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Computational Techniques for Thermochemical Propulsion

Report: Assignment 4

Combustion between air and hydrogen

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1 Introduction

1.1 Physics and quantities of interest

In this assignment the combustion between air and hydrogen is simulated inside the 2D combustor. The spray with the lagrangian particle tracking and the thin liquid film model are deactivated for this purpose. Hence hydrogen is inserted into domain through the fuel inlet boundaries into a gaseous form. To do so the combustion and chemistry mechanisms, which were not implied in the previous assignments, need to be activated.

Since the two models mentioned above are not needed the thickness of the thin film and the thermodynamic properties of the liquid contained by it are not used anymore. For the same reason the dimension and the position of the liquid particles, not present anymore, are not integrated in time anymore.

1.2 Precursor simulation and boundary conditions

As requested the flow is entering the domain at 1050 K, and this high temperature is an important condition to start the reaction, because it enhances the diffusivity and the rate of each elementary reaction. Before simulating the combustion a precursor simulation is done with the air flow entering the domain at the imposed temperature and with no fuel entering through the fuel inlet. To do so the inlet boundary condition for temperature is modified among with the boundary conditions at the fuel inlet, where the the same condition as the walls is set for each field of interest. Additionally the `wall` BC needs to be imposed inside the `blockMeshDict` for the fuel inlet. The problem is integrated for 0.5 seconds and the last timeset is set as initial condition for the new problem by means of the `mapFields` function.

In the main simulation of the actual study case the variable for the mass fraction of C_7H_{16} is substituted by the one for H_2 , the initial condition for the internal field is imposed to be uniform and equal to zero while at the fuel inlet the same velocity of the previous assignments is imposed as boundary condition. As in the third assignment the initialization of the combustion products, which are different for this problem, is not needed and it is automatically done by the solver.

1.3 `physicalProperties` and `speciesThermo`

The `physicalProperties` file does not differ significantly with respect to the baseline. The Heptane fuel is removed from the liquid species specification setting and the `speciesThermo` is introduced as before. In this case the `speciesThermo` specifies the thermodynamic quantities and the interpolation coefficients for the specific heat capacity at constant pressure and it is referred to the reactants and products specific for this problem.

1.4 `CombustionProperties`, `chemistryProperties` and reactions

These input files are needed to introduce the combustion into the problem. In the combustion properties the combustion model is specified as PaSR which is suitable for finite rate combustion problems where neither the reaction rate nor the turbulence mixing rate are infinitely fast.

Inside `chemistryProperties` the settings for the Ordinary differential equations for the chemical reactions are specified while in `reactions` file the elementary reactions for the combustion mechanism are defined among with the empirical coefficients for the reaction rate. These properties, as for the thermodynamic quantities, are valid for a limited range of temperatures.

2 Results

2.1 Setup and Convergence analysis

As in assignment four the adopted solution method is PISO, with two internal loops, alternating the solution of the Helmholtz equation with the equation for the correction of velocity, which value is then used in the former one to have a better estimation of pressure. This is done in one single outer iteration, therefore a different criterion in evaluating the convergence of the solution shall be adopted.

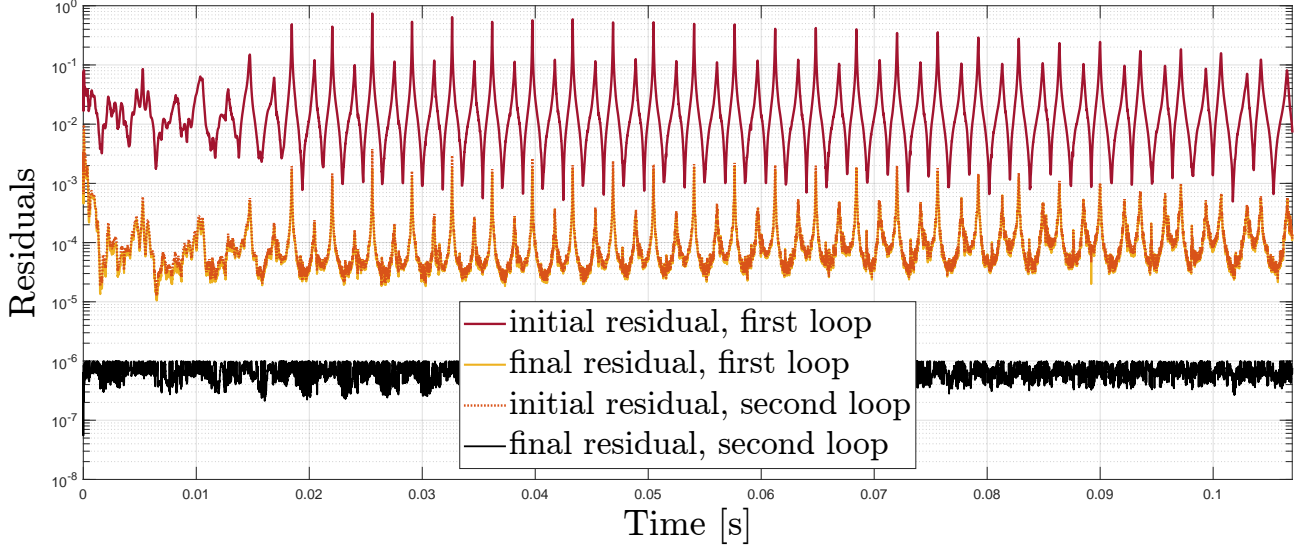


Figure 1: Residuals evolution in time for the pressure field, where the hydrostatic contribution is removed.

Fig. 1 shows the residuals for the pressure field without the hydrostatic contribution (p_{rgh}) for different iterations within each single timestep. Two residuals, the initial and the final one in the Helmholtz solution, are considered for each one of the two internal loops. The red curve is characterized by the highest values, which is reasonable since it's the first iteration of the relative timestep, after the integration in time, and it is strictly related to the evolution of the flow in time. For a steady flow, this term would tend to decrease in time but this system is determined by intense fluctuations. The cause for this could be an interplay between fluidynamics and combustion, hence pressure oscillations are a common phenomenon in combustors. The initial residual is then reduced up to the final one (yellow trace) by iterating the pressure equation. It has been verified that only one iteration is needed in order to satisfy the residual control setting of 0.1. Between the two solutions of the linear system of pressure the velocity is corrected and reinserted inside of it. It can be seen that very small variation on the residual (from yellow trace to the orange one) is achieved by this process and this could be an indication of a good coupling between pressure and velocity.

The residual is then strongly reduced inside the second internal loop, until the pressure residual tolerance of $1e-06$ is reached. And this is achieved for every single timestep of the simulation.

2.2 Post processing

The 2D temperature contour for this simulation is presented in Fig. 2. On top of it the isolines representing the stoichiometric air to fuel ratio and oxydizer to fuel ratio are plotted. The colours characterizing the two isolines are respectively black and white. To retrieve them the two ratios are computed in each single cell of the domain as in 1 and 2:

$$\frac{Y_{O_2} + Y_{N_2}}{Y_{H_2}} - AF_{st} = 0 \quad (1)$$

$$\frac{Y_{O_2}}{Y_{H_2}} - OF_{st} = 0 \quad (2)$$

In this way the two ratios are imposed equal to their stoichiometric values, 31.13 and 8 respectively. In the first case the assumption of constant composition for the air is imposed. For this reason there is small discrepancy between the two definitions in the results and this is due to the finite rate combustion mechanism. Hence the oxidizer and the fuel do not react across a layer with infinitesimal thickness and the oxygen starts reacting as soon as flammability condition is satisfied, before reaching the stoichiometric ratio with the hydrogen mass fraction, which is obtained when part of the reactants have been already consumed and the air composition is different from the original one.

On the contrary the second isoline defines in a proper way when the reactants are in a stoichiometric condition, hence in the same region also the maximum temperatures are reached.

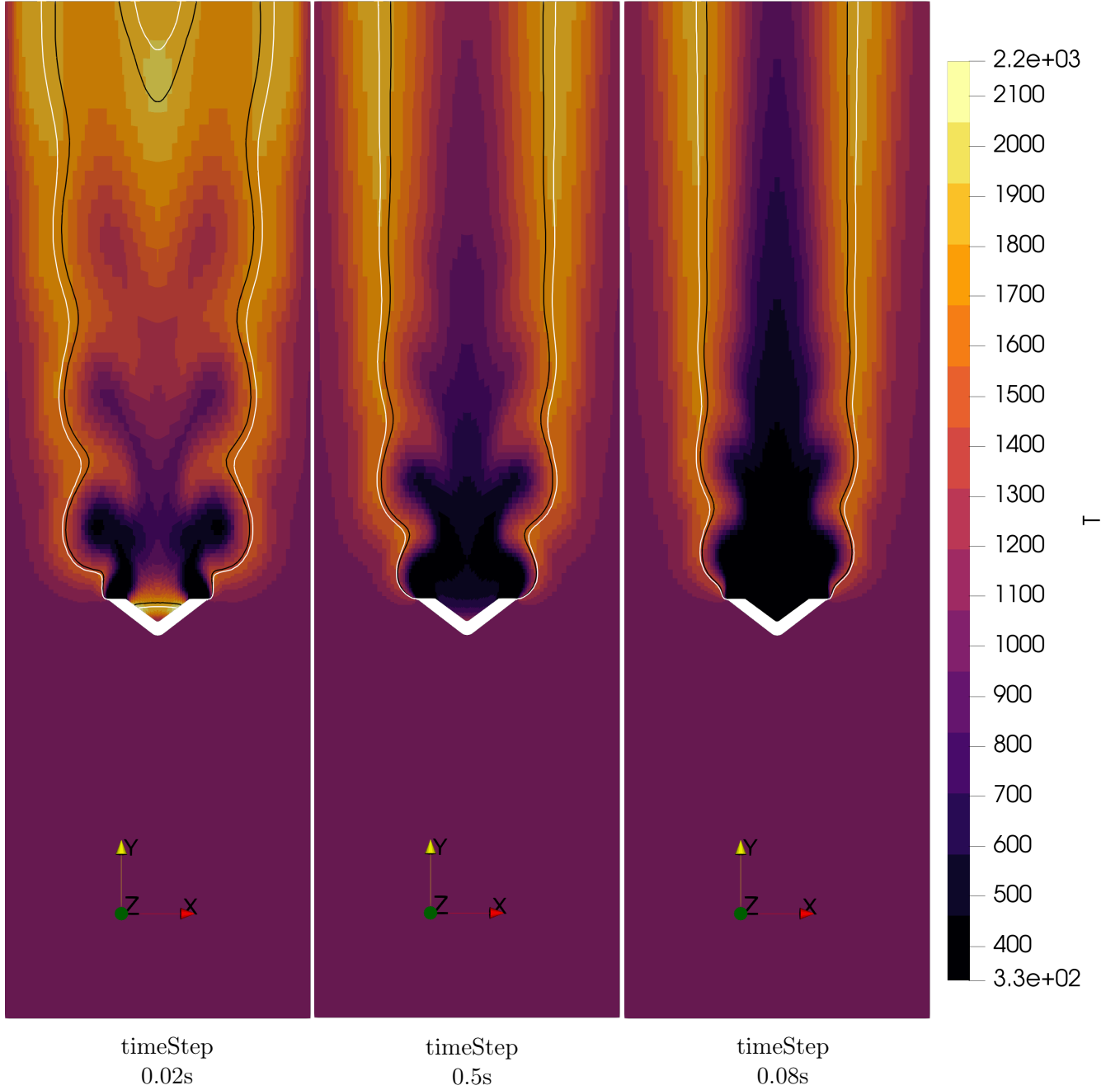


Figure 2: 2D contour for the temperature field expressed in K, for timesteps 0.02s, 0.05s and 0.08s. In addition the isolines for the stoichiometric AF and OF ratio condition, respectively in black and white.