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# Full Length Article A simple model of a water/fuel spray diffusion flame

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#### ABSTRACT

The classical Burke–Schumann diffusion flame is adopted as a paradigm configuration for examining spray diffusion flames in which the spray's droplets are comprised of a mixture of water and a miscible fuel. Building on experimental data and simple modeling predictions from the literature, which testify to the viability of burning fuels heavily diluted with water, a special fuel vaporization Damköhler number was constructed to reflect preferential fuel evaporation and non-ideal solution behavior of the spray's water/fuel droplets. An analytical solution of the governing equations was found. Calculations based on the solution enabled a comparison between water/t-butanol and water/ethylene-glycol spray diffusion flames. The former spray was characterized by strong enhanced fuel evaporation whereas the latter by weak enhanced evaporation. Noticeable differences in flame shapes, heights and temperatures were found for the two spray flames. It is argued that the possibility exists of sustaining water/fuel spray diffusion flames by combining the enhanced fuel evaporation and control of the oxygen supply.

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#### 1. Introduction

The viability of burning fuels heavily diluted with water has been demonstrated by Yi [1] and Yi and Axelbaum [2,3]. The motivation for these studies was the examination of an approach to extract chemical energy by direct combustion from fuels that naturally contain high water content. In contrast to common methods, the suggested approach avoids the energy-demanding process of water removal, thereby increasing the overall energy efficiency. Also, if used in pressurized systems, the latent heat used to evaporate the water can be recovered and utilized. In addition, if oxygen is used as the oxidizer, it allows for efficient carbon capture. Recently, it was reported that utilization of direct steam generation with a natural gas burner to generate power, while enabling carbon capture, is being carried out commercially [4].

Although the combustion of mixtures of water and fuel had been studied in the literature (see Ref. [2,3]) the novel features revealed by Yi and Axelbaum's experiments (backed up by some theoretical support through predictions of an elementary theory of single droplet evaporation/distillation) were that preferential evaporation of, for example, ethanol over water plays a key role in enhancing flame stability in the swirl-stabilized burner configuration, and that non-ideal solution behavior should be accounted

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for when modeling the evaporation process. Preferential evaporation occurs when one chemical substance of a droplet's mixture evaporates more rapidly than another component. In a simple sense, a comparison of the evaporation of pure droplets of two different substances would reveal that one droplet would evaporate more rapidly than the other due to its greater volatility. But, in addition, the greater rate of evaporation may be further enhanced. Generally, in an ideal mixture, the molecular interactions between each pair of chemical species are the same. However, in non-ideal mixtures, molecules of the different components may interact to repel each other. This non-ideal state is expressed through the activity coefficient, which identifies the actual partial pressure of the substance relative to its partial pressure if it were an ideal liquid. Importantly, the activity coefficient is a function of the composition of droplet and in water/fuel mixtures it can be quite large (>3) when the concentration of the fuel is small, particularly for alcohols. To a lesser or greater extent both the aforementioned mechanisms were found to play a role in the water/fuel spray flames considered.

The complex behavior of evaporating (and combusting) multicomponent droplets has been recognized for some time. Newbold and Amundson [5] proposed a model for the evaporation of a multicomponent droplet. Law [6] gave a theory of internal boiling and superheating of vaporizing multicomponent droplets in a quiescent atmosphere and analyzed the different stages of development within the evaporating droplet (see also [7]). An extensive historical overview of, and new advanced developments in this area appear in Sazhin [8].





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In a related theoretical publication Hou et al. [9] presented a mathematical analysis of the interaction between internal heat gain and loss on compound drop spray flames. In these compound droplets a water core is surrounded by *n*-octane fuel. Evaporation occurs sequentially as the water does not begin to evaporate until the "outer shell" of fuel has completely evaporated. For a premixed compound drop spray flame the influence on the burning velocity of the competing heat gain, due to fuel vapor made available for combustion, and heat loss, due to water evaporation, was mapped out in terms of the relative amounts of fuel and water in the droplets.

However, it is well-known that the behavior of a spray of droplets is not always reflected through that of a single droplet multiplied by the number of droplets in the spray. In the current work we consider the aforementioned findings of Yi and Axelbaum, viz. preferential fuel evaporation and non-ideal solution behavior. in a phenomenological manner within the simple modeling context of the classical gas laminar Burke-Schumann diffusion flame [10] subsequently extended in [11,12] to the case of a fuel spray diffusion flame. Here, we investigate a Burke-Schumann type of diffusion flame fired by a water/fuel spray of well-stirred liquid droplets. Although devoid of the intricate details afforded by a more all-encompassing numerical model, experience has shown that relatively simple models of this nature, which enable a mathematical analysis, can serve two main functions: (a) they provide convenient benchmarks for full computational solutions of the problem, and (b) they offer clear, uncluttered insight into the physico-chemical underpinnings of spray-gas interaction and how it impacts combustion. It is from this viewpoint that the current investigation is carried out.

#### 2. Mathematical model - governing equations

The Burke–Schumann spray flame configuration (see Fig. 1) is considered, in which fuel vapor and water/fuel droplets flow in an inner duct (of half width *L*) and oxygen flows in outer ducts (each of width R-L). Under appropriate operating conditions. after diffusive mixing of the two streams, a laminar, spray diffusion flame is established. The velocities of the streams in the inner and outer ducts are taken to be identical and constant, (u, v) = (0, v). A recent sophisticated approach to modeling monodisperse spray combustion is given in [13,14], in which there appears a description of the way in which the different scales relevant to the droplets and the host gas can be thoroughly exploited to formulate spray combustion in both the finite and infinite chemical-Damköhler limit. Advantages of the formulation are the ability to account for non-unity Lewis numbers for the gas phase and heat, mass and momentum transfer between the liquid and gas phases in terms of physically-meaningful mixture fractions and excess enthalpies. However, despite its proven advantages and the insight it affords the approach has yet to be applied to polydisperse and multicomponent spray combustion.

In the current work, the description of the spray that is adopted is based on the alternative proven sectional approach [15] (see also, for example, [11,12,16]). In this approach the pointwise size distribution of droplets in the spray is subdivided into a finite number of size sections each of which contains droplets that fall within a certain size range. The mass balance in any section jaccounts for (a) influx of droplets from the next section up, j + 1, which have diminished in size and have thus become eligible for membership in section j, and (b) convection and mass loss due to evaporation of droplets in section j. Here, for simplicity, we take the spray to be mono-sectional, that is, we assume that a single sectional equation is sufficient to describe the spray's characteristics. Use of a single integral quantity (here the mass fraction of the

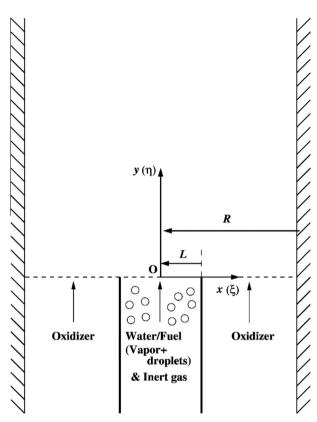


Fig. 1. Configuration for formation of Burke-Schumann spray diffusion flame.

liquid comprising the droplets in the spray) does not negate redistribution of the range of droplet sizes under consideration. However, it does mean that only overall properties of the spray and its effects can be accounted for. In the current context this approach is acceptable. To focus on the essential features of interest it is assumed that the droplets are located in the far-field in relation to the spray source [17] so that they have settled into dynamic and thermal equilibrium with their host gas carrier. In addition, the Lewis number is assumed to be unity. This is generally not too restrictive, but does provide a basis for an analysis for cases of more realistic non-unity Lewis numbers. Also, it is emphasized that changes in the basic flame characteristics (e.g. flame shape, etc.) are not qualitatively effected by Lewis number. The governing equations then assume the following form. For the spray:

$$v\frac{\partial m_{d,F}}{\partial y} = -\tilde{C}_F m_{d,F} H(L-x) \tag{1}$$

$$v\frac{\partial m_{d,W}}{\partial y} = -\tilde{C}_W m_{d,W} H(L-x)$$
<sup>(2)</sup>

in which  $m_{d,F}$  and  $m_{d,W}$  are the mass fractions of liquid fuel and water, respectively, in the sprays droplets and  $\tilde{C}_F$  and  $\tilde{C}_W$  are their sectional vaporization coefficients. The (non-dimensional) form of these vaporization coefficients will be discussed later. Suffice to say now, they contain within them information about such properties as the evaporation properties of the component liquid and the range of droplet sizes under consideration [15]. Coupled to these equations are the conservation equations for the Schwab-Zeldovitch parameters m and  $m_T$  which are derived from the conservation equations for fuel vapor, oxygen and energy

$$v\frac{\partial m}{\partial y} = D_g \left[\frac{\partial^2 m}{\partial y^2}\right] + \tilde{C}_F m_{d,F} H(L-x)$$
(3)

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