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 1. Introduction

Petroleum fuels are widely consumed around the world due to their ease of 2 storage and transportation, especially in the transportation sector, where the 3 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 10 the energy consumed by the transport sector [1], hence there is an increasing 11 concern about their impact on the environment and climate change. Therefore, 12 the use of liquid biofuels (e.g. bioethanol and biodiesel) as an alternative to 13 fossil fuels such as gasoline, kerosene and diesel, is considered to be an excellent 14 option due to their sustainability. Moreover, biofuels are renewable, since they 15 are produced from biomass, and have zero net CO_2 emissions into the atmo-16 sphere when burned, in terms of carbon neutrality. Therefore, the use of biofuels 17 has been expanding worldwide, as they can reduce the net CO_2 emissions by 18 replacing fossil fuels [2]. In the transport sector in particular, the use of blends 19 of fossil fuels and biofuels is being promoted, such as blends of gasoline and 20 bioethanol, and blends of diesel oil and biodiesel. Application of such blended 21 fuels is not limited to the transport sector, but they are being used for electricity 22 generation and heating as well [1, 2]. However, it is known that such liquid fuels 23 consisting of multiple components exhibit complex evaporation behavior and 24

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

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

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

Haelssig et al. [19] proposed a model for calculating the evaporation rate of 73 a liquid consisting of multiple components. They solved a series of equations 74 assuming an equilibrium state at the gas-liquid interface, with both the physical 75 quantities and the evaporation rate at the interface as unknowns. In addition, 76 they used the Volume of Fluid (VOF) method to simulate the evaporation of a 71 liquid composed of two components, treating both the liquid and gas phases as 78 a continuum. Besides, the model was validated using the ethanol-water system 79 for the evaporation of a smooth and stationary liquid. However, verification 80 of the accuracy of the evaporation speed has not been sufficiently carried out. 81 Later on, Strotos et al. [20] applied the VOF method to 2D-axisymmetric sim-82 ulations of bi-component droplet evaporation. However, in their simulations, 83 the evaporation rate was evaluated using the same mathematical model as that 84 in Schlottke and Weigand [21] based on the fuel vapor mass fraction gradient 85 perpendicular to the gas-liquid interface, despite the limitation that this math-86

ematical model is valid only for single-component droplet evaporation. In a 87 more recent work, Soh et al. [22] applied the mass transfer model proposed by 88 Haelssig et al. [19] (for computing the evaporation rate of liquid phase) to 2D 89 micro-scale simulations. However, in their simulations, both the liquid phase 90 and gas phase consist of the same two components (i.e., either n-pentane + CO_2 91 or silicone oil + CO₂), and the gas phase does not comprise air, namely, the 92 components N₂ and O₂. Similarly, in Haelssig et al.'s [19] study which focussed 93 on mass transfer phenomenon under conditions relevant to vapour-liquid con-94 tacting devices, 2D simulations of binary vapour-liquid systems were performed. 95 In these simulations, both the liquid and gas phases comprised the same two 96 components/chemical species (ethanol and water), and air was not present in 97 the gas phase. 98

The objective of our study is to analyze the evaporation phenomenon of a 99 droplet consisting of binary components in air, by solving the gas and liquid 100 phases as a continuum in an Eulerian framework. In this context, the mass 101 transfer model proposed by Haelssig et al. [19] has been extended to two phase 102 systems wherein the gas phase contains two more components/chemical species, 103 viz. N_2 and O_2 (i.e., air), in addition to the vapours of the two components 104 present in the liquid droplet that are formed during evaporation. The compu-105 tation procedure used for this mass transfer/evaporation model, can theoreti-106 cally be applied to evaporating liquid-gas systems with any number of chemical 107 species in both the liquid and gas phases. The aforementioned numerical studies 108 based on the Eulerian framework for simulating the evaporation of bi-component 109 liquid mixtures [19, 20, 22] exclusively use the Volume of Fluid (VOF) method. 110 However, in this study, the Level Set method is used to capture the gas-liquid 111 interface evolution, and a Ghost Fluid method is used to solve the governing 112 equations across the interface. Particularly, the Ghost Fluid Semi-Conservative 113 viscous Method (GFSCM) of Lalanne et al. [23, 24] is employed in the present 114 simulations. The reason for choosing the coupled Level Set method and GF-115 SCM over the VOF method in this study, is that this framework offers some 116 advantages over the VOF method such as: 117

 The ability to accurately reconstruct the gas-liquid interface (i.e., sharp interface representation) [15, 25], which enables accurate evaluation of the interface normal and curvature.

 Accurate computations of species mass fraction gradients perpendicular to the interface are made possible by the accurate evaluation of the interface normal. These are in turn essential for the accurate computations of the evaporation rates of the liquid's components.

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3. Unlike the VOF method used in the aforementioned previous studies 125 [19, 20, 22], the Level Set method avoids the implementation of artifi-126 cial interface thickness when considering the physical properties near the 127 interface. In the VOF method, quantities that are discontinuous across 128 the gas-liquid interface, are smeared out within this artificial interface 129 thickness, which can worsen the resolution of the jump conditions at the 130 interface. But, with the GFSCM applied in this study, it is possible to ac-131 curately discretize the discontinuous quantities across the interface, which 132 improves the resolution of the interfacial jump conditions [17]. 133

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

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 gasliquid 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 u_l , as well as the regression speed of a droplet's surface due to evaporation, and can be captured using the following equation:

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

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

$$\boldsymbol{N} = \frac{\nabla\phi}{|\nabla\phi|} \tag{2}$$

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]:

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

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

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

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

Here, \boldsymbol{u} is the velocity vector, P is the pressure, $\boldsymbol{\tau}$ is the viscous stress tensor, T is the temperature, c_p is the specific heat capacity at constant pressure, λ is the thermal conductivity, and D_k and Y_k are the diffusion coefficient and mass 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]:

$$[P]_{\Gamma} = \sigma \kappa + \left[\mu \frac{\partial (\boldsymbol{u} \cdot \boldsymbol{N})}{\partial N} \right]_{\Gamma} - \sum_{k} \dot{\omega_{k}}^{2} \left[\frac{1}{\rho} \right]_{\Gamma}$$
(7)

$$[\boldsymbol{u}]_{\Gamma} = \sum_{k} \dot{\omega}_{k} \left[\frac{1}{\rho}\right]_{\Gamma} \boldsymbol{N}$$
(8)

$$[T]_{\Gamma} = 0 \tag{9}$$

$$[\lambda \nabla T \cdot \boldsymbol{N}]_{\Gamma} = \sum_{k} L_k \dot{\omega_k} \tag{10}$$

$$[\rho D_k \nabla Y_k \cdot \boldsymbol{N}]_{\Gamma} = -[Y_k]_{\Gamma} \sum_k \dot{\omega_k}$$
(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:

$$\kappa\left(\phi\right) = -\nabla \cdot \boldsymbol{N} \tag{12}$$

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

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

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

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

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 $T = 290 \text{ K}$) [W/m · K]	0.13335	0.13157
Viscosity (at $T = 290$ K) $[\mu Pa \cdot s]$	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:

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

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

Next, we describe the calculation method of the thermophysical properties of the bi-component liquid phase. The thermodynamic properties and transport coefficients of single-component liquid are obtained from the database of NIST [34], taking temperature dependence into account. Typical thermophysical property values of *n*-heptane and *n*-decane at T = 290 K are shown in Table 1. The diffusion coefficient of the bi-component liquid is taken from the 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]:

$$c_{p,l} = \sum_{k} Y_{l,k} c_{p,l,k} \tag{16}$$

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]:

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

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

$$V_{l,k} = \frac{W_k}{\rho_{l,k}} \tag{19}$$

$$\lambda_{l,12} = \frac{2}{1/\lambda_{l,1} + 1/\lambda_{l,2}} \tag{20}$$

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:

$$\nu_{l} = \Psi_{l,1}\nu_{l,1}\exp(\Psi_{l,2}\alpha_{2}) + \Psi_{l,2}\nu_{l,2}\exp(\Psi_{l,1}\alpha_{1})$$
(21)

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

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

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

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

176 2.4. Evaporation rate

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]:

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

$$\dot{\omega_k} - \rho_g D_{g,k} \nabla Y_{g,k} \cdot \mathbf{N} |^{\Gamma} - Y_{g,k}^{\Gamma} \sum_k \dot{\omega_k} = 0$$
(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 2*n* equations. However, these 2*n* 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:

$$p_k^{\Gamma} = P_{sat,k}^{\Gamma} X_{l,k}^{\Gamma} \tag{26}$$

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:

$$\left(P_{sat,k}^{\Gamma}\right)^{0.119} = 11.9 \left(T^{\Gamma}\right)^{0.119} + C$$
 (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:

$$p_k^{\Gamma} = P^{\Gamma} X_{g,k}^{\Gamma} \tag{28}$$

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

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

The evaporation rate $\dot{\omega}_k$ and the mass fractions $Y_{l,k}^{\Gamma}$ and $Y_{g,k}^{\Gamma}$ at the gas-liquid interface, are calculated by solving the coupled nonlinear equations (24), (25), and (29) above, implicitly in conjunction. In the present simulations, the solution to these coupled nonlinear equations is obtained from iterative calculation 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. $\dot{\omega_1}, \dot{\omega_2}, Y_{l,1}^{\Gamma}, Y_{l,2}^{\Gamma}, Y_{g,1}^{\Gamma}, Y_{g,3}^{\Gamma}, Y_{g,4}^{\Gamma}$. Then, Eq. (24) can be written for *n*-heptane and *n*-decane in the liquid phase as follows:

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

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

Furthermore, Eq. (25) can be written for *n*-heptane, *n*-decane, N_2 and O_2 in the gas phase as follows:

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

$$\dot{\omega_2} - \rho_g D_{g,2} \nabla Y_{g,2} \cdot \boldsymbol{N}|^{\Gamma} - Y_{g,2}^{\Gamma} \sum_k \dot{\omega_k} = 0$$
(33)

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

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

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

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

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

$$Y_{l,1}^{\Gamma} + Y_{l,2}^{\Gamma} = 1 \tag{38}$$

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

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

nents (i.e., $\dot{\omega_1}$ and $\dot{\omega_2}$), and the mass fractions of the chemical species in both 187 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 188 of 8 unknowns). However, in Haelssig et al.'s [19] formulation, a set of 7 coupled 189 nonlinear equations are solved for the evaporation rates of the bi-component liq-190 uid mixture's components, mass fractions of the two chemical species (present 191 in both gas and liquid phases) at the interface, and the interface temperature. 192 In the present formulation of the extended evaporation model, the interface 193 temperature is not solved for using the system of coupled nonlinear equations 194 described above. Rather, it is evaluated from the interface jump conditions us-195 ing the GFSCM as described in Section 2.2. For a two-phase system consisting 196 of two components in the liquid phase and four components in the gas phase, 197 the above procedure can be used to solve for $\dot{\omega}_k$, $Y_{l,k}^{\Gamma}$ and $Y_{q,k}^{\Gamma}$. In this study, 198 the same procedure is used for the simulation cases of single-component in the 199 liquid phase and three components in the gas phase. For example, if the liquid 200 droplet were to contain only *n*-heptane, then the surrounding gas phase would 201 contain three components, viz. n-heptane vapour, N₂ and O₂, and n-decane's 202 mass fractions in the liquid and gas phases, and its evaporation rate are set to 203 zero while solving the aforementioned system of equations. Thus, this general 204 computation procedure can theoretically be used to simulate the evaporation 205 of blended liquid fuels in gas, regardless of the number of constituent chemical 206 species in both phases. 207

208 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.

		${ m Remarks}$		Pure n -heptane evaporation	Pure n -decane evaporation		For grid dependency test	Parametric study: Initial composition varied	Parametric study: Initial composition varied	Parametric study: Initial ambient temperature varied	Parametric study: Initial ambient temperature varied				
			Grid points		$108\times108\times108$	$108\times108\times108$		72 imes 72 imes 72	$84 \times 84 \times 84$	$108\times108\times108$	$132\times132\times132$	$108\times108\times108$	$108\times108\times108$	$108\times108\times108$	$108\times108\times108$
	lroplet cases	$\begin{array}{c} \text{Minimum} \\ \text{grid size} \\ [\mu m] \end{array}$		60	60	pplet cases	150	06	60	45	60	60	60	60	
Single-component d	component c	Droplet	diameter	$d_0 \; [\mathrm{mm}]$	1.386	1.520	mponent dre	1.36	1.36	1.36	1.36	1.36	1.36	1.36	1.36
	Ambient	temperature	[K]	294	297	Bi-co	297	297	297	297	297	297	330	360	
		Droplet composition	(Mass fraction ratio)	n-heptane/ n -decane	$100\%\;/\;0\%$	$0\% \ / \ 100\%$		$48\%\ /\ 52\%$	$48\%\ /\ 52\%$	$48\%\ /\ 52\%$	$48\%\ /\ 52\%$	$74\% \ / \ 26\%$	$24\% \ / \ 76\%$	$48\% \ / \ 52\%$	$48\% \ / \ 52\%$
			Simulated Cases		Case S-H	Case S-D		Case B-150	Case B-90	Case B-60	Case B-45	Case BV-60a	Case BV-60b	Case BT-60a	Case BT-60b

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

т



Figure 1: Schematic of the computational domain.

Initial conditions for the simulations of single-component droplet evapora-215 tion are shown in Table 3. Here, Case S-H is the designation for the simulation 216 of evaporation of a pure *n*-heptane droplet (where S stands for single-component 217 and H stands for heptane). The initial droplet diameter d_0 is 1.386 mm, the 218 droplet temperature is 290 K, the ambient temperature is 294 K, and the ambi-219 ent pressure is 0.1 MPa. These conditions are the same as those in Daïf et al.'s 220 experiment [3]. Ambient gas is initially composed of 78% nitrogen and 22% oxy-221 gen by volume. The droplet is placed in the center of a 50 mm \times 50 mm \times 50 mm 222 3D domain as shown in Fig. 1. The computational grid is a non-uniform stag-223 gered Cartesian grid, consisting of 108 grid points in each direction. The min-224 imum grid spacing in each direction is $\Delta x = \Delta y = \Delta z = 60 \ \mu m$, and the 225 computational grid is positioned such that it is densest in the droplet region. 226 The initial velocity is set to zero for both the liquid and gas phases. At the 227 boundaries of the computational domain, Neumann condition is applied to ve-228 locity, and Dirichlet condition is applied to pressure, temperature and species 229 mass fractions (density is computed from the ideal gas equation). 230

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

	Case S-H	Case S-D
Droplet components	n-heptane $100%$	n-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

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

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 239 bi-component droplet's evaporation. The initial ratio of the components in this 240 bi-component droplet is 48% *n*-heptane to 52% *n*-decane by mass, or 50% *n*-241 heptane to 50% *n*-decane by volume. Initial droplet diameter d_0 is 1.36 mm, 242 the ambient temperature is 297 K, the droplet temperature is 290 K, and the 243 ambient pressure is 0.1 MPa. These conditions are once again, the same as 244 those in Daïf et al.'s experiment [3]. In order to investigate the dependence 245 of the simulation results on the grid resolution, 4 cases of the evaporation of 246 the benchmark bi-component droplet are simulated, using different grids by 247 changing the grid size and the number of grid points (but the domain size is the 248 same as that in Fig. 1). The minimum grid size and the number of grid points 249 in each of these grid dependency test cases are summarized in Table 5. The 250 letter B in the designation of cases listed in Table 5 stands for bi-component, 251 and the succeeding numbers such as 150, 90, etc. denote the minimum grid sizes 252 used in the respective simulations. Other conditions are same as those listed in 253 Table 4. 254

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Additionally, two types of parametric simulations are performed in this

Droplet components	n-heptane and n -decane
Droplet composition (mass fraction)	n-heptane $/n$ -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 4: Initial conditions for the benchmark bi-component droplet's simulation cases.

Table 5: Minimum grid size and the number of grid points for the grid dependency test cases of the benchmark bi-component droplet: $n-C_7H_{16}/n-C_{10}H_{22} = 48\% / 52\%$ (by mass).

	Minimum grid size $[\mu m]$	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	$132\times132\times132$

study. In the first type of parametric simulations, the influence of varying 256 the initial composition of the bi-component droplet (i.e., the initial volume or 257 mass fraction ratio of *n*-heptane to *n*-decane) on the evaporation phenomenon 258 is considered. In addition to Case B-60 presented above (see Table 5), two more 259 cases are simulated and their results are compared. Initial volume fraction and 260 mass fraction ratios of n-heptane to n-decane in the droplet for each case are 261 listed in Table 6. Here, the first letter B in the designation of Cases BV-60a and 262 BV-60b, once again implies simulations of the evaporation of droplets composed 263 of bi-components, and the letter V indicates that the initial volume fractions 264 of the two components are varied, while keeping the initial droplet temperature 265 and the initial ambient temperature same as those in Table 4. Other initial 266 conditions are also the same as those shown in Table 4. Computational domain 267 and boundary conditions are also the same as those in Case B-60. The compu-268 tational grid is a non-uniform staggered Cartesian grid, consisting of 108 grid 269 points each in the x-, y- and z-directions. The number 60 in the designation 270 of Cases BV-60a and BV-60b bears the same meaning as that of Case B-60, 271

Simulation cases	Case B-60	Case BV-60a	Case BV-60b	
Volume fraction	50% / 50%	75% / 95%	25% / 75%	
(n-heptane/n-decane)	3070 / 3070	1570 / 2570	2370 / 1370	
Mass fraction	18% / 59%	71% / 26%	24% / 76%	
(n-heptane/n-decane)	40/0 / 52/0	14/0 / 20/0	24/0 / 10/0	
Density ratio (ρ_l/ρ_g)	604.84	595.75	615.31	
Dynamic viscosity	21.64	26.21	20.12	
ratio (μ_l/μ_g)	51.04	20.21	39.13	

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

i.e., the minimum grid spacing is 60 μ m 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 μ m 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 276 evaporation is simulated by varying the initial ambient temperature, while keep-277 ing the initial composition of the droplet fixed, i.e., using the same initial volume 278 or mass fraction ratio of *n*-heptane to *n*-decane as that in Case B-60. Therefore, 279 two more cases are simulated in addition to Case B-60, which are designated 280 as Case BT-60a and Case BT-60b and listed in Table 7. In the nomenclature 281 of Cases BT-60a and BT-60b, the letter B and the number 60 bear the same 282 meanings as those in Case B-60 explained above, and the letter T implies that 283 the initial ambient temperature is varied among these simulations, while keep-284 ing the initial volume fraction ratio of the droplet's components fixed (i.e., 50% 285 *n*-heptane and 50% *n*-decane). The initial ambient temperature in each case is 286 shown in Table 7. Other initial conditions are the same as those in Case B-60 287 (summarized in Table 4). Boundary conditions, computational domain and grid 288 used in Cases BT-60a and BT-60b are also the same as those used in Case B-60. 289 Comparisons of the simulation results among these three cases (listed in Table 290 7) are performed, to understand the influence of initial ambient temperature on 291 the evaporation of bi-component droplet. 292

	Ambient	Density ratio	Dynamic viscosity
	temperature	(ho_l/ ho_g)	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

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

293 2.6. Numerical procedure

Numerical simulations employing the coupled Level Set method and Ghost 294 Fluid Semi-Conservative viscous method (GFSCM) [23, 24], are performed us-295 ing an in-house thermal flow analysis code named FK³ [37]. Second-order accu-296 rate finite difference scheme is used for the spatial discretization of each spatial 297 derivative term in the governing equations. Implicit temporal discretization is 298 employed for time integration of the transport equations of momentum, tem-299 perature and chemical species, while the gas phase density is evaluated with 300 the ideal gas law. Methodology for solving the Poisson equation for pressure 301 by considering jump conditions is described in [24, 38]. Among the cases simu-302 lated in this study, the maximum CPU time incurred is approximately 32,000 303 hours using 64 cores on a CRAY XC40 supercomputer at the Academic Center 304 for Computing and Media Studies (ACCMS), Kyoto University (the wall clock 305 time required for parallel computation of 300,000 time steps using 64 cores is 306 approximately 500 hours). 307

308 3. Results and discussion

³⁰⁹ 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:

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

where, K represents the evaporation speed. Faster evaporation speed of n-310 heptane implies that the volatility of n-heptane is higher than that of n-decane 311 in the room temperature range. Also, both the experimental and simulation 312 results show that the normalized square droplet diameter decreases linearly 313 with time for both fuels, which means that their evaporation speeds are almost 314 constant. This is a typical characteristic of the evaporation of single-component 315 droplets, and is famously known as the D²-law. In addition, by comparing the 316 result of each simulation case with the corresponding experimental result, it can 317 be seen that the predicted evaporation speed of n-decane droplet in Case S-D 318 although marginally slower than that in the experiment, is in good agreement 319



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].

with the measurement. However, the simulation result for evaporation speed 320 of *n*-heptane droplet in Case S-H is visibly slower than that in the experiment. 321 This discrepancy can be attributed to the fact that the simulation does not take 322 into account the natural convection due to gravity, and the heat transfer between 323 the n-heptane droplet and the glass capillary on which it was suspended in the 324 experiment [3]. However, the effect of heat transfer between the glass capillary 325 and the droplet is considered to be small due to the relatively low gas phase 326 temperature. On the other hand, this simulation does not take gravity into 327 account, which may cause the evaporated fuel vapor to stay around the droplet 328 and thus reduce its evaporation speed. In particular, this effect will be more 329 significant in Case S-H owing to the higher volatility of *n*-heptane, which would 330 result in greater amount of fuel evaporation (compared to that of n-decane in 331 Case S-D) and as a result, the deviation from experiment is larger for Case S-H. 332 Figure 3 presents the time variations of the evaporation speed K and evap-333 oration rate $\dot{\omega}$ for Case S-H and Case S-D. Here, evaporation rate $\dot{\omega}$ implies the 334 mass of liquid fuel evaporating per unit of time and per unit of area, and is 335 calculated using the procedure explained in section 2.4. This means that even 336 if the evaporation speed is constant, the evaporation rate will not be constant. 337 Figure 3 shows that in both cases, the evaporation speed and rate are large at 338 the beginning of the simulation (i.e., at t = 0 s), and then decrease significantly. 339



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].

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

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

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

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

Simulation results of the benchmark bi-component droplet evaporating in air (initial conditions listed in Table 4) are presented next. Figure 5 depicts the time variations of the mass fractions of *n*-heptane and *n*-decane in the central x-yplane 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 376 ϕ is zero, i.e., the gas-liquid interface. It can be seen that the droplet diameter 377 decreases with time due to fuel evaporation. As evident from Fig. 5(a), the mass 378 fraction of *n*-heptane in the droplet decreases with time, while the mass fraction 379 of *n*-decane increases with time, as observed in Fig. 5(b). These results show 380 that *n*-heptane, which is more volatile, evaporates preferentially to *n*-decane, 381 and a larger amount of n-decane remains in the droplet. The difference between 382 the mass fractions of the two components becomes more apparent near the gas-383 liquid interface where evaporation occurs, and the mass fraction distribution 384 inside the droplet changes due to the diffusion of chemical species. 385

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.

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

Furthermore, comparing the results of the four simulation cases in Fig. 6, it 405 can be seen that the smaller the minimum grid size is, the faster the evaporation 406 speed and the better the agreement with experiment. To compare the prediction 407 accuracies of Cases B-150, B-90, and B-60 with respect to Case B-45 (which 408 has the finest grid), Table 8 shows the errors in the squared diameter values 409 predicted in Cases B-150, B-90, and B-60 using the values in Case B-45 as the 410 baseline, at various time instances. The table shows that the error in Case B-60 411 is less than 1% throughout the duration of the simulation. On the other hand, in 412 Case B-150, there is an error of more than 1% at t = 50 s, which grows with time. 413 Similarly, the error in Case B-90 increases with time and exceeds 1% at t = 150414 s. Thus, it can be concluded that at least 10 grid points within the droplet 415 diameter are required for accurate computation. Based on the above results 416 and error analysis, the grid used in Case B-60 is employed in the parametric 417

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~%

simulations discussed in section 3.3. Moreover, the parametric simulations are
stopped when the number of grid points within the droplet diameter reaches 10,
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 model proposed in Section 2.4, mass conservation across the gas-liquid interface is respected. To check the mass loss in the various 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:

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

where d(t) is the instantaneous droplet diameter and Δt is the time step value 421 of the simulation. The fuel mass in gas phase obtained from the above equa-422 tion is then added to the fuel mass remaining in the liquid phase to get the 423 instantaneous total fuel mass, whose time variations in the different simulation 424 cases are depicted in Fig. 7. As evident from Fig. 7, the total fuel mass re-425 mains virtually constant with time in all the cases, indicating that the mass 426 loss is negligible in all these cases. Furthermore, numerical errors that manifest 427 as mass loss may also arise in regions where the grid resolution is insufficient. 428 But based on the grid convergence analysis presented above for the benchmark 429 bi-component droplet's evaporation, all the simulations performed in this study 430 were stopped when the droplet size in the respective cases reduced to a value 431 such that 10 grid points were present within the droplet diameter. Hence, the 432 existence of under-resolved regions (which are a source of numerical errors) is 433 extremely unlikely in the present simulations. 434

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:

$$\dot{\omega}_{sum} = \dot{\omega}_{heptane} + \dot{\omega}_{decane} \tag{42}$$

From Fig. 8, it is possible to quantitatively evaluate the instantaneous individual 435 evaporation rates of n-heptane and n-decane. The figure shows that n-heptane 436 evaporates preferentially up to t = 180 s, and *n*-decane evaporates preferentially 437 after that. At t=180 s, the droplet diameter is about 80% of the initial value, and 438 the droplet volume is about half of the initial value. Also, the evaporation rate 439 of n-heptane decreases with time. This is due to the decrease in the quantity of 440 *n*-heptane in the droplet with evaporation. On the other hand, the evaporation 441 rate of n-decane is generally constant regardless of time. The mass fraction of 442 *n*-decane in the droplet increases with evaporation, but since *n*-decane has low 443 volatility, its evaporation rate is almost constant. 444

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

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

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

For further analysis, Fig. 10 depicts the time variations of the evaporation rate of each component (i.e., $\dot{\omega}_{heptane}$ and $\dot{\omega}_{decane}$) and the total evaporation 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: $n\mbox{-heptane}~50\%$ / $n\mbox{-decane}~50\%)$



(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.

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

Next, the effect of initial ambient temperature on the evaporation behaviour
of bi-component droplet is examined using the simulations of Case B-60, Case
BT-60a and Case BT-60b. In these three cases, the initial composition of the
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.

while the initial ambient temperature is different (refer Table 7 and section 484 2.5 for the details of these three cases). Figure 11 shows a comparison of the 485 time variations of the normalized squared droplet diameter among Case B-60, 486 Case BT-60a, and Case BT-60b. As expected, the higher the initial ambient 487 temperature, the higher the evaporation speed of the droplet. Once again, the 488 evaporation speed decreases with time and eventually reaches a constant value 489 in all these three cases. Hence, these simulations are also able to capture this 490 typical characteristic of the evaporation phenomenon of bi-component droplets. 491 Additionally, Fig. 12 shows the time variations of the total evaporation rate 492 and the individual evaporation rates of the droplet's components in Case B-493 60, Case BT-60a, and Case BT-60b. Consistent with the results in Fig. 11, the 494 total evaporation rate $\dot{\omega}_{sum}$ is greater for the case with the higher initial ambient 495 temperature, as evident from Fig. 12. In Case B-60, the total evaporation rate 496 $\dot{\omega}_{sum}$ generally decreases monotonically as depicted in Fig. 12(a). However, 497 from Fig. 12(b) and 12(c), it is evident that $\dot{\omega}_{sum}$ peaks once at $t \approx 15$ s and 498 $t \approx 10$ s in Case BT-60a and Case BT-60b, respectively, before decreasing and 499 then increasing again in these two cases. Such behaviour can be explained by 500 investigating the evaporation rate of each component. In Fig. 12(b) and 12(c), 501



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.

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

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

⁵²⁷ But, it is evident from Fig. 12(b) and 12(c) that the total evaporation rate $\dot{\omega}_{sum}$ 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 $\dot{\omega}_{decane}$ with time in these two cases. With the progress of evaporation of the ⁵³⁰ 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.

537 4. Conclusions

The evaporation phenomenon of bi-component droplets in air was simulated 538 by solving the liquid and gas phases as a continuum using an Eulerian frame-539 work. The Level Set method was employed for capturing the gas-liquid interface 540 evolution, and coupled with the Ghost Fluid Semi-Conservative viscous Method 541 (GFSCM) which allows for the computation of spatial derivatives of discontin-542 uous quantities at the gas-liquid interface. Particularly, the evaporation model 543 proposed by Haelssig et al. [19] has been extended to evaporating liquid-gas 544 systems wherein the liquid phase comprises two components (n-heptane and n-545 decane), and the gas phase comprises four components or chemical species (viz. 546 vapours of n-heptane and n-decane, N₂ and O₂). 3D numerical simulation of the 547 evaporation of a benchmark bi-component droplet (made up of 48% *n*-heptane 548 and 52% *n*-decane by mass) was validated against experimental data. It was 549 confirmed that the simulation can capture the evaporation characteristics of this 550 bi-component fuel droplet as observed in the experiment, such as the preferen-551 tial evaporation of *n*-heptane during the early stages of droplet evaporation, 552 and the gradual reduction in the droplet's evaporation speed with time. These 553 characteristics were also observed in the parametric simulation cases used for 554 investigating the effects of initial composition of the bi-component droplet and 555 the initial ambient temperature on the bi-component droplets' evaporation be-556 haviour. Results of the parametric simulations in which the initial composition 557 of the bi-component droplet was changed, revealed that the larger the initial 558 *n*-heptane concentration in the droplet, the greater the evaporation speed and 559 the total evaporation rate, and the longer the time needed for the evaporation 560 speed to become constant. Additionally, parametric simulations in which the 561

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

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