



# The role of preferential evaporation on the ignition of multicomponent fuels in a homogeneous spray/air mixture

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## Abstract

This work examines the importance of preferential evaporation and liquid species diffusion on the ignition of multicomponent surrogate fuels in homogeneous mixtures. To this end, a model is developed that considers the evaporation of a monodisperse droplet cloud in a homogeneous and isobaric gas-phase environment. The mathematical model accounts for physico-chemical relevant processes, involving (i) species diffusion in the liquid phase, (ii) two-phase thermodynamic equilibrium and (iii) gas-phase chemistry. After evaluating the accuracy of individual model components against available experimental data, the model is applied to investigate the ignition of a surrogate mixture for a Jet-A fuel (POSF 4658) at conditions of interest to gas turbine engines. A parametric study is performed to examine effects on the interaction between multicomponent evaporation and ignition. It is found that the maximum reactivity occurs for conditions at which the ignition time in the gas phase is comparable to the evaporation time. At these conditions, the mixture composition is significantly affected by preferential evaporation, which in turn affects the reactivity of the gas phase. It is shown that intradroplet diffusion plays a major role on the radial droplet composition, thereby conditioning the evaporation rates of single species. A comparison with a zero-diffusivity model for the treatment of droplet internal diffusion emphasizes the importance of liquid diffusion on the autoignition time, and confirms the need for properly accounting for a detailed description of multicomponent evaporation effects.

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**Keywords:** Droplets; Two-phase combustion; Preferential evaporation; Autoignition; Multicomponent diffusion

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## 1. Introduction

The use of surrogates to emulate the characteristic behavior of real fuels is an established methodology [1,2]. However, main topics of discussion have been on the selection of the set of species constituting the surrogate and the specific properties to be matched by a particular surrogate mixture. Ideally, physical (density, molecular weight, H/C ratio, viscosity, etc.) and chemical (ignition delay, flame propagation, soot formation, etc.) targets should be modeled to provide a comprehensive surrogate description. While few studies [3,4] have focused on both target properties, the main emphasis has been attributed to the description of the gas-phase behavior [5,6]. In fact, one of the main complexities in emulating real-fuel properties arises from the strong interaction between the liquid and the gas phase.

Constraining the surrogate formulation to meet specific targets does not imply a complete knowledge of its behavior. Combustion devices operate over a wide range of conditions, and the consideration of conditions that affect the two-phase interaction in combustion, such as temperature, pressure or droplet diameter, introduce a substantial degree of complexity if included in the fuel formulation. For instance, it is widely acknowledged [7] that the ignition delay time is one of the key properties to be reproduced by surrogate fuels. This property is usually contained in frameworks for the surrogate formulation through experimental measurements of the Derived Cetane Number (DCN) [8]. These measurements are carried out through a standardized procedure [9] at specific operating conditions, without providing direct control over specific droplet size distribution or local equivalence ratio. For these cases, an analysis of the influence of different parameters on the ignition delay time can be of primary importance to possibly further constrain a surrogate description.

Recently, particular attention has been devoted to the parametric analysis of the two-phase ignition behavior of different fuels. These studies have been carried out by considering idealized systems, such as spherical droplets in the absence of gravity to isolate chemical processes from other phenomena affecting combustion in real devices, as well as to make the problem computationally tractable using detailed kinetic mechanisms. While experimental [10] and computational [11–15] studies have focused on the ignition behavior of single-component droplets, less attention has been devoted to the investigation of multicomponent fuels. The description of multicomponent fuels requires the consideration of liquid-phase diffusion, non-ideal phase equilibrium, and extended chemical mechanisms for the description of multicomponent gas-phase chemistry. Although the importance of multicomponent evaporation on ignition has been recognized in automotive applications [16–18], the im-

portance for aviation fuels at gas-turbine-relevant conditions has not been considered so far. This is the subject of this work. Specifically, the objective of this study is to investigate effects of multicomponent diffusion and preferential evaporation on the ignition of fuel mixtures. To isolate these effects from the intricate coupling with the gas phase transport, arising in two-phase flow combustion, this study considers an idealized configuration in which the gas phase is represented by a semi-batch reactor. A numerical model is developed to represent the spatial evolution of the liquid phase inside monodispersed droplets, as well as the temporal evolution of the homogeneous gaseous phase. The model formulation is presented in Section 2, where each component of the model is validated. In Section 3, the model is applied to the analysis of the autoignition of the 2nd-generation surrogate of the POSF 4658 Jet-A fuel [8]. A parametric study of effects of droplet diameter and global equivalence ratio on evaporation and ignition is carried out, and the relevance of multicomponent evaporation is quantified through a comparison with a zero-diffusivity model. The manuscript finishes with conclusions.

## 2. Mathematical model

The mathematical model considers the evaporation and ignition of a monodispersed spray cloud in a homogeneous gas phase. To isolate the effect of preferential evaporation from transport in the gaseous mixture we consider the droplet evaporation into a homogeneous gas phase. Indeed, previous numerical studies showed that (i) in non-premixed systems, for low to moderate strain rates, ignition evolves in a manner comparable to that of homogeneous systems, but with slower dynamics because of diffusive losses [19]; and (ii) that in droplet cloud systems, compared to what is analyzed in this work, the ignition process tends to behave in a homogeneous way with decreasing droplet diameters [12]. Since our simulations consider both evaporation and gas-phase chemistry, ignition was considered either during evaporation or after evaporation is completed.

The following assumptions in the model formulation are made:

- Spherically symmetric and monodisperse droplets;
- Absence of chemical reactions in the liquid phase;
- Dynamic equilibrium with the underlying gas phase (no slip velocity);
- Constant pressure;
- Equilibrium conditions at the liquid/gas interface.

In the following subsections, the main model components are described.

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