EMPRESARIOS AGRUPADOS

Project:
Chemical Modeling of Reactions and Processes in Propellant Systems

Title:
Executive Summary Report

Document No: **086-076-F-A50-00004**	Issue: **01**
Purpose of issue: Information	Date: 20/10/2023

Prepared:	SCF	E Shankara	Shankara Coello 2023.10.20 14:17:10 +02'00'
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CLASSIFICATION

Contains information for the design of structures, systems or components: Yes ☐ No ☒

Design verification : Not applicable ☒ Head of OU/Supervisor ☐ Verifier Level 1 ☐ Level 2 ☐

CONTROL OF MODIFICATIONS

Issue	Modifications
01	First issue

PRELIMINARY OR PENDING INFORMATION

Issue	Paragraphs	Subject	Status
01	-	-	

DISTRIBUTION

External	Internal	No. copies/Format
	AGD	1/electronic

ESA STUDY CONTRACT REPORT

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ESA CONTRACT No	SUBJECT	CONTRACTOR
4000136329/21/NL/MG	EVACPRO Chemical Modelling of reactions and processes in propellant systems	EAI

* ESA CR( )No	* STAR CODE	No of TN Executive Summary Report	

ABSTRACT:

This document aims to provide a summary of the activities and findings performed under the ESA CONTRACT No 4000136329/21/NL/MG, corresponding to the project EVACPRO: Chemical Modelling of reactions and processes in propellant systems.

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EVACPRO

ESPSS VALIDATION ACTIVITIES FOR CHEMICAL PROPULSION SYSTEMS

EXECUTIVE SUMMARY REPORT

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ESPSS 3.7.5
Executive Summary

EMPRESARIOS AGRUPADOS

Edition 2023

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Contents

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1. EVACPRO Executive summary Report

1.1 Purpose of the document

This document aims to provide a summary of the activities and findings performed under the ESA CONTRACT No 4000136329/21/NL/MG, corresponding to the project EVACPRO: Chemical Modelling of reactions and processes in propellant systems.

1.2 Reference Documents

[RD-1] ESPSS Libraries User Manual

[RD-2] EVACPRO D1: Propulsion System Models

[RD-3] EVACPRO D2: Model design document

[RD-4] EVACPRO D3: Model Validation Report

[RD-5] Rodriguez F. et. Al, "*IMPROVING LIQUID PROPULSION MODELING CAPABILITIES IN THE EUROPEAN SPACE PROPULSION SYSTEM SIMULATION (ESPSS) LIBRARY*"; 2nd International Conference on Flight Vehicles, Aerothermodynamics and Re-entry Missions & Engineering (FAR) 19 - 23 June 2022. Heilbronn, Germany

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2. Project context

2.0.1 ESPSS

The European Space Propulsion System Simulation (ESPSS) toolkit is developed within EcosimPro by EAI in partnership with ESA. This toolkit provides components and functions for simulating spacecraft and launch vehicle propulsion systems. It includes capabilities to represent models and effects such as liquid, hybrid, or solid rockets, fast transients (water-hammer), design and off-design steady simulations, connection to thermal, mechanical, electrical or control systems, etc. It is the standard tool of the European Space Agency and the European Industry for space propulsion simulation.

2.0.2 EVACPRO

The objective of EVACPRO is to improve ESPSS capabilities applied to transient simulations of complete chemical propulsion systems using novel propellants (LOX/CH4 and H202). This ESPSS extension will enhance the tool fidelity and will better support the design and verification activities of the European propulsion industry. For such purpose, the project is focused in two key application cases to guide ESPSS developments:

- LOX/CH4 application case: activities in the framework of M10 upper stage engine development (being AVIO the prime contractor of this rocket engine development and included in this consortium).
- Green propellant case: Roll and Attitude Control System (RACS) of future version of Vega launchers family.

The above application cases will be used to address the main objective of this project: to demonstrate agreement within 10% between simulated and measured performance along the operation sequence of a propulsion system. This requires determining the modelling capabilities to improve within ESPSS, which are listed hereafter according to the case of application:

- LOX/CH4 application case: this demands enhancements in:
  - Turbo-machinery thermal, mechanical and fluid dynamic transient models.
  - Reduced-order finite rate chemistry models for LOX/CH4.
  - Pyrolysis and coking phenomena within cooling jackets.
  - Heat and mass transfer in novel injectors for LOX/CH4.
- Green propellant case: this demands enhancements in:
  - Instabilities modelling in the catalysts of monopropellant thrusters.
  - Reduced-order finite rate chemistry models for H2O2 and other green propellants.
  - Chemistry models for H2O2 and other green propellants.
  - Injectors modelling for monopropellants.

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3. Project organization and tasks breakdown

The prime contractor for this activity is Empresarios Agrupados Internacional (Spain). 'Sapienza' University of Rome (Italy), AVIO (Italy), Nammo (Norway) and Lukasiewicz Research Network - Institute of Aviation (Poland) act as subcontractors.

The breakdown of the different work packages and milestones, together with the corresponding responsible, is summarised in Fig. 1.1

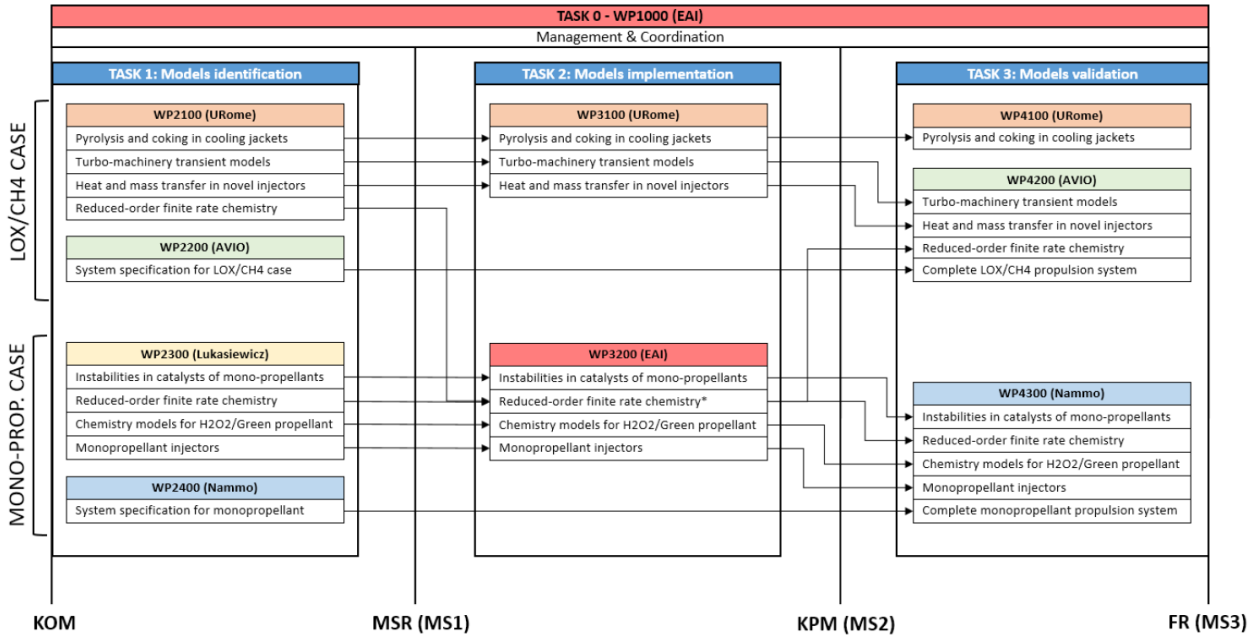

Figure 1.1. Task breakdown

The main reasons to distribute the different tasks between the partners are highlighted herein:

- Task 0: EAI is extensively experienced in ESPSS development projects within ESA frame contracts and it is the official distributor of ESPSS versions. Therefore, the participation of EAI within this project will result in an optimum distribution of resources for the later integration and distribution in the official ESPSS. Lastly, devoting the whole budget of the project to modelling and simulation activities justifies EAI responsibility of WP1000 (non-including experimental activities).
- Task 1: it involves all partners of the project since the identified models must be aligned with those used for the latter validation. Thus, this task requires the involvement of the industrial partners to specify the real components used in the propulsion system and research institutions to carry out the literature research for determining the most suitable models. In this way, the next WPs are included:
  - ◇ 'System specification' (WP2200 and WP2400): the industrial partners describe the characteristics of the components used in the real propulsion system. AVIO will carry out these activities for the case of LOX/CH4 and Nammo for monopropellant case. Both partners are responsible for the development of the complete system and, besides, have experience modelling these systems within ESPSS. Thus, they are fully familiar with the data requested by the simulation tool to address these activities. Lastly, AVIO and Nammo will identify the most suitable validation cases based on their available datasets from other project.

  - ◇ 'Models identification' (WP2100 and WP2300): research institutions will carry out studies to select the most appropriate models based on their experience. On the one hand, it is worth pointing out the relevant background of URome in modelling activities applied to chemical kinetics, turbo-machinery, cooling systems and injectors for rocket engine systems. On the other hand, IoA possesses all the required tools and competence to design a fully functional monopropellant thruster utilizing a catalyst bed. Expertise in this field has been shaped by years of research and testing, during which the phenomena of monopropellant injection and decomposition have been thoroughly understood. Therefore, both partners provide an excellent background to address these activities.

- Task 2: these activities are under the responsibility of EAI and URome, due to their experience as ESPSS developers within multiple ESA framework programs. EAI is the main developer of the ESPSS and it is noteworthy partner of ESA in the area of simulation. URome has carried out multiple ESPSS developments to improve the simulation capabilities of the tool at both numerical and physical level, being a key developer partner of ESPSS. Hence, EAI will be responsible the implementation activities of the green propellant case (WP3200) and URome will be in charge of the implementation related to the LOX/CH4 case (WP3100). Notice that EAI will perform the implementation of the reduced-order finite rate chemistry models for LOX/CH4 in order to exploit the synergies with the green propellant case and, thus, to optimise the time effort for both activities.
- Task 3: the validation activities will be done by the industrial partners of the consortium. They are responsible of the complete system development and have access to all databases required for validation. This approach assures an optimum scenario for validation, since the corresponding partner will not encounter extra-hindrance derived from a potential lack of data. According to it, AVIO will validate the components for the LOX/CH4 propulsion system (WP4200) and Nammo those for monopropellant case (WP4300). Finally, URome is included in this task because it will perform the validation of the pyrolysis and coking phenomena within cooling jackets using open literature (WP4100). The consortium has no experimental data regarding it and it considers that testing it experimentally will consist an on-purpose deterioration of the hardware (implying a relevant economic investment with no direct benefit for the real system). Therefore, these phenomena will be simulated as part of the complete propulsion system validation, but not reaching the coking condition at the test. The validation for coking conditions will be developed against open literature.

4. Project activities summary

4.0.1 Phase 1: models identification [RD-2]

LOX/CH4 injectors

Two aspects must be taken into account for a proper modelling of this kind of injectors: pressure drop models and heat transfer models.

Regarding the pressure losses, the way in which the pressure losses are computed inside ESPSS has been improved to take into account different geometries and types of injectors. Basically, it affects the calculation of the pressure drop coefficient. The following types of injectors are available:

Single jet injectors

Mixed jet injectors

Perforated plate injectors

Furthermore, the inlets can have different geometries: sharp, rounded, slanted or angled.

For the heat transfer, an improved thermal network has been created for the combustor components, which take into account an axial distribution of the injector holes and walls as in the picture below. Several nodes compute dynamically the evolution of the temperatures at the walls, taking into account the conduction among them and the ambient. It is possible to activate convection between the cavities and the walls.

LOX/CH4 reduced order finite rate chemistry

Four Arrhenius schemes have been proposed after a detailed literature review. These schemes for methane oxidation are generated starting from the C1-C4 kinetic mechanism by Zhukov Z-DKM, using the Computational Singular Perturbation and Tangential Stretching Rate algorithms. It leads to four schemes:

TSR-Stoic-21, a general 21-species scheme including initiation chemistry aspects associated to homogeneous ignition, to be operated in the neighbourhood of stoichiometric conditions.

TSR-Stoic-12, a compact 12-species scheme to be operated near stoichiometric conditions, as well.

TSR-Lean-14, a compact 14-species scheme to be operated under fuel-lean conditions.

TSR-Rich-32, a 32-species scheme to be operated under fuel-rich conditions.

All the aforementioned schemes have been tested and validated in terms of equilibrium temperature and composition, counter flow diffusion flames and perfectly stirred reactor calculations. The results showed comparable or superior performance compared to the Zhukov scheme.

Transient model for heating of turbomachines

A model which is significantly suitable to be implemented in the Ecosimpro/ESPSS framework, due to its structure, is present in the open literature. It is a work by a group belonging to the Indian Space Research Organization (ISRO). Such work has been selected to be the starting point for the development of the enhanced pump component in the ESPSS libraries. The scheme is presented in the image below:

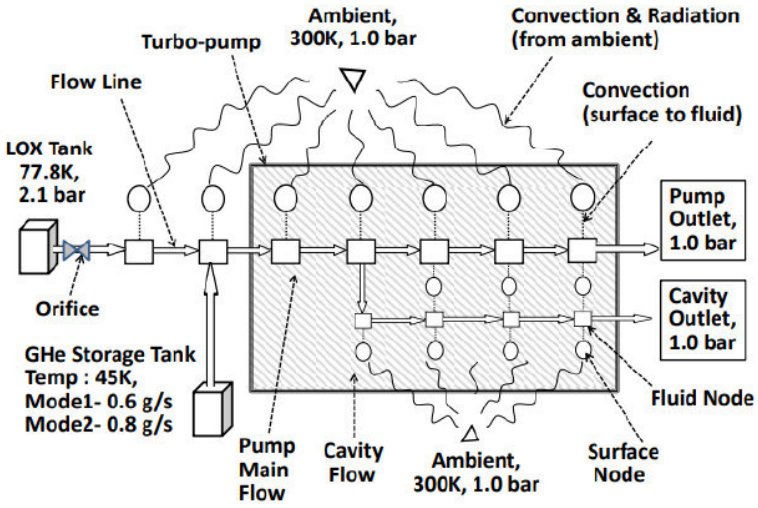

Figure 1.2. Scheme selected for the pump chilldown component

In their framework, fluid nodes solve for the conservation of the mass, of the momentum and of the energy, on a staggered grid. On the other hand, the so-called "surface" nodes, i.e., the thermal nodes, solve for the solid walls exchanging heat both with the fluid and with the external ambient by means of the heat equation. It has to be pointed out that the way in which the authors approach to the problem is significantly similar to the Ecosimpro/ESPSS approach.

Pyrolysis and coking

The model selected takes into account the effects of coke deposition on heat transfer, neglecting the effects on the fluid-dynamics. A time dependant thermal resistance is introduced, according to the carbon deposit build-up rate equation.

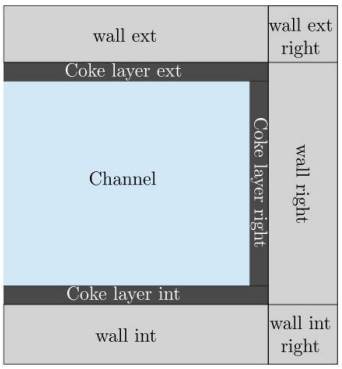

Figure 1.3. Wall structure with coke layer in the cooling jacket assembly

This thermal resistance depends on the Reynolds number, the wall temperature and four experimental coefficients that shall be tuned by the user.

Monopropellant models

This task involves several parts:

Chemical modelling of HTP

It has been decided to model HTP as a Perfect Liquid for lack of available data and for keeping simplicity of the model while fulfilling the requirements.

Several new properties files have been included inside ESPSS, each of them for a different concentration of HTTP: 85, 87.5, 90, 92, 95 and 98%. The range of temperatures goes from 0ºC to 100ºC.

Catalyst bed modelling

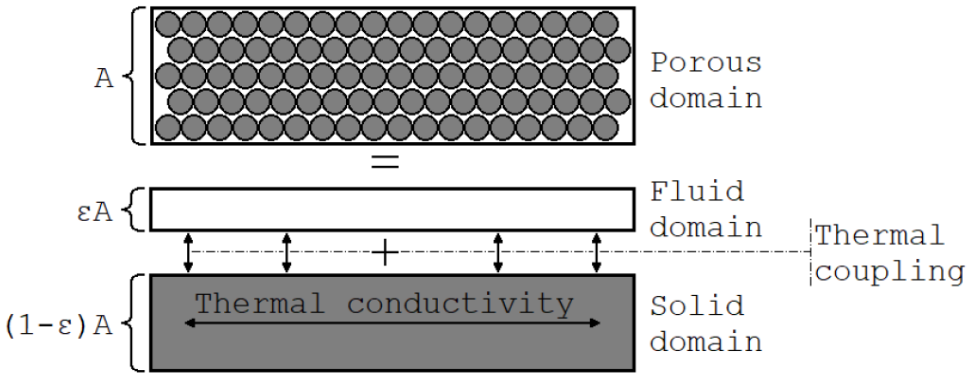

Figure 1.4. Catalyst bed scheme

The liquid and the gas phase are considered to be mechanically coupled. This simplifies the modelling of the multiphase flow, where concentrations of liquid components are parameters which define the properties of the liquid. These parameters are the mass fractions of the components in the flow. The have their own evolution equations.

The components available in the mixture are: liquid HTP, additional water, gaseous hydrogen peroxide, gas water vapor and oxygen vapor.

On the other hand, the fluid phase and the solid phase are considered to be at the same temperature. In the boiling region, liquid components transition into appropriate gas components proportionally to their concentration in the fluid. This stands against the reality of vapour-liquid equilibrium, however, it is compensated by the effective consumption of hydrogen peroxide from the liquid phase. Outside of the boiling region no water vapour is produced and the water produced during decomposition is modelled as additional water.

Delivered data points refer to a given concentration of HTP, which then decreases during the heating period of decomposition (below boiling point). This leads to an interesting challenge in terms of energy transport. As oxygen evolved in the pre-boiling region of decomposition only accounts for 16/34.015 of hydrogen peroxide mass lost, modelling of decomposition without an additional component to take up the remaining 18.015/34.015 of decomposed mass would lead to either mass or energy imbalance. To handle this issue, the additional water liquid component has been introduced, which does not possess the ability to decompose and takes up the mass created in decomposition of HTP.

Thermal losses due to convection and radiation are incorporated into the energy equation.

Proper modelling of finite rate chemistry is done by incorporating a finite rate bulk reaction model which can be easily fed input parameters extracted from the test data. Usage of pressure drop modelling is also crucial as concentration-dependent reaction will also depend on pressure of the gas.

The Ergun equation for the pressured drop, expresses the friction factor as a function of the Reynolds and porosity.

Injectors

The main type of injectors considered in this activity is the showerhead injector, as it is the most prevalent type in monopropellant thrusters.

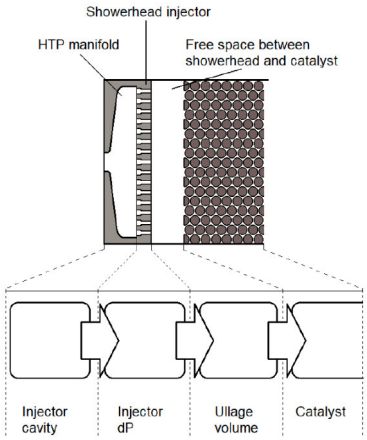

Figure 1.5. Injectors structure for monopropellant combustors

The injection system may be effectively divided into three interconnected components, each with different driving phenomenon and modelling challenges. These components are:

Manifold - injector cavity. Is modelled as a simple, constant 0D volume.

Injector element - set of injection orifices (holes) in case of showerhead injector. It is modelled with a general 1D momentum equation that compute pressure loss as a function of the discharge coefficient.

Ullage volume - non-porous volume between the face of the injector head and the catalyst. It is decided not to model this part due to ambiguities on physical phenomena in this region.

Catalyst bed - as no proven dispersion model has been found and no proposed model can be effectively validated, flow uniformity modelling is skipped to enhance reliability of the entire model. Hence, the model is expected to perform optimally with uniform injection patterns.

This approach enables easier understanding of the coupling between injector design parameters and the performance of a catalyst bed. This functional separation of blocks enables modular approach to modelling and further improvements of the model.

4.0.2 Phase 2: models implementation [RD-1] [RD-3]

LOX/CH4 injectors

A new injector component has been created called "InjectorLoss", more accurate and flexible than the currently existing injector in ESPSS. This new component takes into account a set of possible pressure-loss modes: single jet, mixed jets, swirled, closed swirl, open swirl, bipropellant swirl, gas-swirl and perforated plate.

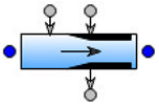

Figure 1.6. New InjectorLoss component

Two new topological macro-combustors have been added to ESPSS: "Preburner_Plate" and "ChamberNozzleDynamic_-Plate". These components incorporate the aforementioned injectors, plus a new heat exchange modelling. It has a detailed thermal network for computing the heat exchanged between the injector plate, the combustor walls and the cavities, as well as their temperatures.

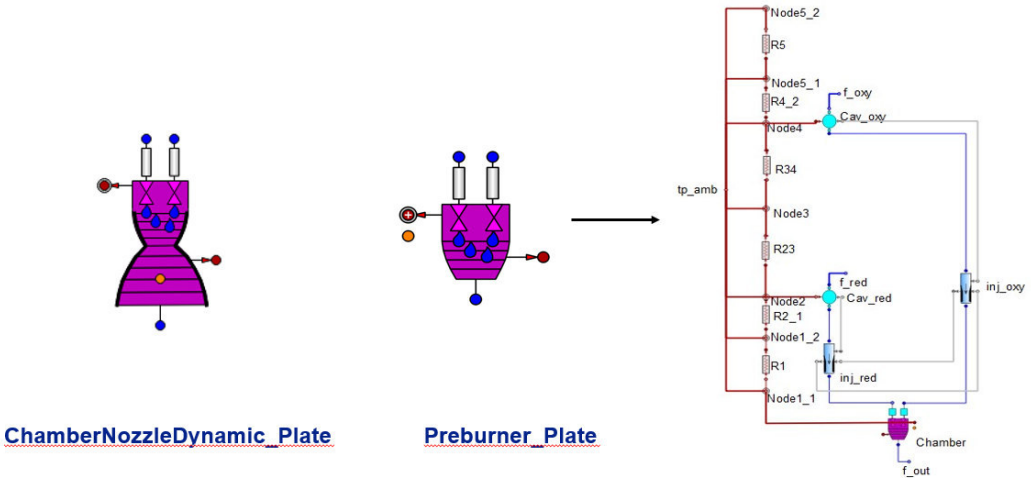

Figure 1.7. New advanced combustors components

LOX/CH4 reduced order finite rate chemistry

This activity consisted in the inclusion in ESPSS of new reduced order kinetic schemes for LOX/CH4 reactions.

During the implementation phase, it was detected that the mechanism TSR-Rich-32 proposed in the literature review phase, offered poor numerical performance, whilst not improving considerably the accuracy for rich mixtures. So, it was decided not to include this mechanism in the next version of the libraries. All in all, future ESPSS versions will have the possibility to compute the following finite rate schemes for LOX/CH4:

TSR-Stoic 21

TSR-Stoic 12

TSR-Lean 14

Global scheme

Each of them has a different number of species and reactions. The user can easily select the desired Arrhenius scheme in the attribute editor of the regular combustors available in ESPSS. No new components have been created at this regard. The necessary new chemicals have been added into the FLUID_PROPERTIES library. The following table shows the main characteristics of the schemes:

	TSR-Stoic-21	TSR-Stoich-12	TSR-Lean-14	TSR-Rich-32	Global
Number of species	21	12	14	32	6
Number of reactions	83	32	48	210	4
MR applicability	0.5 - 55	0.5 - 55	4 - 55	0.5 - 4	0.5-55
Pressure applicability	1 atm - 450 atm	1 atm - 450 atm	1 atm - 450 atm	1 atm - 450 atm	1 atm - 450 atm

Table 1.1. Summary of different schemes' features

First of all, a new ENUMERATIVE variable must be created, for choosing the desired Arrhenius scheme:

```
ENUM Arrh_option = {UsrDf, OX_CH4_12, OX_CH4_21, OX_CH4_Lean14, OX_CH4_Global}
```

Then, in the attribute editor of the component, a new switch will appear called "Arrhenius_inputs", and two possibilities are foreseen:

a) The Arrhenius scheme is a User-defined one, so all the fields for setting up the model are available.

b) The Arrhenius scheme chosen is "OX_CH4_12", "OX_CH4_21", "OX_CH4_Lean14" or "OX_CH4_Global". In these case, the input parameters for the model are read from the library, so the data that is not needed will be locked for the user

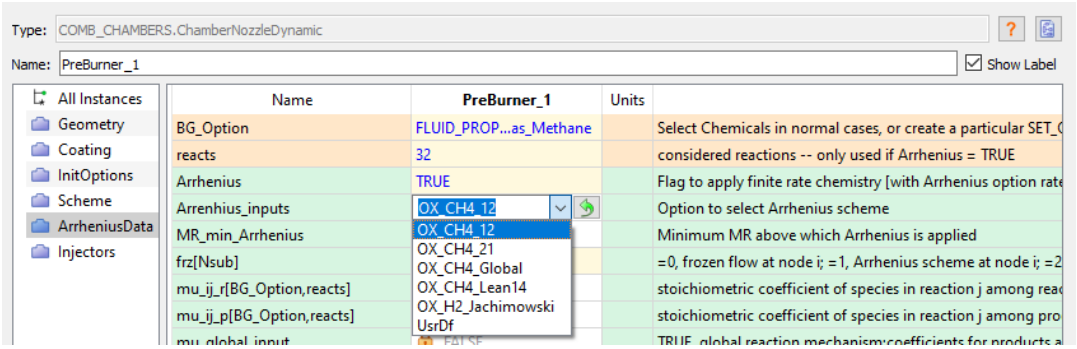

Figure 1.8. Attribute editor options w.r.t. Arrhenius schemes

Transient model for heating of turbomachines

A new component has been added to ESPSS called "Pump_chilldown". It is a topological component that is formed by the main fluid stream, plus a secondary stream in charge of chill down. The proper heat exchange with the inclusion of thermal nodes and conduction elements has been taken into account. A series of discretized volumes have been included to represent the different parts of the pump (impeller, volute, etc.)

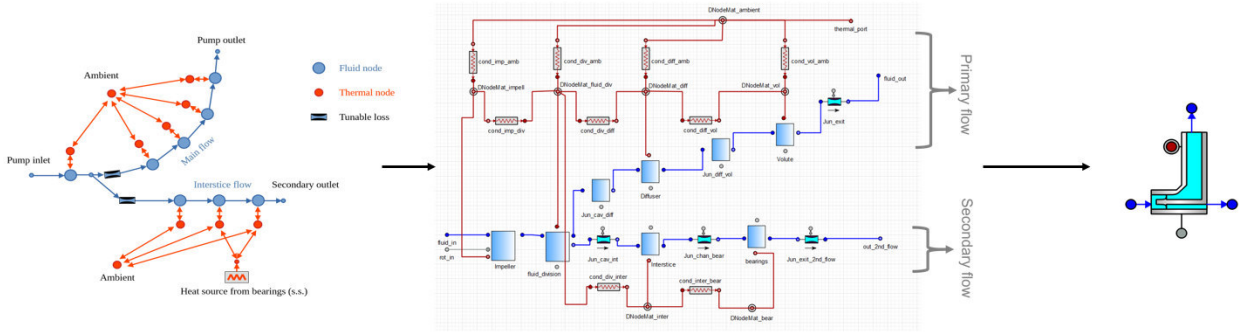

Figure 1.9. Pump chilldown topology

Pyrolysis and coking

Inside ESPSS, three components take this effect into account:

- "Tube_coking": new Tube component with an additional flag for activating/deactivating coking deposition. If the option is deactivated, the component behaves exactly as the regular Tube

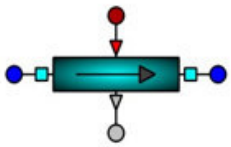

Figure 1.10. New Tube_Coking component

- CoolingJacket: this component has been upgraded to take into account this effect. For each node, the above mentioned thermal resistance is computed and, afterwards, the convective heat transfer coefficient is modified considering this phenomenon.
- CoolingJacket_tore: same considerations than for the CoolingJacket apply.

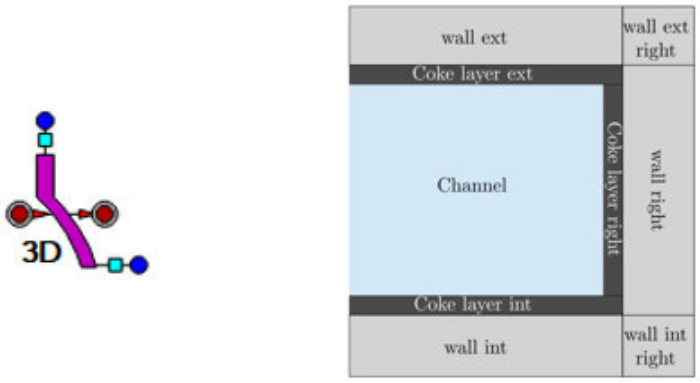

Figure 1.11. Cooling jacket structure sketch with coke layer

Monopropellant components

Three new components have been created inside ESPSS libraries for modelling HTP monopropellant cases:

- InjectorMonoProp: this component inherits equations from the abstract component "AbstractJunction" of the FLUID_-FLOW_1D library. The main difference between this new component and the abstract "AbstractJunctionLoss" is the calculation of the actual throat area as a function of the number of orifices and their geometry, and the calculation of the pressure loss coefficient "zeta" from the discharge coefficient.

There are three possible ways of imposing the discharge coefficient: constant value imposed by the user, a table dependent on the Reynolds number or the correlation of Lichtarowicz et al.

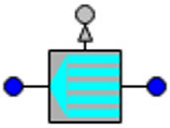

Figure 1.12. New InjectorMonoprop component

- CombustHTP. This component represents a basic HTP catalyst bed. It has several constant parameters for defining the geometry (cross section, length,...), the solid properties, heat coefficients and coefficients for computing the finite rate reactions. It is considered that the combustion and decomposition of the HTP is characterized by a set of volumetric and surface reaction of hydrogen peroxide.

With a 1D discretization, the mass, momentum and energy conservation equations allow to compute the dynamic evolution of the pressure, density, temperature, as well as the concentration of the mixture (HTP, water, vapours of water, vapours of oxygen and vapours of hydrogen peroxide).

For the boiling process, there are several options available for the user, each of them will have certain parameters to be imposed manually.

Figure 1.13. New CombustHTP component for catalyst bed

- CombustMonoprop_HTP. It is equivalent to the former CombustHTP component, but this one includes a nozzle connected downstream to simulate the fluid expansion.

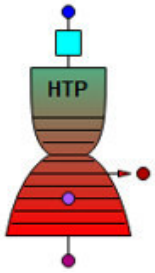

Figure 1.14. New CombustMonoprop_HTP component

4.0.3 Phase 3: models validation [RD-4]

LOX/CH4 Injectors

The appropriate validation of models for pressure losses through injectors two set of experiments were performed, with Reynolds number above 20000 in all cases:

- Water cold-flow tests. The jet injector with sharp edges, rounded inlet and slanted inlet and the perforated plate with slanted inlet have been tested and simulated, considering different mass flow rates at inlet. The perforated plate model shows better performance for the prediction of dP over the range of interest, with a 20% deviation, getting up to 30% for low Reynolds, due to uncertainties of measurements.
- Hot-firing tests. Data coming from DM1 M10 engine hot-firing test have been considered, implemented in coherence with the real hardware, using as BC the sensors data at injector inlet and combustion chamber. The numerical results have very good agreement with experimental data (below 10% for the selected cases) for the steady state values.

For validating the new thermal network, numerical simulations have been implemented considering the relevant dimensions of the components. The comparison between experimental and numerical results shall take into account that sensors are installed on the actual hardware in specific positions which might not be one-to-one useful for direct comparison.

The data from two fluidic thermocouples were available, considering the mean value. The results are really close due to the proximity between the boundary condition and the measurement.

However, the solid temperatures are not well reproduced during transient and steady state. This might be caused by the effective thermal conductivity of the component and to the actual exposed surfaces for the heat exchange between the fluid and the solid. Contac point and interstices are not being considered in the model.

LOX/CH4 reduced order finite rate chemistry

Two finite rate chemistry models were validated TSR-Stoich-21 and TSR-Stoich-12, and compared to the global reaction model of the ESPSS. Two schematics were considered, with a mass flow BC, used for tuning the model at the steady-state, and with a pressure BC, used for validation. Data from the DM1 M10 hot firing test campaign is considered.

Global and TSR-12 models allow to predict the adequate chamber pressure at the steady state, within 10% error wrt experimental data. The predicted chamber pressures are slightly lower than the equilibrium model, which better represents the experimental data at steady state. The running time are important w.r.t the equilibrium model, due to fluctuations of the results. The TSR-12 model allows to estimate the time instant at which ignition occurs.

Transient model for heating of turbomachines

Several simulations have been tested: chilldown, transient phase and transition from chilldown to startup. Test data from the Oxidizer TurboPump Assembly and Fuel TurboPump Assembly obtained during the DM1 experimental test campaign is considered: DM1-02, DM1-04-02.

Chilldown

The mass flow and the most important wall temperatures of ESPSS models can follow the experimental behaviour with a low error. Some differences in other temperatures are observed, due to some uncertanties in the model layout w.r.t. the

real. In addition to that, the real phenomena happening during the chill-down in very complex geometries such as the pump ones are really though to capture with the heat exchange models available in the ESPSS standard tubes.

Transient phase

Several tests have been carried out for the fuel and oxidizer pumps, and different torques. It has been validated the start-up, the shutdown and also the whole transient phase. From the results it is possible to appreciate the match w.r.t the experimental data, presenting a small delay in the mass flow signal due to the location of the mass flow-meter in the testing. A major difference appears during the start-up and shut-down due to a non-perfect characterization of the pump curves near 0-rpm conditions.

Pyrolysis and coking

Three validations cases have been identified: RP-1, Propane and JetA. The model employs a reduced- order approach and requires, due to the complexity of the phenomenon, to be calibrated on the available data. The models show good ability to represent the wall temperature increase due to the increase of thermal resistance with coke formation and deposition inside the cooling channels, with an error less than 10% after calibration.

LOX/CH4: AVIO validation of M10 DM1 test campaign.

The observables variables are the rotational speed, the mass flow and outlet pressure of the fuel and oxidizer pump, and the pressure and mixture ratio of the combustion chamber.

At first step, a calibration at steady state was performed w.r.t experimental test data of all the observables, and then a transient simulation is performed. The results are in line with the experimental data both in terms of absolute values and transient trend: the complete engine model with the new developed pumps is able to reproduce with an high degree of accuracy the experimental transient trend both during the start-up and during the shut-down for all the observable considered. The simulation takes around 7000 seconds to run.

HTP: Nammo validation of PoC1 and PoC4 test campaign

This validation work is focused on the monopropellant combustors and the injector component is also included in the validation.

The decomposition and evolution of pressure, temperature and mass flow is considered. Temperature gradients through the material of the thruster and nozzle is not investigated.

The simulations were done using the perfect liquid 87.5% "PfLiqH2O2_875" from the ESPSS toolkit.

Poc1

Several operation points were considered, for a single thrust OP38 and multiple pulses OP25 and blowdown OP29. Pressure, temperature and thrust data had a good match between test and simulation, mass flow rate was 7-8% too high in SSF, 5 % too high in PMF with the CombustHTP component, which may be caused with problems of the nozzle component for high AR.

The "CombustMonoprop_HTP" gave a better match with the measured mass flow from testing and generally a good match with error <1%. The model was running stable with an acceptable computational time, and it seemed quite robust.

In the simulations the pressure rise is generally faster than in the testing, which may be caused by the model of catalytic decomposition rate for liquid H2O2, thermodynamic effects, flash boiling, Leidenfrost effect, 3D injector effects, small cavity downstream of injector plate that has not been modelled and test sensor delay.

Poc4

There is very good agreement in mass flow, temperature and pressure (<5%) in steady state of the single thrust operation points. Regarding the pulse firing modes, there are some differences in pressure in the start of the pulses, whereas the

levels at the end of the ON-time fit quite well. The peak of water hammer after closing the FCV has quite good accuracy, as well. The maximum error observed in these models is 13% for the temperature in OP5 operation point.

The combustion chamber pressure rise happens more rapid in the simulation than what is recorded from testing, but we also know there are some uncertainties about the delay in the pressure signal from testing caused by the test equipment. The pressure rise time is comparable with what is seen from the previous ESPSS monopropellant component, but there is a greater potential of tuning the EVACPRO-component to fit with test data. The computational speed seems to be in the range of comparable ESPSS-models, which means it is suitable also for simulation of systems with several thrusters.

5. Conclusions and future work

5.1 LOX/CH4 case

Analysis on the chill-down phase show that the new pump model is able to follow the trend of the fluidic nodes in very accurate way, while for the nodal temperature both the nodal geometrical characteristic together with the layout must be as much as possible similar to the real ones to have a representative temperature trend.

Analysis on transient phases showed that the introduced perturbing torque allowed appropriate prediction for LOX pump at start-up, whereas poor predictions of fuel pump and therefore dedicated tuning might be needed in order to fit the results to the specific hardware designed.

The extension of the characteristic pump curves to move from chill-down to start-up condition has been tested. Results show some discrepancies in terms of absolute values which must be attributed to the characteristic curves of the pump and probably also to the turbine, which plays an important role. In fact, the results could be no better of the representation of the characteristic curves during transient, and it is not an easy task. Simulations at engine level were performed. The results were in line with the experimental data both in terms of absolute values and transient trend: the complete engine model with the new developed pumps is able to reproduce with a high degree of accuracy the experimental transient trend both during the start-up and during the shut-down for all the observable considered.

Analyses were performed to validate the proposed models for injector's pressure losses. The comparison with data from hot firing tests showed that the numerical model of perforated plate predicts the appropriate mass flow rate, with an error within the desired 10% range, and typically lower at increasing mass flow rates.

Hence, the implemented model for dP in injectors is an important step and it can support the investigations on performance of LRE at different operating points, taking into account that the Cd is variable at different Re.

The analyses on the implemented chemical models highlighted that the use of finite rate chemistry severely impacts the overall computational time. The great advantage of the use of detailed chemistry is the capability to detect with good accuracy the time of propellants ignition.

5.2 Monopropellant case

The component modelling the catalyst CombustHTP seems to run well in the simulation, and after tuning some of the catalyst reaction rates it gives good agreement with data from testing of two different thrusters. For PoC1 with a high nozzle AR, there was a discrepancy in the massflow up to 8% for SSF. For PoC4 with a more uniform flow into the catalyst and a lower nozzle AR, the temperature, pressure and massflow match quite well with test data, error <3% for the steady-state phase. The combustor and nozzle combined component ("CombustMonoprop_HTP"), also gave better match with the SSF data from PoC1, with error <1%. The simulation of blowdown for 300s also shows good agreement with the test data, which means pressure drop in catalyst pack modelled with Ergun's equation yielded accurate results over the entire mass flow range.

For PMF consisting of a pulsetrain with 20 pulses and 1000ms ON-time, the model showed accumulated propellant mass and total impulse within 2% accuracy for PoC1. PoC4 has only been tested with pulses with ON-time in the range from 20-160ms, hence validation was done with one PMF from each end of this range. The mass bit and impulse bit during 25 pulses were within 10.1% accuracy for both pulsetrains for PoC4.

The combustion chamber pressure rise happens more rapid in the simulation than what is recorded from testing, but we also know there are some uncertainties about the delay in the pressure signal from testing caused by the test equipment. The pressure rise time is comparable with what is seen from the previous ESPSS monopropellant component, but there is a greater potential of tuning the EVACPRO-component to fit with test data. The computational speed seems to be in the range of comparable ESPSS-models, which means it is suitable also for simulation of systems with several thrusters.

5.3 Future work

5.3.1 Regarding the new combustor for LOX/CH4

- The model shall allow to calculate the pressure based on the Dt (without relying on the mesh). This can probably ensure easier simulations and calculations, and more precise predictions.
- The formula for the convective heat transfer rely on the use of the actual diameter, and any error on Dt will propagate also on the prediction of heat transfer and therefore on the coolant state (if any cooling jacket component is implemented).
- Limitation in new chemical schemes: missing N2 and He in the list of non-condensable fluids.
- Probably a dedicated component with finite rate chemistry can be implemented (without all the features for coating, heat exchange, etc.) and only to assess performance in transient phases of small thrusters, which are typically characterized by shorter characteristic time.

5.3.2 Regarding monopropellant components

- Improve the way in which the geometry of the subsonic and supersonic parts are inputed by the user. Currently there are some small inconsistencies.
- Improve robustness when the nozzle type is set as "nozzle_type= NonIsentropic". Now it has been checked that the convergency is much better in the Ideal type of nozzles.
- The "CombustorHTPNozzle" does not seem to handle GN2 as pressurizing gas in the system. Include this future for the next release
- Include an option to be able to specify different porosity along the length of the catalyst

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Edition 2023