemical kinetics and transient heat release. The resulting exhaust species mass fractions are then used to compute emission indices for the main pollutants.

In the present work, Cantera is used to:

1. Define the thermodynamic state of air and fuel streams, through the `Solution` object, which defines the phase of a particulate species, and the `.TPX` command, which is used to set or get the temperature, pressure and mole composition of the defined phase.

```

1      Air = ct.Solution('A2NOx_skeletal.yaml')
2      for i in range(Air.n_reactions):
3          Air.set_multiplier(0.0, i)
4      Air.TPX = T_air, P_air, 'O2:0.21, N2:0.79'
5      Fuel = ct.Solution('A2NOx_skeletal.yaml')
6      for i in range(Fuel.n_reactions):
7          Fuel.set_multiplier(0.0, i)
8      Fuel.TPX = T_fuel, P_fuel, 'POSF10325:1'
9  
```

Chemical reactions are temporarily disabled during the streams preparation stage. This allows the formation of a non-reacting mixture before combustion is initiated.

2. Model mixing prior to combustion.

```

1      res_Air = ct.Reservoir(Air)
2      res_Fuel = ct.Reservoir(Fuel)
3      env = ct.Reservoir(Air)
4
5      mixer = ct.IdealGasReactor(Air)
6      mfc_air = ct.MassFlowController(res_Air, mixer, mdot=
7                                     mdot_air)
8      mfc_fuel = ct.MassFlowController(res_Fuel, mixer, mdot=
9                                     mdot_fuel)
10     outlet = ct.Valve(mixer, env, K=10.0)
11
12     reactor_net = ct.ReactorNet([mixer])
13     reactor_net.advance_to_steady_state()

```

Reservoirs represent infinite supplies of air and fuel at fixed thermodynamic conditions. The `IdealGasReactor` object acts as a perfectly stirred mixing volume, where mass flows from air and fuel streams are combined. At the same time mass flow controllers impose prescribed mass flow rates of air and fuel into the mixer, ensuring control of equivalence ratio and fuel/air mixing conditions. A valve is introduced at the outlet of the mixing reactor to allow mass flow discharge towards an environmental reservoir at fixed pressure. This element ensures mass balance closure and enables the system to reach a steady-state condition by preventing pressure build-up within the mixer. Lastly, the reactor network is advanced in time until steady-state conditions are reached, ensuring that the composition of the mixed stream is independent of initial conditions and representative of a continuously operating mixing process [33].

3. Simulate combustion within a constant-pressure reactor, which reflects the approximately constant-pressure environment of gas turbine combustors. Chemical reactions are enabled at this stage, allowing fuel oxidation and pollutant formation.

```

1      Mixed_state = ct.Solution('A2NOx_skeletal.yaml')
2      Mixed_state.TPX = mixer.T, mixer.thermo.P, mixer.thermo.X
3
4      reactor = ct.IdealGasConstPressureReactor(Mixed_state)
5      def local_heatflux(t):
6          return heatflux_default(t, amp)
7      wall = ct.Wall(left=env, right=reactor, Q=local_heatflux)
8

```

A heat flux is imposed through a wall to control the energy exchange during combustion, allowing the modelling of ignition and heat release effects without explicitly resolving flame propagation [33].

4. Compute the temporal evolution of species mass fractions.

```
1      sim = ct.ReactorNet([reactor])
2
```

The `ReactorNet` object integrates the governing equations in time, providing the temporal evolution of temperature and species mass fractions. These quantities are required for emission indices calculation.

4.3.2 Emission Index

Throughout the years the International Civil Aviation Organization (ICAO) has progressively established regulatory frameworks and monitoring tools aimed at limiting the environmental impact of aircraft engine emissions, with particular emphasis on local air quality and climate-relevant pollutants. These efforts are supported by standardized datasets and certification methodologies, such as those reported in [43], which provide reference emission indices for certified aero-engines under defined operating conditions. Aircraft propulsion consists of the combustion of kerosene with air to generate the thrust required throughout the mission. As a consequence of this process, a variety of chemically active species are released into the atmosphere and, once emitted, these species interact with it, affecting its chemical composition and contributing both to local air quality degradation and to climate change [44].

Emissions of aircraft engines are commonly given in terms of emission indices EI, which describe the amount of a specific compound in g per kg fuel burned [43].

Formally, the emission index is defined as:

$$EI_X = \frac{m_X}{m_{\text{fuel}}} \left[\frac{g_X}{kg_{\text{fuelburnt}}} \right] \quad (4.8)$$

where X is the generic exhaust species. In the context of chemical kinetics simulations, emission indices are evaluated from the exhaust gas composition predicted at the combustor outlet. Using mass fractions, the emission index can be expressed as:

$$EI_X = 1000 \cdot \frac{Y_{X,\text{outletCC}}}{Y_{\text{fuel,inletCC}} - Y_{\text{fuel,outletCC}}} \quad (4.9)$$

Species such as CO₂ and H₂O are directly linked to fuel consumption and combustion stoichiometry; as a result, their emission indices are essentially constant and largely independent of engine operating conditions. Similarly, sulfur oxides emissions scale with the sulfur content of the fuel and are therefore proportional to fuel flow, rather than to combustor thermodynamic conditions. On the other hand, the emission indices of CO and unburned hydrocarbons are strongly dependent on engine power setting and inlet conditions. These species are primarily associated with incomplete combustion and are therefore more present at low power regimes, such as idle or low-thrust operation, where flame temperatures are lower and fuel/air mixing

may be less effective. Conversely, NO_x formation is governed by high-temperature oxidation mechanisms, making its emission index strongly correlated with combustor temperature, pressure and residence time. As a result, NO_x emissions increase substantially at high power settings, where elevated flame temperatures and higher pressures promote thermal NO formation. Lastly, particulate matter emissions arise primarily from incomplete combustion of fuel, leading to the formation of soot and other combustion-generated particles.

Although particulate matter and sulfur oxides emissions are of major environmental relevance, their quantification does not rely on the emission index EI in the same manner as gaseous species. PM emission estimation methodology uses the smoke number as a key parameter (the smoke number is a dimensionless indicator of the optical density of engine exhaust smoke and correlates with the concentration of soot particles), while SO_x emissions are often assessed through sulfur conversion rates and fuel sulfur content [45]. For this reason, the present work does not address the calculation of PM or SO_x emissions, focusing instead on the thermodynamic conditions that govern chemical pollutants formation.

Chapter 5

Results and discussion

This chapter presents the application of the atomization and evaporation models described in Chapter 2. The models are first applied over a range of operating conditions in order to perform a sensitivity analysis. The objective is to investigate how the governing parameters appearing in the relations introduced in Chapter 2 influence droplet size and evaporation dynamics. The evaporation solver is then validated against a documented reference case available in the literature, ensuring consistency of the D^2 -law behaviour and droplet temperature evolution. Lastly, the fully coupled atomization-evaporation model is applied to the CS-1A configuration. After integrating the combustion phase, the model outputs are used to compute emission indices.

5.1 Atomization and evaporation models application

5.1.1 Parametric study

The first application of the model aims at conducting a sensitivity analysis to evaluate how variations in the main physical parameters affect the Sauter Mean Diameter, the evaporation constant K and the droplet evaporation lifetime and temperature. The analysis is performed by varying selected input parameters appearing in the atomization and evaporation equations. The parameters were varied within ranges representative of gas-turbine combustor experimental testing conditions [13]:

- Air temperature $T_{\text{air}} = [300, 500, 800] \text{ K}$;
- Air pressure $P_{\text{air}} = [1, 2, 5] \text{ bar}$
- Air-to-Liquid ratio $ALR = 2 - 8$;;
- Air velocity $U_{\text{air}} = 10 - 120 \text{ m/s}$;
- Fuel temperature $T_{\text{fuel}} = 300 - 420 \text{ m/s}$.

The atomization stage is governed by the Lefebvre correlation, which for plain-jet airblast atomizers can be expressed as:

$$\frac{SMD}{d_o} = 0.48 \left(\frac{\sigma}{\rho_A U_{rel}^2 d_o} \right)^{0.4} \left(1 + \frac{1}{ALR} \right)^{0.4} + 0.15 \left(\frac{\mu_L^2}{\sigma \rho_L d_o} \right)^{0.5} \left(1 + \frac{1}{ALR} \right) \quad (5.1)$$

From this expression, the dominant parameters affecting the Sauter Mean Diameter are the air density and velocity, the ALR and the fuel dynamic viscosity and surface tension. The first plot shown in Fig. 5.1 describes a strong monotonic decrease of D_{32} as U_{air} increases. This behaviour directly follows from:

$$D_{32} \propto (U_{rel})^{-0.8}$$

Since aerodynamic stress scales with $\rho_A U_{rel}^2$, increasing air velocity enhances primary breakup by increasing the Weber number $(\frac{\rho_A U_{rel}^2 d_o}{\sigma})$, which promotes droplet fragmentation, leading to smaller droplets. Physically this means that aerodynamic shear is the dominant atomization mechanism in the investigated range. Even when pressure or temperature vary, the influence of U_{rel} remains the strongest, as visible from the steep slope of the curves; the breakup process is primarily controlled by aerodynamic forces rather than liquid properties.

The decrease of D_{32} with increasing ALR is also evident from the second plot in Fig. 5.1. From the correlation in Eq. 5.1 it can be seen that, as ALR increases, the term $1/ALR$ decreases, reducing the overall droplet size.

$$D_{32} \propto \left(1 + \frac{1}{ALR} \right)^{0.4}$$

Physically, a higher air-to-liquid ratio means more kinetic energy available for atomization, stronger interaction between air stream and liquid jet and improved primary disintegration. However, compared to the velocity effect, the slope is less steep, indicating that ALR contribution to breakup enhancement is secondary with respect to air velocity.

Lastly, a mild reduction of D_{32} with increasing fuel temperature can be seen from the third plot in Fig. 5.1. This trend can be explained through the temperature dependence of liquid properties; in particular, both fuel surface tension and dynamic viscosity reduce as the temperature increases, resulting in smaller droplet.

$$D_{32} \propto \sigma^{0.4}, \quad D_{32} \propto \mu_L^{0.5}$$

The slope is significantly weaker than in the velocity case. This confirms that thermophysical liquid properties play a secondary role compared to aerodynamic forces in the investigated range.

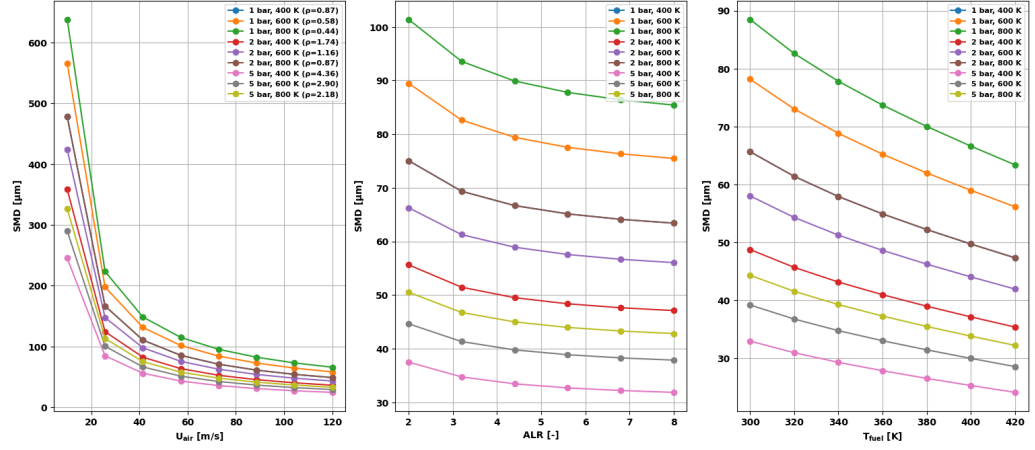


Figure 5.1: SMD as a function of: a) air velocity, b) ALR and c) fuel temperature.

The importance of atomization becomes evident when examining the evaporation results. Since evaporation is governed by the following D^2 -law:

$$D^2(t) = D_0^2 - Kt \quad (5.2)$$

the initial droplet diameter $D_0 = D_{32}$ directly determines the evaporation time:

$$t_{\text{evap}} = \frac{D_0^2}{K} \quad (5.3)$$

Therefore, any parameter reducing SMD also indirectly shortens droplet lifetime. The evaporation rate K in the D^2 -law increases with:

- vapour diffusivity $D_{v,m}$,
- surface vapour pressure p_{sat} ,
- convective enhancement through the Reynolds number.

The evaporation stage is governed by the Abramzon-Sirignano formulation, in which the droplet mass transfer rate can be expressed in proportional form as:

$$\dot{m}_d \propto Sh \ln(1 + B_M) \quad (5.4)$$

where the Spalding mass transfer number is defined as:

$$B_M = \frac{Y_{v,s} - Y_{v,\infty}}{1 - Y_{v,s}} \quad (5.5)$$

and the Sherwood number scales as:

$$Sh \propto Re^{1/2} Sc^{1/3} \quad (5.6)$$

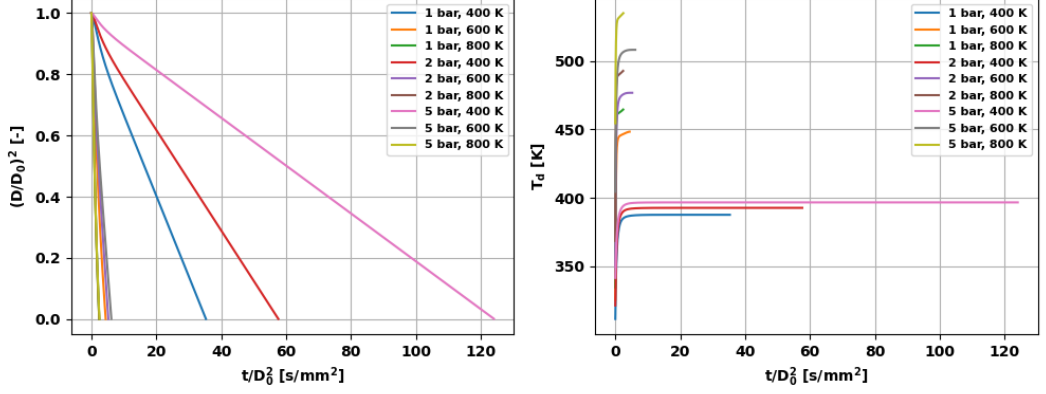


Figure 5.2: Evaporation plots: a) D^2 -law and b) droplet temperature.

The linear decrease of $(D/D_0)^2$ with normalized time confirms diffusion-controlled evaporation, as shown in the first plot in Fig. 5.2. The linearity of the curves validates the implementation of the Abramzon-Sirignano model and confirms that, within the investigated range, droplet regression follows classical theory. An increase in air temperature leads to steeper slopes, corresponding to higher values of K , and therefore shorter evaporation times. From kinetic theory, vapour diffusivity scales as:

$$D_{v,m} \propto \frac{T^{3/2}}{P} \quad (5.7)$$

while the saturation pressure follows an exponential dependence:

$$p_{sat} \propto \exp\left(\frac{L_v}{R} \left(\frac{1}{T_b} - \frac{1}{T_d}\right)\right). \quad (5.8)$$

Increasing air temperature therefore increases diffusivity, surface vapour pressure, the Spalding mass number and the evaporation rate. This explains the strong reduction in droplet lifetime observed in Table 5.1 when temperature increases from 400 K to 800 K. Another parameter that influences evaporation is air pressure. On one hand, diffusivity decreases:

$$D_{v,m} \sim \frac{1}{P} \quad (5.9)$$

which tends to slow down evaporation. On the other hand, air density increases:

$$\rho_g = \frac{P}{RT_g} \quad (5.10)$$

which increases the Reynolds number and enhances convection.

At lower temperatures, diffusion limitation dominates and evaporation slows down with increasing pressure. At higher temperatures, thermal effects and enhanced convection partially compensate for this reduction, leading to a weaker overall pressure dependence. Moreover, cases corresponding to higher pressure exhibit smaller SMD values due to improved atomization. Consequently, even when diffusivity decreases, the reduced initial droplet size significantly shortens the evaporation time. This

highlights the strong coupling between atomization and evaporation phenomena. The droplet temperature profiles in the second plot of Fig. 5.2 show rapid heating towards a quasi-steady value close to the wet-bulb temperature. Higher air temperatures shift this equilibrium upward, resulting in higher steady droplet temperatures. The numerical results of the parametric study are summarized in Table 5.1, while the global sensitivity trends are described in Table 5.2.

Case	T_g [K]	P_g [bar]	ρ_g [kg/m ³]	D_{32} [μ m]	U_{rel} [m/s]	t_{evap} [s]	T_{evap} [K]	P_{evap} [atm]
1	400	1	0.871	65.69	52.69	1.52e-1	387.6	0.057
2	600	1	0.581	78.22	58.99	2.70e-2	448.4	0.369
3	800	1	0.436	88.55	62.46	1.90e-2	464.6	0.558
4	400	2	1.742	48.77	36.43	1.37e-1	392.7	0.069
5	600	2	1.161	58.05	45.14	1.76e-2	476.8	0.749
6	800	2	0.871	65.69	50.61	1.04e-2	492.8	1.077
7	400	5	4.355	32.96	14.79	1.35e-1	396.7	0.079
8	600	5	2.904	39.19	21.85	9.44e-3	508.2	1.495
9	800	5	2.178	44.33	27.40	4.85e-3	535.0	2.525

Table 5.1: Parametric study overall results.

Parameter	Immediate effect	Physical mechanism	Impact on evaporation
T_g	$\uparrow D_{v,m}, \uparrow p_{sat}$	Higher diffusivity and vapour pressure	$\uparrow K, \downarrow t_{evap}$
P_g	$\downarrow D_{v,m}, \uparrow \rho_g$	Diffusion limitation dominates	$\downarrow K$, longer t_{evap} (low T)
U_{rel}	$\uparrow Re, \uparrow Sh$	Enhanced convection	Faster heating and evaporation
ALR	$\downarrow D_{32}$	Improved primary atomization	Shorter lifetime
T_{fuel}	$\downarrow \sigma, \downarrow \mu_L$	Slightly improved breakup	Secondary influence

Table 5.2: Sensitivity analysis for atomization and evaporation.

5.1.2 Validation with documented model in the literature

In order to assess the reliability of the evaporation framework implemented in this work, a reference case was reproduced from the literature. The selected study is the one by Cavalieri et al. [20], where the Abramzon-Sirignano evaporation model is coupled with alternative strategies for thermodynamic and transport properties, including (i) an *ideal-fluid* one based on Raoult’s law for vapour-liquid equilibrium, and (ii) a *real-fluid* one based on the Peng-Robinson equation of state (PR-EoS). In the present validation, only the ideal-fluid formulation reported in the paper was reproduced. Therefore, the vapour-liquid equilibrium at the droplet surface was

computed assuming ideal behaviour, with the surface vapour mole fraction evaluated through Raoult's law:

$$\chi_{v,s} = \frac{p_{\text{sat}}(T_d)}{p_g}, \quad (5.11)$$

and subsequently converted into mass fraction for the evaluation of the Spalding mass transfer number. The benchmark operating point reproduced here corresponds to jet-engine-like conditions, with ambient gas total temperature $T_g = 500$ K and ambient pressure $p_g = 11$ bar. In the present implementation, liquid n-dodecane is used as surrogate consistently with the reference work, and the fuel initial conditions are assigned accordingly to the paper setup, such as $T_{\text{fuel}} = 300$ K.

The atomization SMD is computed through the airblast Rizk-Lefebvre correlation and a Rosin-Rammler distribution is generated using $D_m \equiv D_{32}$ as the scale parameter:

$$F(d) = 1 - \exp \left[- \left(\frac{d}{D_m} \right)^q \right], \quad D_m \equiv D_{32}, \quad (5.12)$$

where q controls the spread of the spray. Typical aviation sprays fall in the approximate range $[2, 6]$ (higher q implies a narrower distribution). The resulting Probability Distribution Function and Cumulative Distribution Function in Fig. 5.3 and Fig. 5.4 show the expected qualitative behaviour:

- the PDF exhibits a single peak around the most probable droplet size, and
- the CDF monotonically approaches unity, representing the cumulative fraction of droplets smaller than a given diameter.

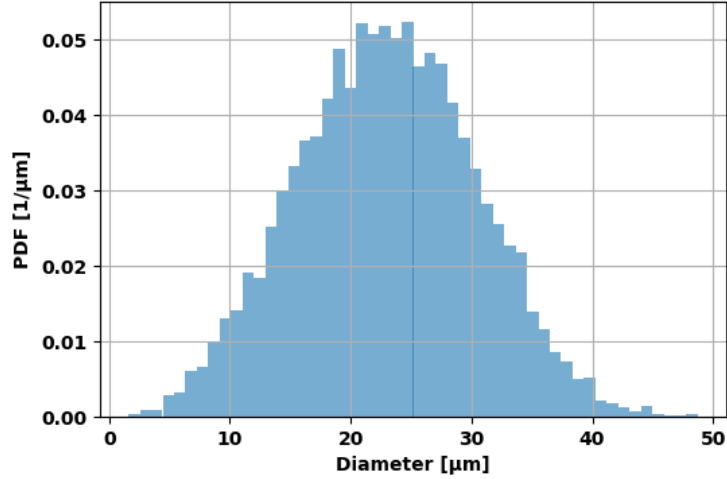


Figure 5.3: Rosin-Rammler distribution, with $D_{32} = 26 \mu m$ and $q = 3.5$.

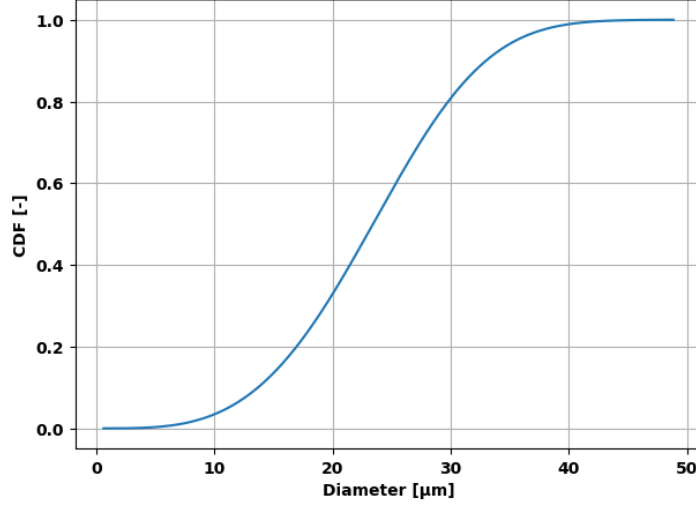


Figure 5.4: Cumulative distribution function.

The evaporation stage is based on the ASM formulation. A key modelling aspect concerns the evaluation of the fuel vapour diffusivity in the surrounding gas mixture. In the reference paper, for the ideal-fluid case, the binary diffusion coefficient is computed using the Fuller-Schettler-Giddings correlation:

$$D_{ij} = \frac{0.00143 T^{1.75}}{p \sqrt{M_{ij}} \left(v_{d,i}^{1/3} + v_{d,j}^{1/3} \right)^2}, \quad (5.13)$$

where $M_{ij} = 2M_i M_j / (M_i + M_j)$ with M_i and M_j being the fuel and gas molecular weights, and v_d is the sum of the atomic diffusion volumes and $v_{d,i} = 246.24$ for n-dodecane [20]. Since a detailed kinetic mechanism was not available in the present implementation, the fuel diffusivity could not be directly evaluated via Cantera transport models. Therefore, the same ideal-gas correlation adopted in the paper was implemented to follow the document formulation. The fuel diffusion coefficient into the gas mixture was then evaluated using the Hirschfelder-Curtiss approximation:

$$D_{i,m} = \frac{1 - Y_m}{\sum_{j \neq i}^{N_s} \frac{X_{j,m}}{D_{ji,m}}}. \quad (5.14)$$

Liquid-phase properties (density, specific heat) were obtained from CoolProp, while gas-phase thermodynamic properties (density, viscosity, specific heat, thermal conductivity) were computed using Cantera.

Fig. 5.5 shows the comparison between the present implementation (blue curve) and the results reported in [20]. The reference curves exhibit a slight initial overshoot above $(D/D_0)^2 = 1$, followed by a quasi-linear decay characteristic of diffusion-controlled evaporation. The blue curve reproduces the overall linear behaviour of the D^2 -law and the correct order of magnitude of the evaporation time. However, two

main differences are observed:

- The initial overshoot is less pronounced;
- The slope of the linear regime is slightly smaller, leading to a marginally longer evaporation time.

The overshoot in the reference curves is associated with the early heat-up transient, during which droplet expansion effects and transient mass transfer corrections can temporarily increase $(D/D_0)^2$. The obtained smoother behaviour may be attributed to small differences in the implementation of film properties, Stefan-flow corrections or transient coupling between heat and mass transfer. Since the diffusion coefficient is evaluated via correlation and the transport properties are obtained from Cantera, minor differences in viscosity or thermal conductivity may alter the Reynolds and Sherwood numbers, thereby slightly modifying the evaporation constant K .

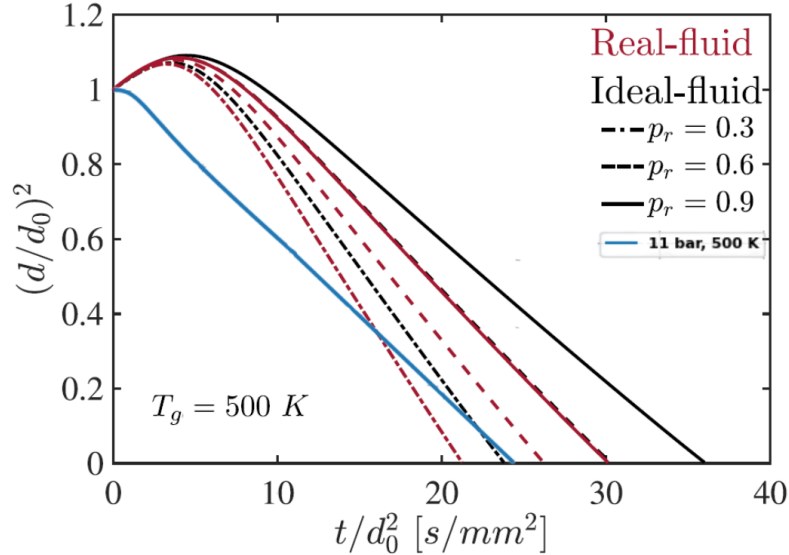


Figure 5.5: Comparison between the D^2 -law of the present validation and documented model.

Fig. 5.6 shows the time evolution of droplet temperature. The reference curves display a progressive heating stage with an asymptotic approach to a wet-bulb-like equilibrium temperature around 470-475 K. The blue curve reproduces the qualitative trend and equilibrium temperature level. However, the heating transient appears slightly faster, and the final droplet temperature is marginally higher (482.27 K).

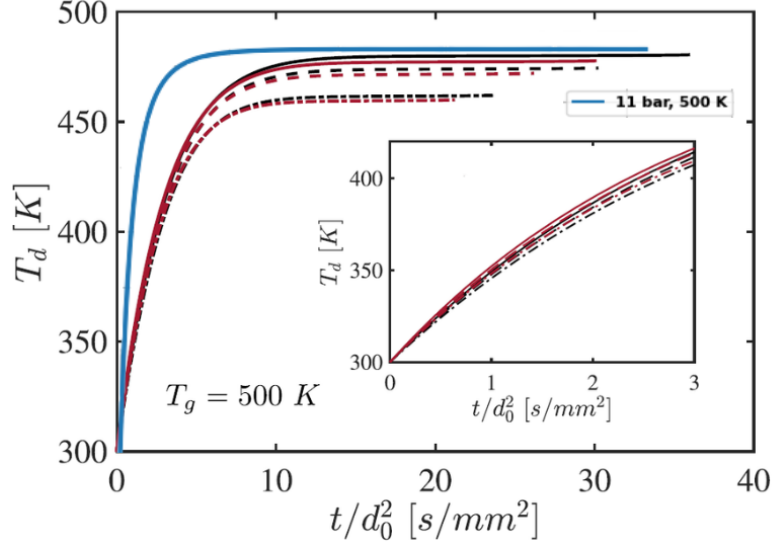


Figure 5.6: Comparison between the droplet temperature evolution of the present validation and documented model.

It is important to remark that in the reference case the initial droplet diameter is $D_0 = 100 \mu\text{m}$, whereas in the present implementation the evaporation stage is initialized with the Sauter Mean Diameter obtained from the atomization model, $D_{32} = 26 \mu\text{m}$. Although the results are presented in normalized form ($(D/D_0)^2$ and t/D_0^2), the evaporation dynamics do not depend solely on D_0^2 . Within the Abramzon-Sirignano framework, convective heat and mass transfer are governed by the Reynolds number:

$$Re = \frac{\rho_g U_{\text{rel}} D}{\mu_m}, \quad (5.15)$$

which depends linearly on the droplet diameter. Consequently, reducing the initial diameter from $100 \mu\text{m}$ to $26 \mu\text{m}$ significantly lowers the Reynolds number, and therefore affects both the Sherwood and Nusselt numbers:

$$Sh \sim 2 + 0.6 Re^{1/2} Sc^{1/3}, \quad Nu \sim 2 + 0.6 Re^{1/2} Pr^{1/3}. \quad (5.16)$$

Since the evaporation constant scales as

$$K \propto \rho_m D_{v,m} Sh \ln(1 + B_M), \quad (5.17)$$

a change in Re directly modifies the convective contribution to mass transfer and, therefore, the slope of the D^2 -law. In addition, smaller droplets heat up faster and this explains the steeper initial temperature rise observed in the present results compared to the reference case. Overall, the comparison confirms the structural correctness and physical consistency of the evaporation model implemented in this work within the ideal-fluid framework.

5.2 Supersonic case study results

The evaporation and emission framework developed in this work is finally applied to the CS-1A supersonic case study along the mission trajectory. The analysis is divided into two parts:

- Atomization and evaporation behaviour across altitude and Mach number,
- Resulting emission indices and their sensitivity to spray modelling.

5.2.1 Atomization and evaporation

The atomization model provides the Sauter Mean Diameter D_{32} as a function of air velocity and pressure, Mach number and altitude. The results show a clear coupling between aerodynamic conditions and spray fineness:

- Increasing Mach number and altitude leads to higher air velocity but lower density.
- The combined effect results in a non-monotonic behaviour of D_{32} along the trajectory.

At low altitude (high pressure and density), primary breakup is enhanced by stronger aerodynamic stresses, leading to smaller droplets. As altitude increases, density decreases significantly, weakening aerodynamic forcing and the velocity increase. The trend observed in the plots is consistent with the Lefebvre correlation:

$$D_{32} \propto \left(\frac{\sigma}{\rho_g U_{\text{rel}}^2} \right)^{0.4} \left(1 + \frac{1}{ALR} \right)^{0.4} \quad (5.18)$$

showing that a reduction in ρ_g at high altitude tends to increase droplet size, while higher U_{rel} promotes breakup. The presence of these double effects explains the moderate variation of D_{32} along the CS-1A trajectory.

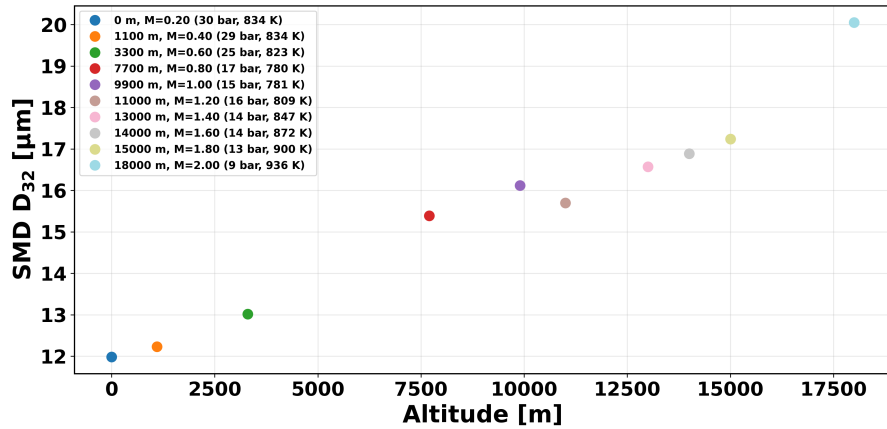


Figure 5.7: SMD vs altitude, using A2 surrogate.

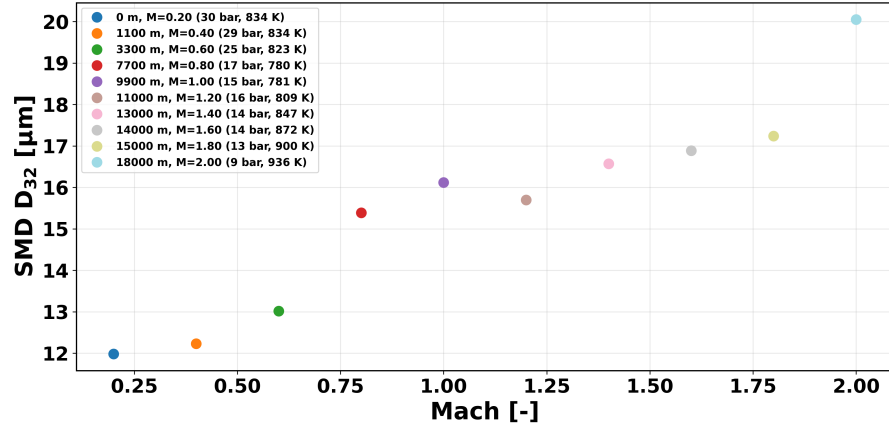


Figure 5.8: SMD vs Mach number, using A2 surrogate.

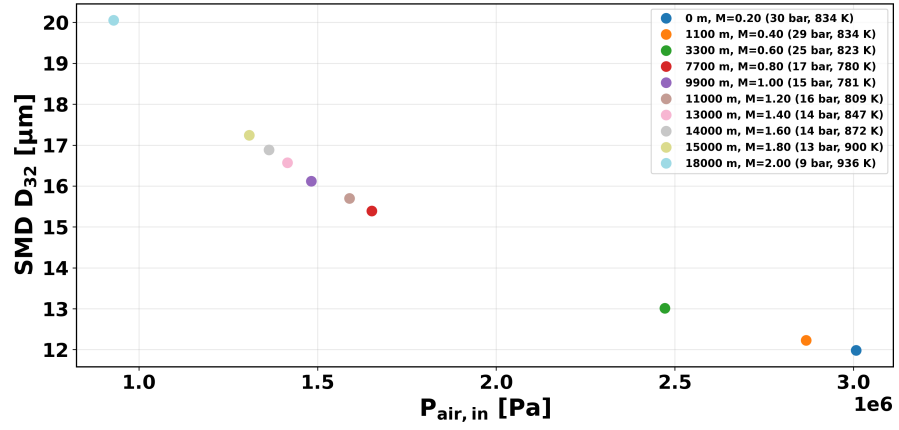


Figure 5.9: SMD vs air pressure, using A2 surrogate.

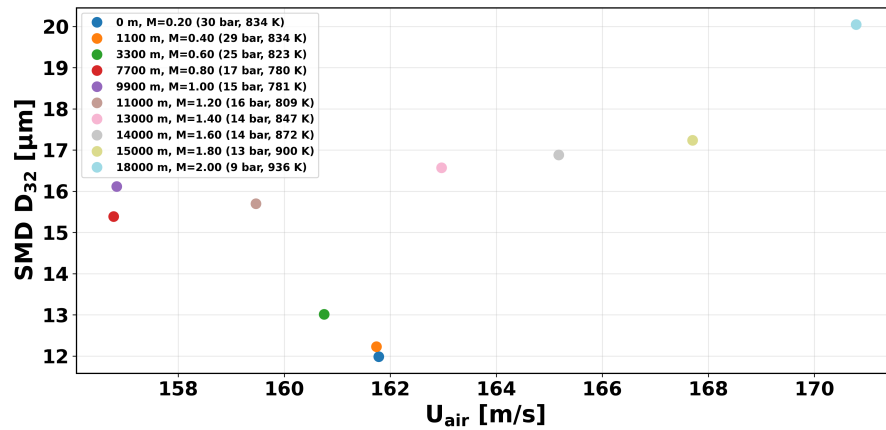


Figure 5.10: SMD vs air velocity, using A2 surrogate.

Evaporation is modelled using the ASM framework under subcritical assumptions, with transport properties from Cantera and liquid properties from CoolProp. The D^2 -law behaviour is preserved in all cases, as shown in Fig. 5.11 below. As altitude

increases gas density decreases and diffusivity increases (approximately $D_{v,m} \propto T^{3/2}/P$). The combined effect leads to faster heating at high T_g , but reduced convective enhancement at very low density.

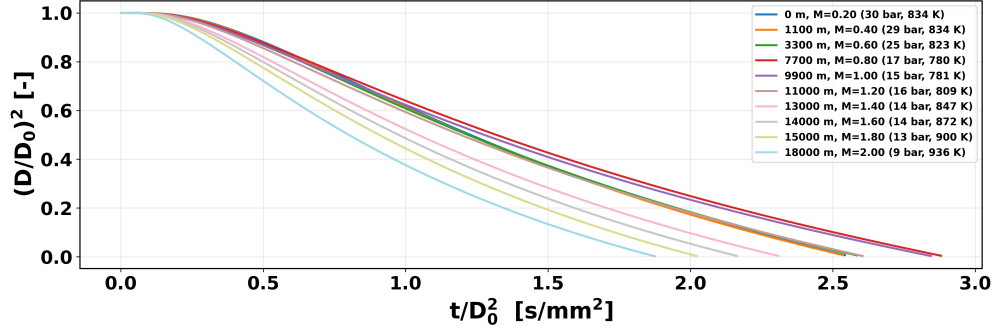


Figure 5.11: D^2 -law, using the A2 surrogate.

Fig. 5.12 shows the evolution of the droplet temperature along the CS-1A trajectory. All cases exhibit the classical two-stage behaviour predicted by the ASM:

1. Rapid heating phase, dominated by convective heat transfer;
2. Asymptotic approach to a quasi steady-state temperature (wet-bulb temperature).

The higher ambient temperature leads to higher asymptotic droplet temperature, as visible in the upper plateau of the curves. However, the reduced density weakens convective heat transfer, slightly moderating the initial heating slope in some cases.

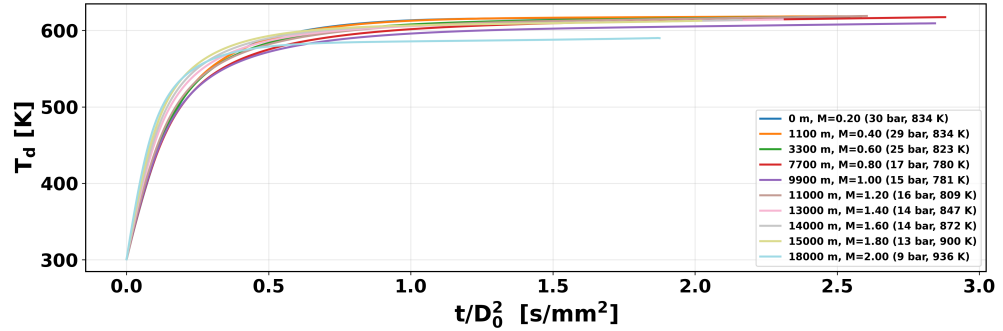


Figure 5.12: Droplet temperature evolution, using the A2 surrogate.

In the evaporation model, the determination of the fuel mass fraction at the droplet surface, $Y_{v,s}$, is a key step. This quantity is obtained by imposing vapour-liquid equilibrium (VLE) at the interface. Two equilibrium closures are implemented in the present code:

- **Peng-Robinson equation of state (fugacity-based)** is used for the first three low-altitude/high-pressure cases, where non-ideal effects are more relevant.

- **Raoult's law (ideal-fluid assumption)** is used for the remaining cases at lower pressure.

The Spalding mass number is computed as:

$$B_M = \frac{Y_{v,s} - Y_{v,\infty}}{1 - Y_{v,s}}, \quad (5.19)$$

with $Y_{v,s}$ obtained either from fugacity equality (PR-EoS) or from

$$\chi_{v,s} = \frac{p_{\text{sat}}(T_d)}{p_g} \quad (5.20)$$

in the ideal case. The results confirm that differences between PR-EoS and Raoult are modest at moderate pressure levels, but become more relevant at higher pressures where PR predicts slightly larger surface fuel fractions [22], as illustrated in Fig. 5.13. This increases B_M and therefore enhances $\dot{m}_d$.

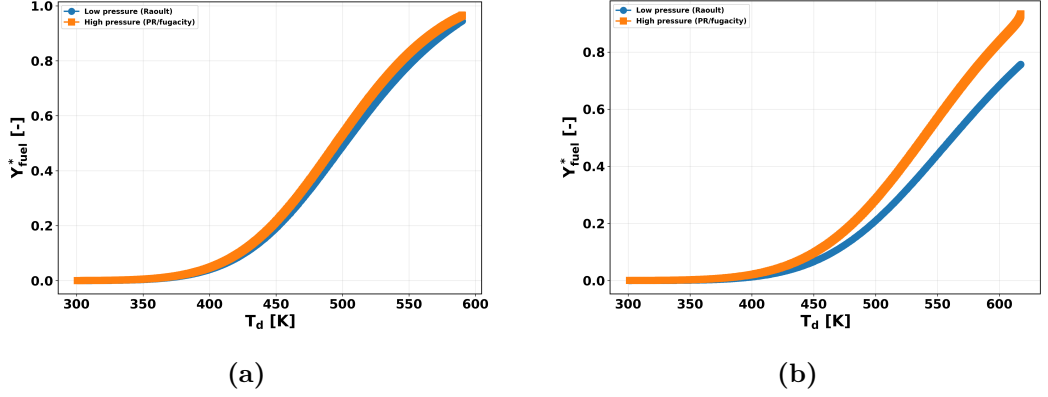


Figure 5.13: Mass fraction of A2 surrogate vapour plotted against the droplet temperature at an ambient pressure of a) 9 bar and b) 30 bar.

The droplet energy balance includes the latent heat term:

$$Q_{\text{lat}} = L_v(T_d) \dot{m}_d, \quad (5.21)$$

which governs the coupling between mass loss and thermal response. Two subcritical approaches were implemented in order to compute the enthalpy of vaporization:

- $L_v(T_d)$ evaluated from CoolProp using saturated liquid and vapour enthalpies;
- Pitzer correlation as an independent sensitivity model.

The enthalpy of vaporization decreases significantly as droplet temperature approaches the critical region. A lower L_v reduces the energy required for phase change and therefore accelerates evaporation at high droplet temperatures.

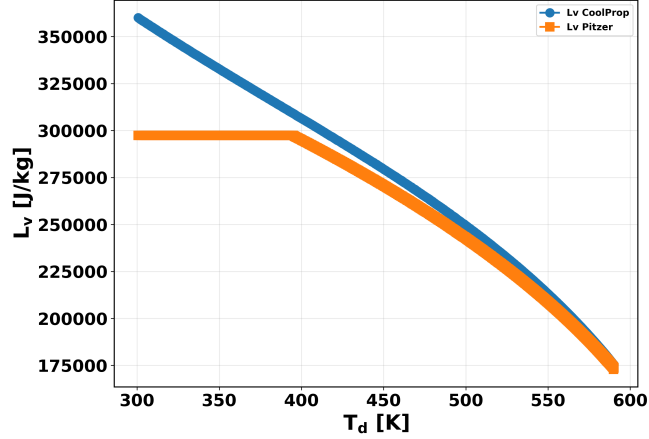


Figure 5.14: Enthalpy of vaporization evolution with droplet temperature, both in CoolProp and Pitzer cases.

5.2.2 Emission indices

All the computed emission indices obtained from the combustion simulations are summarized in Fig. 5.15, where the variation of the emission indices with the flight Mach number is reported for the main chemical pollutants.

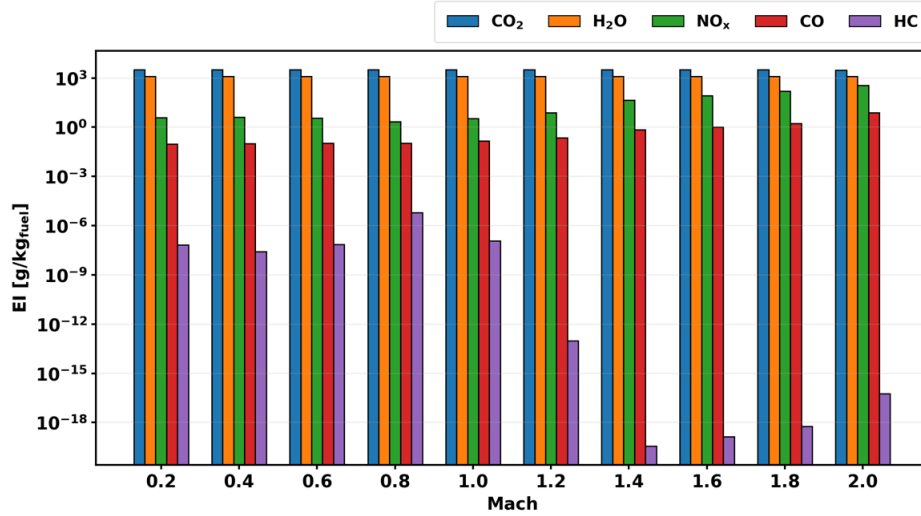


Figure 5.15: Emission indices of the main combustion products as a function of the flight Mach number.

The results are then analysed by comparing full phase-change modelling (atomization + evaporation) and the simplified approach without spray modelling. CO decreases when detailed spray modelling is included, as shown in Fig. 5.16. Improved atomization and evaporation enhance fuel-air mixing and reduce locally rich regions, promoting more complete oxidation and leading to a noticeable decrease in EICO (approximately 25%). Even NO_x shows a reduction between -47% and -13% depending on the flight point. Evaporation modelling takes into account the heat exchange between the colder liquid fuel stream and the hot air stream, reducing the

mixing temperature and, consequently, the peak flame temperature.

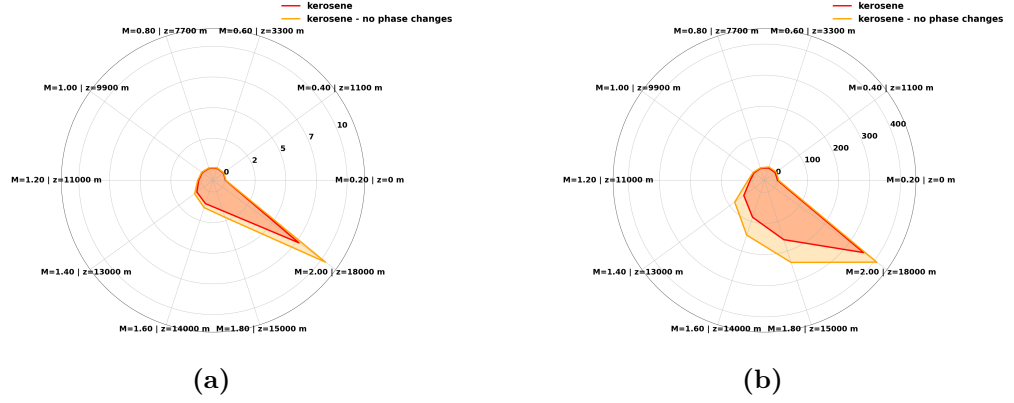


Figure 5.16: Comparison of a) EICO and b) EINO_x, using the A2 surrogate.

The emission indices of CO₂ and H₂O remain nearly unchanged when comparing the detailed spray modelling with the one without phase-change. This behaviour is physically expected. Both CO₂ and H₂O emissions are proportional to fuel burn, which means that their total mass depends on the total amount of fuel burned and its composition (carbon and hydrogen content). Since both modelling approaches use the same chemical surrogates for kerosene and biofuel, the elemental carbon and hydrogen fractions remain unchanged. Consequently, the total production of CO₂ and H₂O per unit mass of fuel is nearly identical. Lastly, when compared with the emission indices reported for the Olympus 593 engine [7], which powered the Concorde aircraft, the present model predicts a slight reduction of CO₂ emissions of approximately 1%, while H₂O emissions show a moderate increase of about 2.8%.

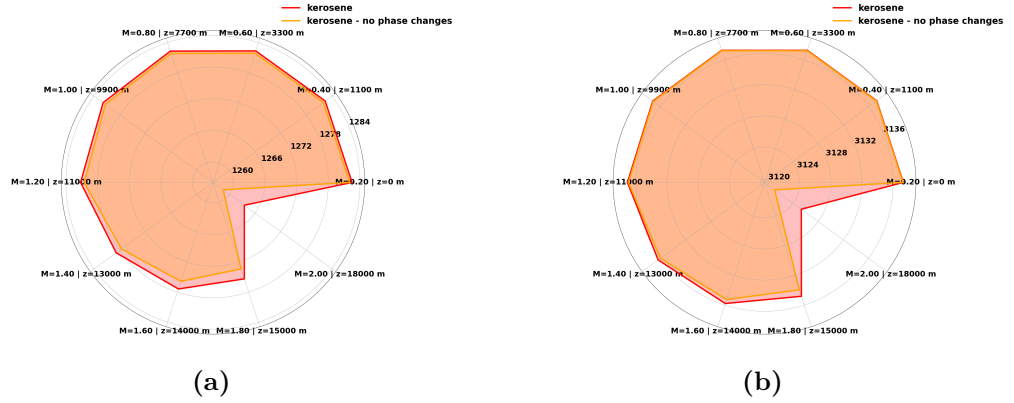


Figure 5.17: Comparison of a) EIH₂O and b) EICO₂, using the A2 surrogate.

The obtained results for HC shown in Fig. 5.18, similarly to the previous modelling approach, are not fully convincing due to their extremely low values. Although atomization and evaporation are now modelled, the absence of a finite combustion chamber volume and data about the geometry prevents a reliable prediction of HC emissions, which are strongly residence-time dependent.

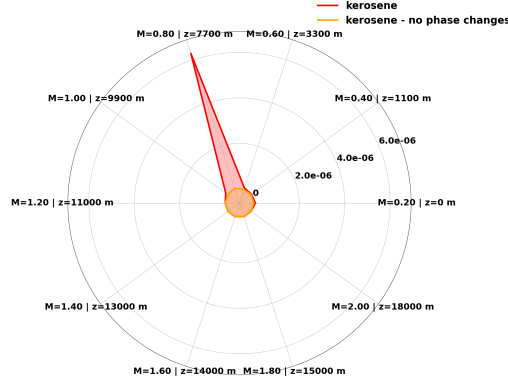


Figure 5.18: Comparison of EIHC, using the A2 surrogate.

Overall, the analysis of the emission indices demonstrates that the inclusion of detailed atomization and evaporation modelling primarily affects temperature- and mixing-sensitive species, while the ones proportional to fuel burn remain unchanged. From a modelling perspective, the results confirm that neglecting atomization and evaporation effects may lead to non-negligible discrepancies in predicting chemical emissions. The comparative sensitivity analysis of all emission indices is summarised in Table 5.3.

Emission Index	Observed Effect	Physical Consequence	Comment
EICO	$\downarrow \sim 25\%$	Improved mixing $\rightarrow$ more complete oxidation	Strongly spray-sensitive
EINO _x	$\downarrow (13\% - 47\%)$	Lower peak T due to evaporation cooling	Temperature-driven species
EICO ₂	$\approx$ constant ($< 0.1\%$)	Stoichiometric dependence	Minor variations
EIH ₂ O	$\approx$ constant ($< 0.4\%$)	Stoichiometric dependence	Minor variations
EIHC	Uncertain	Residence-time controlled	Model limitations

Table 5.3: Sensitivity of emission indices to detailed spray modelling in the CS-1A case study.

The same analysis was performed using the SAF C1 surrogate. The obtained atomization, evaporation and emission trends follow very similar qualitative behaviours. The corresponding plots for the SAF C1 surrogate are reported in Appendix A.

Chapter 6

Comparison between conventional fuels and SAFs

6.1 Sustainable Aviation Fuels

The aviation sector faces a particularly demanding decarbonization challenge. Aircraft propulsion requires liquid fuels with very high gravimetric energy density, excellent low-temperature operability, thermal stability under severe heat loads, and strict safety and materials compatibility requirements. These constraints strongly limit the set of viable energy carriers. As a result, while electrification and hydrogen are long-term research directions, the most technically mature and near-term decarbonization pathway relies on Sustainable Aviation Fuels (SAFs), which are hydrocarbon fuels produced from renewable or non-conventional feedstocks and designed to be compatible with existing aircraft and fuel infrastructure. Their primary characteristic is that they are formulated to meet the property envelope of conventional kerosene, allowing them to function as so-called *drop-in* fuels. This means they can be blended with, distributed as, and ultimately re-identified as conventional jet fuel once they meet specification limits, avoiding parallel logistics chains and aircraft modifications [6]. Conventional fuels are a complex mixture of hydrocarbons spanning a wide carbon-number distribution (C₈-C₁₆), primarily composed of n-paraffins, iso-paraffins, cycloparaffins (naphthenes), and aromatics [6]. The relative proportions of these chemical classes determine key properties such as density, hydrogen content, volatility, viscosity, ignition quality and thermal stability [46]. Any alternative fuel must therefore not only match bulk properties (e.g., freezing point, flash point, heating value), but also provide equivalent functional performances. The qualification pathway for SAFs is codified through ASTM D4054, a rigorous evaluation process assessing fuel properties, material compatibility, operability, emissions and engine performance. Once a pathway is approved, it is incorporated into ASTM D7566 as a synthetic blending component, with defined blending limits and compositional requirements [6].

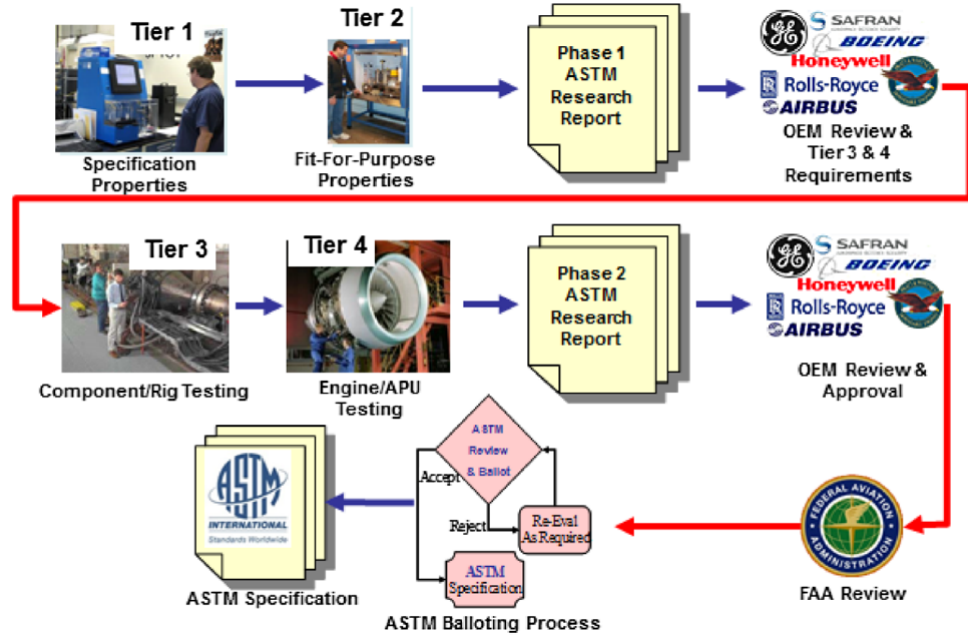


Figure 6.1: D4054 qualification process [6].

Several technological routes have been developed and certified to produce sustainable fuels. Although they differ in feedstock and processing steps, most approved fuels fall into the category of Synthetic Paraffinic Kerosenes (SPK).

- **FT-SPK (Fischer-Tropsch Synthetic Paraffinic Kerosene):** In this pathway, syngas (CO and H_2) is catalytically converted into hydrocarbons. These fuels are typically rich in paraffins, with negligible sulfur and very low aromatic content [47]. This chemical profile leads to high hydrogen content and low soot formation, but also to lower density compared to conventional Jet-A.
- **HEFA (Hydroprocessed Esters and Fatty Acids):** This pathway is currently the most mature and commercially implemented technology for SAF production. This process converts lipid-based feedstocks such as vegetable oils, animal fats, and waste cooking oils into aviation fuel through catalytic hydroprocessing. During the upgrading stage, the oxygen contained in triglycerides is removed through reactions such as hydrodeoxygenation, while additional refining steps, including hydrocracking and isomerization, adjust the hydrocarbon chain lengths to match the kerosene boiling range. The resulting product is a synthetic paraffinic kerosene that can be blended with conventional jet fuel while maintaining compatibility with existing aircraft fuel systems [48].
- **Alcohol-to-Jet (AtJ):** In this route, alcohol intermediates such as ethanol or butanol are first produced through fermentation of biomass-derived sugars or other renewable feedstocks. These alcohol molecules are subsequently upgraded into hydrocarbons through a sequence of catalytic processes including dehydration, oligomerization and hydrogenation. The final product is a paraffinic fuel suitable for aviation applications and compatible with current aircraft engines

when blended with conventional kerosene. The AtJ pathway is considered particularly promising because it can exploit established bioethanol production infrastructures and a wide variety of biomass feedstocks [48].

- **Power-to-Liquid (PtL):** Renewable electricity is used to produce hydrogen through water electrolysis. The hydrogen is then combined with carbon dioxide captured either from industrial sources or directly from the atmosphere to produce synthesis gas. Through catalytic conversion processes, such as Fischer-Tropsch synthesis, this syngas is transformed into liquid hydrocarbons that can be refined into aviation fuels. Although PtL fuels could produce very low lifecycle greenhouse gas emissions, their large-scale deployment is currently limited by high production costs and the significant demand for renewable electricity and carbon capture infrastructure [48].

In the following, the focus is placed on the specific surrogate adopted in this work, designed to represent an AtJ-like paraffinic blend, and on the comparison against the kerosene surrogate of emissions trends.

6.2 Comparison between kerosene and biofuel emission indices

The surrogate employed to represent SAFs is the C1 blend, which represents an Alcohol-to-Jet synthetic fuel developed by Gevo and investigated within the National Jet Fuels Combustion Program. Gevo’s AtJ technology produces sustainable aviation fuel starting from renewable alcohols such as ethanol or isobutanol, obtained through fermentation of biomass-derived sugars. In the industrial process, fermentable sugars derived from agricultural feedstocks are first converted into alcohol via microbial fermentation. The resulting alcohol is then catalytically upgraded into hydrocarbon molecules suitable for aviation fuel through dehydration and oligomerization reactions, followed by hydrogenation and refining steps to obtain a kerosene-range product compatible with conventional jet fuel infrastructure [32].

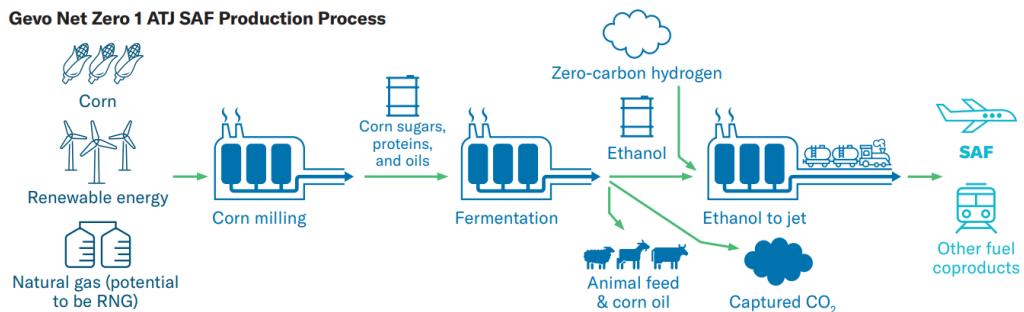


Figure 6.2: Gevo Net Zero 1 AtJ SAF Production Process [32].

In the National Jet Fuels Combustion Program (NJFCP) framework, C1 corresponds to the *Category C* test fuel, formulated as a mixture of C₁₂ and C₁₆ highly branched

paraffins. The NJFCP documentation highlights C1 as a fuel characterized by an extremely low derived cetane number and an unusual/bimodal boiling range, specifically selected to highlight the sensitivity of combustor performance metrics to fuel properties [6]. Fig. 6.3, 6.4 and 6.5 compare the emission indices obtained for the kerosene surrogate and for the biofuel surrogate over the investigated CS-1A operating conditions. The plots indicate that the largest relative differences between the two fuels are observed for CO and NO_x, whereas CO₂ and H₂O remain comparatively weakly sensitive to the fuel switch.

CO and unburned hydrocarbons are commonly interpreted as markers of incomplete oxidation, hence they are sensitive to local quenching, spray evaporation/mixing, and finite-rate chemistry. In the CS-1A set, the biofuel trends for EICO suggest that the AtJ-like surrogate leads, on average, to lower CO than kerosene at several operating points. The physical reason may be that the paraffinic surrogate promotes more effective oxidation pathways under the same residence-time constraints, and that the coupled spray/phase-change modelling yields improved fuel-air mixing, with less locally rich/quenching pockets. The NO_x emission index is largely controlled by the thermal history of the flame (peak temperatures and high-temperature residence time) and, depending on the operating regime, also by mixing-controlled effects that alter local equivalence ratio and hot-spot formation. In the present comparison, the C1 surrogate produces lower EINO_x than A2 across most conditions. This is qualitatively consistent with the following chain of mechanisms:

1. A paraffinic, AtJ-like fuel can alter the adiabatic flame temperature and the heat-release distribution via stoichiometry and kinetic pathways,
2. Coupled spray evaporation/mixing can reduce localized rich regions and mitigate temperature hot-spots,
3. Reduced hot-spot intensity and/or reduced high-*T* residence time leads to lower thermal NO formation.

Even when the inlet conditions are fixed, small variations in peak temperature can significantly affect NO_x formation due to the exponential temperature dependence of thermal NO_x kinetics.

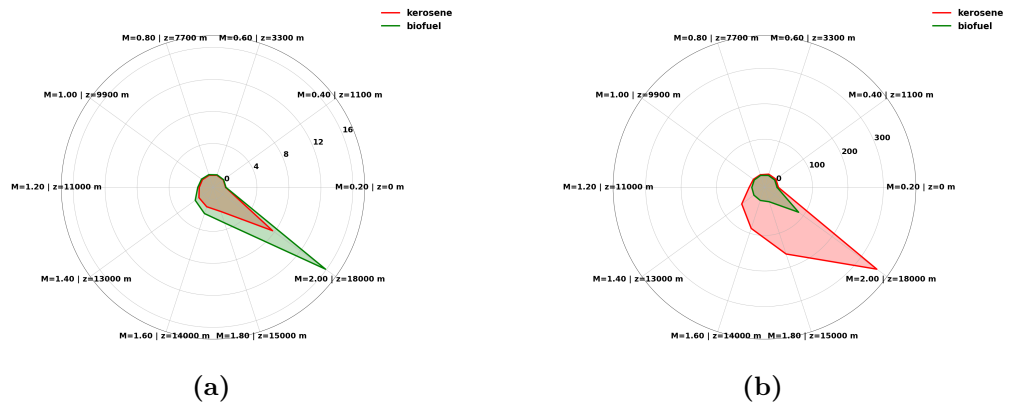


Figure 6.3: Comparison between kerosene and biofuel a) EICO and b) EINO_x.

The modest variation of EICO_2 and EIH_2O between A2 and C1, as shown in the figure below, is consistent with the fact that these species are largely controlled by overall elemental balances at the combustor level. Under comparable thrust/operating point, the total amount of burned fuel (and thus the amount of oxidized carbon and hydrogen) dominates the resulting CO_2 and H_2O . Therefore, when the combustion completeness is high and both simulations use surrogates that reproduce similar overall C/H content at system scale, the corresponding emission indices are expected to vary only mildly [6]. In the present results, the residual differences observed for EICO_2 and EIH_2O can be mainly attributed to stoichiometric considerations and to the elemental composition of the fuel. In particular, a more paraffinic fuel, typically characterized by a higher H/C ratio, tends to produce slightly more water and slightly less carbon dioxide per unit mass of fuel. However, this effect remains relatively small compared to the strong sensitivity of species such as CO or NO_x to local equivalence ratio, mixing conditions, and temperature.

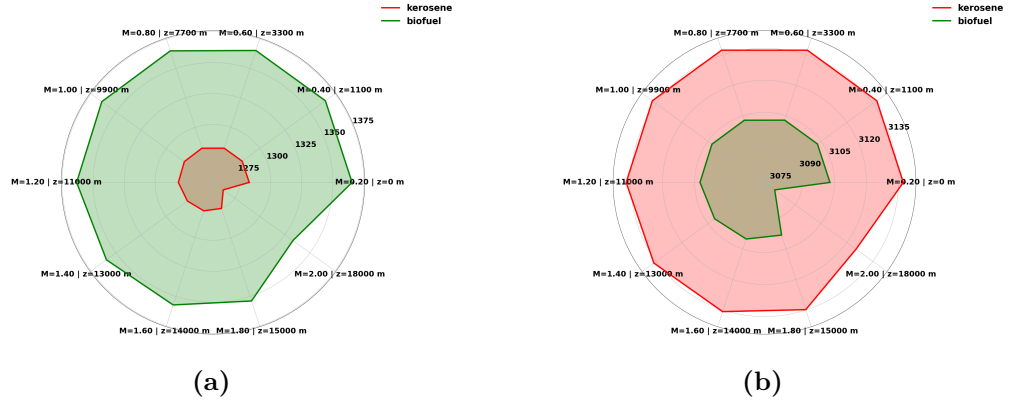


Figure 6.4: Comparison between kerosene and biofuel a) EIH_2O and b) EICO_2 .

UHC trends are typically more difficult to interpret quantitatively in simplified combustor frameworks, because they are strongly affected by residence time in the combustor chamber, wall interactions and local extinction/re-ignition. Accordingly, UHC should be treated as an indicator with higher uncertainty unless detailed geometry and near-wall processes are explicitly resolved.

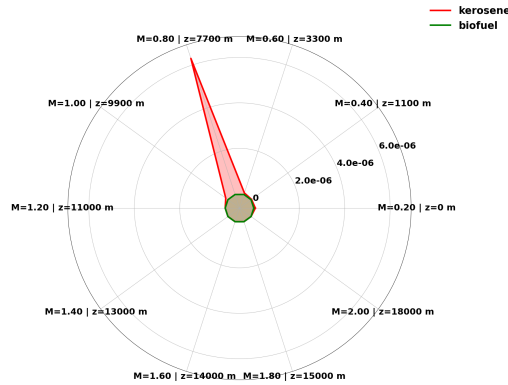


Figure 6.5: Comparison between kerosene and biofuel EIHC .

Overall, the comparison analyses show that switching from a kerosene surrogate to a biofuel surrogate affects primarily the pollutants controlled by local combustion details (CO and NO_x), while the products that are proportional to fuel burn (CO₂, H₂O) remain comparatively stable.

Chapter 7

Conclusions

The present work focused on the development and implementation of a preliminary multi-physics modelling framework aimed at improving the physical representation of liquid fuel combustion processes within early-stage emission estimation methodologies. The main objective of the study was to investigate the influence of phase-change phenomena, specifically fuel atomization and evaporation, on the parameters that mostly influence pollutant emissions in aircraft combustors, and to assess if the proposed approach could capture relevant combustion trends for both conventional kerosene fuels and Sustainable Aviation Fuels (SAFs). The modelling framework developed in this thesis integrates simplified spray atomization models such as Rizk & Lefebvre and Rosin-Rammler, droplet evaporation physics through ASM and PR-EOS formulations and detailed chemical kinetics in a computationally efficient Python code, suitable for conceptual design applications. The inclusion of these physical mechanisms represents a significant step forward compared to simplified emission estimation approaches, which often neglect the liquid-phase behaviour of fuels, assuming them gaseous at the combustor inlet. One of the main outcomes of this work is the demonstration that accounting for phase-change processes improves the physical consistency of the predicted combustion behaviour. In particular, the introduction of atomization and evaporation modelling enables a more realistic representation of fuel/air mixing within the combustor, which directly influences local temperature distributions and reaction rates. This improved description of the combustion phenomenon has a direct impact on the estimation of pollutant formation, especially for species whose formation strongly depends on local mixing conditions and flame temperature. The analysis performed throughout the thesis shows that the proposed modelling approach is able to reproduce emission trends that remain physically coherent across a wide range of operating conditions. Parametric variations in flight Mach number, altitude and operating parameters such as fuel temperature, air velocity and ALR, lead to atomization and evaporation outputs that are consistent with trends reported in literature studies. This shows the robustness of the modelling framework and supports its applicability in preliminary design analyses. A detailed comparison between simplified combustion modelling and the proposed phase-change modelling approach highlights the importance of including spray physics

when analysing emissions generated by liquid fuels. In particular, the results show that improved fuel atomization and evaporation promote more effective fuel/air mixing, reducing locally fuel-rich regions and leading to more complete oxidation processes. As a consequence, a noticeable decrease in CO emissions is observed when detailed spray modelling is included. The analysis also indicates a reduction in NO_x formation, due to lower peak flame temperatures resulting from lower mixing temperatures, caused by the enhanced heat exchange between evaporating droplets and the surrounding hot air stream. The evaluation of emission indices across the considered operating trajectory further confirms the role of phase-change modelling in studying pollutant formation dynamics. CO₂ and H₂O emissions remain largely unaffected by the inclusion of detailed spray physics, since they primarily depend on the overall fuel mass burned and its elemental composition. On the other side significant variations are observed for those pollutants that are affected by incomplete combustion and temperature. These results prove how simplified modelling strategies may provide reasonable predictions for combustion products that are proportional to fuel burn, but can lead to less reliable estimates for species whose formation is strongly influenced by mixing processes and residence times. Another important aspect investigated in this thesis concerns the comparison between conventional kerosene fuels and alternative Sustainable Aviation Fuels. In particular, the analysis focused on the A2, a Jet-A surrogate, and the C1, an Alcohol-to-Jet surrogate formulation. The results obtained from the simulations highlight several differences in emission behaviour. With respect to the A2 surrogate, C1 shows a slight reduction in CO₂ emissions and a moderate increase in H₂O emissions, which is consistent with the differences in fuel stoichiometric composition. At the same time, the simulations indicate lower NO_x emissions for the SAF case, suggesting that the modified combustion characteristics associated with the synthetic fuel can lead to reduced peak flame temperatures. On the other side, the results show an increase in CO emissions, which can be attributed to the complex interaction between mixing processes, reaction kinetics and residence times within the combustor. Overall, the results obtained throughout this work demonstrate that the proposed modelling framework is able to capture the main physical mechanisms governing pollutant formation in aero-engine combustors while maintaining a level of computational cost and efficiency compatible with early design analyses. The methodology therefore represents a valuable tool for preliminary environmental evaluations of propulsion systems. Moreover, the framework can be used for all liquid fuels and this is particularly relevant in the context of the ongoing transition toward more sustainable aviation energy sources.

7.1 Future Works

Although the modelling framework developed in this thesis provides encouraging results, several aspects could be further considered in order to improve the accuracy and applicability of the methodology.

A first possible improvement could be the refinement of the spray modelling ap-

proach. The current implementation studies the main physical mechanisms governing atomization and evaporation; however, additional phenomena such as secondary droplet breakup and droplet-droplet interactions could be incorporated to obtain a more detailed representation of spray dynamics. Moreover, the estimation of the flow conditions at the combustor inlet could be improved. In the present work, a single representative Mach number is assumed for all operating points along the flight trajectory. A more accurate approach could instead compute the combustor inlet Mach number by introducing the efficiency parameters of the upstream engine components.

Another improvement concerns the coupling between the evaporation model and the chemical kinetics description through a more detailed representation of the multi-component nature of surrogate fuels. In the present framework, fuel evaporation is treated in a simplified manner, assuming a fixed fuel composition during the evaporation process. However, surrogate fuels are typically composed of multiple species characterized by different volatility properties. Future developments could therefore incorporate the volatility curves of the individual surrogate components in order to account for their different evaporation rates. As the evaporation process progresses, the relative amount of the various fuel species in the liquid and vapour phases would gradually change, leading to a time-dependent variation of the fuel composition entering the combustion reactions. Including this aspect would provide a more realistic representation of the evaporation process and could improve the accuracy of the predicted combustion behaviour.

Future research could also focus on extending the methodology to additional propulsion systems and operating regimes and updating and upgrading analytical surrogate models used to represent complex fuels. This would allow a more accurate representation of fuel chemical properties and combustion behaviour, especially when analysing different classes of sustainable aviation fuels.

Lastly, it could be useful implementing a three-dimensional geometrical combustor model in order to estimate the residence time distributions within the combustor, which affect the formation of incomplete combustion products such as CO and unburned hydrocarbons (UHC). Incorporating this information would therefore improve the prediction accuracy of these species.

Appendix A

Appendix

A.1 Inputs for the CS-1A supersonic case study

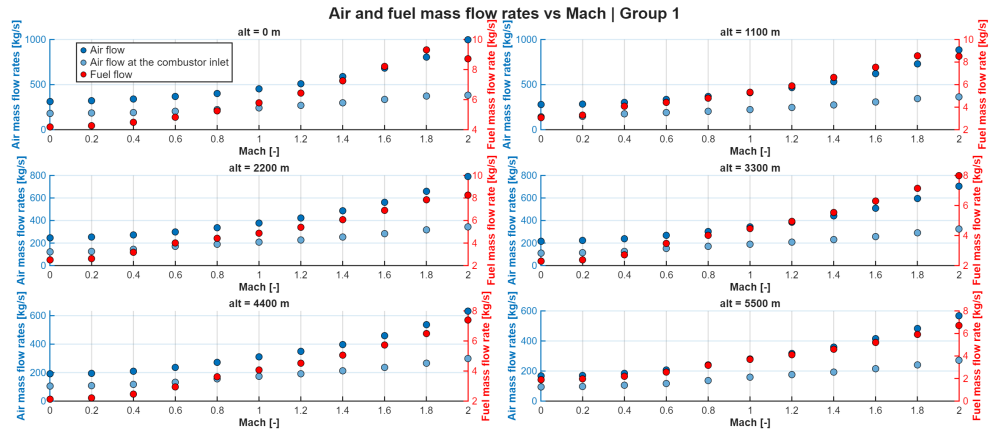


Figure A.1: Air and fuel mass flow rates vs Mach - Group 1.

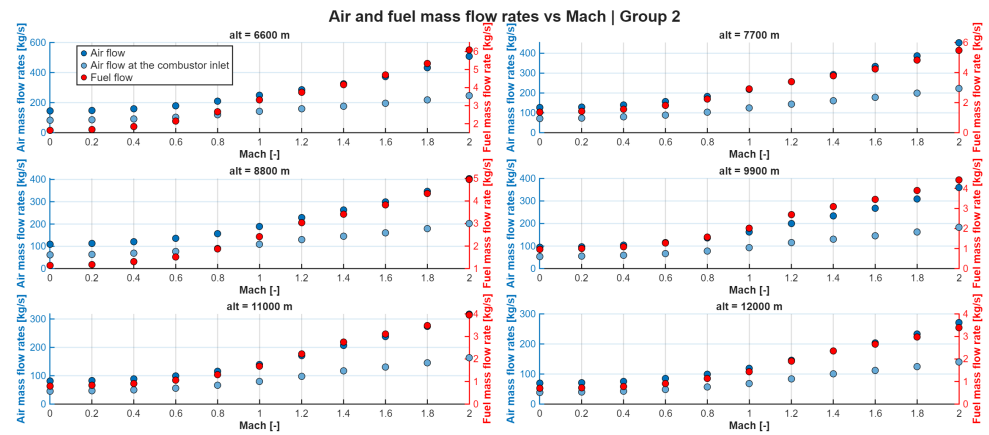


Figure A.2: Air and fuel mass flow rates vs Mach - Group 2.

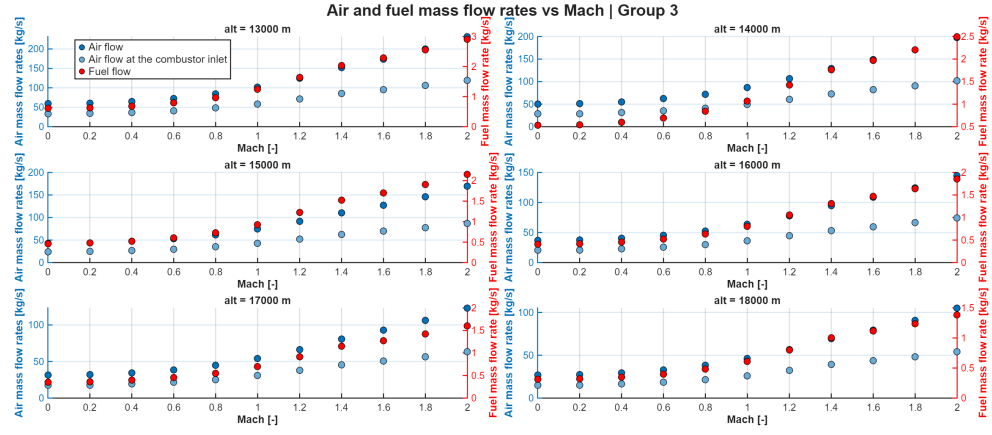


Figure A.3: Air and fuel mass flow rates vs Mach - Group 3.

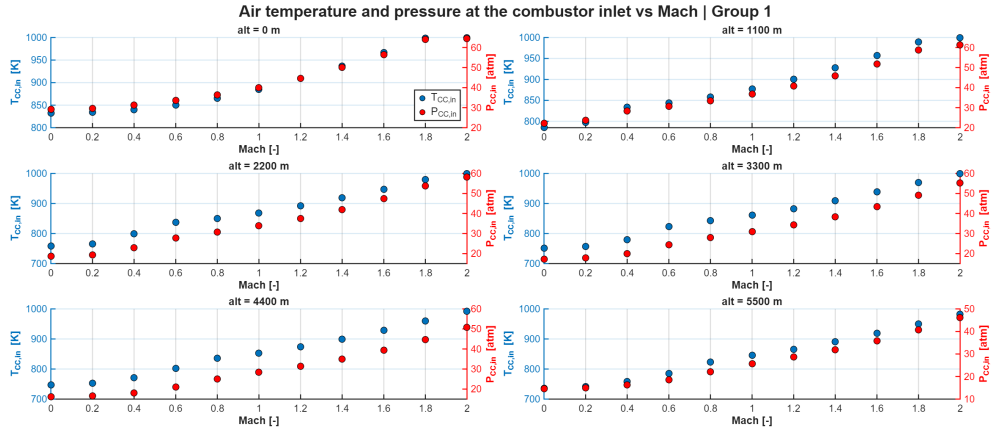


Figure A.4: Air temperature and pressure at the combustor inlet vs Mach - Group 1.

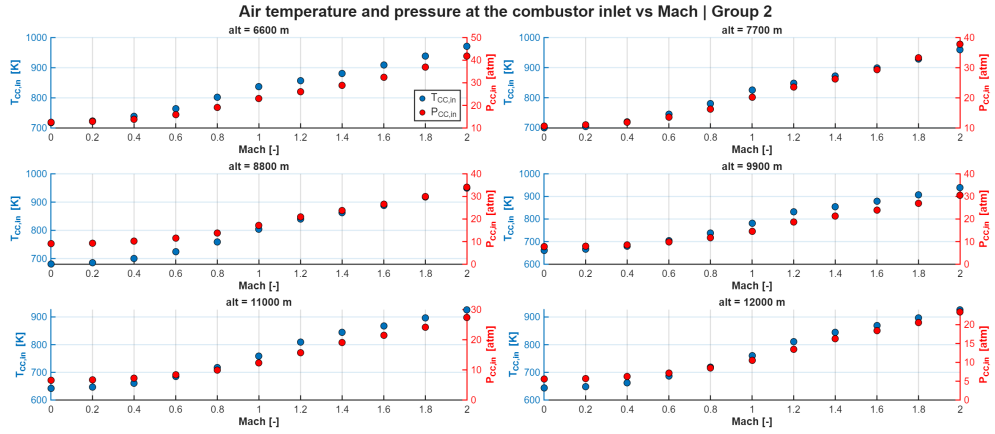


Figure A.5: Air temperature and pressure at the combustor inlet vs Mach - Group 2.

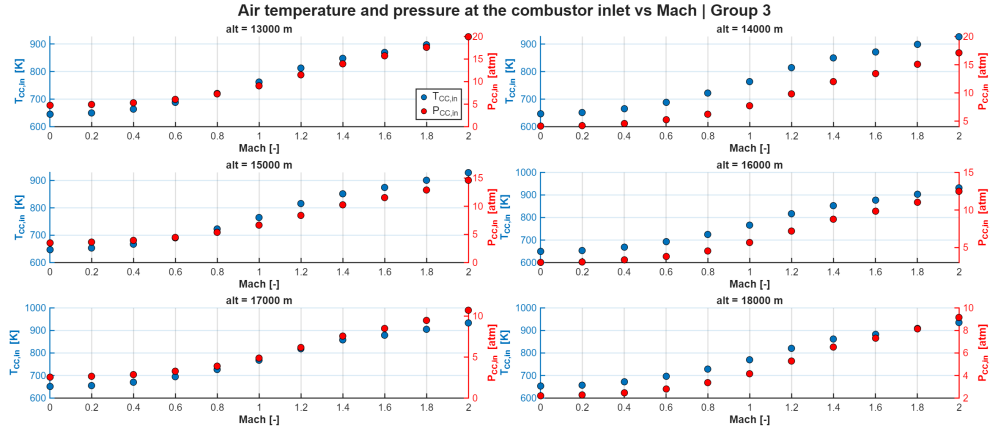


Figure A.6: Air temperature and pressure at the combustor inlet vs Mach - Group 3.

A.2 C1 surrogate results

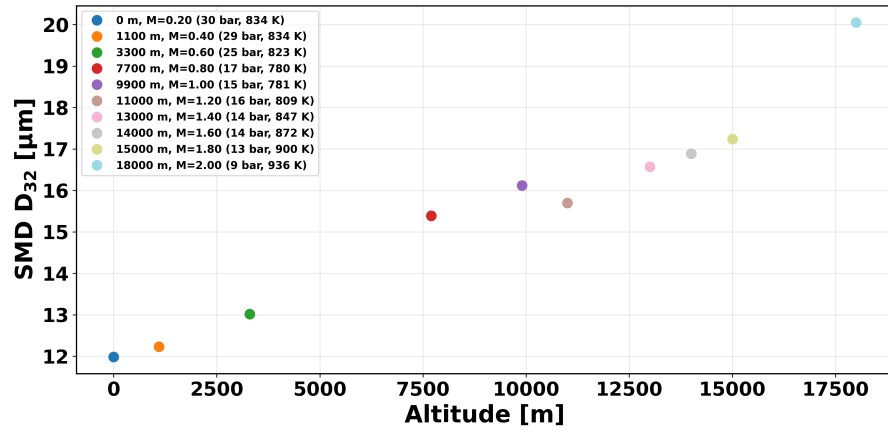


Figure A.7: SMD vs altitude, using C1 surrogate.

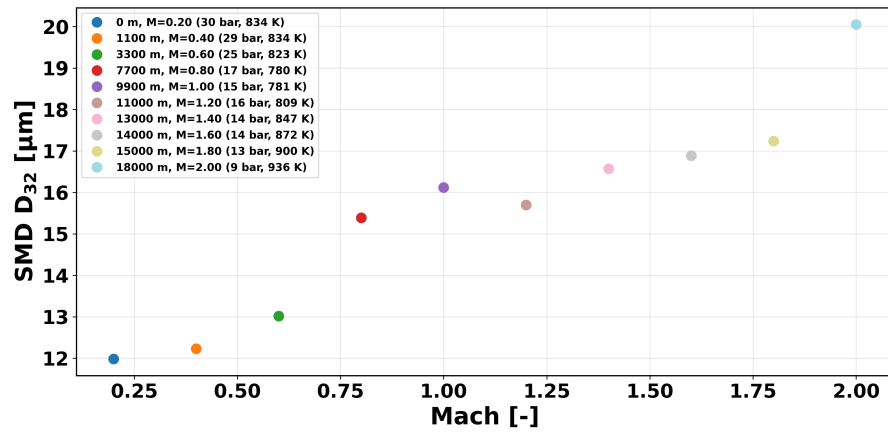


Figure A.8: SMD vs Mach number, using C1 surrogate.

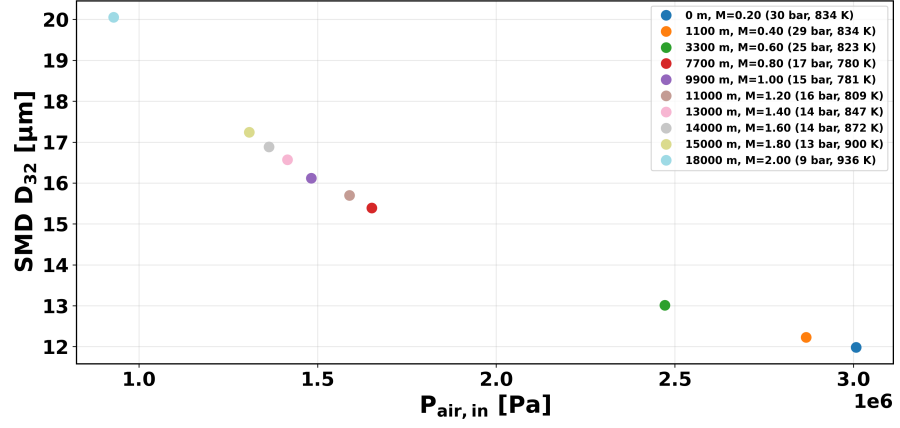


Figure A.9: SMD vs air pressure, using C1 surrogate.

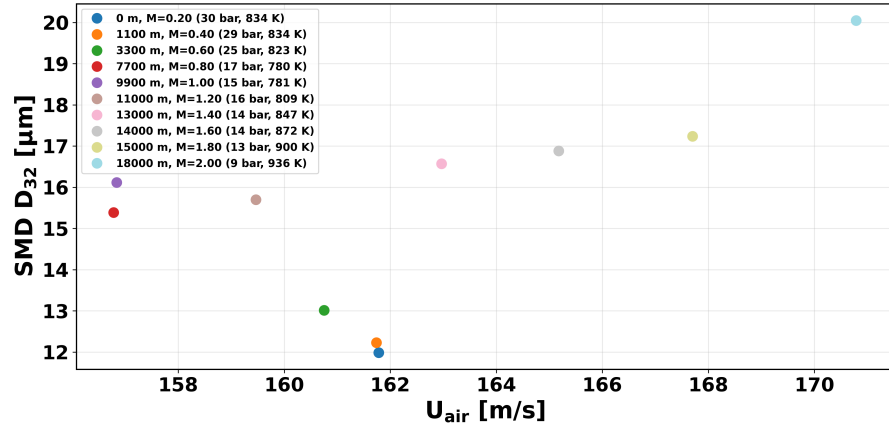


Figure A.10: SMD vs air velocity, using C1 surrogate.

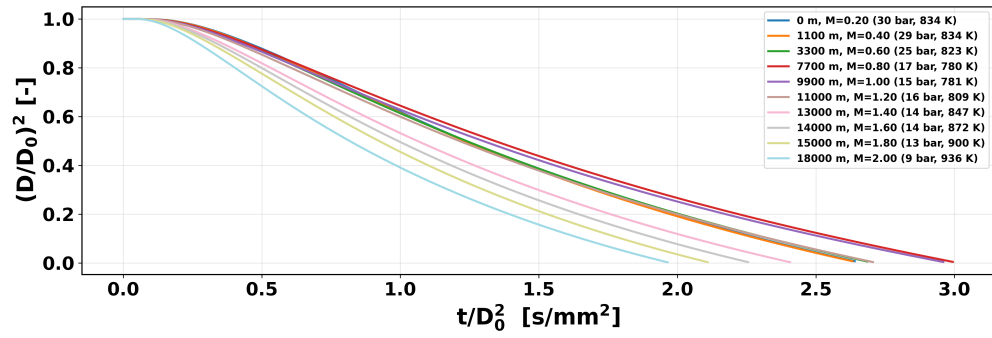


Figure A.11: D^2 -law, using the C1 surrogate.

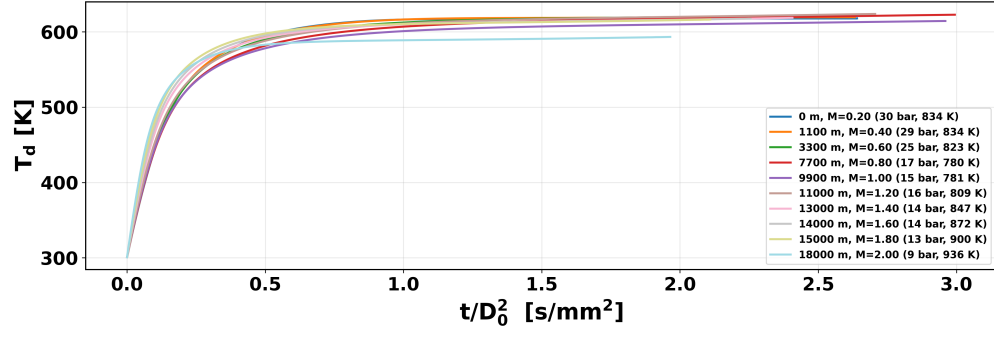


Figure A.12: Droplet temperature evolution, using the C1 surrogate.

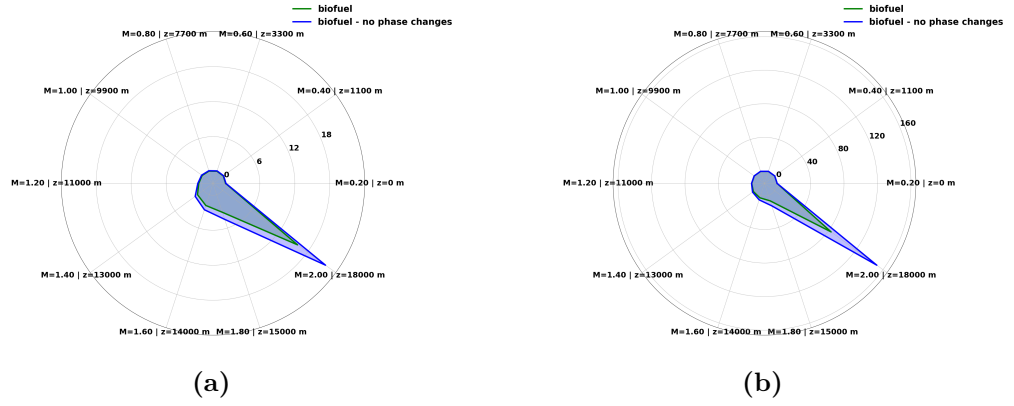


Figure A.13: Comparison of a) EICO and b) EINO_x, using the C1 surrogate.

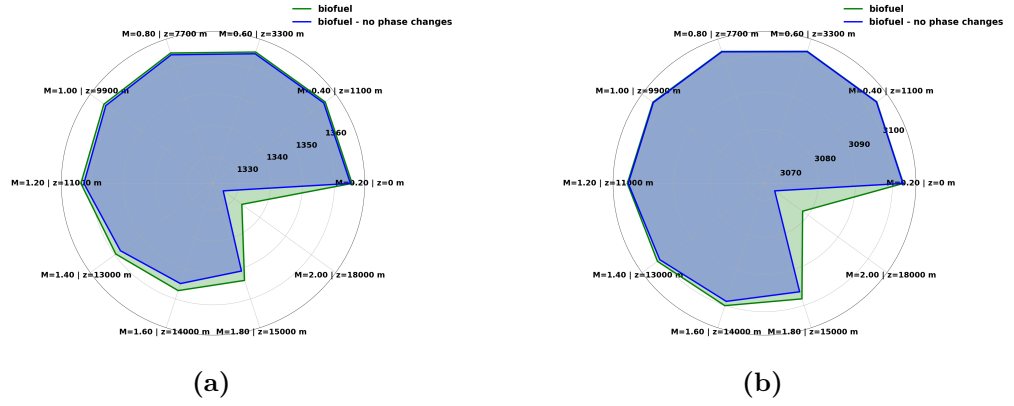


Figure A.14: Comparison of a) EI_{H₂O} and b) EICO₂, using the C1 surrogate.

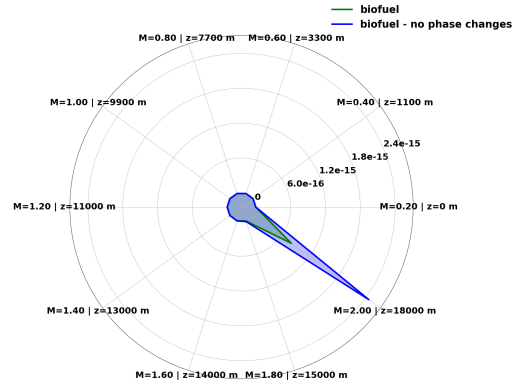


Figure A.15: Comparison of EIHC, using the C1 surrogate.

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