CFD Simulations of Rocket Combustors with Supercritical Injection

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A consistent thermodynamic model is implemented into the finite volume CFD-code TASCOM3D to simulate rocket combustors with supercritical injection conditions. The efficient Soave-Redlich-Kwong cubic equation of state is used in this work to predict the temperature-pressure-density-composition dependency. Empirical models based on the corresponding-states principle are applied to calculate real gas fluid properties. Two non-reacting experiments at supercritical pressure and a model rocket combustor with a single coaxial injector and cryogenic, supercritical injection conditions are simulated to validate the implemented approach. Simulations for all test cases are based on RANS equations keeping computational costs low and allowing investigations of extensive parameter variations. The obtained results generally agree very well with experimental measurements for all test cases. The numerical studies reveal a high sensitivity with respect to the applied turbulence models and turbulent Prandtl and Schmidt numbers. Though quantitatively good results could be obtained with test case dependent, individual numerical setups, a single, unique numerical setup valid for RANS simulations of all test cases cannot be found.

1. Introduction

Rocket engines operate at extreme pressure-temperature conditions so that thermodynamics of the fluid can, at least locally, not be accurately described by formulae valid for ideal gases only. Modifications at various locations in a CFD code are necessary to incorporate deviations from the ideal gas behavior. First, the well-known ideal gas law has to be replaced by a real fluid equation of state (EOS) to describe the temperature-pressure-density-composition dependency in a proper manner. For multi-component problems, a simple cubic thermal EOS like the Soave-Redlich-Kwong (SRK) or the Peng-Robinson (PR) EOS is usually applied in CFD simulations [1–3] to limit the complexity and additional computational cost. Second, all thermodynamic parameters like speed of sound, specific heat, species mass enthalpies, and thermodynamic derivatives like \( \left( \frac{\partial \rho}{\partial p} \right)_T \), which appear in the Jacobian matrices, should be consistently evaluated from the EOS via fundamental thermodynamic relations. Third, transport properties (viscosity, thermal conductivity, binary mass diffusion coefficients) may require modifications depending on the problem of investigation. Fourth, flow phenomena like the Soret and Dufour effect may have to be considered for some problems. Oefelein [4], however, found that their contribution may be neglected for rocket combustors, where propellants are commonly injected through shear-coaxial injectors.

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A real fluid modification was introduced into the finite volume CFD code TASCOM3D considering the aspects mentioned above. Fundamental thermodynamic relations are used for a consistent set of thermodynamic variables.

A supercritical, non-reacting nitrogen jet was extensively investigated by RANS simulation. This test case is widely used in literature for validation of the implemented real fluid formulation [1, 2, 5]. Another validation test case simulated in this work is a supercritical carbon dioxide upward flow in a vertical, heated pipe [6]. Finally, the rocket combustor test case A-60 operated at the Mascotte test facility is investigated [7, 8]. Details of the implementation and CFD results will be presented next.

1.1. Implementation of a Consistent Real Fluid Formulation

Currently, the SRK EOS is implemented into TASCOM3D to account for non-ideal gas behavior. Accordingly, the temperature-pressure-density-composition relation is expressed as

\[ p = \frac{R_u T}{v_m - b} - \frac{a}{v_m(v_m + b)} \]  

where \( p \) and \( T \) are pressure and temperature, \( v_m = M_w / \rho \) is the molar volume with \( M_w \) and \( \rho \) the molecular weight and mass density of the mixture, \( R_u \) is the universal gas constant, and \( a \) and \( b \) are composition-dependent parameters of the mixture. \( a \) also depends on temperature as given in [9]. The mixing parameters are obtained via standard van der Waals mixing rules from their respective pure fluid counterparts \( a_i \) and \( b_i \) (neglecting binary interaction parameters) as

\[ a = \left( \sum_{i=1}^{N_{sp}} X_i a_i^{0.5} \right)^2 \]  

\[ b = \sum_{i=1}^{N_{sp}} X_i b_i \]

with \( N_{sp} \) being the number of species and \( X_i \) the mole fractions of species \( i \). Fig. 1 compares densities of oxygen calculated by the SRK EOS and the ideal gas equation of state (IG EOS) with values from the NIST database. Densities are plotted versus temperature for subcritical, critical, and supercritical conditions w.r.t. the thermodynamic critical pressure of oxygen. A comparable accuracy is obtained for many other unpolar species like nitrogen. A good agreement with NIST data is usually obtained in the gas-like region (high temperatures) for the SRK EOS, but close to the critical point and on the liquid-like side, deviations may be up to 10 - 15%.

The real fluid formulation is implemented into a preconditioning scheme which updates primitive variables \( p \) and \( T \) similar to [10]. Hence, \( v_m (\rho, \text{resp.}) \) must be determined from Eq. 1.1. Depending on the local \( p - T \) combination, up to three possible solutions for the molar volume exist, which are obtained using Cardano’s method [11]. In case more than one root exists (three in practice), the correct solution is the one which, first, is greater than the co-volume parameter \( b \) and, second, minimizes the Gibb’s energy of the mixture. The middle root is always disregarded as it represents an artificial, unstable thermodynamic state. Note that this procedure only works as long as no phase split occurs. For possible multiphase solutions, a much more complicated procedure is necessary. Hence, currently the focus is on test cases within the single phase regime only.
The derivation of all thermodynamic variables and expressions from temperature, pressure, and composition is, except for \( v_m \) (or \( \rho \), resp.), based on Eq. 1.1 in combination with fundamental thermodynamic relations, which are valid for any EOS [12]. For an efficient and flexible implementation, Michelsen and Mollerup [12] suggest to use the reduced residual Helmholtz function

\[
F = -\int_{V'}^{V} \left[ \frac{p(T, V', n_i)}{R_i T} - \frac{n_i V'}{V^2} \right] dV'.
\]  

(1.4)

Eq. 1.1 has to be inserted into Eq. 1.4 to evaluate the integral. All other thermodynamic properties can be derived from \( F \) via differentiation w. r. t. volume, temperature, and species mole numbers \( n_i \). For more details see Michelsen and Mollerup [12].

1.2. Modeling of Transport Coefficients

In addition to deviations of thermodynamic properties from ideal gases, also deviations of molecular transport properties like viscosity, thermal conductivity, and diffusion coefficients from ideal gas values have to be considered. These are usually calculated from empirical models based on the principle of corresponding states [13]. For example, for non-polar fluids or fluid mixtures, the model of Ely and Hanley [14, 15] may be used for the prediction of real fluid viscosities and thermal conductivities. The model of Takahashi [16] is widely accepted for the prediction of binary mass diffusion coefficients at non-ideal gas conditions. In this work, similar models with comparable accuracy but some additional advantages have been implemented into TASCOM3D [17, 18]. Figure 2 shows a comparison of viscosity and thermal conductivity for oxygen between values from the NIST database and values obtained from the model of Ely and Hanley (E & H). The SRK EOS is used to obtain \( v_m = v_m(T, p) \) as input parameter for this model. A good agreement is obtained for a wide range of thermodynamic conditions. However, close to the critical point, for liquid-like conditions, or polar fluids like water, significant
deviations can be observed. For large parts in a RANS or URANS simulation, the turbulent viscosity from the turbulence model will exceed the molecular viscosity by orders of magnitude. A rather inaccurate prediction of transport properties will hardly affect the CFD solution in these regions. For laminar flows, close to the wall, and LES or even DNS computations, this is not true.

2. Simulation of Supercritical Nitrogen Jet

The non-reactive RCM-1-A test case presented at the 2nd International Workshop on Rocket Combustion Modeling [19] was chosen as a validation test case for the implemented real gas model. Cryogenic nitrogen at a temperature of about 120 K is injected through a circular duct of $d = 2.2$ mm diameter into a pressurized chamber at 40 bar. The chamber is filled with gaseous nitrogen at room temperature and has a diameter of 122 mm and a length of 1000 mm. There is some uncertainty concerning the actual injection temperature, which is supposed to lie within a range of 120.9 K and 126.9 K. At the implied injection conditions close to the pseudo-boiling point [20], the density is very sensitive w. r. t. small changes in temperature (see Fig. 1). Axial and radial density distributions were measured in the experiment by Raman images (case 5 in [21]).

Steady-state RANS simulations were performed in this study. Various parameters were investigated to test the sensitivity of the numerical result w. r. t. the implied numerical setup and boundary conditions. Some of these results are presented in this report. The following setup was chosen for the reference simulation:

(a) 2D hexahedral grid with 95,000 elements and $y^+ \approx 1$ resolution at walls,
(b) 2nd order spatial discretization of inviscid fluxes with van Leer limiter and low diffusion multi-dimensional limiting process (MLPld) [22],
(c) $\omega$ - $\omega$ turbulence model [23],
(d) turbulent Prandtl number $Pr_t = 0.9$,
(e) adiabatic walls for injector and faceplate, isothermal chamber wall ($T = 297$ K),
(f) injection temperature $T = 120.9$ K.

Fig. 3 displays the density and temperature distribution close to the injector for the reference simulation. The high sensitivity of density w. r. t. temperature, as discussed before, is reflected in these contours. An increase of 10 K roughly halves the density...
right after the injection. A comparison of axial density profiles at the centerline and radial density profiles at a distance of $x/d = 5.0$ is plotted in Fig. 4. Comparing measured densities with densities obtained from the NIST database at given pressure and minimal/maximal measured temperatures (Fig. 4(a)), discrepancies between measured densities and temperatures become obvious. Densities lie out of the expected range for the given pressure-temperature range. One reason is that Raman measurements are probably biased towards lower values [21]. However, uncertainties in the measured injection
temperatures are likely the main cause due to the aforementioned great temperature-sensitivity of density at these injection conditions.

Fig. 4(a) also provides densities predicted by the SRK EOS at the given pressure and injection temperature range. The density at injection should be underpredicted compared to NIST data by about 9 - 14% depending on the injection temperature. For the reference simulation, the lowest temperature of $T = 120.9$ K was chosen, which was measured within the injector. This results in a predicted density at injection of about $505 \text{ kg/m}^3$, which is clearly above the measured density. Hence, for this injection temperature, the decrease of density along the axis can be compared with the experimental data only in a qualitative manner.

Principally, the RANS simulation resembles the experimental trend. The density at the centerline remains constant until $x/d \approx 10$. Further downstream, the liquid-like cold nitrogen core has dissolved into the warm surrounding nitrogen and density decreases. However, the decrease is slightly more upstream in the reference simulation and initially not as fast as in the experiment. Having a look at the radial density distribution at $x/d \approx 5$ (Fig. 4(b)), deviations compared with the experiment are evident. Radial mixing seems to be much stronger in the experiment and a more diffusive profile is observed. In the simulation, the dense core is still intact until $r/d \approx 0.3$. Also, the mixing layer between the cold and warm nitrogen is much thinner in the simulation.

One reason for the qualitative differences in the radial density profiles may originate from heat transfer from the injector walls to the fluid. This could also partially contribute to the great variations between the measured temperatures within the injector and at the injector exit. Hence, a simulation was performed imposing a linear increasing temperature profile at the injector walls (from 120.9 K to 297 K at the injector exit). Results are shown in Figs. 4(a) and 4(b). As can be seen, the density at the injection is lower, of course, since heat is transferred from the walls to the fluid. The density decrease at the axis already starts prior to the injector exit, though this is not observed in the experimental density values. Further, the radial density profile remains qualitatively the same. Results do not improve with isothermal walls. The use of adiabatic wall boundary conditions within the injector thus seems to be justified.

Further variations of the numerical setup were investigated. The influence of injection temperature was tested by setting it to 122.9 K and 126.9 K, respectively. These temperatures were measured at the injector exit for a parallel and orthogonal oriented thermocouple w. r. t. the axial direction. Using a temperature of 126.9 K, the predicted density of the SRK EOS is close to the measured density. A good match is now obtained, though the decrease in density at the centerline is still slightly too far upstream and too slow. The temperature of the chamber wall was varied in another simulation and set to 250 K to investigate the effect of the assumption of a constant wall temperature of 297 K. The axial density profile remains quite unaffected except downstream of $x/d \approx 25$. However, the radial profile clearly shows that the density of the surrounding nitrogen is now predicted incorrectly due to lower temperatures in the recirculation zone. Therefore, the assumption of a constant chamber wall temperature of 297 K seems appropriate.

It is well known that the modeling of turbulence can have a tremendous influence on calculated turbulent flows. Figs. 4(c) and 4(d) present axial and radial density profiles for simulations with a modified turbulent Prandtl number and alternative $k-\omega$ [24] and SST [25] turbulence models. The turbulent Prandtl number was changed to $Pr_t = 0.7$ in one simulation. This value is regarded in literature as more appropriate for jets, compared to the default value of 0.9, which is often used for the simulation of boundary layer
flows [26]. A smaller turbulent Prandtl number leads to an increased energy transport. This leads to a faster decrease in the axial density profile compared to the reference simulation. A slightly more diffusive radial density profile is also observed, though differences are small.

The two-equation turbulence models have a tremendous effect on the density distribution. The $k - \omega$ model predicts a much slower decrease in the axial density profile compared to the $q - \omega$ model. The reasons for this discrepancy are not obvious. There are probably two effects. First, the heat transfer at the chamber side wall differs. Second, more cool nitrogen seems to enter the recirculation zone, which is much cooler. Hence, also density at $r/d = 2$ is higher than in the experiment and in the reference simulation. Both effects are also observed in the simulation with the SST turbulence model, which predicts a comparable radial density profile as for the $k - \omega$ simulation. However, the axial density profile is totally different and the calculated slope compares favorably well with the measured densities. The different temperatures in the recirculation zone are therefore not the main cause for the great variations between the calculated axial density profiles when using different turbulence models. This is also supported by the results of the simulation with a modified wall temperature of 250 K, which did not considerably influence the axial density profile.

Since the simulation with the SST model agreed qualitatively well with the experiment for the axial density profile, another simulation with the upper temperature limit of 126.9 K used as a constant inlet temperature was performed. For the axial density profile, this numerical setup results in a very good match between the experiment and the simulation. The agreement for the radial profile still shows some discrepancies. The density in the recirculation zone is again too high (due to more cool nitrogen) and mixing close the centerline is delayed compared to the experiment.

### 3. Simulation of Supercritical Carbondioxide in a Heated Pipe

The prediction of wall heat loads in rocket combustors is of great interest. Since no experimental data for wall heat flux and temperature measurements in supercritically operated rocket combustors were available, other test cases had to be considered for validation. Experiments on supercritical fluids in heated pipes provide challenging alternatives for every CFD code. Their results are often used for code validation and to gain a better understanding for applications like supercritical water reactors.

Many of these experiments with a rather high quality of data for comparison exist. Here, a basic experiment [6] at 90 bar pressure with supercritical carbon dioxide (critical pressure 74 bar, critical temperature 304 K) flowing upwards in a vertically, heated pipe is simulated. 2D-axisymmetric simulations were performed. The pipe’s diameter is 22.7 mm. The simulated length of the heated section (imposed wall heat flux) is about 130 diameters long. About 90 diameters with an adiabatic wall precede to obtain a fully developed pipe flow at the entrance to the heated section. Gravity acts in negative x-direction against the flow direction.

Fig. 5 shows simulated temperature and density contours in the test section ($x$-axis compressed by a factor of 50). The established flow field in the heated section is the result of a complex interaction between inertia and gravity forces as well as turbulence and turbulent heat transfer. Simple RANS simulations can only reproduce experimental data in a qualitative way, if at all. Fig. 6 presents simulated and measured wall temperatures in the heated test section. Again, three different turbulence models were
investigated besides further parameter variations (not shown here). The $q$-$\omega$, the $k$-$\omega$ and the SST model predict a qualitatively similar result as the experiment. A sharp rise in temperature at the beginning of the heated section is succeeded by a slower temperature increase until a maximum is reached. Further downstream, temperature decreases again. This detail, a temperature peak with a succeeding decrease, is often not even qualitatively captured with simple turbulence modeling.

From a quantitative point of view, results are not very satisfactory. All simulations predict a too sharp increase in temperature right at the beginning of the heated wall section. Subsequent temperature levels are either too high ($k$-$\omega$ and SST) or too low ($q$-$\omega$). Large-eddy simulations may deliver a better match with experimental data, but at a much higher computational cost. Generally, the implemented real fluid framework seems to be able to predict a meaningful wall heat transfer, but the key issue for good results is apparently appropriate turbulence modeling. Though flow conditions are quite different, one may expect similar problems when it comes to simulating wall heat transfer in rocket engines.
4. Simulation of Supercritical Rocket Combustor Test Case A-60

The A-60 test case [7, 8] operated at the Mascotte rocket engine test facility was simulated. Oxygen and hydrogen are injected through a circular, coaxial injector into a rocket combustion chamber (about 450 mm in length, square cross section with 50 mm edge length). The chamber pressure is about 60 bar and thus above the critical pressure of oxygen (50 bar). Hydrogen is injected at room temperature and acts like an ideal gas, but oxygen is injected cryogenically at 85 K. Hence, the cold oxygen core behaves like a very dense liquid-like fluid and is exposed to significant real gas effects.

2D-axisymmetric RANS simulations were performed. The diameter of the combustor was adjusted to keep the chamber volume equal to the volume of the rectangular model combustor. Fig. 7 shows temperature and density contours for a simulation with the $\omega - \omega$ turbulence model and a turbulent Prandtl and Schmidt number of 0.9. Fig. 8 presents the respective temperatures along the centerline, which are compared to experimental data. A very good match is obtained for this numerical setup. However, one must admit that results are less satisfactory when choosing a different turbulence model or when modifying the turbulent Prandtl and Schmidt numbers (not shown here).

5. Conclusions

Various challenging test cases at supercritical conditions were simulated to validate the real gas framework, which was implemented into the finite-volume CFD Code TAS-
COM3D. The ability of simple RANS models to correctly simulate turbulent jet disintegration, heat transfer and combustion in supercritical environments was investigated in simulations of two non-reacting test cases and a model rocket combustor. Qualitative excellent results could be obtained for all test cases, reproducing experimental data quantitatively with satisfactory accuracy at low computational costs. Sensitivity studies were performed to test the influence of several parameters and boundary conditions. The role of turbulence models and turbulent Prandtl and Schmidt numbers was found to be of great importance for simulating supercritical turbulent flow. No unique numerical setup could be found, which can reproduce experimental data well in a quantitative manner for all test cases. Predictability for alternative test cases with a predefined numerical setup thus seems to be limited to similar operating conditions.

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References

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