Large Eddy Simulation of Super-Critical $CH_4/CO_2/O_2$ Non-Premixed Turbulent Oxy-Combustion

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Summary

- **Technology driving factors for real gas flow investigation.** High-pressure combustion in some industrial applications as in super-critical CO_2 gas turbine cycles, liquid rocket engines, diesel engines exhibit real gas behavior: different fluid properties has to be accounted for by means of real gas equations of state and specific models for molecular transport.
- **Issues in high-pressure combustion.** Physical and numerical models must be able to capture huge variations of fluid properties when crossing the pseudo-boiling line and high-density spatial gradients when dealing with liquid injection, without enhancing wiggle formation in fully compressible multi-species solvers.
- **Affordable equations of state.** Too complex and accurate real gas equations of state cannot be used in already time-consuming simulations, like LES and DNS.
- **Unknowns.** E.g.: the role of radiative transfer of energy; the reliability of chemical mechanims at such extreme conditions.

Numerical Set-Up of the HeaRT Code

- LES (dynamic Smagorinsky for turbulence; LTSM for combustion)
- Peng-Robinson EOS in its improved Translated Volume formulation
- Accurate modelling of diffusive transport mechanisms
- Accurate calculation of diffusive transport coefficients (NIST & kinetic theory)
- Accurate numerical schemes (RK3 in time; AUSM$^+$-up/WENO3-5 & C2nd in space)
- Radiant Transfer of Energy (RTE) through the M1 model:
  effect of increasing pressure strongly simplified: $\kappa_{P,300bar}(T) = 10^3 \times \kappa_{P,1bar}(T)$
- Simplified chemical mechanism: 6 species, 4 steps [Jones & Lindstedt]
- Constitutive relations (molecular diffusion of momentum, mass and energy):

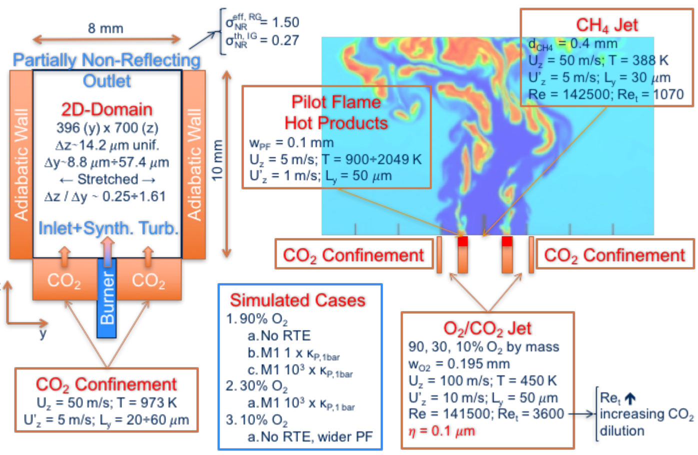
$$\boldsymbol{S} = (-p + \lambda \nabla \cdot \boldsymbol{u})\boldsymbol{I} + 2\mu \boldsymbol{E} = -p\boldsymbol{I} + \boldsymbol{\mathcal{T}}$$

$$\begin{aligned}\boldsymbol{J}_i &= \rho Y_i \boldsymbol{V}_i = \boldsymbol{J}_i^{HC} + \boldsymbol{J}_i^{BD} + \boldsymbol{J}_i^{S} = \\ &= -\rho Y_i D_i \left[\frac{\nabla X_i}{X_i} + \frac{X_i - Y_i}{X_i}\frac{\nabla p}{p}\right] - \mathcal{D}_i^T \frac{\nabla T}{T}\end{aligned}$$

$$D_i = \frac{1 - Y_i}{\sum_{j=1,\, j\neq i}^{N_s} \frac{X_j}{\mathcal{D}_{ji}}}$$

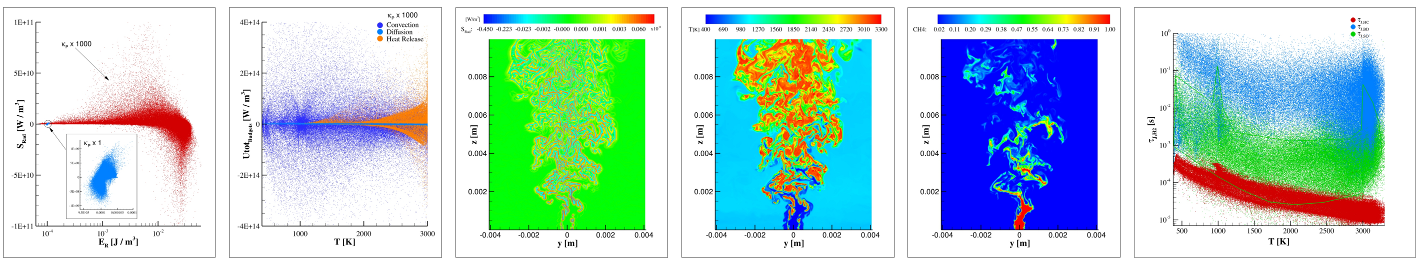
$$\begin{aligned}\boldsymbol{Q} &= \boldsymbol{q}_F + \boldsymbol{q}_{V_i} + \cancel{\boldsymbol{q}_D} = -K\nabla T + \rho \sum_{i=1}^{N_s} h_{s_i} Y_i \boldsymbol{V_i} = \\ &= -\rho\alpha \left[\nabla h_s - \sum_{i=1}^{N_s}\left(1 - \frac{1}{Le_i}\right) h_{s_i} \nabla Y_i\right] \\ &\quad - \sum_{i=1}^{N_s}\left[\rho Y_i D_i \left(\frac{\nabla W_{mix}}{W_{mix}} + \frac{X_i - Y_i}{X_i}\frac{\nabla p}{p}\right) + D_i^T \frac{\nabla T}{T}\right] h_{s_i}\end{aligned}$$

The "Numerical Experiment" Set-Up



- Simple shear-layers at inlet: no strategies to enhance mixing of reactants!
- Only the 90% O_2 case is analysed in detail here, since combustion exhibits anchoring problems and is not efficient in the other present cases.

The Role of Radiant Transfer of Energy and the Flame Structure



1. Very small differences in the flame structure when switching on the RTE model M1, and when intensifying the Planck mean absorption coefficient κ_P.
2. Energy budget analysis shows RTE source/sink term is negligible: in order, convection, heat release, diffusion, radiation, viscous work, gravity work.
3. Peak temperatures do not decrease: radiative cooling / chemical kinetics competition dominated by chemistry ($\omega \propto p$, p^2, p^3 for 1st, 2nd, 3rd order reactions; see energy budgets).
4. The gas becomes "grayer" at HP: negligible RTE effect also in [Caliot, 2014].
5. However, …
   - accurate calculation of κ_P is required from high-resolution spectroscopic databases to check if $10^3 \times \kappa_{P,1bar}$ is sufficient or not
   - … and turbulence / radiation interaction is neglected, although its contribution is expected to be enhanced in high-pressure combustors.
6. Flame stably anchored: small reacting pockets mainly aligned with streamwise direction close to injection, then evolving into larger scales downstream.
   - Reacting structures thinner than at lower pressures: accelerated kinetics
   - Flame corrugated by turbulence without exhibiting any laminar region
   - High momentum ligaments of O_2 and CH_4: isles of fuel (reacting later)
7. Ordered diffusive mechanisms rates: mass, heat, momentum (mass diffusion time is based on H_2 due to its low mass).
8. Among the mechanisms contributing to mass diffusion, the Hirschfelder & Curtiss effect is the most important; the Soret effect can compete with it at intermediate temperatures; the BaroDiffusion effect can be neglected.

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