EFFECT OF RADIANT TRANSFER OF ENERGY IN HIGH-PRESSURE OXY-COMBUSTION

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Abstract
The aim of this work is to investigate the role of radiant transfer of energy in turbulent non-premixed methane oxy-combustion in an atmosphere rich in CO_2 at supercritical conditions by means of Large Eddy Simulation. A simple shear-layer configuration typical of slot burners is considered: the fuel is CH_4 and flows through the central slot, the oxidant O_2/CO_2 (90% O_2 by mass) mixture flows on both sides of the slot, and a pilot flame is imposed at the inlet between the two streams of reactants to force ignition. Another CO_2 stream coflows.
Fully compressible Navier-Stokes equations coupled to the Peng-Robinson cubic equation of state for real gases in its improved translated volume formulation are solved adopting the Large Eddy Simulation approach. The dynamic Smagorinsky and the LTSM subgrid scale models are used for turbulence and combustion closures. Among the diffusive mechanisms only the Dufour effect is neglected; transport properties are accurately calculated. The M_1 radiant transfer of energy model is adopted without considering turbulence-radiation interactions.

Introduction
The Radiative Transfer of Energy (RTE) is a very important mechanism in several applications. At industrial furnace and combustion chamber temperatures the gaseous species that absorb and emit significantly are CO_2, H_2O, CO, SO_2, NO, and CH_4. Other gases, such as N_2, O_2 and H_2, are transparent to infrared radiation and do not emit significantly; however, they become important absorbing/emitting contributors at very high temperatures. A non-negligible contribution to radiation is also provided by hot carbon (soot) particles within the flame and from suspended particulate material (as in pulverized-coal combustion).
Emission and absorption coefficients of gases increase proportionally to the concentration of the participating species, and hence to the mixture pressure for a given species mass or molar fraction. Besides, the spectral coefficients vary with temperature but also with pressure. Increasing pressure results in spectral line broadening, mainly due to molecular collisions (since the gas density increases) [1], up to wider and more overlapping lines than at lower pressures: the result is that the gas becomes ”grayer” (opaque).
When the total emission from a volume element of absorbing medium is to be calculated, the appropriate mean absorption coefficient is the Planck mean

absorption coefficient, k_P. The Planck mean is convenient since it depends only on the local properties and it can be tabulated. Values have been estimated in the past, but these are today known to be seriously in error, especially at higher temperatures and pressures.
This work is devoted to numerical simulation of methane oxy-combustion in supercritical carbon dioxide at 300 bar. Although adopting a simple chemical scheme, simplifying assumptions on the radiative transfer of energy and a two-dimensional computational domain, some interesting observations are highlighted, and needs for future work identified.

Physical and Numerical Models

The compressible Navier-Stokes equations are solved for a reacting real gas flow at supercritical conditions for which the Peng-Robinson cubic equation of state in its improved volume translated formulation is assumed. The mathematical models adopted are derived for a Newtonian fluid with the Stoke's assumption of N_S chemical species. The mass diffusion constitutive law assumed takes into account the Hirschfelder and Curtiss law for multi-component mixtures, the baro-diffusion and Soret effects. The heat diffusion flux takes into account the Fourier law and the mass diffusion fluxes, neglecting the Dufour effect.
Molecular transport properties for individual species are accurately modelled through NIST models for viscosity and thermal conductivity. The diffusion coefficient D_i of the i-th species into the rest of mixture is modelled according to the Hirschfelder and Curtiss expression, where the required binary diffusion coefficient is calculated by means of kinetic theory. The thermo-diffusion coefficient D_T is estimated by means of the EGLIB routines.
A simplified chemical mechanism consisting of 4 reactions and 6 species developed for oxycombustion is adopted [2, Table 2]. Since main radical species are not included in the mechanism, temperature is overestimated by more than 300 K. This is a first step before facing a more complex kinetics.
The transport equations are solved in the framework of Large Eddy Simulation. Unclosed turbulent combustion subgrid terms of the filtered compressible Navier-Stokes equations are modelled through the dynamic Smagorinsky model and the authors' LTSM (Localised Turbulent Scale Model) [3] turbulent combustion model.
The radiant transfer of energy is also taken into account by means of the M_1 diffusive model. For the time being, turbulence-radiation interaction is neglected, although it is expected to play an important role in flame cooling at the high-pressure conditions of the present simulations. Another simplification is the adoption of the individual species' Planck mean absorption coefficients typically used at atmospheric pressure. Since they are expected to increase by increasing pressure, the effect of multiplying them by 1000 is investigated. In the future they will be accurately calculated by using high-resolution spectroscopic databases.

The numerical simulations are performed by means of the in-house parallel code HeaRT and ENEA's supercomputing facility CRESCO [4]. The HeaRT code solves the compressible Navier- Stokes equations discretised through staggered finite-difference schemes. A second-order accurate centered scheme is adopted for diffusive fluxes; convective terms are modelled through the AUSM$^+$-up method coupled with a third/fifth-order accurate WENO interpolation to reduce spurious oscillations (strongly experienced using centered schemes in high-pressure tests); such numerical spatial scheme was extensively tested by the present authors proving its robustness and accuracy. The low-storage third-order accurate Runge-Kutta method of Shu-Osher is used for time integration. The total energy is defined as sum of internal (thermal) and kinetic energy only. The authors found this choice mandatory to avoid, or at least reduce, unphysical energy and temperature oscillations, mainly driving to the divergence of calculation. No spurious waves were experienced in previous simulations of premixed flames, when the total energy was defined including the chemical formation contribution.
Non-reflecting boundary conditions are implemented at open boundaries in their extended form to take into account the effect of variable transport properties, local heat release and real gas effects. It is observed that in previous and present real gas simulations the authors had to impose a higher value of the relaxation constant in the partially non-reflecting treatment of the outlet with respect to the ideal gas theoretical value (1.5 against 0.27) to avoid unphysical pressure drift in the whole computational domain. A synthetic turbulence generator is adopted at flow inlets.

The Numerical Experiment

The numerical experiment here simulated has a nominal pressure around 300 bar and consists in a simple shear-layer; the flow is confined by means of two no-slip adiabatic walls (at left and right of the domain). At the bottom of the computational domain there is the inlet, while the outlet is located at the top. Simulations are perfomed in a two-dimensional framework to reduce computational time. The domain Y x Z is 8 x 10mm, Y and Z being the transversal and the streamwise dircetions, respectively: it is discretised by means of 396 x 700 nodes.
The fuel is CH_4 and is injected centrally at 50m/s and 388K; its width is 4×10^{-4} m. The oxidant O_2/CO_2 mixture flows on both sides of the methane, and a pilot flame is imposed at the inlet between the two streams of reactants to force ignition. Each oxidant jet flows at 100m/s and 450K; their width is 1.95×10^{-4} m. The pilot flames imposed at the inlet exhibit a temperature distribution ranging from 900 to 2049K and a coherent distribution of chemical species; such data come from separate calculations previously performed; these hot gases flow at 5m/s and are 10^{-4} m widen. Adjacent to each of the oxidant streams, there is a coflowing stream of CO_2 at 50m/s and 973K. The (isotropic) turbulence characteristics of the jets are specified in terms of velocity fluctuations and auto-correlation length-scales: $u' = 5$m/s and $l_y = 3 \times 10^{-5}$ m for the methane jet; $u' = 1$m/s and $l_y = 5 \times 10^{-5}$ m for the pilot flames; $u' = 10$m/s and $l_y = 5 \times 10^{-5}$ m for the oxidant jets; $u' = 5$m/s and l_y

ranging from 2 to 6 x 10^{-5} m for the CO_2 coflowing streams. The length-scale l_y is the (transversal) scale on the inlet plane, while the orthogonal one is $l_z = 2l_y$. The methane jet Reynolds number (based on its bulk velocity and diameter) is nearly 142500 while its turbulent counterpart (based on the imposed velocity fluctuation and length-scale) is around 1070. The oxidant jet Reynolds number is nearly 141500, while its turbulent counterpart ($Re_{t\,Ox}$) is around 3600. The smallest dissipative scale expected comes from the $Re_{t\,Ox}$ and is nearly 10^{-7} m.
Three simulations are performed. The first, without considering the radiant transfer of energy (case NO-RTE); the second, switching on the M1 model with two different levels of absorption: in the case named 1 x k_P the individual species Planck mean absorption coefficients used at atmospheric pressure are adopted, while in the case 10^3 x k_P they are intensified by a factor 10^3.

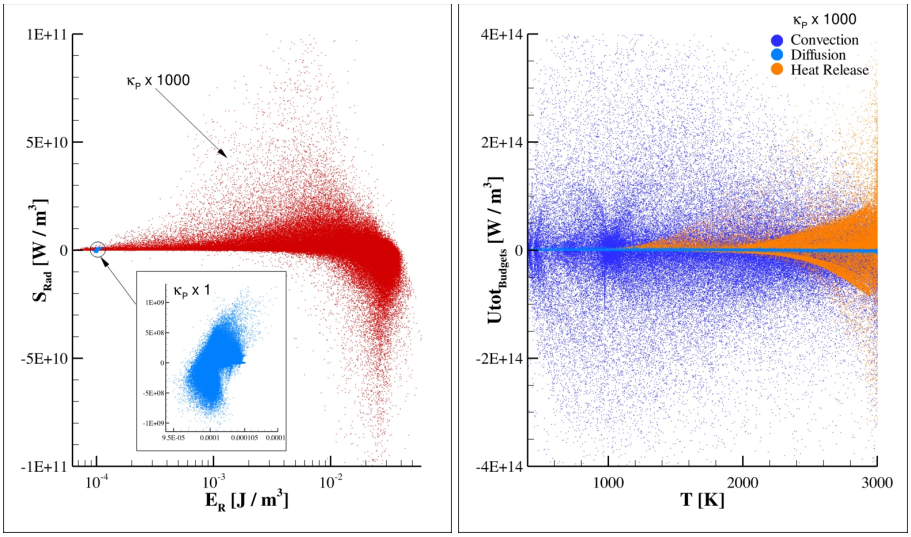

Figure 1. Instantaneous distributions of the radiative source term in the total energy transport equation versus the radiant energy density for two intensifying factors of the Planck mean absorption coefficient k_P (left). Instantaneous distributions of energy budgets related to convection, diffusion and heat release terms contributing to the total energy transport equation (right); contributions from viscous and gravity force works are lower and hence not reported.

Effect of Radiant Transfer of Energy

Comparing results obtained without considering the RTE model with those obtained using different intensification factors of the Planck mean absorption coefficients, very little differences appear in the flame. This happens despite the large differences in the radiation source/sink term of the energy transport equation shown in Fig. 1 (left). This behaviour can be easily understood by comparing the energy budgets of the different terms contributing to the total energy transport and shown in Fig. 1 (right). The order of magnitude of the work done by the gravity

force is 10^5W/m^3; the viscous work is of the order of 10^8W/m^3; since they are order of magnitudes lower than the other terms, they are not shown. Then, in the ordered list of budgets there is the radiative source term with 10^{10}W/m^3, followed by the heat diffusion term with 10^{11}W/m^3. It can be concluded that in the present simulation the effect of radiant transfer of energy is negligible even with the intensifying factor 10^3 for the k_P . However, accurate calculation of the Planck mean absorption coefficients from high-resolution spectroscopic databases is necessary to really understand if the intensification factor 10^3 here adopted is justifiable, sufficient or not. Besides this, it is reminded that turbulence/radiation interaction has not been taken into account in this work, although its contribution is expected to be enhanced in high-pressure combustors [5, 6].

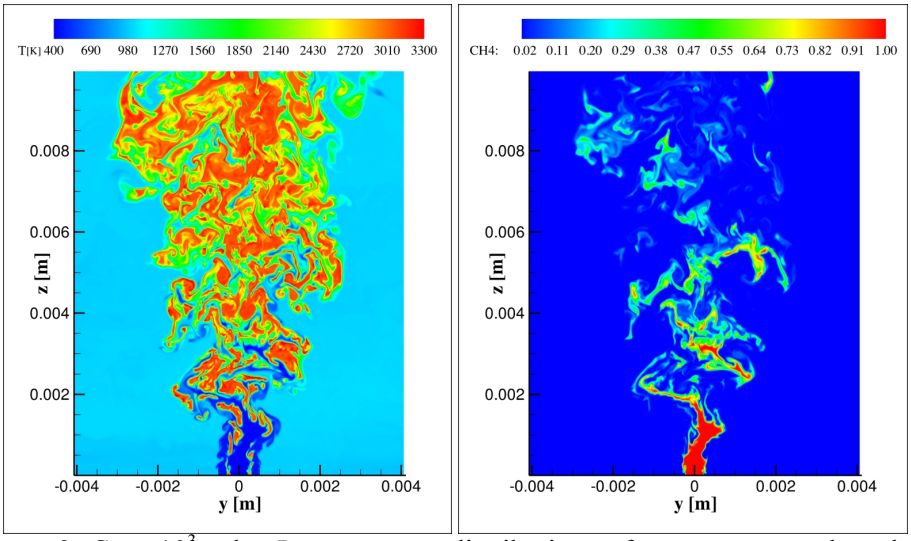

Figure 2. Case 10^3 x k_P. Instantaneous distributions of temperature and methane mass fraction.

It is observed that radiation cooling is active in the hottest regions of the flame but it produces a negligible effect, i.e., peak temperatures do not decrease due to radiation transport. As a matter of fact, the competition between the enhanced radiative cooling expected and the enhanced chemical kinetics (both due to the high pressure) is here dominated by chemistry, in agreement with the heat release budget that is four order of magnitudes greater than the radiative budget. Instantaneous distributions of the radiative source/sink term show that it is localized in thin layers. Although not shown, the results evidenced that radiative cooling (associated to negative values of S_{rad}) in this flame is limited to a very thin layer localized around the stoichiometric mixture fraction and it is more frequent in the hot products side ($Z < Z_{st}$).

Once clarified that in the present simulations the effect of radiation is negligible, let's examine the structure of the flame. The flame is stably anchored, showing

small reacting pockets mainly aligned in the streamwise direction close to the injection, and evolving into larger scale reacting regions moving downstream, as revealed by the temperature snapshot in Fig. 2 (left). The reacting structures are thinner than those typically encountered at lower pressures: this is due to the accelerated chemical kinetics promoted by the high-pressure condition. The methane distribution associated to the same instant is reported in Fig. 2 (right) showing that the jet is corrugated by turbulence without exhibiting any laminar region on its boundaries. High-momentum O_2 ligaments penetrate the methane jet as well as CH_4 fingers also develop into the coflowing stream, thus producing isles of fuels later developing in reacting pockets.

Conclusions

The present real gas simulations prove the robustness of the numerical schemes implemented in the HeaRT code to simulate high-pressure oxy-combustion in s-CO_2 atmosphere. Neglecting turbulence-radiation interaction and with the simplified assumptions on the k_P, it was shown that RTE is negligible; in the future high-resolution spectroscopic databases will be adopted. A further improvement will be a chemical mechanism with radical species.

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