

Numerical simulation of bi-component fuel droplet evaporation using Level Set method

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Abstract

Fuel droplets consisting of multiple components are known to exhibit complex evaporation behavior. The Eulerian framework employed in Computational Fluid Dynamics (CFD) which treats the droplets as a continuum, is effective for simulating the complex evaporation behavior of such multicomponent droplets. In this study, the evaporation of binary-component or bi-component fuel droplets (which consist of two chemical species) in air, is simulated using the Eulerian framework with an extended evaporation model and its validity is examined. Spatio-temporal evolution of the gas-liquid interface is captured using the Level Set method, and a Ghost Fluid method is incorporated to consider the jump conditions at the interface. The computed evaporation speed of a fuel droplet consisting of a mixture of *n*-heptane and *n*-decane is compared with that of a previous experiment. Results show that *n*-heptane evaporates preferentially and the total evaporation speed is in an overall good agreement with that in the experiment. This confirms that the numerical framework used in the present simulation is capable of capturing the evaporation phenomenon of a bi-component fuel droplet. Additionally, several parametric simulations with different initial compositions (i.e., mass ratio of the constituent chemical species) of the bi-component fuel droplet and different initial ambient temperatures are performed, to investigate their influences on the evaporation character-

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istics of bi-component fuel droplet. The applicability of the proposed extended evaporation model and the numerical framework under these various simulation conditions are verified.

Keywords: Bi-component fuel droplet evaporation, Eulerian framework, Level Set method

1. Introduction

Petroleum fuels are widely consumed around the world due to their ease of storage and transportation, especially in the transportation sector, where the majority of energy consumption is derived from fossil fuels. In 2018 alone, the share of fossil fuels (crude oil, natural gas and coal) in the global energy consumption was about 81% [1]. Based on the energy consumption trends worldwide, it appears that the energy supplied by fossil fuels will continue to dominate the power generation and transport (including aerospace propulsion) sectors for the time being [1, 2]. However, the main problem with burning fossil fuels is the emission of greenhouse gases such as CO_2 . Fossil fuels account for 92% of the energy consumed by the transport sector [1], hence there is an increasing concern about their impact on the environment and climate change. Therefore, the use of liquid biofuels (e.g. bioethanol and biodiesel) as an alternative to fossil fuels such as gasoline, kerosene and diesel, is considered to be an excellent option due to their sustainability. Moreover, biofuels are renewable, since they are produced from biomass, and have zero net CO_2 emissions into the atmosphere when burned, in terms of carbon neutrality. Therefore, the use of biofuels has been expanding worldwide, as they can reduce the net CO_2 emissions by replacing fossil fuels [2]. In the transport sector in particular, the use of blends of fossil fuels and biofuels is being promoted, such as blends of gasoline and bioethanol, and blends of diesel oil and biodiesel. Application of such blended fuels is not limited to the transport sector, but they are being used for electricity generation and heating as well [1, 2]. However, it is known that such liquid fuels consisting of multiple components exhibit complex evaporation behavior and

25 have therefore been studied experimentally. For example, Daïf et al. [3] inves-
 26 tigated the evaporation behavior of two-component fuel droplets consisting of
 27 *n*-decane and *n*-heptane, in their experimental study. In those experiments [3],
 28 no aggressive behavior of the droplet occurred, and the diameter of this droplet
 29 which was suspended on one end of a glass capillary, was observed to reduce
 30 due to surface evaporation. Although experimental techniques have improved
 31 over the years, there are still limitations to the data that can be obtained from
 32 experiments.

33 In order to compensate for the limitations of experiments, numerical studies
 34 have been conducted. Numerical simulation is an effective approach to ana-
 35 lyze the mechanisms of these complex phenomena because it can provide more
 36 detailed data on all the relevant quantities compared with experiments. For
 37 example, Ebrahimi et al. [4] developed a new evaporation model for multi-
 38 component hydrocarbon droplets, by considering the Stefan flow caused by the
 39 density difference at the gas-liquid interface, and the heat flux between the gas
 40 and liquid phases due to the diffusion of chemical species. Also, Kitano et al.
 41 [5] performed numerical simulations of the evaporation of multicomponent fuel
 42 droplets comprising a mixture of *n*-dodecane, iso-octane, and toluene (used as
 43 a surrogate fuel for Jet-A), based on the non-equilibrium Langmuir-Knudsen
 44 evaporation model [6, 7]. Another approach to modelling heating and evap-
 45 oration of multicomponent droplets which takes into account the diffusion of
 46 species in the liquid phase (i.e., inside the droplet) and thermal diffusion, called
 47 the Discrete Component Model (DCM), has been developed [8, 9]. The DCM
 48 has been applied to simulations of biodiesel fuel droplet heating and evaporation
 49 [10, 11], but its applicability is limited to cases in which the number of compo-
 50 nents in the liquid mixture is small [9]. Therefore, to overcome the limitations
 51 of the DCM, an improved model for heating and evaporation of complex multi-
 52 component hydrocarbon fuel droplets, called the quasi-discrete model, has been
 53 proposed [9, 12] and applied to analyse diesel and gasoline fuel droplets' heating
 54 and evaporation [13]. Reviews of the aforementioned models and other models
 55 for multicomponent droplet evaporation that are not mentioned here can be

56 found in [9, 14]. Although these models [4, 5, 8, 9, 12] are widely used for spray
 57 simulations based on the conventional Eulerian-Lagrangian framework, wherein
 58 the gas phase is treated as an Eulerian continuum and the multicomponent
 59 droplets are treated as Lagrangian particles (i.e., spherical point-masses), they
 60 also have inherent assumptions/simplifications in their formulations. There-
 61 fore, these models may not be adequate for clarifying all the physical mecha-
 62 nisms involved in multicomponent droplet heating and evaporation over a range
 63 of conditions. So, it can be difficult to accurately capture the spatio-temporal
 64 variations of local temperature and species mass fractions inside the droplet, and
 65 these models also cannot capture the changes in the droplet's shape (since it is
 66 assumed to be a spherical point-mass). Hence, the Eulerian framework, wherein
 67 a droplet is treated as a continuum and fully resolved (i.e., discretized by the fine
 68 computational grid), is necessary for accurately capturing such local changes in
 69 the droplet's physical properties. Although this method has been widely used in
 70 numerical simulations of single-component droplets [15–18], studies employing
 71 the Eulerian framework in numerical simulations of multicomponent droplets
 72 are limited.

73 Haelssig et al. [19] proposed a model for calculating the evaporation rate of
 74 a liquid consisting of multiple components. They solved a series of equations
 75 assuming an equilibrium state at the gas-liquid interface, with both the physical
 76 quantities and the evaporation rate at the interface as unknowns. In addition,
 77 they used the Volume of Fluid (VOF) method to simulate the evaporation of a
 78 liquid composed of two components, treating both the liquid and gas phases as
 79 a continuum. Besides, the model was validated using the ethanol-water system
 80 for the evaporation of a smooth and stationary liquid. However, verification
 81 of the accuracy of the evaporation speed has not been sufficiently carried out.
 82 Later on, Strotos et al. [20] applied the VOF method to 2D-axisymmetric sim-
 83 ulations of bi-component droplet evaporation. However, in their simulations,
 84 the evaporation rate was evaluated using the same mathematical model as that
 85 in Schlottke and Weigand [21] based on the fuel vapor mass fraction gradient
 86 perpendicular to the gas-liquid interface, despite the limitation that this math-

87 ematical model is valid only for single-component droplet evaporation. In a
 88 more recent work, Soh et al. [22] applied the mass transfer model proposed by
 89 Haelssig et al. [19] (for computing the evaporation rate of liquid phase) to 2D
 90 micro-scale simulations. However, in their simulations, both the liquid phase
 91 and gas phase consist of the same two components (i.e., either *n*-pentane + CO₂
 92 or silicone oil + CO₂), and the gas phase does not comprise air, namely, the
 93 components N₂ and O₂. Similarly, in Haelssig et al.'s [19] study which focussed
 94 on mass transfer phenomenon under conditions relevant to vapour-liquid con-
 95 tacting devices, 2D simulations of binary vapour-liquid systems were performed.
 96 In these simulations, both the liquid and gas phases comprised the same two
 97 components/chemical species (ethanol and water), and air was not present in
 98 the gas phase.

99 The objective of our study is to analyze the evaporation phenomenon of a
 100 droplet consisting of binary components in air, by solving the gas and liquid
 101 phases as a continuum in an Eulerian framework. In this context, the mass
 102 transfer model proposed by Haelssig et al. [19] has been extended to two phase
 103 systems wherein the gas phase contains two more components/chemical species,
 104 viz. N₂ and O₂ (i.e., air), in addition to the vapours of the two components
 105 present in the liquid droplet that are formed during evaporation. The compu-
 106 tation procedure used for this mass transfer/evaporation model, can theoret-
 107 ically be applied to evaporating liquid-gas systems with any number of chemical
 108 species in both the liquid and gas phases. The aforementioned numerical studies
 109 based on the Eulerian framework for simulating the evaporation of bi-component
 110 liquid mixtures [19, 20, 22] exclusively use the Volume of Fluid (VOF) method.
 111 However, in this study, the Level Set method is used to capture the gas-liquid
 112 interface evolution, and a Ghost Fluid method is used to solve the governing
 113 equations across the interface. Particularly, the Ghost Fluid Semi-Conservative
 114 viscous Method (GFSCM) of Lalanne et al. [23, 24] is employed in the present
 115 simulations. The reason for choosing the coupled Level Set method and GF-
 116 SCM over the VOF method in this study, is that this framework offers some
 117 advantages over the VOF method such as:

- 118 1. The ability to accurately reconstruct the gas-liquid interface (i.e., sharp
119 interface representation) [15, 25], which enables accurate evaluation of the
120 interface normal and curvature.
- 121 2. Accurate computations of species mass fraction gradients perpendicular to
122 the interface are made possible by the accurate evaluation of the interface
123 normal. These are in turn essential for the accurate computations of the
124 evaporation rates of the liquid’s components.
- 125 3. Unlike the VOF method used in the aforementioned previous studies
126 [19, 20, 22], the Level Set method avoids the implementation of artificial
127 interface thickness when considering the physical properties near the
128 interface. In the VOF method, quantities that are discontinuous across
129 the gas-liquid interface, are smeared out within this artificial interface
130 thickness, which can worsen the resolution of the jump conditions at the
131 interface. But, with the GFSCM applied in this study, it is possible to ac-
132 curately discretize the discontinuous quantities across the interface, which
133 improves the resolution of the interfacial jump conditions [17].

134 To the best of the authors’ knowledge, this is the first study to implement
135 the coupled Level Set method and GFSCM along with the extended evapora-
136 tion model, in the context of bi-component droplet heating and evaporation.
137 Specifically, three-dimensional numerical analyses are performed for droplets
138 comprising a binary mixture of *n*-heptane and *n*-decane, and the calculation
139 accuracy is verified by comparing the evaporation speed with the experimental
140 result of Daïf et al. [3]. Furthermore, we perform parametric simulations to
141 investigate the influence of varying the initial mass/volume fraction ratio of the
142 droplet’s components and the initial ambient temperature on the evaporation
143 characteristics of bi-component droplet.

144 2. Numerical methods

145 2.1. Level Set method

In the present simulations, both the gas and liquid phases are treated as an Eulerian continuum and their interface is captured using the Level Set method [15, 26]. The Level Set method is often used in numerical simulations of gas-liquid two-phase flows, because it can accurately capture the gas-liquid interface and rigorously solve the velocity, temperature, and concentration fields near the droplet. The Level Set method defines a Level Set function ϕ , which is a function representing the distance from the gas-liquid interface. It is defined as $\phi = 0$ on the gas-liquid interface, $\phi > 0$ on the liquid side, $\phi < 0$ on the gas side, and its gradient is 1. Movement of the gas-liquid interface depends on the liquid phase velocity $\mathbf{u}_l$, as well as the regression speed of a droplet's surface due to evaporation, and can be captured using the following equation:

$$\frac{\partial \phi}{\partial t} + \left(\mathbf{u}_l + \frac{1}{\rho_l} \sum_k \dot{\omega}_k \mathbf{N} \right) \cdot \nabla \phi = 0 \quad (1)$$

Here, $\dot{\omega}_k$ is the evaporation rate of chemical species k . ρ is the density and the subscript l represents the liquid phase. $\mathbf{N}$ is the normal vector to the gas-liquid interface and is calculated using the equation below:

$$\mathbf{N} = \frac{\nabla \phi}{|\nabla \phi|} \quad (2)$$

146 2.2. Governing equations of gas and liquid phases

Governing equations used in the simulations, are the transport equations of mass, momentum, temperature and mass fraction of chemical species, for both the liquid and gas phases as shown below [27]:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \quad (3)$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla P + \nabla \cdot \boldsymbol{\tau} \quad (4)$$

$$\rho c_p \frac{\partial T}{\partial t} + \rho c_p \mathbf{u} \nabla T = \nabla \cdot (\lambda \nabla T) + \left(\rho \sum_k c_{p,k} D_k \nabla Y_k \right) \nabla T \quad (5)$$

$$\frac{\partial \rho Y_k}{\partial t} + \nabla \cdot (\rho Y_k \mathbf{u}) = \nabla \cdot (\rho D_k \nabla Y_k) \quad (6)$$

147 Here, $\mathbf{u}$ is the velocity vector, P is the pressure, $\boldsymbol{\tau}$ is the viscous stress tensor,
 148 T is the temperature, c_p is the specific heat capacity at constant pressure, λ is
 149 the thermal conductivity, and D_k and Y_k are the diffusion coefficient and mass
 150 fraction, respectively, of the k^{th} chemical species.

These governing equations are solved by considering the discontinuity of physical quantities at the gas-liquid interface. The discontinuity/jump conditions (which serve as boundary conditions at the interface) of pressure, velocity, temperature, and mass fraction, needed to account for the conservation of mass, momentum and energy across the gas-liquid interface, are expressed by the following equations [23, 28, 29]:

$$[P]_{\Gamma} = \sigma \kappa + \left[\mu \frac{\partial(\mathbf{u} \cdot \mathbf{N})}{\partial N} \right]_{\Gamma} - \sum_k \dot{\omega}_k^2 \left[\frac{1}{\rho} \right]_{\Gamma} \quad (7)$$

$$[\mathbf{u}]_{\Gamma} = \sum_k \dot{\omega}_k \left[\frac{1}{\rho} \right]_{\Gamma} \mathbf{N} \quad (8)$$

$$[T]_{\Gamma} = 0 \quad (9)$$

$$[\lambda \nabla T \cdot \mathbf{N}]_{\Gamma} = \sum_k L_k \dot{\omega}_k \quad (10)$$

$$[\rho D_k \nabla Y_k \cdot \mathbf{N}]_{\Gamma} = -[Y_k]_{\Gamma} \sum_k \dot{\omega}_k \quad (11)$$

where, $[]_{\Gamma}$ represents the difference between the value on the liquid side and the value on the gas side of the fuel droplet surface, and is defined as $[\alpha]_{\Gamma} = \alpha_l - \alpha_g$, for a physical quantity α . The subscript g represents the gas phase. μ is the

dynamic viscosity, σ is the surface tension, and κ is the curvature. κ of the gas-liquid interface is obtained from the following equation:

$$\kappa(\phi) = -\nabla \cdot \mathbf{N} \quad (12)$$

The latent heat of vaporization L can be calculated by solving the Watson's equation:

$$L = L_{B,atm} \left(\frac{T_c - T^\Gamma}{T_c - T_{B,atm}} \right)^{0.38} \quad (13)$$

151 where, $L_{B,atm}$ is the latent heat of vaporization at the normal boiling point
 152 temperature, $T_{B,atm}$ is the normal boiling point temperature, T_c is the critical
 153 temperature and T^Γ is the gas-liquid interface temperature. Here, the super-
 154 script Γ represents the gas-liquid interface.

155 In this study, the Ghost Fluid method [28, 30, 31] is used to discretize these
 156 discontinuous physical quantities across the interface when solving the governing
 157 equations (3)-(6). In the Ghost Fluid method, two-phase flows are considered
 158 as two types of single-phase flows and calculated separately by defining a virtual
 159 fluid across the interface for each phase, that takes into account the discontinu-
 160 ity/jump conditions at the interface, i.e., Eqs. (7)-(11). By using this method,
 161 spatial differentiation at the interface position becomes possible for the physical
 162 quantities that are discontinuous across the gas-liquid interface. In particular,
 163 simulations are performed in this study using the Ghost Fluid Semi-Conservative
 164 viscous Method (GFSCM) developed by Lalanne et al. [23, 24].

165 2.3. Thermophysical properties

First, we describe the calculation method of the thermophysical properties of the multicomponent gas phase. The thermodynamic properties and transport coefficients of the gas phase are computed as functions of temperature and species mass fractions as per CHEMKIN [32, 33]. The diffusion coefficient of each component/chemical species, $D_{g,k}$, is calculated using a two-component diffusion coefficient $D_{g,jk}$ for the j^{th} and k^{th} chemical species, with the following

Table 1: Thermophysical properties of *n*-heptane and *n*-decane

Thermophysical property	<i>n</i> -heptane	<i>n</i> -decane
Density (at $T = 290$ K) [kg/m ³]	686.46	732.78
Heat capacity (at $T = 290$ K) [J/gK]	2.2104	2.1628
Thermal conductivity (at $T = 290$ K) [W/m · K]	0.13335	0.13157
Viscosity (at $T = 290$ K) [μ Pa · s]	426.88	957.69
Surface tension (at $T = 290$ K) [N/m]	0.020890	0.024115
Boiling temperature [K]	371.53	447.27
Critical temperature [K]	540.1	617.7
Saturated vapor pressure [Pa]	4000.6	101.41

equation:

$$D_{g,k} = \frac{1 - Y_{g,k}}{\sum_{j \neq k} X_{g,j} / D_{g,jk}} \quad (14)$$

where, $X_{g,j}$ is the mole fraction of the j^{th} gaseous chemical species, and is calculated using the molar weight W_k of each gaseous chemical species from the following equation:

$$X_{g,j} = \frac{Y_{g,j} / W_j}{\sum_k Y_{g,k} / W_k} \quad (15)$$

166 Next, we describe the calculation method of the thermophysical properties
167 of the bi-component liquid phase. The thermodynamic properties and trans-
168 port coefficients of single-component liquid are obtained from the database of
169 NIST [34], taking temperature dependence into account. Typical thermophys-
170 ical property values of *n*-heptane and *n*-decane at $T = 290$ K are shown in
171 Table 1. The diffusion coefficient of the bi-component liquid is taken from the
172 experiments of Lo [35].

The specific heat capacity at constant pressure $c_{p,l}$ of a mixture solution is given by the following equation, using the specific heat at constant pressure $c_{p,l,k}$ of each constituent component [36]:

$$c_{p,l} = \sum_k Y_{l,k} c_{p,l,k} \quad (16)$$

The thermal conductivity λ_l of a liquid consisting of binary components is given

by the following equation using the thermal conductivity $\lambda_{l,k}$ of each component [36]:

$$\lambda_l = (\Psi_{l,1})^2 \lambda_{l,1} + 2\Psi_{l,1}\Psi_{l,2}\lambda_{l,12} + (\Psi_{l,2})^2 \lambda_{l,2} \quad (17)$$

Here, $\Psi_{l,k}$ is the k^{th} liquid component's volume fraction, and $\Psi_{l,k}$ and $\lambda_{l,12}$ are calculated from the following equations:

$$\Psi_{l,k} = \frac{Y_{l,k}/\rho_{l,k}}{\sum_j Y_{l,j}/\rho_{l,j}} = \frac{X_{l,k}V_{l,k}}{\sum_j X_{l,j}V_{l,j}} \quad (18)$$

$$V_{l,k} = \frac{W_k}{\rho_{l,k}} \quad (19)$$

$$\lambda_{l,12} = \frac{2}{1/\lambda_{l,1} + 1/\lambda_{l,2}} \quad (20)$$

173 where, $V_{l,k}$ is the k^{th} liquid component's molar volume.

In addition, the kinematic viscosity coefficient ν_l of a liquid consisting of binary components is calculated using the kinematic viscosity coefficient $\nu_{l,k}$ of each constituent component [36] as:

$$\nu_l = \Psi_{l,1}\nu_{l,1} \exp(\Psi_{l,2}\alpha_2) + \Psi_{l,2}\nu_{l,2} \exp(\Psi_{l,1}\alpha_1) \quad (21)$$

Here, $\nu_{l,1} < \nu_{l,2}$, and α_1 and α_2 are given by the following equations:

$$\alpha_1 = -1.7 \ln \frac{\nu_{l,2}}{\nu_{l,1}} \quad (22)$$

$$\alpha_2 = 0.27 \ln \frac{\nu_{l,2}}{\nu_{l,1}} + \left(1.3 \ln \frac{\nu_{l,2}}{\nu_{l,1}}\right)^{\frac{1}{2}} \quad (23)$$

174 Thus, governing equations (3) - (6) are solved using the thermophysical prop-
175 erties obtained from the above calculations in Eqs. (14) - (21).

In order to compute the evaporation rate, first, the jump condition for the mass fraction of each chemical species at the gas-liquid interface given by Eq. (11), is rewritten separately for the liquid and gas phases as follows [19]:

$$\dot{\omega}_k - \rho_l D_{l,k} \nabla Y_{l,k} \cdot \mathbf{N}|^\Gamma - Y_{l,k}^\Gamma \sum_k \dot{\omega}_k = 0 \quad (24)$$

$$\dot{\omega}_k - \rho_g D_{g,k} \nabla Y_{g,k} \cdot \mathbf{N}|^\Gamma - Y_{g,k}^\Gamma \sum_k \dot{\omega}_k = 0 \quad (25)$$

Assuming there are n chemical species in both the gas phase and the liquid phase, then, writing Eqs. (24) and (25) for each of the n chemical species will result in a system of total $2n$ equations. However, these $2n$ equations alone are not sufficient to calculate the evaporation rate $\dot{\omega}_k$. This is because the mass fractions $Y_{l,k}^\Gamma$ and $Y_{g,k}^\Gamma$ at the gas-liquid interface are also unknown. Then, assuming that the liquid phase is an ideal solution (i.e, the activity coefficient γ_k of the k^{th} chemical species in the liquid phase is assumed to be unity), and further assuming a vapor-liquid equilibrium state, the following Raoult's law is applicable:

$$p_k^\Gamma = P_{sat,k}^\Gamma X_{l,k}^\Gamma \quad (26)$$

where, p_k^Γ is the partial pressure of chemical species k in the gas phase at the gas-liquid interface. $P_{sat,k}^\Gamma$ is the saturation vapor pressure of chemical species k when it exists as a single substance, and it is given by Sato's equation below:

$$(P_{sat,k}^\Gamma)^{0.119} = 11.9 (T^\Gamma)^{0.119} + C \quad (27)$$

Here, C is a constant, and the unit of $P_{sat,k}^\Gamma$ is [mmHg]. Also, from Dalton's law, the following relationship is obtained:

$$p_k^\Gamma = P^\Gamma X_{g,k}^\Gamma \quad (28)$$

Using Eqs. (15), (26) and (28), the following relationship can be obtained:

$$P_{sat,k}^{\Gamma} \frac{Y_{l,k}^{\Gamma}/W_k}{\sum_j Y_{l,j}^{\Gamma}/W_j} = P^{\Gamma} \frac{Y_{g,k}^{\Gamma}/W_k}{\sum_j Y_{g,j}^{\Gamma}/W_j} \quad (29)$$

177 The evaporation rate ω_k and the mass fractions $Y_{l,k}^{\Gamma}$ and $Y_{g,k}^{\Gamma}$ at the gas-liquid
 178 interface, are calculated by solving the coupled nonlinear equations (24), (25),
 179 and (29) above, implicitly in conjunction. In the present simulations, the solu-
 180 tion to these coupled nonlinear equations is obtained from iterative calculation
 181 using Newton's method.

In this study, we simulate the evaporation of two-component droplets consisting of *n*-heptane and *n*-decane. As an initial condition, the gas phase surrounding the bi-component fuel droplet consists of nitrogen (N₂) and oxygen (O₂). The liquefaction of nitrogen and oxygen is not taken into account. In other words, in our simulations, there are two chemical species, viz. *n*-heptane and *n*-decane in the liquid phase, and four chemical species, viz. *n*-heptane, *n*-decane, nitrogen and oxygen in the gas phase. If these chemical species are numbered as: (1) *n*-heptane, (2) *n*-decane, (3) nitrogen and (4) oxygen, there will be eight unknowns, viz. $\omega_1, \omega_2, Y_{l,1}^{\Gamma}, Y_{l,2}^{\Gamma}, Y_{g,1}^{\Gamma}, Y_{g,2}^{\Gamma}, Y_{g,3}^{\Gamma}, Y_{g,4}^{\Gamma}$. Then, Eq. (24) can be written for *n*-heptane and *n*-decane in the liquid phase as follows:

$$\omega_1 - \rho_l D_{l,1} \nabla Y_{l,1} \cdot \mathbf{N}|^{\Gamma} - Y_{l,1}^{\Gamma} \sum_k \omega_k = 0 \quad (30)$$

$$\omega_2 - \rho_l D_{l,2} \nabla Y_{l,2} \cdot \mathbf{N}|^{\Gamma} - Y_{l,2}^{\Gamma} \sum_k \omega_k = 0 \quad (31)$$

Furthermore, Eq. (25) can be written for *n*-heptane, *n*-decane, N₂ and O₂ in the gas phase as follows:

$$\omega_1 - \rho_g D_{g,1} \nabla Y_{g,1} \cdot \mathbf{N}|^{\Gamma} - Y_{g,1}^{\Gamma} \sum_k \omega_k = 0 \quad (32)$$

$$\dot{\omega}_2 - \rho_g D_{g,2} \nabla Y_{g,2} \cdot \mathbf{N} |^\Gamma - Y_{g,2}^\Gamma \sum_k \dot{\omega}_k = 0 \quad (33)$$

$$-\rho_g D_{g,3} \nabla Y_{g,3} \cdot \mathbf{N} |^\Gamma - Y_{g,3}^\Gamma \sum_k \dot{\omega}_k = 0 \quad (34)$$

$$-\rho_g D_{g,4} \nabla Y_{g,4} \cdot \mathbf{N} |^\Gamma - Y_{g,4}^\Gamma \sum_k \dot{\omega}_k = 0 \quad (35)$$

Additionally, Eq. (29) can be written for *n*-heptane and *n*-decane (species no. 1 and 2, respectively) as follows:

$$P_{sat,1}^\Gamma \frac{Y_{l,1}^\Gamma/W_1}{\sum_j Y_{l,j}^\Gamma/W_j} = P^\Gamma \frac{Y_{g,1}^\Gamma/W_1}{\sum_j Y_{g,j}^\Gamma/W_j} \quad (36)$$

$$P_{sat,2}^\Gamma \frac{Y_{l,2}^\Gamma/W_2}{\sum_j Y_{l,j}^\Gamma/W_j} = P^\Gamma \frac{Y_{g,2}^\Gamma/W_2}{\sum_j Y_{g,j}^\Gamma/W_j} \quad (37)$$

The eight unknowns are obtained by solving these eight equations, i.e. Eqs. (30) - (37), implicitly. However, in practice, instead of solving Eqs. (31) and (35), the following Eqs. (38) and (39) can be solved, which state that the sum of mass fractions of chemical species is unity in both the gas phase and the liquid phase:

$$Y_{l,1}^\Gamma + Y_{l,2}^\Gamma = 1 \quad (38)$$

$$Y_{g,1}^\Gamma + Y_{g,2}^\Gamma + Y_{g,3}^\Gamma + Y_{g,4}^\Gamma = 1 \quad (39)$$

182 It is worth noting that there is a distinction between the formulation/methodology
 183 adopted for the evaporation model in this study and by Haelssig et al. [19].
 184 Specifically, for the implementation of the evaporation model in this study, 8
 185 coupled nonlinear equations, viz. Eqs. (30), (32), (33), (34), (36) - (39) are
 186 solved implicitly to compute the evaporation rates of the droplet's two compo-

nents (i.e., ω_1 and ω_2), and the mass fractions of the chemical species in both liquid and gas phases at the interface, i.e., $Y_{l,1}^\Gamma, Y_{l,2}^\Gamma, Y_{g,1}^\Gamma, Y_{g,2}^\Gamma, Y_{g,3}^\Gamma, Y_{g,4}^\Gamma$ (a total of 8 unknowns). However, in Haelssig et al.'s [19] formulation, a set of 7 coupled nonlinear equations are solved for the evaporation rates of the bi-component liquid mixture's components, mass fractions of the two chemical species (present in both gas and liquid phases) at the interface, and the interface temperature. In the present formulation of the extended evaporation model, the interface temperature is not solved for using the system of coupled nonlinear equations described above. Rather, it is evaluated from the interface jump conditions using the GFSCM as described in Section 2.2. For a two-phase system consisting of two components in the liquid phase and four components in the gas phase, the above procedure can be used to solve for $\omega_k, Y_{l,k}^\Gamma$ and $Y_{g,k}^\Gamma$. In this study, the same procedure is used for the simulation cases of single-component in the liquid phase and three components in the gas phase. For example, if the liquid droplet were to contain only *n*-heptane, then the surrounding gas phase would contain three components, viz. *n*-heptane vapour, N_2 and O_2 , and *n*-decane's mass fractions in the liquid and gas phases, and its evaporation rate are set to zero while solving the aforementioned system of equations. Thus, this general computation procedure can theoretically be used to simulate the evaporation of blended liquid fuels in gas, regardless of the number of constituent chemical species in both phases.

2.5. Computational configuration and conditions

In this study, 3D numerical simulations are performed for the evaporation phenomenon of bi-component (*n*-heptane + *n*-decane) and single-component (either pure *n*-heptane or pure *n*-decane) droplets. Table 2 shows a summary of all the simulation cases performed in this study. All the relevant details of each simulation case are described in this table and their nomenclature is explained in the following.

Table 2: Summary of initial conditions and computational details of all the simulations performed in this study.

Single-component droplet cases						
Simulated Cases	Droplet composition (Mass fraction ratio) <i>n</i> -heptane/ <i>n</i> -decane	Ambient temperature [K]	Droplet diameter d_0 [mm]	Minimum grid size [μm]	Grid points	Remarks
Case S-H	100% / 0%	294	1.386	60	$108 \times 108 \times 108$	Pure <i>n</i> -heptane evaporation
Case S-D	0% / 100%	297	1.520	60	$108 \times 108 \times 108$	Pure <i>n</i> -decane evaporation
Bi-component droplet cases						
Case B-150	48% / 52%	297	1.36	150	$72 \times 72 \times 72$	For grid dependency test
Case B-90	48% / 52%	297	1.36	90	$84 \times 84 \times 84$	For grid dependency test
Case B-60	48% / 52%	297	1.36	60	$108 \times 108 \times 108$	For grid dependency test
Case B-45	48% / 52%	297	1.36	45	$132 \times 132 \times 132$	For grid dependency test
Case BV-60a	74% / 26%	297	1.36	60	$108 \times 108 \times 108$	Parametric study: Initial composition varied
Case BV-60b	24% / 76%	297	1.36	60	$108 \times 108 \times 108$	Parametric study: Initial composition varied
Case BT-60a	48% / 52%	330	1.36	60	$108 \times 108 \times 108$	Parametric study: Initial ambient temperature varied
Case BT-60b	48% / 52%	360	1.36	60	$108 \times 108 \times 108$	Parametric study: Initial ambient temperature varied

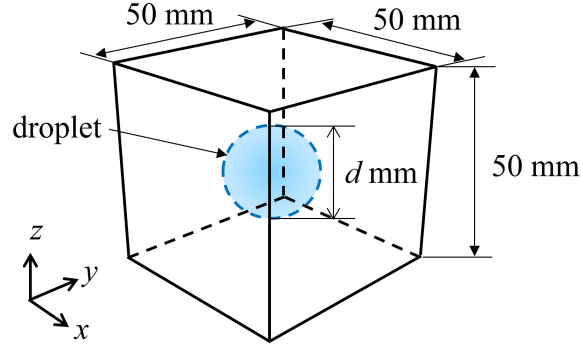


Figure 1: Schematic of the computational domain.

Initial conditions for the simulations of single-component droplet evaporation are shown in Table 3. Here, Case S-H is the designation for the simulation of evaporation of a pure *n*-heptane droplet (where S stands for single-component and H stands for heptane). The initial droplet diameter d_0 is 1.386 mm, the droplet temperature is 290 K, the ambient temperature is 294 K, and the ambient pressure is 0.1 MPa. These conditions are the same as those in Daïf et al.'s experiment [3]. Ambient gas is initially composed of 78% nitrogen and 22% oxygen by volume. The droplet is placed in the center of a 50 mm $\times$ 50 mm $\times$ 50 mm 3D domain as shown in Fig. 1. The computational grid is a non-uniform staggered Cartesian grid, consisting of 108 grid points in each direction. The minimum grid spacing in each direction is $\Delta x = \Delta y = \Delta z = 60 \mu\text{m}$, and the computational grid is positioned such that it is densest in the droplet region. The initial velocity is set to zero for both the liquid and gas phases. At the boundaries of the computational domain, Neumann condition is applied to velocity, and Dirichlet condition is applied to pressure, temperature and species mass fractions (density is computed from the ideal gas equation).

Similarly, the simulation of evaporation of a pure *n*-decane droplet is designated as Case S-D. The initial droplet diameter d_0 is 1.52 mm, and the ambient temperature is 297 K. Other conditions (such as ambient pressure, initial composition of ambient gas, initial droplet temperature, initial density ratio ρ_l/ρ_g

Table 3: Initial conditions for the single-component droplet simulations: Case S-H and Case S-D.

	Case S-H	Case S-D
Droplet components	<i>n</i> -heptane 100%	<i>n</i> -decane 100%
Droplet temperature [K]	290	290
Droplet diameter d_0 [mm]	1.386	1.520
Ambient gas composition [vol. %]	N ₂ /O ₂ = 78/22	N ₂ /O ₂ = 78/22
Ambient temperature [K]	294	297
Ambient pressure [MPa]	0.1	0.1
Field velocity [m/s]	0	0
Density ratio (ρ_l/ρ_g)	572.05	627.45
Dynamic viscosity ratio (μ_l/μ_g)	23.39	49.74

and initial dynamic viscosity ratio μ_l/μ_g) are listed in Table 3, and they match those in the experiment of Daïf et al. [3] for a pure *n*-decane droplet. Boundary conditions, computational domain and grid are the same as those used in Case S-H.

Table 4 shows the initial conditions for the simulations of the benchmark bi-component droplet’s evaporation. The initial ratio of the components in this bi-component droplet is 48% *n*-heptane to 52% *n*-decane by mass, or 50% *n*-heptane to 50% *n*-decane by volume. Initial droplet diameter d_0 is 1.36 mm, the ambient temperature is 297 K, the droplet temperature is 290 K, and the ambient pressure is 0.1 MPa. These conditions are once again, the same as those in Daïf et al.’s experiment [3]. In order to investigate the dependence of the simulation results on the grid resolution, 4 cases of the evaporation of the benchmark bi-component droplet are simulated, using different grids by changing the grid size and the number of grid points (but the domain size is the same as that in Fig. 1). The minimum grid size and the number of grid points in each of these grid dependency test cases are summarized in Table 5. The letter B in the designation of cases listed in Table 5 stands for bi-component, and the succeeding numbers such as 150, 90, etc. denote the minimum grid sizes used in the respective simulations. Other conditions are same as those listed in Table 4.

Additionally, two types of parametric simulations are performed in this

Table 4: Initial conditions for the benchmark bi-component droplet’s simulation cases.

Droplet components	<i>n</i> -heptane and <i>n</i> -decane
Droplet composition (mass fraction)	<i>n</i> -heptane/ <i>n</i> -decane = 48% / 52%
Droplet temperature [K]	290
Droplet diameter d_0 [mm]	1.36
Ambient gas composition [vol. %]	N ₂ /O ₂ = 78/22
Ambient temperature [K]	297
Ambient pressure [MPa]	0.1
Field velocity [m/s]	0
Density ratio (ρ_l/ρ_g)	604.84
Dynamic viscosity ratio (μ_l/μ_g)	31.64

Table 5: Minimum grid size and the number of grid points for the grid dependency test cases of the benchmark bi-component droplet: *n*-C₇H₁₆/*n*-C₁₀H₂₂ = 48% / 52% (by mass).

	Minimum grid size [μm]	Grid points
Case B-150	150	$72 \times 72 \times 72$
Case B-90	90	$84 \times 84 \times 84$
Case B-60	60	$108 \times 108 \times 108$
Case B-45	45	$132 \times 132 \times 132$

study. In the first type of parametric simulations, the influence of varying the initial composition of the bi-component droplet (i.e., the initial volume or mass fraction ratio of *n*-heptane to *n*-decane) on the evaporation phenomenon is considered. In addition to Case B-60 presented above (see Table 5), two more cases are simulated and their results are compared. Initial volume fraction and mass fraction ratios of *n*-heptane to *n*-decane in the droplet for each case are listed in Table 6. Here, the first letter B in the designation of Cases BV-60a and BV-60b, once again implies simulations of the evaporation of droplets composed of bi-components, and the letter V indicates that the initial volume fractions of the two components are varied, while keeping the initial droplet temperature and the initial ambient temperature same as those in Table 4. Other initial conditions are also the same as those shown in Table 4. Computational domain and boundary conditions are also the same as those in Case B-60. The computational grid is a non-uniform staggered Cartesian grid, consisting of 108 grid points each in the *x*-, *y*- and *z*-directions. The number 60 in the designation of Cases BV-60a and BV-60b bears the same meaning as that of Case B-60,

Table 6: Initial conditions of volume fraction, mass fraction, density ratio and viscosity ratio for each case in the first type of parametric simulations.

Simulation cases	Case B-60	Case BV-60a	Case BV-60b
Volume fraction (<i>n</i> -heptane/ <i>n</i> -decane)	50% / 50%	75% / 25%	25% / 75%
Mass fraction (<i>n</i> -heptane/ <i>n</i> -decane)	48% / 52%	74% / 26%	24% / 76%
Density ratio (ρ_l/ρ_g)	604.84	595.75	615.31
Dynamic viscosity ratio (μ_l/μ_g)	31.64	26.21	39.13

i.e., the minimum grid spacing is 60 μm in each direction. The computational grid is positioned such that it is densest in the droplet region. It will be shown later in section 3.2 that using a grid spacing smaller than 60 μm in the droplet region, does not offer any appreciable improvement in the results.

In the second type of parametric simulations, the bi-component droplet's evaporation is simulated by varying the initial ambient temperature, while keeping the initial composition of the droplet fixed, i.e., using the same initial volume or mass fraction ratio of *n*-heptane to *n*-decane as that in Case B-60. Therefore, two more cases are simulated in addition to Case B-60, which are designated as Case BT-60a and Case BT-60b and listed in Table 7. In the nomenclature of Cases BT-60a and BT-60b, the letter B and the number 60 bear the same meanings as those in Case B-60 explained above, and the letter T implies that the initial ambient temperature is varied among these simulations, while keeping the initial volume fraction ratio of the droplet's components fixed (i.e., 50% *n*-heptane and 50% *n*-decane). The initial ambient temperature in each case is shown in Table 7. Other initial conditions are the same as those in Case B-60 (summarized in Table 4). Boundary conditions, computational domain and grid used in Cases BT-60a and BT-60b are also the same as those used in Case B-60. Comparisons of the simulation results among these three cases (listed in Table 7) are performed, to understand the influence of initial ambient temperature on the evaporation of bi-component droplet.

Table 7: Initial conditions of ambient temperature, density ratio and viscosity ratio for each case in the second type of parametric simulations.

	Ambient temperature	Density ratio (ρ_l/ρ_g)	Dynamic viscosity ratio (μ_l/μ_g)
Case B-60	297 K	604.84	31.64
Case BT-60a	330 K	660.84	30.55
Case BT-60b	360 K	720.73	28.66

2.6. Numerical procedure

Numerical simulations employing the coupled Level Set method and Ghost Fluid Semi-Conservative viscous method (GFSCM) [23, 24], are performed using an in-house thermal flow analysis code named FK³ [37]. Second-order accurate finite difference scheme is used for the spatial discretization of each spatial derivative term in the governing equations. Implicit temporal discretization is employed for time integration of the transport equations of momentum, temperature and chemical species, while the gas phase density is evaluated with the ideal gas law. Methodology for solving the Poisson equation for pressure by considering jump conditions is described in [24, 38]. Among the cases simulated in this study, the maximum CPU time incurred is approximately 32,000 hours using 64 cores on a CRAY XC40 supercomputer at the Academic Center for Computing and Media Studies (ACCMS), Kyoto University (the wall clock time required for parallel computation of 300,000 time steps using 64 cores is approximately 500 hours).

3. Results and discussion

3.1. Validation of evaporation speed of single-component droplet

Prediction accuracies of the simulations for a pure *n*-heptane and a pure *n*-decane droplet evaporating in air, i.e., Case S-H and Case S-D, respectively, are verified first. Figure 2 shows comparisons of the time variations of the squared value of droplet diameter of pure *n*-heptane and pure *n*-decane obtained from the simulations of Case S-H and Case S-D, respectively, with the corresponding experiment data of Daïf et al. [3]. Here, the instantaneous droplet diameter d

has been normalized by the initial droplet diameter d_0 in both cases. Comparing the results for n -heptane droplet with those for n -decane droplet in Fig. 2, it is evident that the evaporation speed of n -heptane is greater than that of n -decane in both the experiment and the simulations. Here, evaporation speed is defined as the absolute value of the slope of the lines in the graph of Fig. 2, in the following manner:

$$K = \left| \frac{\partial (d/d_0)^2}{\partial t} \right| \quad (40)$$

where, K represents the evaporation speed. Faster evaporation speed of n -heptane implies that the volatility of n -heptane is higher than that of n -decane in the room temperature range. Also, both the experimental and simulation results show that the normalized square droplet diameter decreases linearly with time for both fuels, which means that their evaporation speeds are almost constant. This is a typical characteristic of the evaporation of single-component droplets, and is famously known as the D²-law. In addition, by comparing the result of each simulation case with the corresponding experimental result, it can be seen that the predicted evaporation speed of n -decane droplet in Case S-D although marginally slower than that in the experiment, is in good agreement

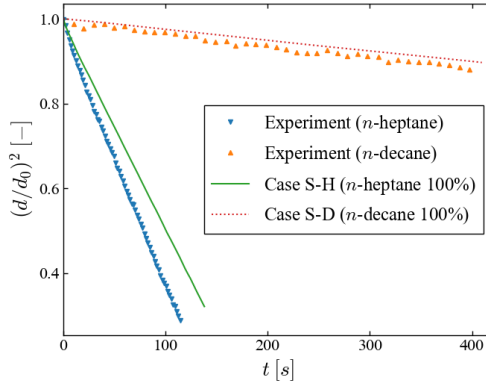


Figure 2: Comparisons of time variations of normalized squared droplet diameter of pure n -heptane in Case S-H and pure n -decane in Case S-D, with the corresponding experimental data [3].

320 with the measurement. However, the simulation result for evaporation speed
 321 of n -heptane droplet in Case S-H is visibly slower than that in the experiment.
 322 This discrepancy can be attributed to the fact that the simulation does not take
 323 into account the natural convection due to gravity, and the heat transfer between
 324 the n -heptane droplet and the glass capillary on which it was suspended in the
 325 experiment [3]. However, the effect of heat transfer between the glass capillary
 326 and the droplet is considered to be small due to the relatively low gas phase
 327 temperature. On the other hand, this simulation does not take gravity into
 328 account, which may cause the evaporated fuel vapor to stay around the droplet
 329 and thus reduce its evaporation speed. In particular, this effect will be more
 330 significant in Case S-H owing to the higher volatility of n -heptane, which would
 331 result in greater amount of fuel evaporation (compared to that of n -decane in
 332 Case S-D) and as a result, the deviation from experiment is larger for Case S-H.

333 Figure 3 presents the time variations of the evaporation speed K and evap-
 334 oration rate $\dot{\omega}$ for Case S-H and Case S-D. Here, evaporation rate $\dot{\omega}$ implies the
 335 mass of liquid fuel evaporating per unit of time and per unit of area, and is
 336 calculated using the procedure explained in section 2.4. This means that even
 337 if the evaporation speed is constant, the evaporation rate will not be constant.
 338 Figure 3 shows that in both cases, the evaporation speed and rate are large at
 339 the beginning of the simulation (i.e., at $t = 0$ s), and then decrease significantly.

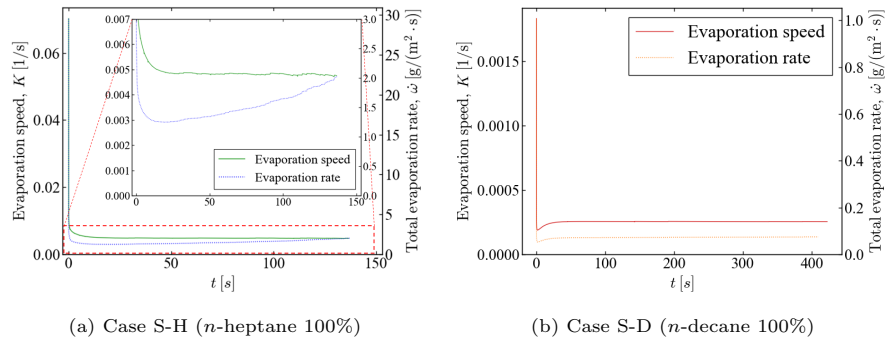


Figure 3: Time variations of evaporation speed K and total evaporation rate $\dot{\omega}$ for (a) Case S-H and (b) Case S-D.

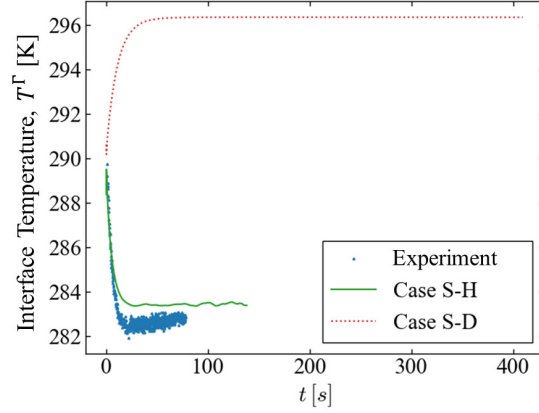


Figure 4: Time variations of temperature at the gas-liquid interface T^Γ for single-component droplet simulation cases (Case S-H and Case S-D), and experimental data for n -heptane droplet [3].

340 This is due to the fact that the simulations start with no fuel vapor in the gas
 341 phase, and therefore the liquid fuel tends to evaporate suddenly, resulting in
 342 large values of K and $\dot{\omega}$ at $t = 0$ s. Then, as the fuel evaporates into the sur-
 343 rounding gas phase, a quasi-steady state is reached and the evaporation speed
 344 becomes nearly constant.

345 Time variations of the temperature at the gas-liquid interface T^Γ for Case
 346 S-H and Case S-D are shown in Fig. 4. Temperature at the surface of an
 347 evaporating n -heptane droplet (i.e., gas-liquid interface temperature) measured
 348 in the experiment is also shown in this figure for comparison. The T^Γ values
 349 presented for Case S-H and Case S-D in Fig. 4, are averaged over the droplet
 350 surface (i.e., gas-liquid interface) at each time instance. This figure shows that
 351 in Case S-H, T^Γ decreases rapidly at the beginning of the simulation and then
 352 becomes approximately constant. The reduction in interface temperature is due
 353 to the loss of heat from the evaporation of n -heptane (i.e., latent heat transfer),
 354 and this characteristic is consistent with that observed in the experiment. Also,
 355 the gas-liquid interface temperature predicted in Case S-H is about 1 K higher
 356 than that in the experiment. This minor discrepancy can be attributed to the
 357 fact that the simulation of Case S-H under-predicts the evaporation speed (see

358 Fig. 2) and hence the amount of fuel evaporation. Consequently, the total
 359 amount of heat lost due to evaporation in the simulation will also be lower
 360 than that in the experiment. On the other hand, in Case S-D, the gas-liquid
 361 interface temperature T^Γ increases with time and eventually becomes constant.
 362 This is because the evaporation rate of *n*-decane in Case S-D is much smaller
 363 than that of *n*-heptane in Case S-H (see Fig. 3). Consequently, the amount of
 364 fuel evaporation, and hence the total amount of heat lost due to evaporation
 365 will also be smaller in Case S-D. Thus, T^Γ of the *n*-decane droplet in Case S-D
 366 initially rises due to the heat transfer from the surrounding ambient gas, whose
 367 temperature is higher than that of the droplet (initial ambient temperature =
 368 297 K). However, once the sensible heat transfer rate from the ambient gas to
 369 the droplet becomes equal to the heat loss rate due to evaporation (i.e., latent
 370 heat transfer rate), T^Γ becomes constant.

371 3.2. Validation of evaporation speed of bi-component droplet

372 Simulation results of the benchmark bi-component droplet evaporating in air
 373 (initial conditions listed in Table 4) are presented next. Figure 5 depicts the time
 374 variations of the mass fractions of *n*-heptane and *n*-decane in the central *x-y*
 375 plane in Case B-45 (for the meaning of this designation, refer Table 5 and section

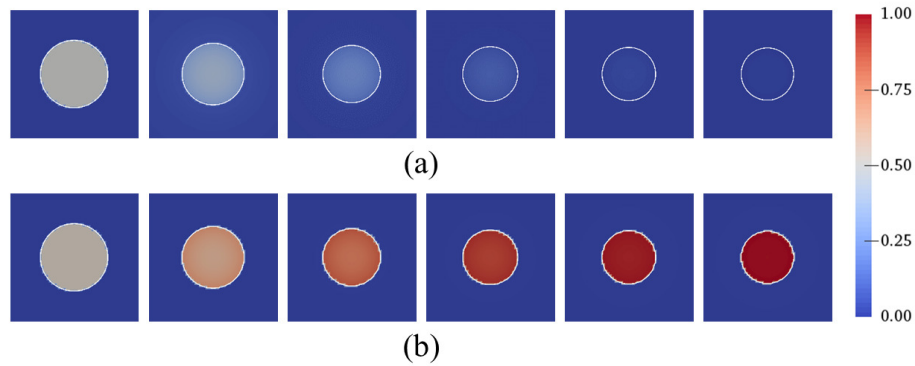


Figure 5: Time variations of mass fraction distributions of (a) *n*-heptane and (b) *n*-decane from left to right ($t=0$ s, 50 s, 100 s, 150 s, 200 s, 250 s) in Case B-45. The white iso-line represents the gas-liquid interface.

2.5). The white iso-line represents the iso-surface where the Level Set function ϕ is zero, i.e., the gas-liquid interface. It can be seen that the droplet diameter decreases with time due to fuel evaporation. As evident from Fig. 5(a), the mass fraction of *n*-heptane in the droplet decreases with time, while the mass fraction of *n*-decane increases with time, as observed in Fig. 5(b). These results show that *n*-heptane, which is more volatile, evaporates preferentially to *n*-decane, and a larger amount of *n*-decane remains in the droplet. The difference between the mass fractions of the two components becomes more apparent near the gas-liquid interface where evaporation occurs, and the mass fraction distribution inside the droplet changes due to the diffusion of chemical species.

To examine the dependence of simulation results of the benchmark bi-component droplet evaporation on the grid resolution, Fig. 6 shows a comparison of the time variations of the squared value of normalized droplet diameter, among the experiment [3] and the simulations of Case B-150, Case B-90, Case B-60 and Case B-45. These four cases serve as a grid dependency test. It can be seen that the evaporation speed decreases with time in all the four cases as well as the experiment. This is a characteristic of the evaporation phenomenon of

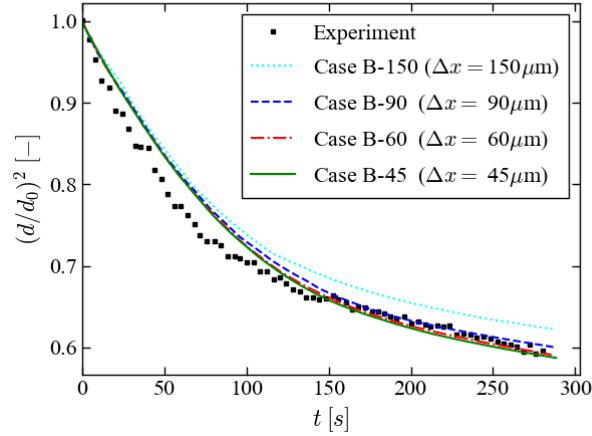


Figure 6: Comparison of time variations of normalized squared droplet diameter among experiment [3] and simulations of Case B-150, Case B-90, Case B-60 and Case B-45.

393 bi-component droplets, and the results of the simulations are in good qualita-
 394 tive agreement with the experimental data. However, the evaporation speed
 395 predicted by each simulation is slower than that in the experiment, especially
 396 in the early stages of evaporation, when the deviation from the experiment is
 397 clearly discernible for all the four cases. This is once again attributed to the
 398 fact that the simulations do not take into account the natural convection due to
 399 gravity, and the heat transfer between the bi-component droplet and the glass
 400 capillary on which it was suspended in the experiment, similar to the single-
 401 component droplet cases. Consequently, the simulations will underestimate the
 402 evaporation rate of *n*-heptane during the early stages of evaporation of the bi-
 403 component droplet, a trend that was also observed in the result of Case S-H
 404 (see Fig. 2).

405 Furthermore, comparing the results of the four simulation cases in Fig. 6, it
 406 can be seen that the smaller the minimum grid size is, the faster the evaporation
 407 speed and the better the agreement with experiment. To compare the prediction
 408 accuracies of Cases B-150, B-90, and B-60 with respect to Case B-45 (which
 409 has the finest grid), Table 8 shows the errors in the squared diameter values
 410 predicted in Cases B-150, B-90, and B-60 using the values in Case B-45 as the
 411 baseline, at various time instances. The table shows that the error in Case B-60
 412 is less than 1% throughout the duration of the simulation. On the other hand, in
 413 Case B-150, there is an error of more than 1% at $t = 50$ s, which grows with time.
 414 Similarly, the error in Case B-90 increases with time and exceeds 1% at $t = 150$
 415 s. Thus, it can be concluded that at least 10 grid points within the droplet
 416 diameter are required for accurate computation. Based on the above results
 417 and error analysis, the grid used in Case B-60 is employed in the parametric

Table 8: Errors in squared diameter values of Case B-150, Case B-90, and Case B-60 relative to the values of Case B-45, at various time instances.

	$t = 50$ s	$t = 100$ s	$t = 150$ s	$t = 200$ s	$t = 250$ s
Case B-150	1.1%	2.1 %	4.2 %	5.0 %	5.5 %
Case B-90	0.21%	0.82 %	1.4 %	1.5 %	2.0 %
Case B-60	0.05%	0.08 %	0.50 %	0.46 %	0.53 %

418 simulations discussed in section 3.3. Moreover, the parametric simulations are
 419 stopped when the number of grid points within the droplet diameter reaches 10,
 420 to ensure adequate simulation accuracy.

In the present simulations, the evaporating droplets are not subjected to any appreciable deformation, so regions of high curvature where numerical errors arise due to discretization of the transport equation of the Level Set function do not occur, and hence mass loss due to such numerical errors is expected to be negligible [15, 17, 24, 25]. Also, in a previous work of ours [18], the Level Set method and the Ghost Fluid method were used for simulating flame propagation in fuel droplet arrays, and the simulations were rigorously validated against experimental data, with the simulation results showing good agreement with measurements. Although only single-component droplets' evaporation was considered in these previous studies [15, 18, 24], the present study deals with the evaporation of bi-component droplets. So, in the formulation of the extended evaporation model proposed in Section 2.4, mass conservation across the gas-liquid interface is respected. To check the mass loss in the various simulation cases discussed thus far (including the single-component droplet simulations, i.e., Cases S-H and S-D), Fig. 7 shows the time variations of the total fuel mass

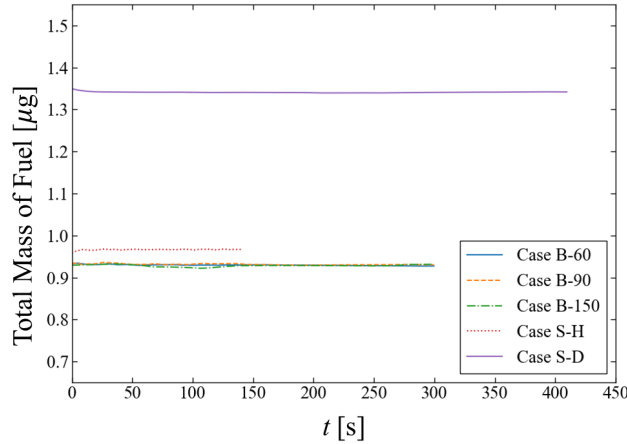


Figure 7: Time variations of the total fuel mass, i.e., sum of mass of n -heptane and mass of n -decane in both the liquid and gas phases, for the different simulation cases.

in these simulation cases. Here, total fuel mass implies summation of the masses of n -heptane and n -decane in both the liquid and gas phases. For the results shown in Fig. 7, the masses of n -heptane and n -decane that are converted into vapour form (i.e., gas phase), have been calculated using the time series data of their respective evaporation rates. Since the evaporation rates of n -heptane $\dot{\omega}_{heptane}(t)$ and n -decane $\dot{\omega}_{decane}(t)$ vary with time, the total fuel mass that has evaporated $M_{vap}(t)$ from the start of the simulation to any given time instance t_{ins} can be evaluated using the following equation:

$$M_{vap}(t_{ins}) = \sum_{t=0}^{t=t_{ins}} [\dot{\omega}_{heptane}(t) + \dot{\omega}_{decane}(t)] \times \pi[d(t)]^2 \times \Delta t \quad (41)$$

where $d(t)$ is the instantaneous droplet diameter and Δt is the time step value of the simulation. The fuel mass in gas phase obtained from the above equation is then added to the fuel mass remaining in the liquid phase to get the instantaneous total fuel mass, whose time variations in the different simulation cases are depicted in Fig. 7. As evident from Fig. 7, the total fuel mass remains virtually constant with time in all the cases, indicating that the mass loss is negligible in all these cases. Furthermore, numerical errors that manifest as mass loss may also arise in regions where the grid resolution is insufficient. But based on the grid convergence analysis presented above for the benchmark bi-component droplet's evaporation, all the simulations performed in this study were stopped when the droplet size in the respective cases reduced to a value such that 10 grid points were present within the droplet diameter. Hence, the existence of under-resolved regions (which are a source of numerical errors) is extremely unlikely in the present simulations.

Time variations of the evaporation rates of each component of the benchmark bi-component droplet, and the total evaporation rate in Case B-45 are also examined and these results are presented in Fig. 8. Here, $\dot{\omega}_{heptane}$ represents the evaporation rate of n -heptane, and $\dot{\omega}_{decane}$ represents the evaporation rate of n -decane. $\dot{\omega}_{sum}$ represents the total evaporation rate and is calculated from

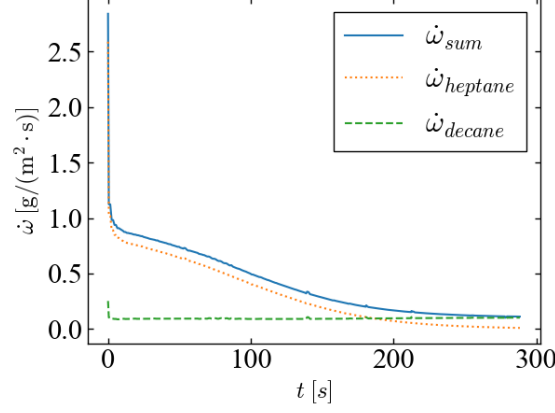


Figure 8: Time variations of total evaporation rate $\dot{\omega}_{sum}$, and evaporation rate of each component ($\dot{\omega}_{heptane}$ and $\dot{\omega}_{decane}$) of the benchmark bi-component droplet, in Case B-45.

the following equation:

$$\dot{\omega}_{sum} = \dot{\omega}_{heptane} + \dot{\omega}_{decane} \quad (42)$$

From Fig. 8, it is possible to quantitatively evaluate the instantaneous individual evaporation rates of n -heptane and n -decane. The figure shows that n -heptane evaporates preferentially up to $t = 180$ s, and n -decane evaporates preferentially after that. At $t=180$ s, the droplet diameter is about 80% of the initial value, and the droplet volume is about half of the initial value. Also, the evaporation rate of n -heptane decreases with time. This is due to the decrease in the quantity of n -heptane in the droplet with evaporation. On the other hand, the evaporation rate of n -decane is generally constant regardless of time. The mass fraction of n -decane in the droplet increases with evaporation, but since n -decane has low volatility, its evaporation rate is almost constant.

3.3. Effects of initial composition of bi-component droplet and initial ambient temperature

Parametric simulations for investigating the influences of initial composition of the bi-component droplet and the initial ambient temperature, on the

449 evaporation behaviour of bi-component droplets are analysed next. First, the
 450 effect of initial composition of the bi-component droplets on their evaporation
 451 characteristics is examined for Cases B-60, BV-60a and BV-60b (refer section
 452 2.5 for the meaning of the designations of these cases). In these three cases,
 453 the initial composition of the droplet is different (see Table 6), but the initial
 454 ambient temperature is fixed at 297 K. Comparison of the time variations of
 455 normalized squared droplet diameter among Case B-60, Case BV-60a, and Case
 456 BV-60b is presented in Fig. 9. It can be seen that the evaporation speed (i.e.,
 457 $K = |\partial(d/d_0)^2/\partial t|$) is higher for the case in which more *n*-heptane is initially
 458 present in the bi-component droplet. In all these three cases, the evaporation
 459 speed decreases with time and eventually approaches a constant value (i.e., the
 460 slope of each curve becomes constant towards the end). Also, the greater the
 461 initial *n*-heptane volume fraction in the droplet, the longer it takes for the evap-
 462 oration speed to become constant.

463 For further analysis, Fig. 10 depicts the time variations of the evaporation
 464 rate of each component (i.e., $\dot{\omega}_{heptane}$ and $\dot{\omega}_{decane}$) and the total evaporation
 465 rate $\dot{\omega}_{sum}$ in Case B-60, Case BV-60a, and Case BV-60b. It is observed that

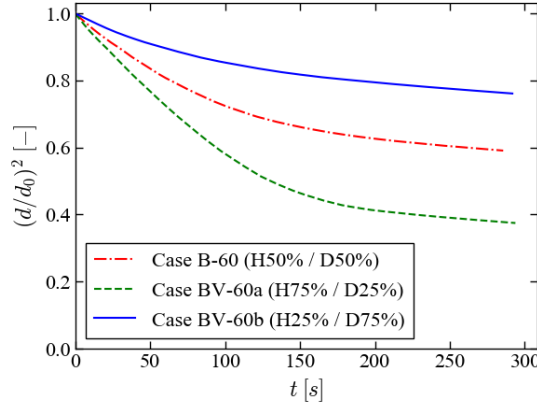
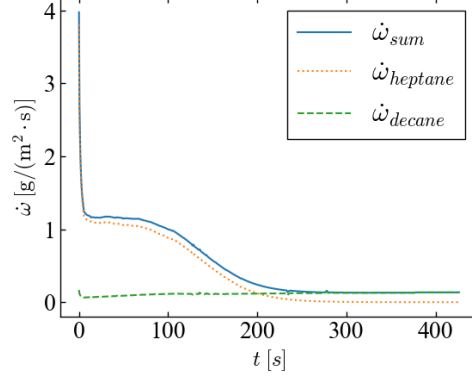
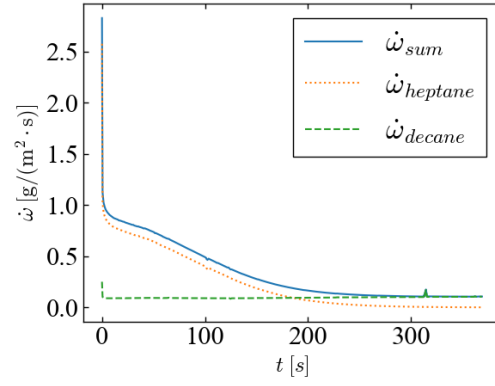


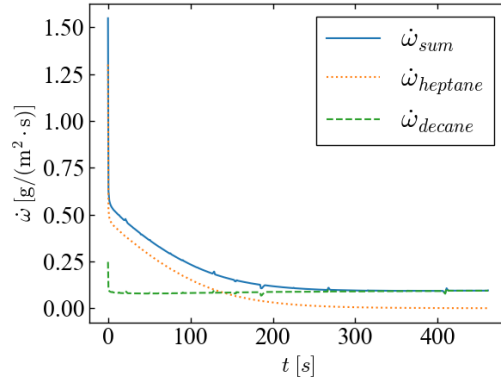
Figure 9: Time variations of normalized squared droplet diameter for Cases B-60, BV-60a and BV-60b. In the legend, H stands for *n*-heptane and D stands for *n*-decane, and the percentages denote the volume fractions of these two components in each simulation case.



(a) Case BV-60a (Initial volume fraction ratio: *n*-heptane 75% / *n*-decane 25%)



(b) Case B-60 (Initial volume fraction ratio: *n*-heptane 50% / *n*-decane 50%)



(c) Case BV-60b (Initial volume fraction ratio: *n*-heptane 25% / *n*-decane 75%)

Figure 10: Time variations of total evaporation rate and the individual evaporation rate of each component of the bi-component droplet in (a) Case BV-60a, (b) Case B-60 and (c) Case BV-60b.

466 the evaporation rate of *n*-heptane decreases with time in all three cases, while
 467 the evaporation rate of *n*-decane increases very gradually in each case, such
 468 that it appears to be virtually constant. However, the time it takes for the
 469 evaporation rate of *n*-decane to exceed that of *n*-heptane, i.e., the cross-over
 470 point between the curves of $\dot{\omega}_{heptane}$ and $\dot{\omega}_{decane}$ in the graphs of Fig. 10, is
 471 longer for the case in which the initial volume/mass fraction of *n*-heptane is
 472 higher. Furthermore, since the evaporation rate of *n*-heptane is greater than
 473 that of *n*-decane during the early stages of droplet evaporation in each case, the
 474 shape of the total evaporation rate curve looks similar to that of the $\dot{\omega}_{heptane}$
 475 curve. Thus, the results in Figs. 9 and 10 show that the numerical framework
 476 (i.e., methods described in sections 2.1, 2.2, 2.3 and 2.4) employed in this study,
 477 is capable of simulating the evaporation characteristics of a droplet composed of
 478 two components which is suspended in air, regardless of its initial composition
 479 (i.e., the initial volume or mass fraction ratio of the two components).

480 Next, the effect of initial ambient temperature on the evaporation behaviour
 481 of bi-component droplet is examined using the simulations of Case B-60, Case
 482 BT-60a and Case BT-60b. In these three cases, the initial composition of the
 483 bi-component droplet is fixed at 50% *n*-heptane and 50% *n*-decane by volume,

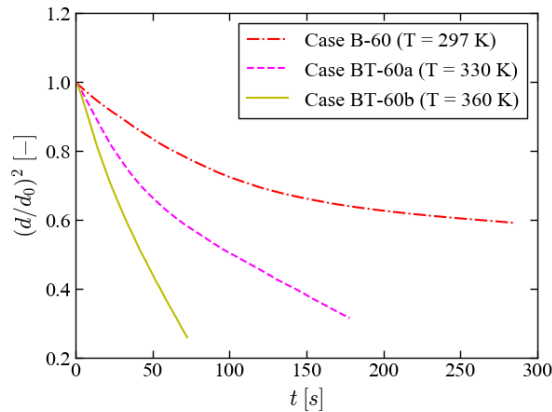
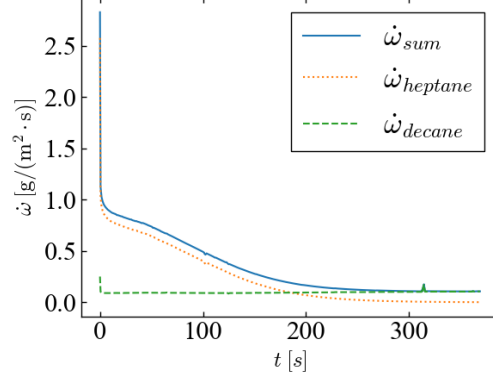
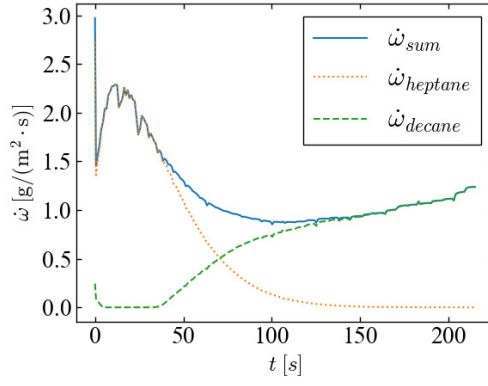


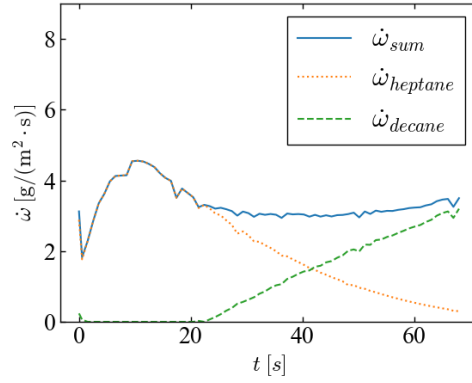
Figure 11: Time variations of normalized squared droplet diameter for Cases B-60, BT-60a and BT-60b.



(a) Case B-60 (Initial ambient temperature, $T = 297$ K)



(b) Case BT-60a (Initial ambient temperature, $T = 330$ K)



(c) Case BT-60b (Initial ambient temperature, $T = 360$ K)

Figure 12: Time variations of total evaporation rate and the individual evaporation rate of each component of the bi-component droplet in (a) Case B-60, (b) Case BT-60a and (c) Case BT-60b.

484 while the initial ambient temperature is different (refer Table 7 and section
 485 2.5 for the details of these three cases). Figure 11 shows a comparison of the
 486 time variations of the normalized squared droplet diameter among Case B-60,
 487 Case BT-60a, and Case BT-60b. As expected, the higher the initial ambient
 488 temperature, the higher the evaporation speed of the droplet. Once again, the
 489 evaporation speed decreases with time and eventually reaches a constant value
 490 in all these three cases. Hence, these simulations are also able to capture this
 491 typical characteristic of the evaporation phenomenon of bi-component droplets.

492 Additionally, Fig. 12 shows the time variations of the total evaporation rate
 493 and the individual evaporation rates of the droplet's components in Case B-
 494 60, Case BT-60a, and Case BT-60b. Consistent with the results in Fig. 11, the
 495 total evaporation rate $\dot{\omega}_{sum}$ is greater for the case with the higher initial ambient
 496 temperature, as evident from Fig. 12. In Case B-60, the total evaporation rate
 497 $\dot{\omega}_{sum}$ generally decreases monotonically as depicted in Fig. 12(a). However,
 498 from Fig. 12(b) and 12(c), it is evident that $\dot{\omega}_{sum}$ peaks once at $t \approx 15$ s and
 499 $t \approx 10$ s in Case BT-60a and Case BT-60b, respectively, before decreasing and
 500 then increasing again in these two cases. Such behaviour can be explained by
 501 investigating the evaporation rate of each component. In Fig. 12(b) and 12(c),

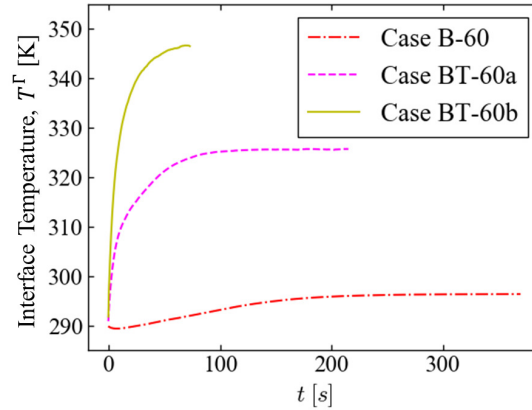


Figure 13: Time variations of temperature at the gas-liquid interface T^Γ of the bi-component droplet in Case B-60, Case BT-60a and Case BT-60b.

502 it is observed that the first peak of the total evaporation rate $\dot{\omega}_{sum}$ coincides
503 with the peak of the evaporation rate of n -heptane $\dot{\omega}_{heptane}$ in both Case BT-60a
504 and Case BT-60b. In Case B-60, it is found that $\dot{\omega}_{heptane}$ becomes smaller with
505 time as the amount of n -heptane in the droplet decreases with evaporation, and
506 $\dot{\omega}_{decane}$ which is much smaller than $\dot{\omega}_{heptane}$ in the beginning, remains virtually
507 constant in time. Therefore, $\dot{\omega}_{sum}$ also decreases with time in Case B-60.

508 However, in Case BT-60a and Case BT-60b, even though the amount of
509 n -heptane in the droplet decreases with evaporation, the total evaporation rate
510 first increases in these two cases, contrary to the behaviour of $\dot{\omega}_{sum}$ in Case B-
511 60. This increase in $\dot{\omega}_{sum}$ in Case BT-60a and Case BT-60b can be understood
512 by examining the temperature at the gas-liquid interface T^Γ of the droplet. For
513 this purpose, Fig. 13 shows the time variations of the gas-liquid interface tem-
514 perature T^Γ for Cases B-60, BT-60a and BT-60b. In Cases B-60, the interface
515 temperature T^Γ drops slightly at the beginning of the simulation due to the
516 latent heat of evaporation (since $\dot{\omega}_{sum}$ is large at $t = 0$ s, see Fig. 12(a)), then
517 increases gradually due to sensible heat transfer from the ambient gas and even-
518 tually levels off. But in Cases BT-60a and BT-60b, T^Γ rises rapidly from the
519 beginning of these simulations, because of the greater difference between the ini-
520 tial ambient temperature and the initial droplet temperature resulting in more
521 sensible heat transfer from the ambient gas to the droplet. As a consequence of
522 this rapid increase in T^Γ , the evaporation rate of n -heptane $\dot{\omega}_{heptane}$ increases
523 at the beginning of the simulations of Cases BT-60a and BT-60b. However,
524 $\dot{\omega}_{heptane}$ starts to decrease after reaching a peak value in these two cases as the
525 rate of increase of T^Γ (i.e., $\partial T^\Gamma / \partial t$) starts to slow down, which causes $\dot{\omega}_{sum}$ to
526 decrease as well.

527 But, it is evident from Fig. 12(b) and 12(c) that the total evaporation rate
528 $\dot{\omega}_{sum}$ starts to increase again, after $t \approx 100$ s in Case BT-60a and $t \approx 35$ s in
529 Case BT-60b. This is caused by the increase in the evaporation rate of n -decane
530 $\dot{\omega}_{decane}$ with time in these two cases. With the progress of evaporation of the
531 bi-component droplet, there is an increase in the mass fraction of n -decane in
532 the droplet arising from the preferential evaporation of n -heptane in the early

stages. This coupled with the rapid increase in T^{Γ} in Cases BT-60a and BT-60b (see Fig. 13), leads to a rise in $\dot{\omega}_{decane}$ and hence $\dot{\omega}_{sum}$ in these two cases. The higher the initial ambient temperature, the more pronounced the increase in the evaporation rate of n -decane.

4. Conclusions

The evaporation phenomenon of bi-component droplets in air was simulated by solving the liquid and gas phases as a continuum using an Eulerian framework. The Level Set method was employed for capturing the gas-liquid interface evolution, and coupled with the Ghost Fluid Semi-Conservative viscous Method (GFSCM) which allows for the computation of spatial derivatives of discontinuous quantities at the gas-liquid interface. Particularly, the evaporation model proposed by Haelssig et al. [19] has been extended to evaporating liquid-gas systems wherein the liquid phase comprises two components (n -heptane and n -decane), and the gas phase comprises four components or chemical species (viz. vapours of n -heptane and n -decane, N_2 and O_2). 3D numerical simulation of the evaporation of a benchmark bi-component droplet (made up of 48% n -heptane and 52% n -decane by mass) was validated against experimental data. It was confirmed that the simulation can capture the evaporation characteristics of this bi-component fuel droplet as observed in the experiment, such as the preferential evaporation of n -heptane during the early stages of droplet evaporation, and the gradual reduction in the droplet's evaporation speed with time. These characteristics were also observed in the parametric simulation cases used for investigating the effects of initial composition of the bi-component droplet and the initial ambient temperature on the bi-component droplets' evaporation behaviour. Results of the parametric simulations in which the initial composition of the bi-component droplet was changed, revealed that the larger the initial n -heptane concentration in the droplet, the greater the evaporation speed and the total evaporation rate, and the longer the time needed for the evaporation speed to become constant. Additionally, parametric simulations in which the

562 initial ambient temperature was varied, correctly predicted that the higher the
563 initial ambient temperature, the greater the evaporation speed and the total
564 evaporation rate of the bi-component droplet. Furthermore, in the two simula-
565 tion cases where the initial ambient temperature (330 K and 360 K) was much
566 higher than the initial droplet temperature (290 K), the total evaporation rate
567 first increased with time to reach a peak value and then decreased, following
568 which it started to increase again. Such a peculiar behaviour of the total evap-
569 oration rate in these two cases was attributed to the temporal behaviour of the
570 gas-liquid interface temperature, and to that of the individual evaporation rates
571 of the droplet’s components, i.e., *n*-heptane and *n*-decane. Thus, the numerical
572 framework demonstrated in this study is promising and will be applied to fur-
573 ther investigations of multicomponent evaporating liquid-gas problems in future
574 studies.

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