realGasReactingFoam: 높은 압력의 압축성 반응 유동장을 위한 OpenFOAM 기반의 해석 솔버

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realGasReactingFoam: an OpenFOAM-based solver for compressible reacting flow at high pressure

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reactingFoam is a typical solver for simulations of multi-dimensional compressible reacting flows with using detailed chemical mechanism in OpenFOAM [1], but it is limited to low pressure simulations due to lack of real gas models. This work introduces a novel solver, *realGasReactingFoam* for studying of reacting flows at supercritical conditions. It is developed based on the study by Li et al. [2] and original *reactingFoam* solver with updated *thermophysicalModels* library including widely used real gas models such as modified Soave-Redlich-Kwong (SRK) equation of state, Chung model for dynamic viscosity and thermal conductivity and Takahashi model for binary diffusion coefficients [3]. In this solver, the following assumptions are applied. First a mixture with zero bulk viscosity assumption is adopted in which all thermodynamic and transport properties of a mixture are evaluated by using real gas models mentioned above. Second, mass diffusivity is based on mixture averaged model in which diffusion velocity is based on Fick's law with a consideration of correction velocity to ensure the global mass conservation [4]. Third, Soret effect, diffusion due to pressure gradient and body force are neglected in species conservation. Finally, Dufour effect and radiative heat transfer are also omitted in the conservation of energy.

The implementation of real gas models is first validated by comparing the generated thermophysical properties of major species against the experimental data of NIST [5], as shown in Figure 1. A good agreement between generated and benchmark data is observed, implying the excellent performance of the developed library in evaluating transport and thermodynamic properties of species.

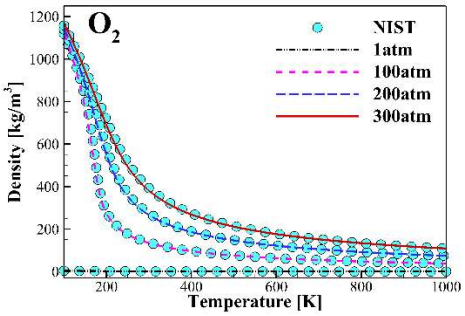

Figure 1. The density profile of pure oxygen species obtained from present work and NIST data [4] from 1 atm to 300 atm at different temperature.

The developed solver is then validated by performing two dimensional (2-D) simulations of laminar counterflow non-premixed flames of CH_4 versus O_2/CO_2 mixture at various pressures from atmospheric to supercritical pressure. However, only results at 200 atm is presented here. The results then are compared to those obtained using the OPPDIF [6] which has been incorporated the same set of real gas models and has been validated by a previous study [7].

In the present counterflow configuration, the fuel of CH_4 is issued from the lower nozzle while the oxidizer composed of 21% O_2 and 79% CO_2 by volume is supplied from the upper nozzle. The temperature of the fuel and oxidizer are 300 K and 1000 K, respectively. At both inlets, plug-flow boundary conditions are utilized. The flame and flow are characterized by using global strain rate, $\boldsymbol{a}$, which is defined as $\boldsymbol{a} = (|\boldsymbol{U_F}| + |\boldsymbol{U_O}|)/\boldsymbol{L}$, where U is the axial velocity, and L is the distance between the two inlets. The subscripts F and O represent the fuel and oxidizer inlets, respectively.

Figure 2 shows the streamlines of the flow

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and temperature field of 2-D steady laminar counterflow non-premixed CH_4 versus O_2/CO_2 flame at 200 atm with a global strain rate of 100 s^{-1} obtained from *realGasReactingFoam* solver using GRI-Mech 3.0 detail chemical mechanism.

Figure 3 presents the comparisons in the flame structure between data extracted along the central line of 2-D counterflow flame at 200 atm with the benchmark data computed by real-fluid based OPPDIF [7]. The results show a good agreement between two solvers, indicating the applicability of the developed solver for laminar reacting flows over the wide range of pressure. As a future work, the present platform will be further developed and validated for turbulent simulations at supercritical conditions.

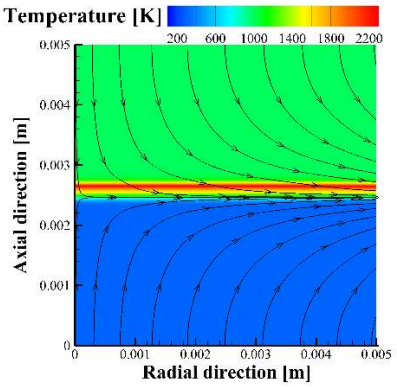

Figure 2. Streamlines and temperature isocontours of the 2-D laminar counterflow non-premixed CH_4 versus O_2/CO_2 flame at 200 atm obtained from *realGasReactingFoam* solver.

Acknowledgements

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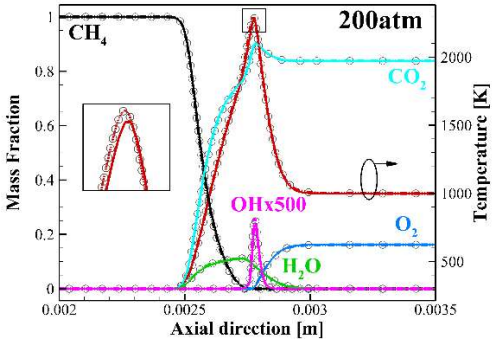

Figure 3. The profiles of temperature and species mass fraction of 1-D laminar counterflow non-premixed CH_4 versus O_2/CO_2 flame at 200 atm. Solid lines and symbols represent the data obtained from *realGasReactingFoam* solver and real-fluid based OPPDIF, respectively.

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