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# Comparison of droplet evaporation models for a turbulent, non-swirling jet flame with a polydisperse droplet distribution

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ABSTRACT

The current investigation aims to present the numerical results of a turbulent spray jet flame in the framework of Large Eddy Simulation. The injection of *n*-heptane liquid fuel is achieved through the use of a pressure-swirl atomiser generating a lifted spray flame. The evolution of the sub-grid probability density function of relevant scalars is accounted for by the Eulerian stochastic field method. A non-reactive spray computation is conducted in a preliminary stage. The simulation allows for a stochastic breakup formulation in combination with a stochastic dispersion model to confirm their predictive capabilities. This is achieved as the liquid properties such as droplet diameter and velocity profiles are found to be in excellent agreement between the simulated results and measurements. The main target of the work is to assess the performance of the most widely accepted evaporation models in a turbulent droplet-laden flame. In this paper, a detailed comparison of the evaporation models is conducted thanks to a recent development in measurement techniques which allow to permit the spray temperature profiles. The time-averaged droplet temperature across the spray flame is therefore investigated in order to validate several droplet vaporisation models. All the models under consideration are found to capture the formation of a double reaction zone flame and the measured lift-off height is reproduced within a satisfactory level of accuracy. This good reproduction of the flame morphology additionally confirms the performance of the *pdf* approach as a closure for the unknown turbulence–chemistry interaction in this type of spray flames. However, the simulated wet-bulb temperature in the hot burnt gas between the two reaction zones in addition to the profile along the spray centreline show a large discrepancy when compared to measurements. This large difference thus requires further investigation both in the modelling of evaporation and in the accuracy of measurement techniques.



## 1. Introduction

The evaporation and combustion of a cluster of liquid droplets, forming a turbulent spray, have been the subject of interest for many investigators owing to a wide range of their practical applications, including spark ignition engines, aircraft propulsion systems and liquid-fuelled rockets, among others. The combustion properties such as efficiency, stability and pollutant formation rate are often controlled by the nature of the turbulent spray in terms of size and velocity distributions predominantly affecting its dispersion and vaporisation. A better understanding towards the characteristic behaviour of the reactive spray in a turbulent flame is therefore essential to improve the quality of two-phase combustion systems. However, many important questions still remain unanswered with regard to the modelling of turbulent spray combustion because of the occurrence of complex phenomena - turbulence, heat and mass transfers between phases, small-scale influence on droplet evolution and chemical reactions. An additional difficulty arises since such processes are likely to take place in a coupled manner. In spite of numerous past works (please see review papers [1,2]), therefore, the development of computational flow solvers yielding a reliable prediction for the properties of spray flames is still challenging. The main focus of this work is, in particular, made on the transport (heat and mass transfer) rates between the spray flame and liquid droplets.

The pioneering work of Maxwell [3] goes back to 1877, when he proposed a simple model for the rate of droplet evaporation controlled exclusively by the diffusion process. Since then, the vaporisation of a single and multicomponent droplet has been mainly investigated due to various modelling challenges when considering a cloud of droplets in turbulent flames. They include droplet dispersion in a turbulent gaseous flow, droplet–droplet interaction, spray formation through the use of atomisers and coupling between flame and spray. The fundamental knowledge obtained from

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the consideration of single droplets might then be used to advance modelling approaches to the prediction of spray combustion phenomena. To provide a detailed physical insight into the evaporation process of single droplets, numerical attempts have been performed through the application of models based on the *exact solution* of a complete set of the unsteady Navier–Stokes, species and energy equations, for instance, in [4,5]. All the computations therein were carried out under the assumption that the shape of droplets remains spherical. In contrast, a comprehensive model for the direct numerical simulation (DNS) of three-dimensional evaporating, deforming droplets was introduced in the work of Schlottke and Weigand [6]. The model is based on the Volume-Of-Fluid approach through which strong droplet deformations can be captured while the influence of the Stefan flow is correctly represented by calculating the velocities of the gaseous and the liquid-phase at the interface.

The evaporation of a single droplet or droplet arrays burning in a convective environment has attracted several numerical studies; a fuel spray can be simplified as an aggregation of individual liquid droplets. Raghavan et al. [7] numerically investigated the transient behaviour of spherical droplets in terms of flame shape and burning rate using DNS with a global single step reaction. The predictions were validated against measurements obtained from a porous sphere experiment. The burning of a single droplet considerably differs from that of a droplet array – droplets in a closely packed situation burn as a group rather than individually [8]. As a result, the modelling of droplet array combustion is of interest by many researchers. The interaction of two burning fuel drops of arbitrary size was studied by Brzustowski et al. [9] without the consideration of Stefan convection. There exist only few models (e.g., [10,11]) by which the combustion of multiple-droplet arrays as well as the influence of droplet–droplet interactions on burning rates can be examined. A more complete information on the modelling of burning droplets packed in a predetermined array can be found in a review paper by Sirignano [12]. Unfortunately, all the aforementioned models cannot be directly employed for the purpose of many droplet calculations mainly due to a great demand for the computational analysis of each droplet. In addition, they are not suitable for the Lagrangian spray approach with a point-source approximation which is of concern in the current work.

For the simulation of practical applications with many droplets, most evaporation models assume infinite liquid thermal conductivity due to their low cost. The well-established equilibrium models include the classical rapid mixing model [13,14] and Abramzon–Sirignano model [15]. Bellan and Harstad [16] considered non-equilibrium evaporation effects based on the Langmuir–Knudsen law via the definition of a surface mole fraction. Miller et al. [17] compared several evaporation models and their performance for single droplet evaporation. Although no direct evidence in relation to experimental measurements was obtained therein, they highlighted based on sensitivity analysis that non-equilibrium effects should be taken into account for droplets with the initial diameter of less than 50 μm and with increased slip velocity because they have significant contributions to the surface mole fraction and hence affect the evaporation process.

Due to a lack of experimental measurements for droplet diameters less than 100 μm (common in many practical sprays), comparisons of the rate of change of droplet diameter and temperature have been performed only for relatively large droplets (initial sizes $\sim$1 mm), see for example, [18]. In the case of spray flames, however, the validation of evaporation models has been rather limited to mean droplet diameters as measurements for droplet temperature are rare. Novel laser-based techniques such as Global Rainbow Technique (GRT) [19] allow to measure mean fuel droplet temperature profiles within a turbulent spray flame and therefore determine the heat and mass transfer rates between the gaseous flow and droplets. The present work therefore aims to assess several evaporation models in two-phase reacting flows. The experimental configuration [20] under investigation consists of an *n*-heptane spray flame, where the fuel is injected by a simplex nozzle. The most commonly used evaporation models (classical rapid mixing and Abramzon–Sirignano models) will be adopted to confirm their predictive capabilities in the two-phase reactive flow. In addition, the influence of non-equilibrium evaporation and internal temperature variation on droplet statistical quantities and the global behaviour of the spray flame will be assessed. Although numerous attempts to simulate two-phase reactive flows in the context of Large Eddy Simulation (LES) exist, no strong evidence to support the selection of one evaporation model over another in turbulent reactive environments is available. In most of similar LES studies [21,22], only equilibrium evaporation models have been employed. In addition, to the best of authors' knowledge, only little work [23] has accounted for non-equilibrium effects on the evaporation process of reactive droplets, but made no direct comparison to other models. Therefore, this work also attempts to make a suggestion for the choice of suitable evaporation models for the LES computation of spray flames.

In the current work, the probability density function (*pdf*) method formulated within the LES framework is applied to predict various physical mechanisms including turbulence–chemistry interaction, droplet dispersion and evaporation, and spray atomisation. The unknown interaction between turbulent motions and combustion is represented by the Eulerian stochastic field method [24] while the evolution of the spray properties is treated in a Lagrangian framework. The Eulerian–Lagrangian approach for particulate flows has been successfully applied to study a wide range of turbulent spray flames such as gas turbine combustors [25,26], swirl-stabilised flames [27], a methanol spray flame [28] and an ethanol flame under MILD conditions [29]. The liquid fuel injection is characterised by the use of a stochastic breakup model [30], which does not require an approximation of initial droplet distributions in the vicinity of the nozzle exit. To the authors' knowledge, the spray burner of interest here has been numerically investigated only in the work of Shum-Kivan et al. [31] where the focus was made on the analysis of the flame structure and stabilisation. In this investigation, the performance of several evaporation models will therefore be validated in terms of variations of the wet-bulb temperature of *n*-heptane fuel in different flame regions.

## 2. Mathematical modelling

### 2.1. Gas-phase governing equations

In the LES approach, a filtering operator is applied to a set of the governing equations in order to separate the resolved, large-scale turbulent motions from scales smaller than the filter width. As a result, the large-scale contributions to the velocity and scalar fields can be solved for directly while the influence of the sub-grid scale (*sgs*) fluctuations on the resolved flow variables has to be closed through the choice of suitable models. To take into account the strong density fluctuations that arise in chemically reacting flows, the most practical approach is the use of a density-weighted (or Favre) filtering operation, defined as $\tilde{f}(\boldsymbol{x},t)=\overline{\rho f}/\bar{\rho}$. Additional unclosed terms in the mass conservation equation are thus prevented. Further details on the filtered governing equations of mass, momentum and scalars with liquid-phase source terms can be found in [26,30]. The unknown contribution to the filtered chemical source term ($\overline{\rho\dot{\omega}_\alpha}$) is taken into account using a joint sub-grid scale *pdf* for all the scalar variables required to describe chemical reaction as proposed in [32]. In this work, the evolution