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Evaluation of real-fluid flamelet/progress variable model for laminar hydrothermal flames

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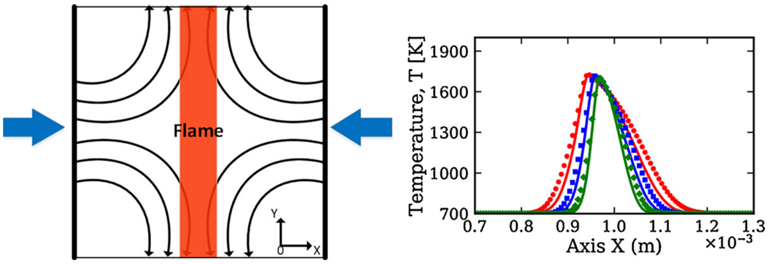
GRAPHICAL ABSTRACT



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ABSTRACT

In this article, hydrothermal flames were studied and an extended flamelet model was developed accounting for the real-fluid effects. The newly formulated real-fluid flamelet/progress variable (FPV) model was evaluated in a laminar counterflow configuration through both *a priori* and *a posteriori* analyses. At supercritical conditions, the ideal-gas model results showed a higher flame temperature and intermediate species mass fractions compared to the real-fluid model results in both the detailed chemistry (DC) and FPV approaches. To thoroughly evaluate the real-fluid flamelet library, the *a priori* tests were carried out under atmospheric and supercritical conditions with different strain rates. The comparisons of tabulated quantities and reference values from DC simulations showed that the real-fluid FPV model can correctly predict the thermal properties and species mass fractions in hydrothermal flames. Finally, the *a posteriori* analysis showed overall good agreement between the FPV and DC results, verifying the newly proposed real-fluid FPV approach.

1. Introduction

Hydrothermal flames are flames that are operated in supercritical aqueous environments ($P > 22.1$ MPa and $T > 647$ K) [1]. Under atmospheric circumstances, water is a kind of polar substance while it becomes non-polar under supercritical condition, which profits it to be an ideal medium for oxidation or combustion. In this case, non-polar gases such as O_2, H_2 and CO_2, and organic compounds such as CH_4 and CH_3OH can be miscible with supercritical water completely, forming a single homogeneous phase that has no inter-facial resistances. In that single-phase combustion, the combustion time scales are shortened and the reaction efficiency is improved compared with those in multi-phase combustion. Thus hydrothermal combustion is a promising solution for treating toxic organic wastes because of its high efficiency and ability to generate clean energy [1]. However, the underlying physics of hydrothermal combustion are not well understood yet. Improving the understanding of hydrothermal combustion is of great significance to enable the design and optimization of practical hydrothermal

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combustion devices.

The hydrothermal flames are difficult to study experimentally because the operating pressure is extremely high and measurement techniques are strictly restricted. The researchers at Swiss Federal Institute of Technology (ETH) successfully operated continuous hydrothermal flames in both transpiring-wall reactors (TWR) and wall-cooled hydrothermal burners (WCHB) [2–4]. In Ref. [4], several flames for different concentration of methanol in the supercritical water were studied and the flame temperature at the axis of the reactor was measured. Zhang et al. [5,6] developed a new transpiring wall reactor in which the fuel was preheated by the hot water to the ignition temperature of hydrothermal flames. The hydrothermal flame characteristics such as ignition and extinction processes were investigated. Concerning numerical studies, hydrothermal flames have been simulated to explore the operating characteristics of the reactors [7–9]. However, these simulations only considered one- or two-step reaction mechanism, in which no information of important intermediate species was available.

The flamelet model proposed by Peters et al. [10] is popular when dealing with combustion process because it consumes less computation resource without sacrificing detailed chemistry. It assumes that the local turbulent flame structure is thin and can be approximated by 1-D flamelets. This assumption is valid at sufficiently large Damkhler number and low Karlovitz number [11]. The task for simulating hydrothermal flames is more challenging because under such high-pressure circumstances the ideal-gas equation of state is no longer valid [12]. Proper equations of state (EOS) to predict the thermodynamic properties as well as the real-fluid models for transport properties of the mixture are necessary.

Recently, the aerospace community made a lot of efforts in improving the prediction of the combustion processes using the flamelet model coupled with real-fluid equation of state in rocket engines. Kim et al. [13] studied H_2/liquid O_2 flamelets at high pressures with a 1-D real-fluid flamelet model and the influence of real-fluid effects, pressure and O_2 inlet temperature on the flame structure were investigated. Lacaze et al. [14] studied the H_2/liquid O_2 flames under supercritical conditions in a 2-D laminar counterflow configuration and the results showed that the assumption of the flamelet model is satisfied under such conditions and the flame topology is strongly influenced by the real-fluid effects. More recently, Chong et al. [15] investigated the supercritical combustion of CH_4 and O_2 which is diluted by CO_2 using direct numerical simulations (DNS) and compared the DNS predictions with the generated 1-D diffusion flamelet results. It suggested that the dilution process weakens the heat release and broadens the flame zone, which may challenge the flamelet assumption.

Despite of the progresses for supercritical flames mentioned above, to the best of the authors' knowledge, there is no numerical study of hydrothermal flames using the flamelet method before. To apply the flamelet method for hydrothermal flames, there are three main aspects to be considered. First, because of the dilution of water, hydrothermal flames have lower flame temperatures which are close to the critical temperature of the mixture. Thus, the real-fluid effects may be significant and the influence of gas state models on the flamelet model performance needs to be investigated. Second, to evaluate the real-fluid flamelet method, the validity of the flamelets should be examined rigorously in the hydrothermal flames. Finally, the sensitivity of real-fluid flamelet model to parameters such as the strain rate should be understood and detailed comparisons of specie and thermal property distributions between the flamelet and reference results are desirable.

In the above context, this study is aimed to develop and evaluate the real-fluid flamelet/progress variable model (FPV) for hydrothermal flames under different operating conditions. To this end, a real-fluid FPV model is formulated, and then the performance of the FPV model is evaluated through both the *a priori* and *a posteriori* analyses in a laminar counterflow flame configuration. Particularly, in the *a priori* tests, the trajectory variables are obtained from the detailed chemistry (DC) simulation results and used to extract the thermochemical quantities from the flamelet library. The extracted quantities are compared with those in the detailed chemistry simulations to evaluate the accuracy of the flamelet library. In contrast, the trajectory variables are calculated by solving the corresponding transportation equations in the *a posteriori* tests, thus the performance of the flamelet model coupled with the flow solver is evaluated. The tests are operated under atmospheric and supercritical conditions at different stain rates to study different influencing factors on the FPV model performance.

2. Theoretical basis

In this section, the fundamental theory of the present study, including the real-fluid equation of state, formulas for thermodynamic and transport properties, governing equations for detailed chemistry model and flamelet/progress variable model, is provided.

2.1. Real-fluid equation of state and thermodynamic properties

It was shown that cubic equations of state (EOS) can well balance the conflicting of accuracy and computational cost [16]. In the present study, the Peng–Robinson (PR) cubic EOS [17] is employed to describe thermodynamic quantities, which can be written as:

$$P = \frac{R_g T}{V_m - b_m} - \frac{a_m}{V_m^2 + 2V_m b_m - b_m^2} \tag{1}$$

where R_g is the molar gas constant, T is the temperature and V_m is the molar volume. The parameters a_m and b_m account for the intermolecular attractive and repulsive forces, respectively, which are calculated with the mixing rules suggested by Poling et al. [18]:

$$a_m = \sum_i \sum_j X_i X_j a_{ij}(T) \tag{2}$$

$$b_m = \sum_i b_i \tag{3}$$

where X_i is the molar fraction of species i. The coefficient a_{ij} is a function of the mixture temperature and the critical point properties. Both a_{ij} and b_i were described in Ref. [18] and are not repeated here for the sake of brevity.

In order to ensure the self-consistency, other thermophysical properties of interest such as the specific enthalpy h and constant-pressure specific heat capacity c_p should be calculated from the same equation of state and these properties are given by:

$$h = G - T\left(\frac{\partial G}{\partial T}\right)_{p,X} = h^0 + \mathrm{pv} - \mathrm{RT} + K_1\left(a_m - T\frac{\partial a_m}{\partial T}\right) \tag{4}$$

$$c_p = \left(\frac{\partial h}{\partial T}\right)_{p,X} = c_p^0 - T\frac{(\partial p/\partial T)^2_{V_m,X}}{(\partial p/\partial V_m)_T} - R - T\frac{\partial^2 a_m}{\partial T^2}K_1 \tag{5}$$

$$K_1 = \frac{1}{2\sqrt{2}b}\ln\left[\frac{V_m + (1-\sqrt{2})b}{V_m + (1+\sqrt{2})b}\right] \tag{6}$$

where G is the Gibbs energy. h^0 and c_p^0 denote the low-pressure reference enthalpy and heat capacity, respectively, which can be calculated form the NASA thermodynamic data coefficients [19].

2.2. Real-fluid transport properties

In the present study, the Chung's [20] method based on the Chapman–Enskog theory is employed to predict the real-fluid transport properties. For supercritical fluid, the dynamic viscosity predicted by the Chung's method is a correction of the low-pressure viscosity η_0, which is given by: