



A mathematical model for heating and evaporation of a multi-component liquid film



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ABSTRACT

A new model for heating and evaporation of a multi-component liquid film, based on the analytical solutions to the heat transfer and species diffusion equations inside the film, is suggested. The Dirichlet boundary condition is used at the wall and the Robin boundary condition is used at the film surface for the heat transfer equation. For the species diffusion equations, the Neumann boundary conditions are used at the wall, and Robin boundary conditions are used at the film surface. The convective heat transfer coefficient is assumed to be constant and the convective mass transfer coefficient is inferred from the Chilton-Colburn analogy. The model is validated using the previously published experimental data for heating and evaporation of a film composed of mixtures of isooctane/3-methylpentane (3MP). Also, it is applied to the analysis of heating and evaporation of a film composed of a 50%/50% mixture of heptane and hexadecane in Diesel engine-like conditions.

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1. Introduction

The importance of modelling liquid film heating and evaporation in various engineering applications is well known [1]. Recently, most of the attention has been focused on the application of these models to the analysis of the processes in internal combustion engines (see [2] and the references therein).

The formation of liquid films in engine combustion systems is known to lead to detrimental processes, including the formation of smoke-inducing piston fuel films in spark-ignited engines [3], and the initiation of fuel films on the surface of Diesel injectors [4]. The accumulation of deposits inside and on the surface of fuel injector nozzles is associated with reduced engine performance and lifetime. This reduction in performance is known to manifest in a variety of ways including increased acoustic and pollutant emissions [5–7]. The deposits can also reduce the hydraulic diameter of the nozzle orifices, resulting in a reduction in the quantity of injected fuel and reduced repeatability of injection [7–9], all of which cause a reduction in engine power [10]. The deposits can also increase cavitation, which can then lead to further choking of the nozzle [11]. Injector needle sticking can occur and eventually lead to injector failure [12,13]. Accurate mathematical modelling of the heating and evaporation of multi-component liquid films can help us to improve our understanding of the formation and

decomposition processes of fuel films, and lead to the development of more efficient prevention and control strategies.

The modelling of heating and evaporation of liquid films has been considered in a number of papers some of which are reviewed in [2]. The simplest model of these processes is based on the assumption that the liquid is well mixed and the thermal diffusion inside it can be considered infinitely fast (zero-dimensional model). In [14] the temperature gradients inside the liquid film were taken into account, but based on a rather simplistic assumption that the temperature distribution can be approximated by the piecewise linear function (linear temperature model). The model based on the assumption of a more complex polynomial distribution of temperature inside the liquid film is known as the quasi-dimensional model [2]. Finally the model based on the rigorous solution to the heat conduction equation inside the liquid film and the assumption that temperature gradients in the direction perpendicular to the wall are much larger than those along the wall is known as the one-dimensional model [2]. Our analysis is focused on the latter model, as the most general one.

In contrast to most previously suggested models of the phenomenon, we will take into account the presence of multiple components in the liquid film, which is typical for automotive fuels. Both thermal and species diffusion inside the liquid film will be taken into account. As in the case of the analysis of multi-component droplet heating and evaporation (see [15]), the model is based on the analytical solutions to the heat transfer and species diffusion equations. The film will be assumed to be thin which will

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Nomenclature

| | |
|-------------|--|
| c | specific heat capacity |
| c_{μ} | constant equal to 0.09 |
| D | diffusion coefficient |
| f_n | parameter introduced in (4) |
| h | convection heat transfer coefficient |
| h_0 | $h\delta_0/k_l$ |
| k | thermal conductivity |
| L | specific heat of evaporation |
| Le | Lewes number |
| M | molar mass |
| \dot{m}_f | evaporation mass flux |
| N | total number of evaporating species |
| Nu | Nusselt number |
| p | pressure or parameter introduced in Eq. (20) |
| Pr | Prandtl number |
| q | heat flux |
| q_n | parameter introduced in Eq. (4) |
| q_{Yn} | parameter introduced in Eq. (27) |
| R_u | universal gas constant |
| Re | Reynolds number |
| Sc | Schmidt number |
| t | time |
| T | temperature |
| u | parameter defined by Eq. (14) |
| u^* | friction velocity |
| v_n | eigenfunction defined by Eq. (23) |
| x | distance from the wall |
| X | x/δ_0 or molar fraction |
| y | distance from the surface of the film |
| Y | mass fraction |

Greek symbols

| | |
|---------------------|-----------------------------|
| δ | film thickness |
| ϵ_i | parameter defined by (13) |
| Θ | function introduced in (19) |
| κ | thermal diffusivity |
| $\kappa_{\delta 0}$ | $k_l/(c_l\rho_l\delta_0^2)$ |
| λ_n | eigenvalues |
| μ | dynamic viscosity |
| ν | kinematic viscosity |
| ρ | density |

Subscripts

| | |
|-----|--|
| a | ambient |
| eff | effective |
| e | evaporation |
| f | film |
| g | gas |
| i | species |
| in | inner |
| l | liquid phase |
| m | mass transfer |
| out | outer |
| p | constant pressure |
| s | surface of the film |
| T | turbulent |
| v | vapour phase |
| w | wall |
| 0 | value at the beginning of a time step or initial value |

allow us to use the one-dimensional model in which both temperature and liquid species mass fractions depend only on the distance from the wall.

We start our analysis with the case of mono-component liquid films (Section 2). In Section 3 this analysis is generalised to the case of multi-component liquid films. The solution algorithm is described in Section 4. The validation of the model against published experimental data and its application to the analysis of specific cases of bi-component fuel film heating and evaporation in engine-like conditions is described in Section 5. The main results of the paper are summarised in Section 6.

2. Heating and evaporation of a liquid film (mono-component liquid)

The analyses of the processes in liquid and gas phases, described within this model, are presented in the following subsections.

2.1. Liquid phase

Assuming that the gradients of temperature in the film in the direction perpendicular to the wall are much greater than those in the direction parallel to the wall, the heat conduction equation inside the film can be simplified to:

$$\frac{\partial T}{\partial t} = \kappa_1 \frac{\partial^2 T}{\partial x^2}, \quad (1)$$

where $\kappa_1 = k_l/(c_l\rho_l)$ is the liquid thermal diffusivity, k_l , c_l , and ρ_l are the liquid thermal conductivity, specific heat capacity, and density, respectively, x is the distance from the wall.

Eq. (1) is expected to describe the heat conduction process in this film except in the vicinity of its edges. Also, in the case of thin films, the contribution of the convective term, ignored in Eq. (1), is expected to be very small.

Following [16], we assume that the liquid temperature at the wall is equal to the constant wall temperature: $T(x=0, t) = T_w$ (Dirichlet boundary condition).

Yan et al. [17] specified heat flux rather than temperature at the wall (Neumann boundary condition). This heat flux was estimated as $q_w = k_w(T_{\text{out}} - T_{\text{in}})/\delta_w$, where k_w is the thermal conductivity of the wall, δ_w is the wall thickness, T_{out} and T_{in} are wall temperatures at the outer and inner boundaries. This approach to the estimation of the heat flux is applicable only in the case of steady state problems, which is not compatible with the modelling of the transient process in the liquid film. The rigorous approach to this problem would require a coupled solution for the liquid film and the wall similar to the one considered in [15] for spherical layers. To the best of our knowledge, this approach to the problem of liquid film heating and evaporation has not been investigated.

Following [16], the boundary condition at the surface of the liquid film ($x = \delta_0$) is presented as:

$$h(T_{\text{eff}} - T_s) = k_l \left. \frac{\partial T}{\partial x} \right|_{x=\delta_0-0}, \quad (2)$$

where

$$T_{\text{eff}} = T_g + \frac{\rho_l L \dot{\delta}_{0e}}{h}, \quad (3)$$

the value of $\dot{\delta}_{0e}$ (the derivative of the film thickness with respect to time), controlled by film evaporation (indicated by the additional subscript e), is taken from the previous time step, L is the specific

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