Modelling of Combustion and Heat Transfer in Rocket Combustion Chambers Using CFX

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Summary

The paper presents a review of three successful works done at the Institute of Space Propulsion (DLR-Lampoldshausen) on modelling processes in rocket combustion chambers. ANSYS CFX was used for CFD modelling of combustion and heat transfer in all three cases. The first work is a methodological study on problems associated with the usage of finite rate chemistry model in CFD simulation. The second work is an example of modelling of flow and heat transfer in porous media using CFX. The third work is devoted to modeling of combustion in a subscale rocket combustion chamber. In all considered works the good agreement of the numerical results with experimental data was obtained. The good agreement with experimental data was achieved by extending functionalities of CFX with the help of user defined CEL (CFX Expression Language) functions. For rocket engines heat transfer predictions are of particular importance. For this reason, the transport properties were modelled using empirical equations which are more accurate than the built-in function of mass averaging.

Keywords

Combustion modelling, Heat transfer, Liquid rocket engines, Hydrogen, ANSYS CFX

1. Motivation

Accurate prediction of heat loads is one of the key problems of rocket engine design. At the current moment the design of rocket combustion chambers requires an extensive trial-and-error testing. CFD (computational fluid dynamics) modelling offers a means to reduce the amount of expensive hot-fire tests while the abilities of computing machines and programs are constantly growing. The goal of the current work is the accurate predictions of the wall heat fluxes in a rocket combustion chamber.

2. Combustion modelling using Finite Rate Chemistry model

The active use of ANSYS CFX [1-2] began at the Institute of Space Propulsion (DLR-Lampoldshausen) ten years ago. At that time, the task of CFD modelling of rocket combustion chamber was considered as impossible. For this reason, a small subscale combustion chamber operated at low pressures was set as the first target for CFD modelling. The chamber had small dimensions: 60 × 60 × 140 mm^2 and operated with hydrogen and oxygen and had two different ignition regimes: smooth and strong ignition [3]. The strong ignition was characterised by a strong pressure peak, so there was a need of CFD modelling in order to understand the origin of the ignition regimes.
The finite-rate chemistry model was chosen as combustion model for the CFD modelling, as the most universal model. There are many different reaction kinetic models of hydrogen oxidation ranging from global reaction model to detailed reaction mechanisms. Therefore, before carrying out the CFD modelling the testing of different hydrogen kinetic schemes was done [4]. A one-step, a two-step, an abridged, a skeletal and four detailed kinetic schemes of hydrogen oxidation were tested.

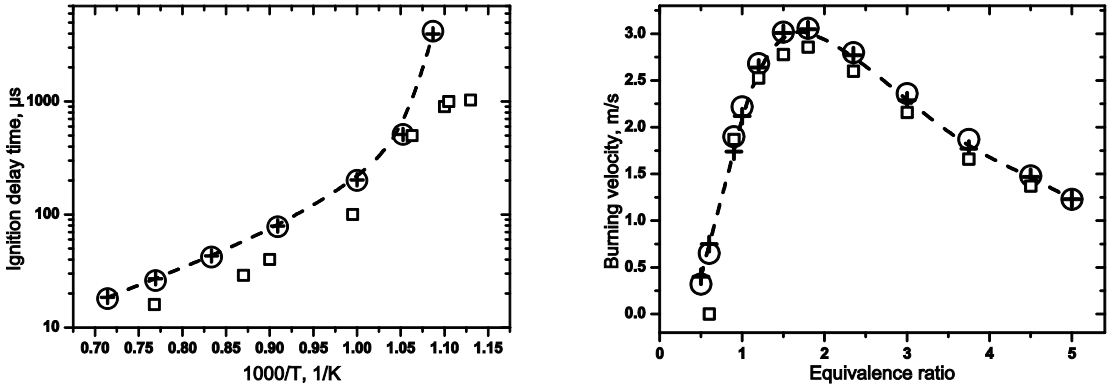

Figure 1: Comparison of the simulating data obtained using ANSYS CFX and CHEMKIN. Squares – the experimental data on ignition and burning of a stoichiometric hydrogen-air mixture at 1 atm [5,6]; dash line (B-spline) and crosses – modelling with the use of ANSYS CFX, big circles – modelling with the use of CHEMKIN [7].

First, all tested kinetic models models were verified against calculations with the use of 0D and 1D numerical codes. The ignition of H_2-O_2 mixture at constant volume and hydrogen freely propagating flame, which are two the most typical combustion problems, were simulated using ANSYS CFX for the verification of the reaction models, see Fig. 1. The verification showed that kinetic equations ("chemical source") may be solved correctly only with a proper numerical setup. Foremost, the finite rate chemistry model requires the use of the special solver option: "stiff chemistry". The need for the use of this option emanates from the fact that chemical reactions are characterised by different timescales. Therefore, to solve kinetic equations correctly it necessary to integrate equations using a time step related to the smallest timescale over a time interval related to the largest timescale. As was shown in work [4], the difference between reaction rates (i.e. time scales) of some reactions can reach ten orders of magnitude in hydrogen flames. This leads to the need for the use of a very small time step for solving the Navier–Stokes equations while the option "stiff chemistry" allows using a larger time step.

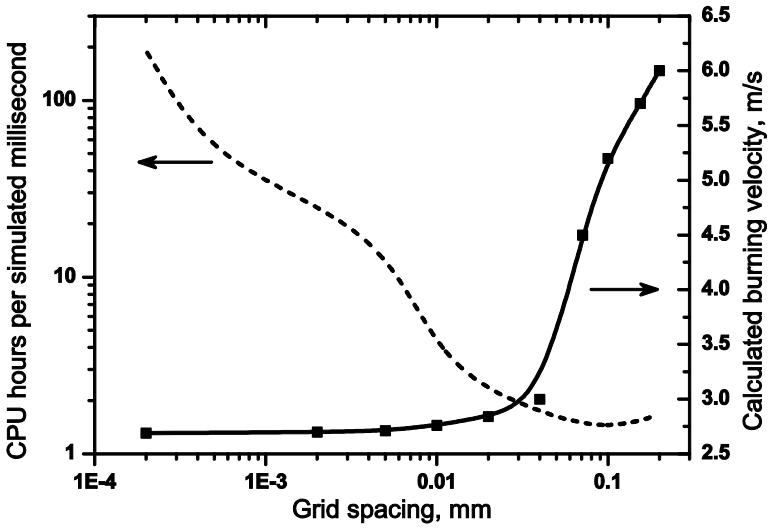

Figure 2: Simulating results and computational cost as the function of grid spacing. (Hydrogen–air mixture at 1 atm, kinetic model [4]).

The second requirements for the correct calculations of the chemical source in the Navier–Stokes equations in CFX is that the numerical mesh should be fine enough in order to resolve the flame front, which has a thickness from 1 μm to 100 μm. (The thickness of flame front depends on pressure and mixture composition.) The use of fine grid, of course, increases the required computational time, see Fig. 2; however, it is the only way to obtain the correct value of burning velocity in simulations. As one can see on Fig. 2, the burning velocity virtually becomes independent on mesh resolution after resolving flame front which is about 40 μm at given conditions and approaches asymptotically to the correct value of burning velocity which equals to ~2.5 m/s at these conditions.

The comparison of the different hydrogen kinetic mechanisms with the experimental data is presented in Fig. 3. The comparison showed that the detailed kinetic schemes are more accurate than the reduced ones. The simulations showed the common trend for kinetic models: more details – higher computational cost – higher precision. The simulations of the combustion of hydrogen-air mixture showed that the accuracy of global reaction mechanisms is not enough for the simulations of ignition; however, hydrogen flame can be adequately simulated with the use one-step and two-step kinetic models.

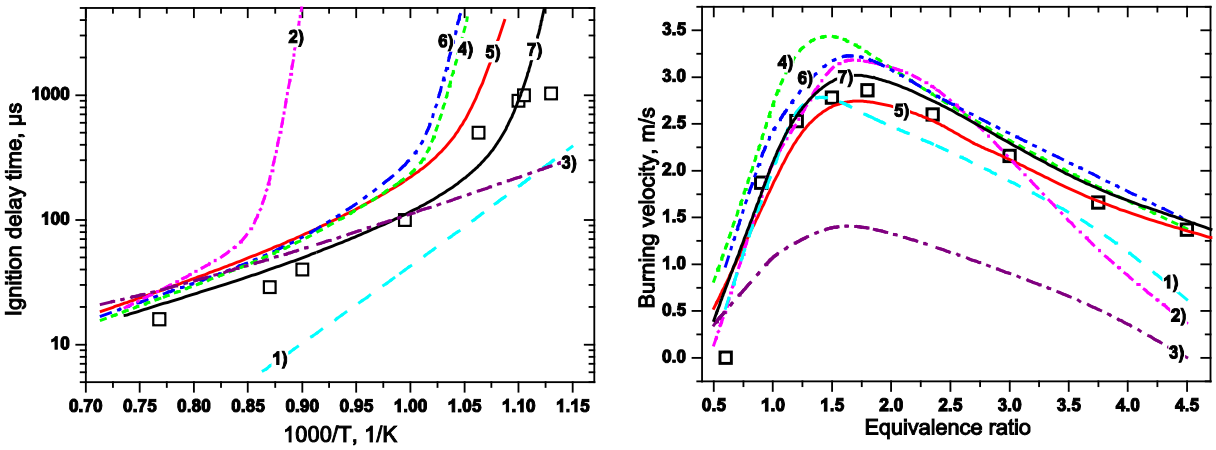

Figure 3: Ignition delay times and burning velocities of a hydrogen-air mixture at 1 atm. Squares – experimental data [5,6]; (1) dash cyan line – one-step kinetic model; (2) dash dot magenta line – two-step kinetic model; (3) dash dot purple line – abridged reaction mechanism (6 species, 7 reactions); (4) dash line green – skeletal mechanism (8 species, 13 reactions); (5-8) solid red line, dash dot dot blue line, solid black line, and dot orange line – different detailed hydrogen mechanisms (21–29 reactions).

The good agreement with the experimental data would be impossible without the accurate modelling of the transport properties of gas mixture and mixture components. According to the analysis of Zeldovich and Frank-Kamenetskii, the laminar burning velocity is proportional to the square root of the diffusivity in burning gases [8]. Therefore, it is important to model correctly the transport properties of gas mixture when the flame propagates in CFD simulations through the heat and mass transfer

3. Modelling of heat transfer in porous materials

The application of porous materials can improve the performance of rocket combustion chambers. A porous injector head can provide effective mixing of fuel and oxidizer at low pressure drop in the injector head. This new injection concept is being under development at the German Aerospace Center (DLR-Lampoldshausen) [9,10]. Nowadays the porous injector faceplates are used in some rocket engines (for example: SSME and J-2) where the small fraction of the fuel flow is fed through the porous injector faceplate in order to cool it; whereas, the main part of the fuel is still injected through coaxial injectors. Coaxial injectors proved their efficiency, but they require a very precise manufacture and keep their efficiency in the narrow range of mass flows, which is bounded from above and below. These problems can be easily solved by the application of a porous injector head. According to the hot-tests at DLR-Lampoldshausen the porous injector head (Fig. 4) allows to maintain the high combustion efficiency over the wide throttling range from 37.5% to 125% [10]. Besides the manufacture costs and the throttling capability, porous injector head has two additional advantages over conventional coaxial injectors. Porous injector head operates at a smaller pressure drop than injector heads with coaxial injectors. The small diameter of the injectors in a porous head results in a small jet break-up distance which allows reducing the chamber length. Such features improve the performance of rocket engines.

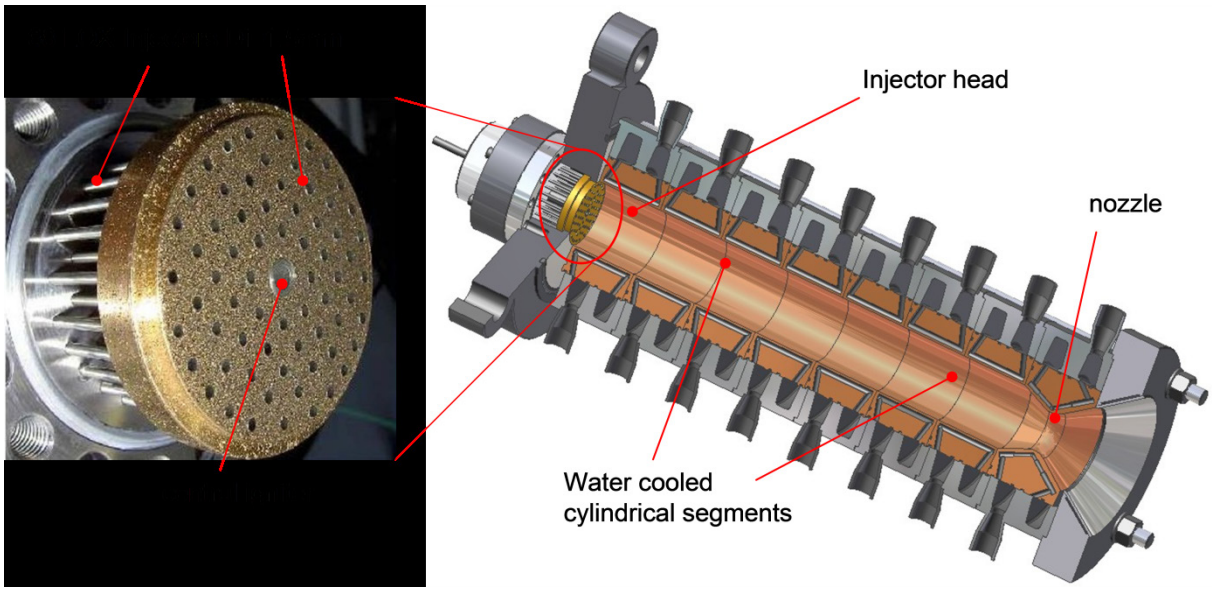

Figure 4. Photo of porous injector head API-68 and the cross-section of the sub-scale combustion chamber model ”B” [11].

Rocket combustion chambers are exposed to severe thermal loads during the burn. The components of a thrust chamber assembly (injector head, side walls, and nozzle) require adequate cooling. The proper design of an injector head needs the knowledge of the heat fluxes inside the chamber. The problem of heat management in a porous injector head was studied theoretically in work [12] by Zhukov and Haidn. They considered the heat conduction problem in porous material in one-dimensional settings, see Fig. 5. The problem had the following boundary conditions. Heat flux Φ was incident on the porous wall of the thickness l from one side. From the other side the cold fluid with temperature T_0, density ρ, and velocity v flowed into the porous wall.

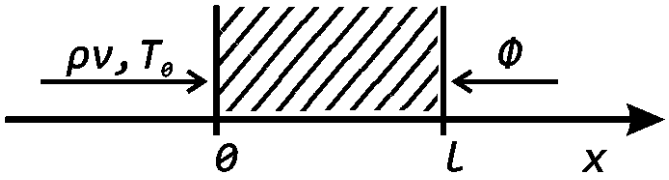

Figure 5. Schematic representation of the boundary conditions.

The equations for the heat transfer in the cooling media and porous matrix can be reduced significantly when the following considerations are taken into account:

- the flow and boundary conditions are stationary;
- the thermal conductivity of cooling fluid is negligible in comparison with the thermal conductivity of the porous material and the advection of heat by the flow.

The last condition requires that the velocity of the flow is large enough, namely,

$$\rho_f v_f c_f \gg 0.5\sqrt{\alpha\lambda}\,,$$

where c_f is the heat capacity of the cooling fluid, α is the heat transfer coefficient between porous media and fluid, and λ is the thermal conductivity of porous material. This condition is hold well in rocket injector heads, through which propellants are fed at very large flow rates. After the simplification and the reduction of order of the equations, they were solved analytically. The analytical solution gave the expression for the temperature inside porous media as well as for the temperature at the hot gas side:

$$T_{hot} = T_0 + {\Phi}/{\rho_f v_f c_f} + {\Phi}/{\sqrt{\alpha\lambda}}\,,$$

which connects the temperature of the hot-gas wall with the incident heat flux, and the properties of fluid flow and porous matrix.

To support the obtained results the modelling of conjugate heat transfer in porous materials was performed using ANSYS CFX. In contrast to the analytical solution, the numerical solution neither required the additional assumptions about the properties of the fluid and the flow nor imposed the constraints on the thermal conductivity of coolant and the flow velocity. The typical conditions of the hot tests of the combustion chamber “B” with the porous injector head API-68 [11] were taken as the boundary conditions. In the modelling the properties of porous media corresponded to the properties of sintered bronze SIKA-B 150. The comparison of the analytical solution with the numerical solution is presented in Fig. 6.

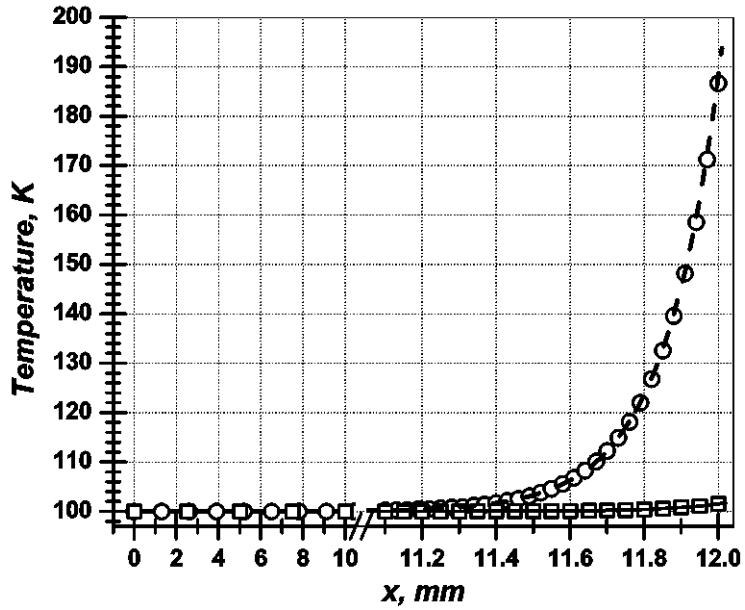

Figure 6. Comparison of the numerical (points) and analytical (lines) solutions. Temperature of the cooling fluid – solid line and squares, temperature of the porous media – dash line and circles.

As one can see, the temperatures obtained analytically and numerically coincide with each other very well. The analytical solution disregards the thermal expansion of cooling fluid. This simplification is valid in this particular case; however, the numerical solution is also valid in the case when the temperature and the properties of cooling fluid at the different ends of porous material differ significantly from each other. The both solutions capture the physics of the process. The temperature of fluid equals to the temperature of porous material everywhere except a very narrow layer of around 1 mm near the hot gas side. This is due to the fact that the porous material has a very developed surface and, correspondingly, features by a large interfacial area. The sharp temperature increase of the porous wall near the hot gas side reflects the fact that all heat incident on the porous wall is transported back towards the hot wall by the cooling fluid. The temperature increase of the cooling fluid is low because the heat flux incident on the porous wall is not enough to heat the massive flow of the cooling fluid, which is actually not a cooling fluid in the rocket engine but one of the injected propellants.

4. Penn State test case

The Penn State test case is a widely cited experiment carried out at the Pennsylvania State University. In the experiments wall heat flux measurements were performed in a cylindrical rocket chamber with a single coaxial injection element [13]. The experimental setup consisted of two preburners and a main combustion chamber. The configuration of the experimental setup corresponded to a stage combustion cycle operating with gaseous oxygen and hydrogen propellants. Zhukov [14] carried out CFD modelling of the Penn State preburner in order to validate his CFD model.

The CFD simulations of the Penn State preburner were performed in a quasi-three-dimensional domain, which represents a sector of 1 degree and one element thick. The domain included the combustion chamber, the converging-diverging nozzle, and a small part of the coaxial injector.

The turbulent combustion was modelled with the use of the SST turbulence model and the eddy dissipation model (EDM) [1]. In work [14] Zhukov extended the EDM model primarily in order to get the correct flame temperature. The correct value of flow temperature is very important for the accurate prediction of heat fluxes in combustion chamber. One of the advantages of the EDM model is its simplicity; however, the global reaction used in the EDM model results in the flame temperature of around 5000 K. Indeed, at high temperatures the dissociation of H_2O and other species starts playing a significant role, so the hydrogen-oxygen flame has temperature around 3500 K. To resolve the issue with the flame temperature, an additional parameter (“Flame Temperature”) is employed. The reaction rate is set to zero when the temperature exceeds the value of this parameter. The model has also three other additional parameters (chemical timescale, extinction temperature, and mixing rate limit) for modelling different phenomena of turbulent combustion. The distinctive feature of the new EDM type model is that all of these parameters, including “Flame Temperature”, are not constant but functions of the local mixture ratio. However, the advantages of the developed combustion model over the standard EDM are not visible in the Penn State test case because in this test case the propellants are injected at very high temperatures (at 720 K and 811 K), and flame extinction does not play a significant role in contrast to cryogenic rocket engines. Nevertheless, the new model was used because it results in a smooth distribution of reaction rate in combustion chamber without critical points and thus shows a better convergence by one order of magnitude than the standard EDM model.

In order to get a mesh independent solution, the mesh was successively uniformly refined five times. During the refinement the spacing was reduced twofold in the axial and radial directions. In addition, the structure of the mesh (i.e. blocking) was kept the same. It is necessary to note that the initial coarse mesh already had refinement around the side walls, the injector post, and in the shear layer between the jets of fuel and oxidizer. In CFD simulations the accurate prediction of wall heat fluxes requires high mesh resolution near the walls. For this reason, the near-wall grid resolution was improved approximately three times at each step refinement (i.e. with the higher rate than the mesh itself). The amount of mesh points was increased four times at each step from 30k nodes to 4.1M nodes. The near-wall resolution was improved during the grid convergence study in terms of maximum y^+ from 20 to 0.7. At the last step the spacing was reduced by only a factor of 1.4, and the near-wall resolution was improved by a factor of 2. The mesh convergence study showed that the solution became practically mesh-independent in the volume of the chamber after the second refinement on a mesh with 126k nodes. However, for the used near-wall treatment the mesh with y^+ around 1 is recommended for accurate heat transfer predictions [1]. Hence, the mesh-independent solution

required further mesh refinement, and it was obtained with the mesh which had a near-wall resolution of y^+ = 1.4 and consists of 1.5M nodes.

Combustion in a liquid rocket engine is characterized by many processes. The detailed modelling of all processes is challenging and requires great effort. In order to find a minimum modelling level required for accurate predictions of wall heat fluxes, the complexity of the numerical mode was gradually increased within eight steps from the simplest models and settings up to the inclusion of a radiation heat transfer model at the final step. The CFD simulations showed that the use of the basic and default settings result in significantly lower wall heat fluxes than in the experiment. It was also shown that the modelled wall heat fluxes are strongly influenced by the thermal conductivity of gas mixture. Therefore, a special attention was paid to modelling of the thermodynamic properties and particularly to modelling of the transport properties. In order to take into account the increase of the thermal conductivity with temperature, Sutherland's equations were employed for modelling of the transport properties of individual components of mixture. The presence of hydrogen increases the thermal conductivity of mixture; thus, a new mixing rule was used for modelling the transport properties of gas mixture. The detailed discussion about modelling the transport properties can be found in the followed section.

The simulation results obtained in work [14] agree well with the experimental data and CFD results of other groups [15], see Fig. 7. All simulations compared in Fig. 7 were obtained with the use of the RANS simulations and correlate with each other well. However, the results obtained with the use of the CFD code Rocflam3 have excellent agreement with the experimental data, which is the result of the fitting of the turbulent Schmidt and Prandtl numbers [15]. The other simulations lie below the experimental points and outside the margins of the experimental error at x < 50 mm, and above the experimental points at x ≥ 175 mm. Unfortunately, the comparison of the different simulations does not allow us to make any conclusions except for the fact that it is possible to predict wall heat fluxes in rocket combustion chambers using RANS simulations. All four simulations presented in the figure were performed using different turbulent and combustion models, different turbulent Prandtl and Schmidt numbers, and slightly different boundary conditions. This is the reason why it is so difficult to draw conclusions from the comparison of the different CFD simulations. Even the comparison of the results obtained with the use of the same code (CFX) does not give us the opportunity to explain the difference in the results. There are also other CFD simulations of the Penn State combustor performed with the use of RANS, URANS, DES, and LES.

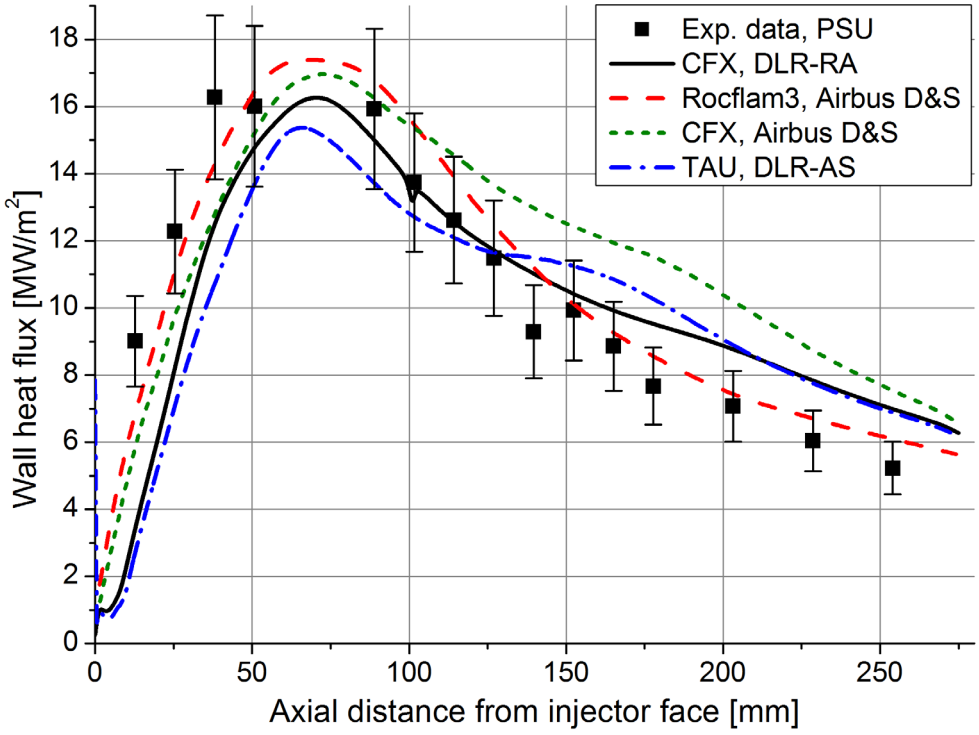

Figure 7. Comparison of the results of work [14] (black line) with experimental data [13] and simulation results of other groups [15].

5. Thermal conductivity of gas mixture

In all considered CFD simulations [4,12,14] thermal conductivity plays a significant role. In all mentioned cases hydrogen is a working fluid or an essential component of gas mixture. Hydrogen has the highest thermal conductivity among gases, and its presence significantly increases the thermal conductivity of the mixture. CFX defines the property of multicomponent mixture using a mass averaging [1], by which the contribution of the individual components to the properties of the mixture is directly proportional to the mass fraction, i.e.

$$\lambda_{mix} = \sum w_i \lambda_i \ ,$$

where w_i is the mass fraction of i species, and λ is the thermal conductivity. This leads to underestimating the transport coefficients for the mixture of hydrogen with oxygen. The mass averaging eliminates completely the influence of hydrogen on the thermal conductivity of the mixture; for example, in an equimolar mixture of hydrogen and oxygen the hydrogen mass fraction amounts only 6%. The inadequacy of the mass averaging clearly follows from the data of works [16,17] where the experimental data on the viscosity and thermal conductivity of H_2-O_2 mixtures at standart conditions were presented. For this reason, the thermal conductivity of the gas mixture was modelled in works [4,12,14] using the CFX Expression Language CFX [2] by empirical formulas suggested in [18]:

$$\lambda_{mix} = \frac{1}{2}\left[\sum x_i \lambda_i + \left(\sum {}^{x_i}/_{\lambda_i}\right)^{-1}\right],$$

where x_i is the mole fraction of i species.

6. Concluding remarks

Three different cases have been considered: modelling of combustion with the use of detailed reaction models, modelling of the heat transfer in a porous media, and wall heat flux predictions in a rocket combustion chamber. It was shown that it is possible to model accurately the processes of combustion and heat transfer in rocket combustion chambers using CFX. However, getting reliable results requires the accurate modelling of the main processes in the combustion chambers: turbulence, combustion and heat transfer. The modelling of such processes requires a detailed approach because these processes cannot be described by two or three, or five constants using values by default.

The transport properties of multicomponent mixtures are described with the use of the mass averaging in CFX. The use of mass-averaging leads to a significant discrepancy of the transport properties in mixtures with hydrogen. Therefore, the transport properties in such cases should be programmed by user itself using CFX Expression Language (CEL).

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