

Mass transfer and combustion in transcritical non-premixed counterflows

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1 Introduction

Many practical systems like gas turbines, aero and automotive engines operate at elevated pressures. In the case of cryogenic rocket engines, which motivates the present investigation, pressure takes values as high as 40 MPa. The propellants, usually oxygen, hydrogen or methane are injected in a transcritical or supercritical state. Combustion under such extreme conditions is a topic of current interest and much progress has been made in the recent period. Experiments carried out in model scale facilities have provided information on the combustion process. This is exemplified in Juniper et al. [1] who provide results on high pressure liquid oxygen/ gaseous hydrogen (LOx/GH₂) combustion and by Singla et al. [2] who consider combustion of transcritical oxygen with supercritical or transcritical methane. The flame structure in the last case is quite unusual comprising two conical regions of light emission indicating chemical conversion of reactants, one close to the oxygen boundary and the other, near the outer methane boundary. The structure of such flames clearly differs from those observed in more standard conditions.

There are many recent numerical simulations of high pressure flames. These reflect the real gas behavior of supercritical fluids. For example, Harstad et al. [3] propose an improved equation of state for supercritical fluids. Direct numerical simulations of mixing layers under high pressure and temperature are carried out in [4]. Large eddy simulations of transcritical reactants are reported by Oefelein and Yang [5] and Zong et al. [6] in a coaxial configuration. A number of studies have focused on spherical droplets placed in a supercritical environment, see [7]. However, it is known from experiments that there are no droplets under transcritical conditions but that a highly wrinkled frontier separates the dense propellant from the surrounding lighter fluid. Mass transfer takes place from the dense region and is essentially governed by the amount of exchange area and the local turbulent state of the flow which can be described by the local strain rate. It is known that strained flames can be used to represent local elements of the turbulent flame so that this geometry is directly useful for modeling purposes. Some work is already available on high pressure counterflow flames fed by non-premixed reactants but under high temperature injection conditions. This geometry is considered in this article, but in the case of transcritical injection. Oxygen is injected at low temperature while methane is injected either in a

supercritical state or in a transcritical state.

This article begins with the treatment of real gas effects of transcritical fluids (section 2). Modifications of the balance equations to include real gas effects and corresponding mixing rules are briefly reviewed section 3. Results of simulations are discussed in section 4.

2 Thermodynamic and transport of transcritical fluids

In transcritical combustion, the reactants evolve from cryogenic temperatures, about 80K, to flame temperatures of about 3000K. This temperature range is quite large and it is important to predict accurately the fluid behaviour over the whole temperature range at a given pressure.

This requires a unified thermodynamic representation of transcritical fluids. This has been accomplished by developing a package of routines designated as TransChem describing real gas effects in ranges where the fluid departs from ideal gas behavior. In the case of ideal gases this set of routines coincides with the standard Chemkin library. Systematic tests of state equations were carried out for pure oxygen, hydrogen and methane. The conclusion of these tests is that the modified Peng-Robinson equation of state (eq. 1) [3]

$$p = \frac{RT}{V - b_m} - \frac{a_m}{V(V + b_m) + b_m(V - b_m)} \quad (1)$$

can be used to accurately represent the fluid behavior over the considered temperature range at high pressure. Mixtures of high pressure fluids are considered by means of mixing rules which apply to the coefficients of the equation, a_m and b_m . Thermodynamic properties are determined using the departure function formalism where any property is defined as a deviation from its standard state value.

3 Modelling strained flames under transcritical conditions

The modeling of transcritical flow or combustion poses a challenge because of thermodynamic departures from perfect gas behavior and transport anomalies. Balance equations and, if necessary, numerical methods have to be modified to take into account these phenomena. These problems are tackled by Meng and Yang [10] who developed a unified treatment of general fluid thermodynamics and transport in combination with a preconditioning scheme. The energy balance, developed in [10], is formulated in terms of temperature and, because of real gas effects this equation features many additional terms. The treatment proposed in the present article takes a different track. To avoid complexities of the temperature equation one may use an enthalpy formulation so that real gas thermodynamics only appears in the determination of the mixture enthalpy h , and of the species enthalpies, h_k ($k = 1, N$). This alternative formulation has been validated, and shown to be equivalent to the standard description and the modified flow solver can be used equally in real and perfect gas cases. Using standard notations [11] and equation of state (1), the corresponding set of equations for laminar transcritical strained flames is, as follows (ϵ is the imposed strain rate) :

$$\rho\epsilon\hat{U} + \frac{\partial(\rho v)}{\partial z} = 0 \quad (2)$$

$$\epsilon(\rho\hat{U}^2 - \rho_{+\infty}) + \rho v \frac{\partial\hat{U}}{\partial z} - \frac{\partial}{\partial z} \left(\mu \frac{\partial\hat{U}}{\partial z} \right) = 0 \quad (3)$$

$$\rho v \frac{\partial Y_k}{\partial z} + \frac{\partial}{\partial z} (\rho Y_k V_k) - \omega_k W_k = 0, \quad (k = 1, N) \quad (4)$$

$$\rho v \frac{\partial h}{\partial z} - \frac{\partial}{\partial z} \left(\lambda \frac{\partial T}{\partial z} \right) + \frac{\partial}{\partial z} \left(\sum_{k=1}^N \rho Y_k h_k V_k \right) = 0 \quad (5)$$

4 Results and discussion

Three cases are considered in this article : (1) Non-reacting opposite transcritical and supercritical oxygen flows, (2) Non-premixed strained laminar flames of transcritical oxygen against gaseous methane, (3) Flames formed by transcritical oxygen impinging on transcritical methane. The reaction mechanism, taken from reference [12] features 29 species and 141 reactions. Real gas thermodynamics and transport are obtained from TransChem library while complex chemistry is handled with Chemkin software [8]. The first problem is studied in order to examine the mass transfer between a dense low temperature fluid and the surrounding vapor. When the pressure is above critical, this mechanism replaces vaporization phenomenon. This analysis determines the rate at which transfer takes place under transcritical injection of oxygen. The mass transfer rate is obtained as a function of the strain rate for a chamber pressure of 7MPa. Transcritical oxygen is injected at 80K while the impinging oxygen jet is injected at 1000K. Results (not shown here) indicate that a strong density gradient, due to transcritical effects, appears in the mixing zone. The density evolves from a liquid-like density in the transcritical region to a gas-like density in the supercritical zone.

In the second case a flame is produced between oxygen injected at $z = +\infty$ in a transcritical state ($T = 80\text{K}$), with a liquid-like density of 1200 kg m^{-3} whereas methane, injected at $z = -\infty$ at 300K, has a density close to that of a gas (Fig. 1 (left)) for a chamber pressure of 7MPa. Simulations, carried out with these injection conditions, feature a large gradient of density between the oxygen injection zone and the flame region. This phenomenon is highlighted in transcritical flame experiments and is well retrieved numerically. The flame develops in the light-density region.

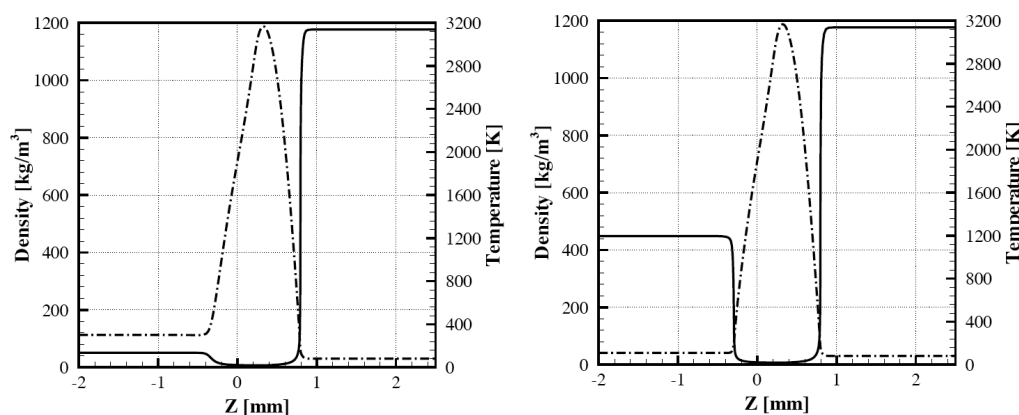


Figure 1: Density (solid) and temperature (— · —) profiles for oxygen / methane strained flames at 7MPa and $\epsilon = 20 \text{ s}^{-1}$ for different injection conditions : (left) oxygen is injected in a transcritical state, (right) oxygen and methane are injected in transcritical conditions.

In the third case which is relatively non-standard, both reactants are injected under transcritical conditions (Fig. 1 (right)). The chamber pressure is still 7MPa, and the methane temperature is reduced to 110K, the reactant densities of methane and oxygen are similar. The temperature profile is more symmetric than in the previous case. The flame thickness is slightly lower than that of the simple transcritical flame. The density profile features two strong gradient zones which confine the flame. Combining the temperature and density profiles one finds that the flame develops in the gaseous region as in the previous case, and the rate of burning is controlled by mass transfer from the two dense reactants.

5 Conclusion

A numerical study of non-premixed strained flames at high pressure is proposed in this paper. Methane / oxygen flames are treated for a pressure above critical and at least one reactant is injected at a temperature below its critical value. Transcritical fluids depart from perfect gases and feature transport anomalies. These phenomena are taken into account by using appropriate equations of state and transport laws which give accurate results at high pressure and in a large range of temperature. TransChem is new version of Chemkin developed to include these transcritical effects. In this context, it is convenient to use an enthalpy form for energy balance. This avoids inclusion of many additional real gas terms. With this unified treatment, simulations of high pressure strained flows and flames are carried out. A cold counterflow of transcritical oxygen against supercritical oxygen is chosen to simulate the behavior of a dense pocket surrounded by its own vapor. The mass transfer rate from the dense region is determined as a function of the strain rate. Reactive flow simulations are carried out at high pressure with a case where only oxygen is injected in transcritical conditions and also in the most extreme case where both methane and oxygen are injected in a transcritical state. The calculations feature strong density gradients. It is found that the flame develops in the gaseous region adjacent to the dense reactant (or reactants) and that the rate of burning is controlled by mass transfer from these region (or regions).

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