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Semi-analytical and numerical investigation of a reactive gaseous film between two evaporating liquids

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ABSTRACT

Reactive gaseous films between two evaporating liquids are studied both analytically and numerically, under simplifying assumptions. For high enough heats of reaction, a semi-analytical solution is exhibited. This solution is used to validate an Arbitrary Lagrangian–Eulerian method. Computations are carried out for low heats of reaction, showing how the system behavior is strongly influenced by the value of the heat of reaction compared to the heats of vaporization of reactants.

1. Introduction

Electricity production through a water-steam cycle in a sodium-cooled fast reactor leads to consider the risks associated with the consequences of a sodium-water reaction which can occur in accident conditions. The phenomenon is complex as it involves chemical reactions, phase change and hydrodynamics [13]. A deep understanding of these processes helps predict the dynamics of sodium-water reaction.

When liquid water and liquid sodium are put into contact, a gaseous film appears [2,13], in which the reaction takes place. The main reaction writes:

$$\mathrm{Na} + \mathrm{H_2O} \rightarrow \mathrm{NaOH} + \frac{1}{2}\mathrm{H_2}. \quad (1)$$

To our knowledge, the position of the reaction zone inside this film has not yet been experimentally observed. In [17], an experiment is carried out, in which water vapor is blown on the surface of liquid sodium. The authors observe a reaction zone above the sodium pool and an aerosol of condensed particles. By analogy, a diffusion-flame model of the gaseous film between liquid sodium and liquid water can be suggested. In this model, sodium and water react in gaseous form and product hydrogen and sodium hydroxide. Sodium hydroxide is generated both in vapor and condensed phase.

In [2], liquid sodium is injected into water through a capillary. The author observes the growth of the gaseous film around the liquid metal jet, followed by fragmentation of the jet and detachment of bubbles. In [13], a Pyrex sphere containing liquid sodium is immersed into water. The sphere is broken, putting both reactants into direct contact, and the reaction is filmed. A model taking into account Rayleigh–Taylor instability is developed to interpret the destabilization of the film.

To this day, the chemical kinetics of sodium-water reaction remains largely unknown. In [13], the sole reaction (1) is considered, and is assumed to be irreversible and infinitely fast.

As a result of the high temperatures of the flame and of the evaporation front of sodium, radiative heat transfer happens. A complete evaluation of the effect of this heat transfer would in particular require taking into account absorption and emission by the aerosol of condensed particles, which is beyond the scope of this work. A model of this interaction is presented in [17].

Similarly, it seems difficult to evaluate the importance of turbulence in the dynamics of the phenomenon. In the phenomena studied in [2,13], turbulence may have a larger time scale than the film growth and destabilization, whereas the gas-phase experiment in [17] is simulated taking into account turbulent diffusivities. Turbulence is not taken into account in this work.

The interaction of gaseous films and evaporating liquids is also studied in film boiling problems. Numerical simulations of film

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List of symbols

A_2	dimensionless number defined in Section 3.2
A_3	dimensionless number defined in Section 3.2
α_F^l	liquid fuel thermal diffusivity (m^2/s)
α_O^l	liquid oxidizer thermal diffusivity (m^2/s)
β	dimensionless number defined in Section 3.2
γ	dimensionless number defined in Section 3.2
C_v	gas mixture heat capacity at constant volume ($J\,.\,kg^{-1}\,.\,K^{-1}$)
$C_{v,F}^l$	liquid fuel heat capacity at constant volume ($J\,.\,kg^{-1}\,.\,K^{-1}$)
$C_{v,O}^l$	liquid oxidizer heat capacity at constant volume ($J\,.\,kg^{-1}\,.\,K^{-1}$)
D	diffusion coefficient in the gaseous film (m^2/s)
δ	gaseous film thickness (m)
Δx_F	space step in liquid fuel near the evaporation front (m)
Δx_O	space step in liquid oxidizer near the evaporation front (m)
Δx_g	space step in the gaseous film (m)
Δx_w	space step in liquid fuel near the wall (m)
Δx_∞	space step in liquid oxidizer near the outer boundary (m)
e_F	liquid fuel thickness (m)
e_O	liquid oxidizer thickness (m)
F	fuel
H	height of the two-dimensional computational domain (m)
k_F^l	liquid fuel thermal conductivity ($W\,.\,m^{-1}\,.\,K^{-1}$)
k_O^l	liquid oxidizer thermal conductivity ($W\,.\,m^{-1}\,.\,K^{-1}$)
k_g	gas mixture conductivity ($W\,.\,m^{-1}\,.\,K^{-1}$)
K_F	conductivity ratio defined as k_F^l/k_g
K_O	conductivity ratio defined as k_O^l/k_g
L_F	fuel latent heat of vaporization (J/kg)
L_O	oxidizer latent heat of vaporization (J/kg)
O	oxidizer
Q	heat of reaction per unit mass of fuel consumed (J/kg)
R_F	diffusivity ratio defined as α_F^l/D
R_O	diffusivity ratio defined as α_O^l/D
ρ_F^l	liquid fuel density (kg/m^3)
ρ_O^l	liquid oxidizer density (kg/m^3)
ρ_g	gas mixture density (kg/m^3)
s	stoichiometric mass ratio defined as $\nu_O W_O/(\nu_F W_F)$
T	temperature (K)
$T_{\text{sat},F}$	fuel evaporation front temperature (K)
$T_{\text{sat},O}$	oxidizer evaporation front temperature (K)
T_w	wall temperature (K)
T_∞	temperature at $x = e_O + \delta(t)$ (K)
t	time (s)
Θ_F	defined as $C_v T_{\text{sat},F}/Q$
Θ_O	defined as $C_v T_{\text{sat},O}/Q$
Θ_∞	defined as $C_v T_\infty/Q$
Θ_w	defined as $C_v T_w/Q$
U	defined as $C_v T/Q$
v_g	gas velocity (m/s)
x	abscissa (m)
Y_F	fuel mass fraction
Y_F^0	fuel mass fraction at $x = 0^+$
Y_O	oxidizer mass fraction
Y_O^0	oxidizer mass fraction at $x = \delta^-$
Z_2	passive scalar defined as $U + Y_F$
Z_3	passive scalar defined as $sU + Y_O$

boiling have been carried out [11,7], assuming constant densities of liquid and vapor phases.

In this work, reactive gaseous films between two evaporating liquids are studied both analytically and numerically, under simplifying assumptions. The main (and crudest) assumptions of our model are: (i) all products are gaseous; (ii) the gaseous film has constant density; (iii) the evaporation front temperatures are constant; (iv) the phenomenon is one-dimensional; (v) the chemical reaction is single-step, irreversible and infinitely fast; and (vi) radiative heat transfer is not taken into account, since the aerosol of condensed particles is not modeled. One of our main purposes is to exhibit a reference semi-analytical solution, for high enough heats of reaction. This solution can be used (and is then used in this work) to validate an Arbitrary Lagrangian–Eulerian code. Numerical computations are carried out, showing how the system behavior is strongly influenced by the value of the heat of reaction compared to the heats of vaporization of reactants. A more realistic simulation of sodium - water reaction would require production of condensed sodium hydroxide, as well as gas compressibility, to be taken into account. Therefore, this work can be seen as a first step towards a more complete model.

2. Governing equations

We consider an exothermal, single-step, irreversible, and infinitely-fast reaction between a fuel (F) and an oxidizer (O). At the reaction zone, reactants and products are assumed to be in gaseous form.

$$\nu_F F_{(g)} + \nu_O O_{(g)} \rightarrow \nu_{P_1} P_{1(g)} + \ldots + \nu_{P_n} P_{n(g)}. \qquad (2)$$

The one-dimensional problem under consideration is represented in Fig. 1. Liquid fuel and liquid oxidizer are separated by a gaseous film where reaction (2) takes place. The heat released by the reaction allows reactants to evaporate. They migrate towards each other by molecular diffusion and react. As shown in Fig. 1, the reaction zone has no thickness: fuel and oxidizer cannot be found together at the same location because their reaction rate is infinite. The gaseous products $P_1, \ldots P_n$ released then diffuse through the film.

Because of evaporation, the gaseous film expands. Liquid fuel is delimited by a fixed wall at constant temperature T_w, while liquid oxidizer is delimited by an inert gas at constant temperature T_∞ and pressure p_∞. The oxidizer is therefore pushed towards the inert gas. The phenomenon is one-dimensional and gravity is neglected.

Liquids are assumed incompressible, of respective densities ρ_F^l and ρ_O^l. Given the high density ratio between liquids and gas under consideration (typically 1000), the liquid fuel thickness e_F and the liquid oxidizer thickness e_O are regarded as constant. In other words, the variation of thickness due to phase change is neglected.

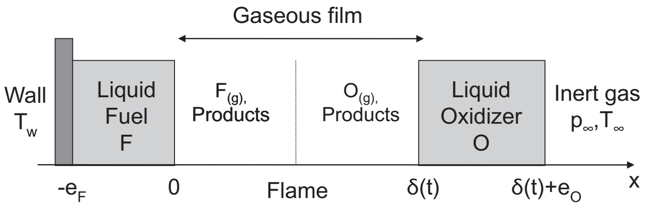

Fig. 1. Gaseous diffusion flame between two evaporating liquids.