Numerical Simulation of LOx/CH$_4$ Supercritical Combustion in a non-Homogenous Mixture

Florian Monnier and Guillaume Ribert
CORIA - CNRS, Normandie Université, INSA de Rouen Normandie
76000 Rouen, France

1   Introduction

To ensure a correct description of the combustion process in a liquid rocket engine (LRE), validated chemistry is required as well as adequate thermochemistry and transport properties suitable for high-pressure conditions. In the literature, the kinetic schemes describing the combustion of methane with air are well validated at low-pressure, see for example the considerable work carried out on the GRI3.0 [15] mechanism, but studies remain scarce for higher pressure levels [12, 15, 20]. The present work concerns the design of the future European rocket which will require the use of methane as fuel and pure oxygen as oxidizer [11], for a pressure in the combustion chamber greater than 5.0 MPa. The RAMEC mechanism [12] or the one developed by Zhukov and Kong [20] can be used for such extreme thermodynamic conditions. However, the number of chemical species involved makes the numerical simulation of detailed or skeletal kinetic mechanism highly prohibitive [2, 3] in the case of high performance computing. As a consequence, a reduced CH$_4$/O$_2$ combustion mechanism has been recently designed [10] from RAMEC kinetic (38 species and 190 reversible reactions) [12] using the ORCh procedure [9]. The performances of this reduced mechanism (17 species and 44 reversible reactions) were examined through the computation of canonical cases to recover auto-ignition delays as well as the structure of laminar premixed and non-premixed flames, obtained with the detailed chemistry. A more severe test case, consisting in simulating the evolution of a O$_2$-CH$_4$ premixed flame in a homogeneous isotropic turbulent (HIT) environment at 56 bar, was also successfully performed. In the present study, the reduced chemistry is evaluated on a O$_2$-CH$_4$ non-homogeneous high-pressure mixture. Such a situation is closer to the cases encountered in real LRE where the methane is injected separately from the oxygen by means of a coaxial injector. In non-homogeneous mixtures, triple flames appear, which is a severe setup for testing the accuracy of reduced kinetic schemes over the entire range of equivalence ratio.

2   Configuration and Numerical Setup

Simulations are performed with the numerical code SiTCom-B [1, 6], which solves the conservation equations of species mass fractions, with complex molecular transport properties, momentum and total sensible

energy in their fully compressible form over the structured mesh in a finite volume formulation resorting to a skew-symmetric-like scheme for the convective fluxes [4] and to a fourth-order centred scheme for the viscous and diffusive fluxes. An addition of second and fourth-order artificial dissipation terms [16, 17, 19] is used to overcome spurious oscillations [13]. Time is advanced with a fourth order Runge-Kutta scheme. Navier-Stokes characteristic boundary conditions [13] are applied to describe in/outflows. Code acceleration for the calculation of chemical source terms follows the recommendations of [3].

The fully coupled conservation equations are thus summarized:

$$\frac{\partial U}{\partial t} + \frac{\partial F_c^j}{\partial x_j} + \frac{\partial F_d^j}{\partial x_j} = S \tag{1}$$

where the vector of conservative variables (U), the conservative variables flux vectors (F_c^j), the diffusive fluxes (F_d^j), and the source term vector (S), are expressed as,

$$
\begin{aligned}
U &= [\rho u_i, \rho E, \rho Y_k]^T, &(2)\\
F_c^j &= [\rho u_j u_i + \delta_{ji} p, \rho u_j E + u_j p, \rho u_j Y_k]^T, &(3)\\
F_d^j &= [-\tau_{ij}, -u_i \tau_{ij} + q_j, -\rho V_{k,j} Y_k]^T, &(4)\\
S &= (0, \dot\omega_E, \dot\omega_k)^T. &(5)
\end{aligned}
$$

u_i are the velocity components, E is the total non chemical energy decomposed as the sum of sensible energy and kinetic energy. Y_k is the kth chemical species in a pool of N_{sp} species. τ_{ij} is modeled with the Newtonian viscous stress tensor, and q_j, the jth component of the heat flux vector, is given for a multi-component flow in [7]. $\dot\omega_k$ is the chemical rate of species k and $\dot\omega_E$, the heat release due to combustion. To complete the above set of equations, the Soave-Redlich-Kwong (SRK) equation of state (EoS) is used

$$p = \frac{\rho R_u T}{W - b\rho} - \frac{\rho^2 a \alpha(T, \omega)}{W(W + b\rho)}, \tag{6}$$

instead of the ideal EoS, which is unable to predict correctly dense fluids. Eq. (6) links pressure, p, temperature, T and density, ρ. R_u is the universal gas constant and W the molecular weight of the fluid mixture, $W = \sum_{k=1}^{N_{sp}} X_k W_k$ with X_k the mole fraction of species k (among N_{sp} species). The Van der Waals mixing rules are used for mixtures:

$$a\alpha = \sum_{i=1}^{N_{sp}} \sum_{j=1}^{N_{sp}} X_i X_j \sqrt{\alpha_i \alpha_j a_i a_j} (1 - \kappa_{ij}) \quad \text{and} \quad b = \sum_{i=1}^{N_{sp}} X_i b_i. \tag{7}$$

κ_{ij} is the binary interaction coefficient. The constants a_i (attractive forces), b_i (co-volume of particles) and α_i are determined from universal relationships [14], involving the critical temperature and partial pressure of species k, T_{c_k} and p_{c_k}, respectively, as well as the acentric factor. The evaluation of such coefficients at high pressure is based on kinetic theory considerations for dense gas mixtures. They are expressed as $D_{kl}^{bin} = F_c \times D_{kl}^{bin,\circ}$, with $D_{kl}^{bin,\circ}$, the binary diffusion coefficients at standard pressure given by the kinetic theory of dilute gases [8], i.e. using polynomial fits, or coming from the empirical correlation of Fuller et al. [5, 14]. F_c is a correction factor that takes into account for volume effects. Using the Takahashi approach [18], the scaling factor F_c is tabulated as a function of the reduced temperature and pressure.

3   Results

The reduced chemistry proposed in [10] was used to follow the evolution of a premixed flame over time, but without any chance of observing non-premixed combustion. However, this combustion regime is that
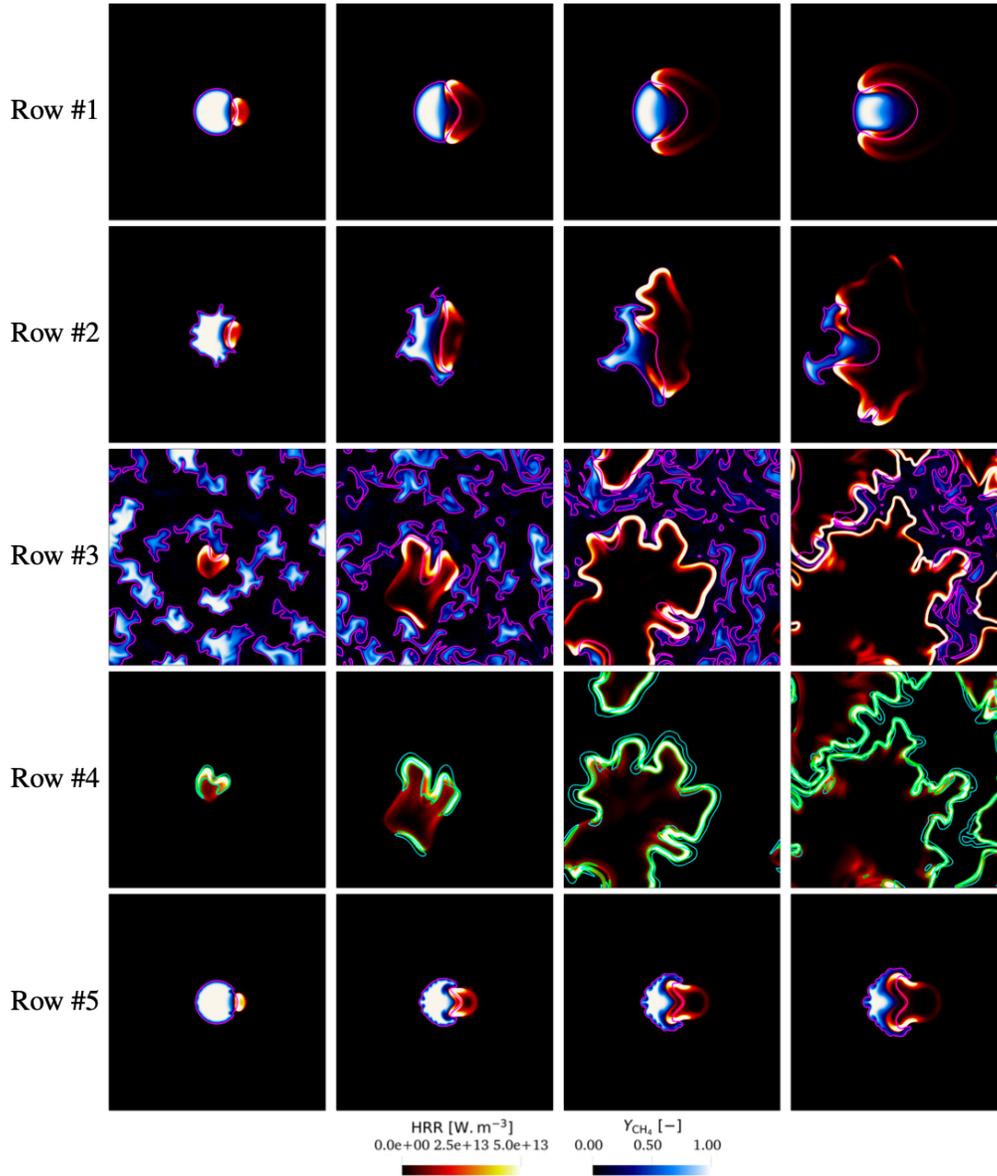

Figure 1: Temporal evolution of O_2/CH_4 combustion at 56 bar. Row #1: $T_{CH_4} = T_{O_2} = 300$ K, HIT *off*, 1 blob. Row #2: $T_{CH_4} = T_{O_2} = 300$ K, HIT *on*, 1 blob. Row #3: $T_{CH_4} = T_{O_2} = 300$ K, HIT *on*, multi-blob. Row #4: same as Row #3, comparison between reduced (green) and detailed (blue) chemistry on the heat release rate (line for $HRR = 2e13$). Row #5: $T_{CH_4} = 288$ K, $T_{O_2} = 85$ K, HIT *off*, 1 blob. Stoichiometric isoline in pink.

expected in the context of combustion in LREs, and one way of approaching this reality, but keeping a

feasible configuration in order to validate the new reduced scheme, is to consider one (or more) blob of methane surrounded by oxygen, and analyze the flame propagation mode once the mixture is ignited. A triple flame must thus appear, i.e. a non-premixed reaction zone will separate the lean premixed branch located on the oxygen side from the rich premixed branch located on the methane side. This benchmark will thus be decisive in the validation of the reduced kinetic scheme. In Fig. 1, a pocket of methane having a diameter of 3.0×10^{-5} m is fired using a hot spot of diameter 1.5×10^{-5} m. A two-dimensional uniform structured mesh is used (box 0.15 mm long) and each direction is discretized with 600 mesh cells, i.e. the mesh resolution is 0.25 μm. The pressure is set to 56 bar.

In Row #1, a twin flame spreads all around the pocket of methane from right to left before merging again. Each flame has three reaction zones, clearly visible on the field of heat release rate: one is on the methane side, the other one on the oxygen side, and the latter between the two first and located on the stoichiometric isoline and corresponding to a diffusion flame. The field of temperature develops around the pocket of methane and reach a value close to the one observed in 1D counterflow flames. The addition of turbulence (HIT parameters are similar to those used in [10]) to the velocity field (Row #2) results in multiple triple flames which follow the pockets of methane that break away from the initial methane blob. The complexity of the flow is exacerbated when multiple methane blobs are added to the turbulent velocity field (Row #3). Here again, triple flames appear and disappear locally according to the local composition of methane and oxygen. This case has been simulated with both reduced and detailed chemistry and a good comparaison can be observed in Row #4 on the heat release rate. The flame front location found with the reduced chemistry is somewhat delayed in time compared to the one found with the detailed chemistry. This behavior has already been observed in [10] on the simulation of premixed flames. Finally, in Row #5, when firing the dense ($\rho \approx 1200$ kg/m^3) and cryogenic ($T_{O_2} = 85$ K) oxygen, Rayleigh-Taylor-like instabilities, i.e. instabilities due to the difference in density of two fluids, appear prior to the flame propagation. Such instability is initiated by the pressure wave resulting from the addition of the hot spot to the cold flow at ignition. The flame propagation is similar to the one observed in Row #1 with a twin triple flame developing around the methane pocket. However, the propagation velocity is modified due to the fact that the flame is unable to surround the methane pocket, i.e. to follow the pseudo interface separating the oxygen from the methane. Rather, the flame pushes the dense blob to the left while consuming it.

4 Conclusion

The good performance of the reduced scheme proposed by Monnier and Ribert in [10] is evaluated on non-homogeneous O$_2$/CH$_4$ mixtures at high-pressure. When firing such mixtures, triple flames appear separating the methane blob from the surrounding oxygen. The behavior of the reduced scheme is compared with the results obtained using the detailed kinetic from which it was created. A very good agreement is observed on a configuration where multi-blob of methane interact with oxygen in a turbulent environment. Finally, when decreasing the temperature of the oxygen up to 85 K leads to the appearance of instabilities of Rayleigh-Taylor type which modify the propagation velocity of the resulting triple flame.

The present study shows that the reduced chemistry of Monnier and Ribert can be used to simulate high-pressure non-premixed flames.

5 Acknowledgments

References

[1] Bouheraoua L, Domingo P, Ribert G. (2017). Large-eddy simulation of a supersonic lifted jet flame: Analysis of the turbulent flame base. Combust. Flame 179: 199–218.

[2] Duboc B, Ribert G, Domingo P. (2019). Evaluation of chemistry models on methane/air edge flame simulation. Proc. Combust. Inst. 37: 1691-1698.

[3] Duboc B, Ribert G, Domingo P. (2019). Hybrid transported-tabulated chemistry for partially premixed combustion. Comput. Fluids. 179: 206-227.

[4] Ducros F, Ferrand V, Nicoud F, Weber C, Darracq D, Gacherieu C, Poinsot T. (1999). Large-eddy simulation of the shock/turbulence interaction. J. Comput. Phys. 152: 517–549.

[5] Fuller E, Schettler P, Giddings J.C. (1966). New method for prediction of binary gas-phase diffusion coefficients. Industrial and Eng. Chem., 58(11): 18–27.

[6] Guven U, Ribert G. (2018). Large-eddy simulation of supersonic hydrogen/oxygen combustion: application to rocketlike igniter. J. Propul. Power 34: 291–307.

[7] Guven U, Ribert G. (2019). Impact of non-ideal transport modeling on supercritical flow simulation. Proc. Combust. Inst. 37: 3255–3262.

[8] Hirschfelder J, Curtiss C, Bird R. (1954). Molecular theory of gases and liquids. New York: Wiley edition.

[9] Jaouen N, Vervisch L, Domingo P, Ribert G. (2017). Automatic reduction and optimisation of chemistry for turbulent combustion modeling: Impact of the canonical problem. Combust. Flame. 175: 60–79.

[10] Monnier F, Ribert G. (2021). Simulation of high-pressure methane-oxygen combustion with a new reduced chemical mechanism. *Combust. Flame*. DOI: 10.1016/j.combustflame.2021.111735.

[11] Patureau de Mirand A, Bahu J.-M, Gogdet O. (2020). Ariane Next, a vision for the next generation of Ariane Launchers. Acta Astronaut. 170: 735–749.

[12] Petersen E, Davidson D, Hanson R. (1999). Kinetics modeling of shock-induced ignition in low-dilution CH4/O2 mixtures at high pressures and intermediate temperatures. Combust. Flame. 117: 272–290.

[13] Petit X, Ribert G, Lartigue G, Domingo P. (2013). Large-eddy simulation of supercritical fluid injection. J. Supercritical Fluids. 84: 61–73.

[14] Poling B, Prausnitz J, O'Connell J. (2001). The properties of gases and liquids. McGraw Hill, 5th edition.

[15] Smith G, Golden D, Frenklach M, Moriarty N, Eiteneer B, Goldenberg M, Bowman C, Hanson R, Song S, Gardiner W, et al., GRImech 3.0 reaction mechanism, Sandia National Laboratory

[16] Swanson R, Turkel E. (1992). On central-difference and upwind schemes. J. Comput. Phys. 101: 292–306.

[17] Swanson R, Radespiel R, Turkel E. (1998). On some numerical dissipation schemes. J. Comput. Phys. 147: 518–544.

[18] Takahashi S. (1974). Preparation of a generalized chart for the diffusion coefficients of gases at high pressures. J. Chem. Eng. Jap., 7: 417-420.

[19] Tatsumi S, Martinelli L, Jameson A. (1995). Flux-limited schemes for the compressible Navier-Stokes equations. AIAA J. 33: 252–261.

[20] Zhukov V, Kong A. (2018). A Compact Reaction Mechanism of Methane Oxidation at High Pressures. Prog. React. Kinet. Mec. 43: 62–78.