Spray Combustion and Heat Transfer Modelling in LOX/H2, LOX/HC and MMH/NTO Combustion Chambers

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Abstract
For over two decades, EADS/Astrium supported the design and development of its rocket combustion chambers with two in-house RANS codes: ROCFLAM, a multi-phase RANS code developed especially for storable MMH/NTO engines and CryoROC, a ROCFLAM derivate for cryogenic LOX/H2 combustion. Both numerical codes had in common that they are limited to a very special use in the frame of their incorporated chemistry, since both of them are equipped with global reaction schemes, adapted to specific load points. To enlarge the general applicability towards various combinations of fuel and oxidiser, it was decided to, firstly, merge these two codes and then to implement as additional (chemical) alternative a generally applicable tabulated equilibrium-based chemistry, open to any kind of fuel/oxidiser combinations. The new code was named Rocflam-II and it has meanwhile replaced its predecessors. Some of its applications are presented in this paper.

Nomenclature

ATV	Automated Transfer Vehicle	PB	Pre-Burner
CFD	Computational Fluid Dynamics	PDF	Probability Density Function
CFX	commercial CFD code, ANSYS Ltd. (1997-2004)	MMH	Monomethylhydrazine
HC	Hydrocarbons, here Kerosene or Methane	PPDF	presumed Probability Density Function
Isp	specific Impulse [s]	RANS	Reynolds Averaged Navier-Stokes
LOX	Liquid Oxygen	RCFS	Regenerative Coolant Flow Simulation
NTO	Nitrogen Tetroxide	ηc*	combustion efficiency

Introduction
Cryogenic oxygen-based as well as storable rocket propulsion systems are one of the major business fields of the Space Transportation Division of EADS/Astrium. Products representing Astrium's experience in this field are the thrust chambers of the Vulcain, Vulcain-2, HM-7 and VINCI engine systems on the cryo-genic oxygen/hydrogen side and AESTUS as well as numerous in-orbit propulsion systems on the stor-able side. Additionally, hydrocarbon applications, i.e. LOX/Methane and LOX/Kerosene, have been and are under investigation on subscale and fullscale level.

One of the main problem areas for actively cooled thrust chambers is the extreme heat flux along the wall due to the high combustion temperatures occurring at high chamber pressure. Tailoring the channel cross sections of the regenerative cooling circuit to optimize the consumption of pressure drop, requires precise information about the wall heat flux distribution (and, of course, the corresponding wall temperature, which is most critical for the chamber's lifetime). Moreover, the near-throat region is supposed to be the thermally highest loaded section of the combustion chamber which makes the choice of appropriate cooling systems a challenging task.

In recent years, it became commonly agreed, that the most resource effective way in developing and assessing new propulsion systems led through the path of computational fluid dynamics (CFD), i.e. the numerical simulation with 2- or 3-dimensional Navier-Stokes codes incorporating the latest models in turbulence and combustion research. Thus, 1-D Nußelt-based correlations and the previously applied trial and error approaches associated with expensive experimental testing programs could be reduced significantly during the development phase. While nowadays the employment of numerical methods to predict rocket engine performance is state-of-the-art, their use to determine heat loads in thrust chambers is still a challenging topic. The reason is that for heat fluxes steep gradients have to be resolved

which especially in combustion chambers depend on the complex interaction of multiple physi-cal phenomena such as turbulence, multi-phase flow and combustion.
Over the last two decades, EADS/Astrium developed two similar in-house Navier-Stokes codes to meet these aforementioned purposes: the CryoROC code (Cryogenic ROcket Combustion), for LOX/H_2 applications only [4], and the ROCFLAM code (ROcket Combustion FLow Analysis Module), a tool exclusively used for storable engines [5]. These two codes were replaced recently by one single code, the improved Rocflam-II code, which comprises the advantages of the two predecessors and which can be applied to both cryogenic and storable engines. This tool incorporates state-of-the-art models of many physical disciplines such as aerothermodynamics, multi-phase flows, turbulence and multi-species chemistry. The objective is not to resolve each single sub-process occurring in thrust chambers in too far-reaching detail but to reflect the global operational behaviour of such rocket motors. Balancing model accuracy and computational effort, the major assignment of this sophisticated engineering tool is to provide heat flux distributions along (regeneratively) cooled combustion chamber walls as well as global performance data.

Test data obtained by means of EADS/Astrium's calorimeter model combustor as well as full-scale ground test and flight operational data has been used to anchor and adapt the Rocflam-II simulations.
This paper's objective is to present an introduction and overview of the Rocflam-II code, its modelling philosophy and to discuss typical applications demonstrating the potential of the code to support modern rocket engine design. Special focus of the paper will be the effect of staged combustion injection conditions on combustion and heat transfer, the new Rocflam-II features to simulate LOX/Hydrocarbons (with methane as example) as well as storable MMH/NTO thrusters.

The Rocflam-II Code

EADS/Astrium's in-house code Rocflam-II is a structured, finite volume, compressible and axisymmetric/2-D, multiphase Navier-Stokes solver which supports multi-block capabilities. A standard 2-equation k-ε turbulence model (Chien 1982, [1]) is incorporated with a 2-layer approach at the wall [8].

Most important and outstanding feature is the Lagrange module for particle injection and tracking. Bi-propellant and multi-class droplets or particles can be injected in a gaseous environment that way. They will be tracked, heated up and finally vaporised before they go into the RANS equations of state as right-sided source terms. The Lagrange module can be considered the heart of the Rocflam-II code. It enables the code to handle the boundary conditions along which the propellants are injected, as solid walls rather than an opening. The injected liquid droplets (or better to speak of "particles") are indeed injected as disperse droplets, i.e. they are not building up a continuous phase, only when entering into the gaseous phase the (mass, impulse, energy) equations of state are to be fulfilled.

As a practical consequence, the actual boundary conditions to be imposed are therefore only the corresponding mass flow rates of fuel and oxidiser, their injection velocities and their injection temperatures, respectively. Especially the face plate pressure is *not* to be a-priori imposed but a computational variable. In fact, this approach offers a variety of modelling possibilities to all kind of rocket engines, even in circumstances where the thermodynamic conditions are not really refer to "particles" or "droplets".

The Lagrange module additionally incorporates a secondary droplet break-up and a supercritical gasification model for cryogenic propellants as LOX and Methane. Turbulent combustion can be modelled by either a presumed PDF approach with tabulated equilibrium chemistry (the preferred choice) or global reaction schemes together with an eddy dissipation concept, which are available for diverse fuel/oxidiser combinations. A comprehensive summary of all the code's features and capabilities can be found in the following Table 1.

▪ compressible, sub- and supersonic steady-state flows ▪ k - ε turbulence model (Chien 1982) ➢ 2 layer model ➢ logarithmic wall function ➢ compressibility effects (Sarkar) ▪ chemical reaction models ➢ multi-step global reaction schemes (turbulence & kinetically controlled) • Hydrazine/NTO • MMH/NTO • LOX/H_2 ➢ presumed PDF with tabulated chemistry • LOX/H_2 • LOX/CH_4 and LOX/Kerosene ▪ Lagrangian partical tracking (Stochastic Separated Flow model) ➢ multi-class, bi-propellant, discrete particle injection and sequential tracking approach ➢ mass, momentum, enthalpy and turbulence coupling with gas phase	▪ supercritical LOX gasification model ▪ annular liquid film cooling model ▪ advanced droplet-to-wall / film interaction model ▪ secondary droplet break-up ▪ viscous heating, species diffusion ▪ heat conduction in solid walls ▪ porous walls and crack simulation ▪ standard Jannaf property data base ▪ special real gas data treatment for cryogenic, low temperatures ▪ coupling with EADS/Astrium's RCFS-II code (Regenerative Coolant Flow Simulation) ▪ coupling with 3D CFX code for conjugate heat transfer computations ▪ 2D, axi-symmetric, finite volume ▪ Favre-averadged Navier-Stokes ▪ SIMPLE algorithm (pressure correction) ▪ implicit Stone solver ▪ 2nd order upwind spatial discretisation ▪ structured, non-orthogonal, curvilinear meshes ▪ multi-block

Table 1: Technical features of the Rocflam-II code

Cryogenic LOX/H2 Simulations

In terms of chemical reaction schemes, the Rocflam-II code basically offers two alternatives for common LOX/H2 simulations. One choice is a 5-species global reaction scheme combined with an eddy dissipation concept for the turbulent combustion (which actually comes from the preceding CryoROC code), the second and, however, preferable choice will be a tabulated equilibrium-based chemistry, with a variety of species, together with a PPDF approach for the turbulent combustion. Practically, a six species equilibrium-based chemistry, as depicted in Table 2, turned out to be suitable for standard applications. If necessary, additional species as liquid (water) or even solid H_2O (ice) can be taken into account, as e.g. in case of condensation problems [2].

	Species	
1.	oxygen	O_2
2.	hydrogen	H_2
3.	(gaseous) water / steam	H_2O
4.	hydrogen radical	OH
5.	atomic hydrogen	H
6.	atomic oxygen	O

Table 2: Species considered for LOX/H2 equilibrium chemistry combustion

Heat flux management of high performance launcher propulsion systems is usually governed by regenerative cooling circuits. Heat fluxes induced by hot combustion gases are transferred into and carried away by the cooling fluid, as it is illustrated in Figure 1. A major challenge of liquid propellant thrust

chamber layout is thus the precise quantification of local heat fluxes in a multi-phase, multi-species and chemically reacting hot flow environment. In particular for LOX/HC combustion the physical-chemical processes are manifold and complex. Figure 1 illustrates some of various possible phenomena in such an environment.

EADS/Astrium has several numerical codes to simulate the coolant flow, e.g. the RCFS-II code [7], a one dimensional code based on Nusselt-type correlations (used for cooling channels design) or CFX, a fully 3-D commercial RANS solver. The Rocflam-II code is loosely coupled to one of these, with a mutual exchange of wall temperature and wall heat flux values.

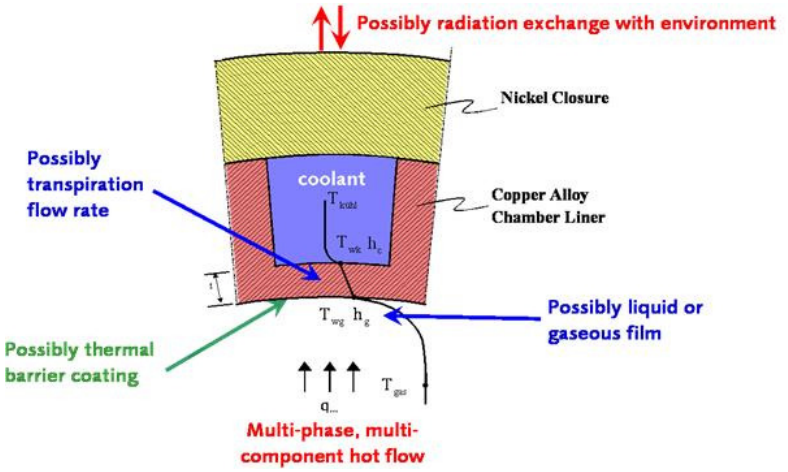

Figure 1: Sketch of possible head load management in liquid propellant rocket combustion chambers

A usual way at EADS/Astrium developing rocket combustion chambers is via subscale model chambers, which are to be thoroughly tested before going into the design of corresponding fullscale engines. Equipped with numerous local heat flux and temperature measurements, as well as global numbers as combustion efficiency, the numerical tools are that way easily verified and validated and thus able to make fullscale predictions on a high confidence level.

Recently, EADS/Astrium's Rocflam-II code has been extended and adapted to encounter a so-called "warm injection", i.e. a fuel-rich, heated-up pre-burner gas mixture is injected into the combustion chamber as "fuel" – instead of pure, cryogenic hydrogen (addressed in the following as "cold" injection). This warm injection (with an inflow temperature $T_{inj,PB}\approx$600-700 K) is principally not handled differently from the cold injection ($T_{inj,H2}\approx$120 K). In both cases ("cold" over-critical hydrogen or "warm" PB-gas), gaseous source terms are going directly into the RANS equations of state. The core flow (liquid oxygen) is modelled in both cases as liquid particles or droplets. This approach seemed, from an engineering point of view, a feasible mode to predict excellent results.

In case of this modelling approach, a simple boundary condition, namely a closed wall, can be addressed. Moreover, since we don't have pure hydrogen as fuel, but a gas mixture of a certain pre-burner mixture ratio, a new, so-called "partly premixed" injection type was introduced. Here, the real fuel-rich pre-burner gas mixture, which consists, cum grano salis, of only H_2 and H_2O, will be replaced and modelled by molecular H_2 and O_2 (but according to the correct pre-burner mixture ratio) in a thermodynamic state before reaching the gas generator combustor (but taking into account the estimated turbine losses). Downstream of the fuel sleeve of the injection element, they are both injected then via the Lagrange module as gaseous source terms into the chamber (see Figure 2 right). Immediately after reaction, the thermodynamic state of the "warm injection" is achieved.

Figure 2: traditional non pre-mixed injection (left) and the partly pre-mixed injection, designed for warm injection (right)

It was of course an option as well to simulate the outcome of the pre-burner gases by a real gaseous medium flowing into the chamber. However, the results were not satisfying. In direct comparison, the partly pre-mixed approach described above turned out to be the far better approach. The “best” naturally refers to the measured wall heat flux distribution and the total heat load as measure. During a thorough study, which tried out several different possibilities, e.g. gaseous injection, the shortcomings of all these alternatives seemed to be much more evident.

The Figure 3 depicts the temperature flowfield, comparing the cold and the warm injection type. As it can be recognised, the warm, partly premixed injection, leads to a slightly earlier onset of the combustion processes, finally resulting in a less stratified flowfield up to the throat, which that way will lead to a higher combustion efficiency ηc* and performance.

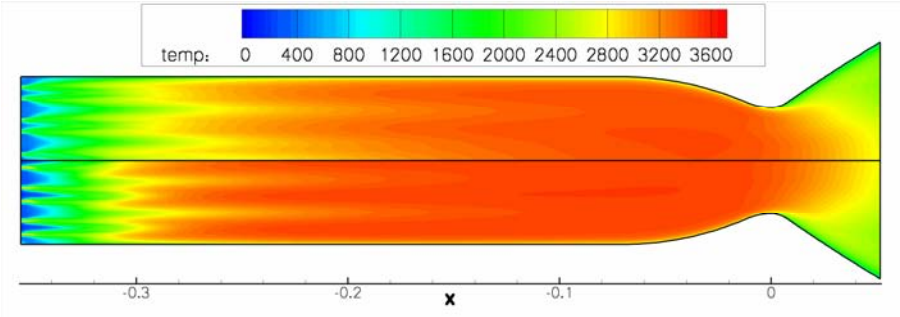

Figure 3: Subscale chamber, temperature flowfield, “cold injection” (upper half) and “warm injection” (lower half)

The corresponding wall heat fluxes are shown in the following Figure 4. Numerous subscale measurements are plotted in comparison with coupled Rocflam-II/RCFS-II predictions in case of standard “cold” injection, for the just recently performed “warm injection” measurements from only one campaign are available. Notice, that both "cold" and "warm" cases reflect identical chamber conditions in terms of pressure and mixture ratio.

Remarkable here is the fact that the absolute level of the heat flux (in the cylindrical part of the chamber as well as at the throat area) is higher in case of warm injection. In the measurements as well as in the Rocflam-II predictions! A possible explanation could be that due to the much broader “warm” injection elements, the actual element-to-wall-distance, i.e. the edge of the outer element to the wall, is reduced. However, the shear layer between fuel and oxidiser, where the major part of the combustion process is supposed to take part, remained more or less the same. In any case, the “warm" injection seems to lead to higher temperatures of unburned gases near the chamber walls and a better distribution of the spray, which both leads to higher fluxes.

A second observation, which can be made from Figure 4, is that the “warm injection” leads to a significantly steeper increase of the local heat flux at the rear part of the combustion chamber, i.e. in the vicinity of the face plate. This again is shown by both measurements and numerical simulation.

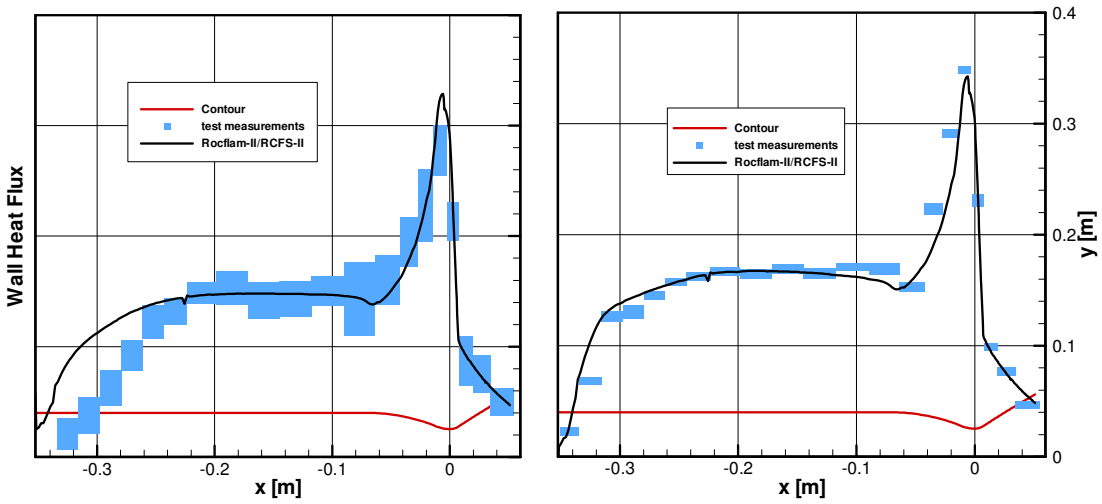

Figure 4: Subscale chamber, wall heat flux profiles for "cold injection" (left) and "warm injection" (right)

After the successful simulation of combustion chambers with warm pre-burner gases on subscale level, The Rocflam-II code was applied to a generic (fullscale) thrust chamber design for a warm injection concept in the frame of an internal study. A comparison between subscale and fullscale level for an envisaged load point of 150 bar is shown in Figure 5. The onset of the hot combustion zone appears to be a bit later on fullscale level. This is at a first glance a surprising result, which requires further investigations. The wall heat fluxes, on the other hand, are as expected, with its maximum values near the throat. Here, the fullscale flux is somewhat "broader", due to the contour geometry, and lies, in absolute values, under the subscale flux (due to the much higher fullscale throat diameter).

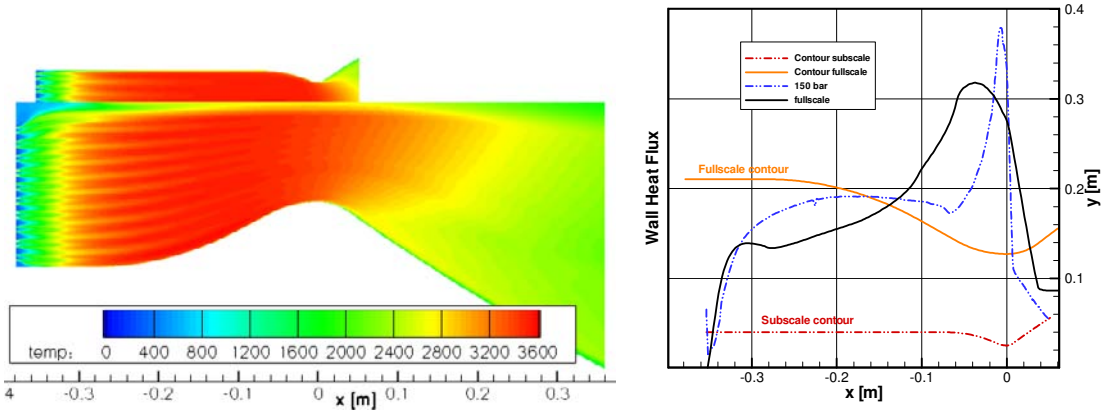

Figure 5: left: temperature flowfield, "warm injection" for subscale (upper half) and a generic thrust chamber (lower half); right: corresponding heat fluxes along the walls

Hydrocarbon LOX/CH4 Simulations

Another field of applications at EADS/Astrium is the design of hydrocarbon engines. The term "hydrocarbon" basically means LOX/Methane or LOX/Kerosene engines. Here, only examples of methane-driven motors are discussed. As for standard LOX/H_2 engines the development strategy foresees first testing on subscale level. In the frame of the TEHORA project LOX/Kerosene and LOX/Methane hot firing tests were conducted on subscale level at the Russian company KBKhA in Voronezh/Russia. These tests had two major goals, namely to compare the efficiency parameters and the heat flux distributions resulting from various injector head configurations. Details of the development and the test programmes are described e.g. in [3] or [6].

Such subscale tests were recalculated using the Rocflam-II code. The applied equilibrium-based chemistry considers eight different species. The following Table 3 gives an overview:

	Species	
1.	methane	CH_4
2.	oxygen	O_2
3.	carbon monoxide	CO
4.	carbon dioxide	CO_2
5.	hydrogen	H_2
6.	water	H_2O
7.	hydrogen radical	OH
8.	atomic hydrogen	H

Table 3: Species considered for LOX/Methane equilibrium-based chemistry combustion

In case of supercritical methane (pinj > pcrit, Tinj≈250 K > Tcrit), the fuel is injected as gaseous source terms as H_2 in the case of LOX/H_2, whereas the oxygen is modelled as liquid droplets.

The following Figure 6 depicts the temperature flowfield of a LOX/Methane subscale chamber. A long stratified flowfield becomes visible in the first half of the thrust chamber, which almost completely disappears in the second thrust chamber half.

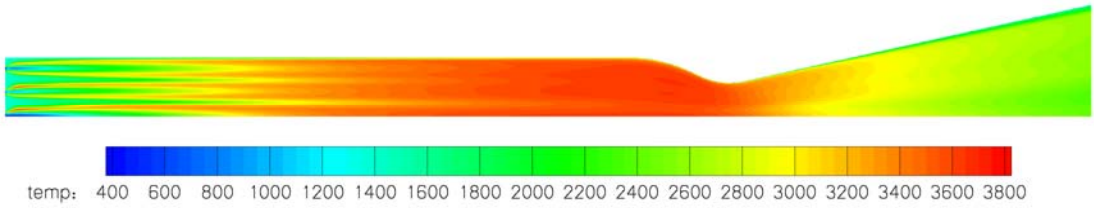

Figure 6: TEHORA subscale chamber, LOX/Methane, temperature flow field

A comparison with the heat flux measurements from two different TEHORA test campaigns is given in the next Figure 7 for coupled Rocflam-II/RCFS-II and RCFS-II/RCFS-II simulations. It is recognised from a first glance that the agreement is very good between the measurements and the computational predictions at the throat and beyond as well as for the face plate vicinity. However, minor discrepancies exist along the cylindrical part of the combustion chamber.

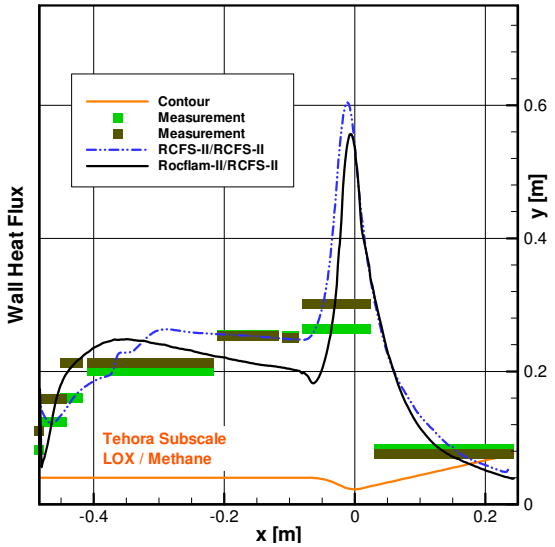

Figure 7: TEHORA subscale chamber, LOX/Methane, wall heat flux distributions

An example for a fullscale application including a large nozzle is shown in the following Figure 8. The stratified temperature flowfield with ten injection element rows is clearly visible, even along the supersonic nozzle.

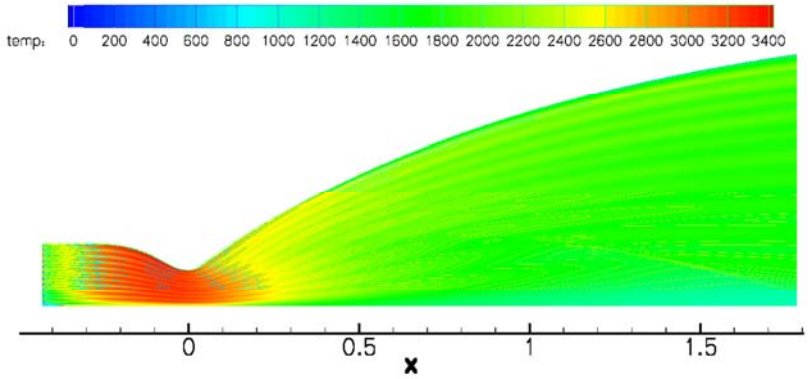

Figure 8: Fullscale engine, LOX/Methane, temperature flowfield

Storable MMH/NTO Simulations

Different to what was shown in the previous sections, storable engines are simulated with a global reaction scheme rather than a tabulated equilibrium-based chemistry (since the assumption of chemical equilibrium does not suit well for common MMH/NTO reaction rates). Here, one conservation equation is solved for each species (the species, which are considered in the global reaction scheme, are depicted in Table 4). The global chemistry for MMH and NTO mainly consists of three chemical reactions treating common combustion, reaction of residuals and dissociation. MMH and NTO are both injected as droplets. It is emphasized here, that the simulation of two liquid phases by a spray combustion approach was originally the motivation for the ROCFLAM development. To the authors´ knowledge, up to now no commercial approach offering these capabilities is available.

	Species	
1.	methane	CH_4
2.	nitrogen dioxide	NO_2
3.	water	H_2O
4.	nitrogen	N_2
5.	hydrogen	H_2
6.	hydroxyl radical	OH
7.	atomic hydrogen	H
8.	carbon dioxide	CO_2
9.	carbon monoxide	CO

Table 4: Species considered for the 3-step MMH/NTO global chemistry scheme

For the anchoring of the MMH/NTO chemistry the Aestus engine was used. Aestus powers the Ariane 5 upper stage for the insertion of payloads into LEO, SSO and GTO. Aestus is also used on the ES-ATV version of Ariane 5 for the placement of ESA's ATV into a low Earth orbit.

The Rocflam-II simulation was coupled with RCFS-II (as described above) in the combustion chamber. A load point marked by a mixture ratio O/F = 2.05 and a total mass flow rate of 8.77 kg/s was simulated. Figure 9 shows the temperature and mixture ratio flowfield for the Aestus engine. A zoom on the combustion chamber is shown in Figure 10. Near the face-plate, cold areas (green) can be observed. Hot streaks (yellow and red) indicate shear layers of the injection rows where the MMH and NTO droplets

are initialised. Further downstream the propellants mix and react with each other. This can also be observed in the mixture ratio distribution in the lower part of the figure. The red streaks near the face plate show oxidizer rich regions which indicate the NTO injection jets. The thin green streaks in between mark the shear layer between the two propellants which start to mix in these regions. Further downstream the high gradients in mixture ratio are reduced, and the green colour close to the convergent part of the combustion chamber indicates a mixture ratio close to the design mixture ratio O/F = 2.05. Only small stratification remains which, however, is responsible for a corresponding decrease in ηc*. As mentioned before, only the propellant mass flow rates are prescribed as inflow condition. Hence, the chamber pressure is a result of the evaporation and combustion computation. For the present Aestus case Rocflam-II predicts 10.12 bar, which corresponds to an imperfect combustion of ηc*=97.1%., a value which is also confirmed by Aestus engine operation.

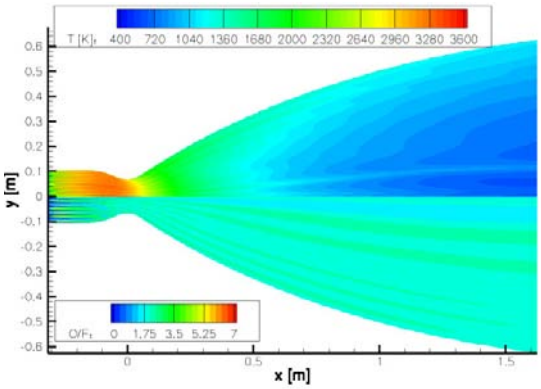

Figure 9: Aestus, temperature (upper half) and mixture ratio (lower half) flowfield, simulated with Rocflam-II

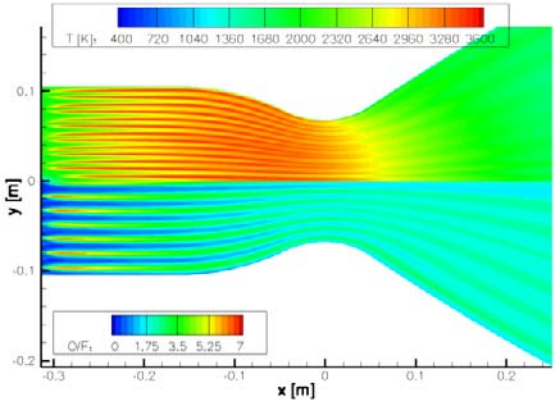

Figure 10: Aestus combustion chamber, temperature (upper half) and mixture ratio (lower half) flowfield, simulated with Rocflam-II

The predicted local wall heat flux and wall temperature distribution (Figure 11) cannot be compared to test data since no local measurements exist; only the integrated heat load picked up by the regenerative cooling system of the combustion chamber is available. The predicted integral heat pick-up lies about 1.1 % above the measured value, which is considered an excellent agreement. Regarding standard performance data, as e.g. the Isp, the numerical predictions show very good agreement with the measurements as well.

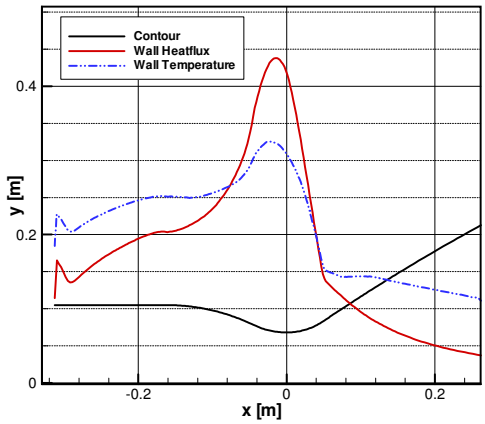

Figure 11: Aestus, Wall heat flux and wall temperature, simulated with Rocflam-II/RCFS-II

Summary & Outlook

Over the last two decades, EADS/Astrium developed and applied two similar in-house Navier-Stokes codes to account for heat transfer problems in (regeneratively) cooled rocket thrust chambers: the Cryo-

ROC code, for LOX/H2 applications only and the ROCFLAM code, a tool exclusively used for storable engines. These two codes were replaced recently by one single code, the improved Rocflam-II code, which comprises the advantages of the two predecessors and which can be applied to both cryogenic and storable engines. This tool incorporates state-of-the-art models of many physical disciplines such as aerothermodynamics, multi-phase flows, turbulence and multi-species chemistry. The objective is not to resolve each single sub-process in too far-reaching detail but to reflect the global operational behaviour of such rocket thrust chambers.

Some examples of the Rocflam-II code, applying to classical cryogenic LOX/H_2 engines as well as to LOX/Methane and MMH/NTO motors are presented here. Basically, the code is verified and validated on subscale model chambers, where detailed measurements are available. In a second step, fullscale predictions are given and compared, where available, to test data.

For the cryogenic LOX/H_2 engines, an approach is introduced to simulate the wall heat transfer of staged combustion engines with warm fuel injection. The Rocflam-II code delivers very good results comparing the heat flux predictions with subscale measurements. The capability of Rocflam-II to predict the heat flux for LOX/Methane engines is proved by the simulation of TEHORA subscale tests. Also here, good agreement is shown. Finally, the upper-stage engine Aestus, using the hypergolic propellant combination MMH/NTO, is simulated in coupled Rocflam-II/RCFS-II simulations. The comparison of integral heat flux shows almost perfect agreement and confirms the versatility of the code.

Acknowledgement
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