

1-D Simulation of Solid and Hybrid Combustors with EcosimPro/ESPSS

J. Moral⁽¹⁾, F. Rodríguez⁽¹⁾, J. Vilá⁽¹⁾, F. Di Matteo⁽²⁾, J. Steelant⁽²⁾

(1) Empresarios Agrupados Internacional. S.A. Magallanes, 3. 28015 Madrid. Spain. (email: frj@empre.es)

(2) Aerothermodynamics and Propulsion Analysis Section (TEC-MPA), ESTEC-ESA, Keplerlaan 1, P.O. Box 299, 2200 AG Noordwijk, The Netherlands (email: Johan.Steelant@esa.int / Francesco.Di.Matteo@esa.int)

Abstract

The configuration of the Ariane 6, which foresees a consistent use of solid rocket motors (SRM), and the increasing effort of some companies in hybrid propulsion systems support the necessity to have fast and accurate modelling tools. In this paper, the developments carried out for the 1D simulation of solid and hybrid rocket motors in the ESPSS/EcosimPro [1] environment are described.

The proposed 1-D formulation for the solid and hybrid propulsion is firstly presented; the main hypothesis used and its limitations are discussed, as well as its implementation and integration in the ESPSS code. In this context, a non-causal and object oriented modelling approach is used in order to obtain a flexible frame for future improvements. The results of simulations with the new components are finally presented. A sensitivity analysis is performed in order to evaluate the effect of different parameters (data, mesh discretization) on the simulation results.

Since the source code is available, an ESPSS user can adapt or extend the libraries in order to fulfil his specific needs.

INTRODUCTION

A continuous and fruitful collaboration between ESA, industry and research centers have developed ESPSS as a state of the art tool for the simulation of space propulsion systems. It consists of a set of system libraries compatible with EcosimPro, which main target is the simulation of liquid and recently first basic models for solid rocket engines. They feature 0/1-D models for tanks, pipes, turbo machinery, valves, fitting, nozzles, combustion chambers, etc.

ESPSS libraries provide palettes of components that can be used to build graphically complex systems. EcosimPro basically incorporates the following features: an object-oriented programming language which enables encapsulation, inheritance and aggregation, a powerful DAE solver and a friendly Graphic User Interface (GUI).

ESPSS version 3.0 accounts for important upgrades. Between many others, it includes new components for the simulation of scramjet & solid/hybrid combustors:

- Solid/hybrid combustor components include an “evaporation” model for the solid (and liquid) propellants together with a 1D reaction delay model for the combustor core.
- Airbreathing combustor components including an intake, a 1D model for the liquid fuel injections and evaporation together with a 1D reaction delay model.

ESPSS OVERVIEW

ESPSS Software can be used for system concept definition, mission analysis, impact studies, investigation of anomalies and optimization, testing and pressuring/propellant loading. It is structured in different project areas (libraries):

- The Fluid Properties library allows, among other capabilities, calculating real properties of the typical working fluids in propulsion systems as it is done by the well-known NIST code [3].
- The Fluid Flow library simulates complex two-phase, two fluid systems, dealing in particular with two-phase discontinuities and shock waves. It uses improved algorithms for fast transient 1D fluid flow, performing better tracking of the pressure and phase discontinuities (priming conditions for example).
- The Combustion Chamber library simulates 1D liquid, solid and hybrid rocket engines, including the calculation of the chemical equilibrium of an arbitrary mixture of chemicals as the well-known CEA code does, but in transient and non-adiabatic conditions.
- The Tanks and Turbo-Machinery Libraries allow integrating the state of the art of these rocket subsystems.
- Special dedicated libraries for orbital and attitude motion and for electrical propulsion systems are also part of the tool.

In transient conditions, the convection and mixing of burned gases is calculated dynamically (using the transport equations) for any component downstream a combustion chamber (staged engines). These components calculate the fluid thermodynamic properties in accordance with the local current chemical composition at a point.

Finally, the STEADY library contains a complete set of the components of the previous libraries, but for the direct calculation of the steady performances of any cycle type under design and off-design conditions. This means that the “sizing” of the cycle can be calculated under steady conditions by the code giving some design conditions such as the chamber pressures, mixture ratio, efficiencies, etc.

HYBRID COMBUSTOR FORMULATION

The transient conditions (pressures, temperatures, mass flows and heat exchanged with the walls) will be derived from general 1D area varying transient conservation equations. The composition of the combusted gases is obtained according to the minimum Gibbs energy method [2].

A) Topology

The schematic of “*CombustChamberNozzle_hybrid*” type component is shown below. This component represents a non-adiabatic 1D combustor-nozzle chamber for solid and hybrid propellants built by means of a hybrid combustor, an oxidizer injector with its cavity and a Nozzle.

The “*CombustChamber_hybrid*” component has an outlet fluid port to be connected to other ESPSS components. The properties and composition of combusted gases can be transmitted by the outlet fluid port to another ESPSS component (see the application examples).

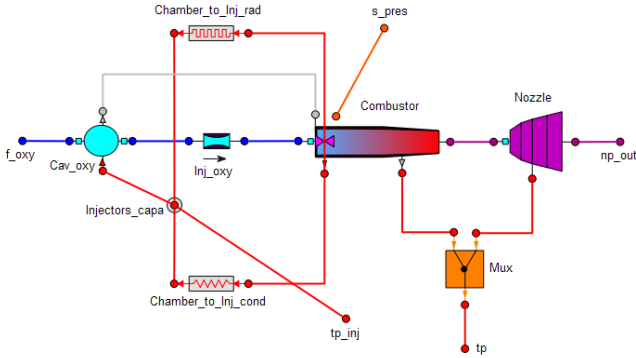


Figure 1 Schematic of a hybrid combustion chamber

B) 1D Conservation equations

In the gas core of the combustor, similar equations as in the ESPSS “Pipe” component are used, whereas extra terms are added to mimic the rubber and droplets vaporization, and the production of combusted gases. The following system of governing equations, here in area-scaled matrix conservation form, is modeled:

$$\frac{\partial \omega}{\partial t} + \frac{\partial f(\omega)}{\partial x} = \Omega(\omega)$$

where:

$$\omega = A \begin{pmatrix} \rho \\ \rho x \dots \\ \rho v \\ \rho u \end{pmatrix}; f(\omega) = A \begin{pmatrix} \rho v \\ \rho v x \dots \\ \rho v^2 + P + qn \\ \rho v(u + P/\rho) \end{pmatrix}$$

$$\Omega(\omega) = \begin{pmatrix} \Sigma S_{vap} \\ S_{vap} \\ -0.5(\Delta \xi / \Delta x) \rho v |v| A + P(dA/dx) \\ \Delta Q / \Delta x + \rho g v A \end{pmatrix}$$

A is the variable flow area and v the velocity. ρ , $x \dots$, P, u are the gas mixture density, vapor mass fractions (from the oxidizer and the grain), the pressure and the total energy respectively. “qn” is the artificial dissipation term. Previous equations need to be closed with the gases state equations (pressure calculation coupled with the products calculation as explained below).

Next paragraphs describe the numerical approach for the calculation of the different source (S) terms together with similar simplified equations for the liquid phase if any (hybrid combustors) along a 1D mesh. A *centered scheme* within a *staggered grid* is used, in

which the continuity and energy equations are evaluated at the center of the volumes, and the momentum equation at the junctions between the volumes.

The DASSL [6] solver is used for integrating the transient terms.

Mass and energy equations:

$$V_i \rho'_i + V_i \rho_i = m_{jun,i-1} - m_{jun,i} + m_{vap_sp,i} + m_{vap_oxy,i}$$

$$(u'_i \rho_i + u_i \rho'_i) V_i + V_i \rho_i u_i = m h_{jun,i-1} - m h_{jun,i} + q_{vap_sp,i} + q_{vap_oxy,i}$$

- $m_{jun,i}$: Gas mixture mass flow at the exit of volume i
- $m h_{jun,i}$: Gas mixture total enthalpy flow at the exit of volume i
- ρ_i, u_i : Gas mixture density and total energy at volume i. ($u = u_{st} + 0.5 vel^2$). “vel” is the mean velocity calculated from the adjacent junctions, see the momentum equations
- $m_{vap_oxy,i}$: Mass flows of vaporized oxidizer at volume i
- $q_{vap_oxy,i}$: Heat and enthalpy flows of vaporized oxidizer at volume i
- $m_{vap_sp,i}$: Mass flows of “vaporized” solid propellant (grain) at volume i
- $q_{vap_sp,i}$: Heat and enthalpy flows of “vaporized” solid propellant (grain) at volume i

The derivative of volume i is calculated in paragraph “*Solid propellant consumption*”. Vaporization terms are calculated in paragraphs “*Solid and liquid evaporation models*”.

In the case of a hybrid combustor, the gas mass (vapors and non-condensable gases) and enthalpy flows ($m_{jun,0}$, $m_{hjun,0}$ terms) at injector level ($i=0$) are calculated by the Injector component taking into account the quality calculated in the Cavity component.

$$m_{jun,0} = m_{oxy,inj} x_{oxy}; \quad m h_{jun,0} = m_{jun,0} h_{oxy,mix_gas}$$

where $m_{oxy,inj}$ is the injector mass flow (liquid plus gas) and x_{oxy} is the gas mixture mass fractions (vapor plus non condensable gases) in the cavity. Enthalpies “ h_{jun} ” are calculated using the upstream cell conditions: $h_{jun,i} = h_{i-1} = (u + P/\rho)_{i-1}$. P, T conditions are derived from the combustion equations (see below).

Momentum equations:

Momentum equations for a 1D area varying tube are:

$$0.5(L_{i-1} + L_i) \cdot m'_{jun,i} = A_{i-1} [P + qn + \rho v^2 - 0.25 \xi \cdot \rho v |v|]_{i-1} - A_i [P + qn + \rho v^2 + 0.25 \xi \cdot \rho v |v|]_i - 0.5(P_{i-1} + P_i)(A_{i-1} - A_i)$$

- P_i : Gas pressure at node i
- L_i : Length of each chamber at node i

The artificial dissipation, $qn(i)$, is used for avoiding numerical spikes and calculated as follows [4, 5]:

$$qn(i) = -Damp \frac{m_{jun}(i+1) - m_{jun}(i)}{A} V_{sound}(i)$$

Damp is a global constant to be defined in the experiment file. Momentum equations are applied to the exit of any volume in which the combustor is discretized.

Liquid oxidizer “evaporation” model

Vaporization flows, “ m_{vap_oxy} ”, and enthalpies flows, “ q_{vap_oxy} ” (source term for the gas mixture conservation equations), are calculated by the droplet vaporization model:

Assuming a very thin saturated layer between the oxidizer droplets and the surrounding gases, the conservation equations establish that the sum of convective heat plus enthalpy mass flow are the same at both sides of the layer. Then, the following set of equations is applied at each combustor volume i , allowing the calculation of the mass and energy exchanges through this layer:

$$m_{vap_oxy,i} = A_{liq_oxy,i} \left(hc_i (T_i - T_{sat_oxy,i}) + hk_i (T_{liq_oxy,i} - T_{sat_oxy,i}) \right) / (h_{vap_oxy,i} - h_{liq_oxy,i})$$

$$q_{vap_oxy,i} = m_{vap_oxy,i} h_{vap_oxy,i} - A_{liq_oxy-gas,i} hc_i (T_i - T_{sat_oxy,i})$$

$$hk_i = 2\lambda_{liq_oxy,i} / D_{droplet_oxy}$$

$$A_{liq_oxy,i} = f_{vap,i} 6M_{liq_oxy,i} / \rho_{liq_oxy} / D_{droplet_oxy}$$

- $M_{liq_oxy,i}$: Liquid mass at volume i , see the equations for liquids later on
- $T_{liq_oxy,i}$: Liquid droplet temperatures at volume i
- τ_{vap} : Characteristic vaporization time (input data)
- $D_{droplet}$: Mean droplet diameter
- $A_{liq_oxy,i}$: Equivalent exchange area between the droplets and the gas
- $f_{vap,i}$: Vaporization factor (time dependant input data)
- T_i : Gas temperatures at volume i
- hc_i : Heat exchange coefficient at gas side (Dittus correlation)
- λ_{oxy} : Droplet conductivity
- $T_{sat_oxy,i}$: Saturation temperature calculated at the partial vapor pressure of volume i
- $h_{vap_oxy,i}$, $h_{liq_oxy,i}$: Saturation enthalpies calculated at the partial vapor pressure of volume i

The droplet diameter has been modulated by the vaporization factor f_{vap} . This factor is an input datum depending on the time and on the volume number. In theory, assuming a known droplet size at the injection plate, the droplet diameter evolution could be determined by “simple” equations relating the evaporated mass flow with the liquid mass conservation equations. Nevertheless, due to the high penetration and breakup of the liquid jets, it seems more realistic to assume a known (adjusted, f_{vap} factors) droplet size at each chamber volume, the number of droplets being determined by the current liquid mass.

Solid propellant “evaporation” model

The solid propellant evaporation and consumption models are based on an equivalent cylindrical shaped grain. The thickness of the cylinder (“equivalent thickness”) is such that the actual mass of the cylindrical grain matches the mass of the actual grain.

Mass fractions of the solid propellant constituents are input data within a predefined set of constituents {HTPB, IPDI, RubUsr, KNO3_a, Al_cr, S_a, NH4NO3_IV, NH4CLO4_l}. *Note that the solid propellant “constituents” are reactants that will be “evaporated” before reacting in the core of the combustor.*

Two models are available for the source terms in the gas mixture conservation equations (“ m_{vap_oxy} ”, “ q_{vap_oxy} ”) corresponding to the solid propellant contribution:

1/ User defined model

The solid propellant consumption for each node “ i ” is calculated assuming an empirical regression law, function of the mass flow or the pressure for the hybrid or solid option respectively:

$$r_{sp,i} = a_{sp} G_i^{b_{sp}} \text{ (stdHybrid)}; \quad r_{sp,i} = a_{sp} P_i^{b_{sp}} \text{ (stdSolid)}$$

$$m_{vap_sp,i} = r_{sp,i} \rho_{sp} A_{sp,i}; \quad A_{sp,i} = f_{sp} \pi D_{sp,i} L_i$$

a_{sp} , b_{sp} : Regression rate constants (input data)

ρ_{sp} : Grain density (input data)

G/P: Gas mass flow per unit area or Pressure at volume i

$D_{sp,i}$: Current equivalent internal diameter of the solid propellant grain at volume i

L_i : Length of node i of the chamber

$A_{sp,i}$: Actual exchange area between the grain and the gas at volume i

f_{sp} : grain/fluid interface factor

The actual solid-gas exchange area of the grain is related with the equivalent one through the adaptation factor “ f_s ”, which is calculated according to a parabolic relation depending on the grain thickness:

$$f_s = A_{wet}/A_{cyl} = f_{sp}[1] + f_{sp}[2]*th + f_{sp}[3]*th^2$$

where $f_{sp}[i]$ are input data coefficients. *These coefficients resume the geometrical calculation of the grain perimeter changing with the grain consumption, thus allowing the adjustment of the thrust profile for not cylindrical grains.*

2/ Advanced model

Similarly than in the injected liquid “evaporation” model, and assuming a thin vapor layer between the grain and the surrounding gases, the conservation equations establish that the sum of convective heat plus enthalpy mass flow are the same at both sides of the layer. Then, the following set of equations is applied at each combustor volume i , allowing the calculation of the mass and energy exchanges through this layer:

$$m_{vap_sp,i} = A_{sp,i} (hc_i (T_i - T_{sat}) + hk_i (T_{sp,i} - T_{sat})) / LH_{sp}$$

$$q_{vap_sp,i} = m_{vap_sp,i} LH_{sp} - A_{sp,i} hc_i (T_i - T_{sat})$$

$$hk_i = 2\lambda_{sp,i} / th_{sp,i}$$

T_{sat_sp} : “Saturation” temperature of grain (input data)

LH_{sp} : “Latent” heat for grain evaporation (input data)

λ_{sp} : Grain conductivity (input data)

$T_{sp,i}$: “Liquid” grain temperatures at volume i

T_i : Gas temperatures at volume i

hc_i : Heat exchange coefficient at gas side at volume i

- hk_i: Heat exchange coefficient by conduction at volume i
th_{sp,i}: Grain thickness at volume i

As in the User defined model, the exchange area A_{sp,i} between the grain and the gas is modulated by the grain/fluid interface factors f_{sp}. The heat and enthalpy exchange with the gas phase is evaluated with the same formula in both cases:

$$q_{\text{vap_red},i} = m_{\text{vap_red},i} \text{LH}_{\text{sp}} - A_{\text{sp},i} hc_i (T_i - T_{\text{sat}})$$

In this respect, the importance of the values of LH_{sp} ("Latent" heat for the grain evaporation) and T_{sat} ("liquid" grain temperature) is pointed out. Both variables are input data in the current model.

Burning rate:

The burned gas mass flow is calculated assuming a global characteristic burning time. It is assumed that any species (vapor or burned gas) present in the gas mixture contributes to the global reaction rate, so the burning rate will be proportional to the total gas mixture density:

$$m_{\text{bu},i} = f_{\text{bu},i} \rho_i V_i / \tau_{\text{bu}} \tanh((t - t_{\text{burn}}) / \tau_c)$$

- m_{bu,i}: Burned gases mass flow at volume i
τ_{bu}: Characteristic burning time
τ_c: Ignition time delay with respect to the ignition order
f_{bu,i}: Burning factors at volume i

The burning factors are automatically set to one if the burning conditions are true: mixture ratio within the allowed limits and ignition flag activated. Otherwise the burning factors are set to zero.

Conservation of vapors, solid propellant gases and products mass fractions:

The vapor mass conservation equations take into account the burned gas production and the vaporization terms previously calculated:

$$(x'_{\text{sp},i} \rho_i + x_{\text{sp},i} \rho'_i) V_i + x_{\text{sp},i} \rho_i V_i' = x_{\text{sp},i-1} m_{\text{jun},i-1} - x_{\text{sp},i} m_{\text{jun},i} + m_{\text{vap_sp},i} - x_{\text{sp},i} m_{\text{bu},i}$$

$$(x'_{\text{oxy},i} \rho_i + x_{\text{oxy},i} \rho'_i) V_i + x_{\text{oxy},i} \rho_i V_i' = x_{\text{oxy},i-1} m_{\text{jun},i-1} - x_{\text{oxy},i} m_{\text{jun},i} + m_{\text{vap_oxy},i} - x_{\text{oxy},i} m_{\text{bu},i}$$

- X_{oxy,i}: Oxidizer vapor mass fraction at volume i
X_{sp,i}: Solid propellant "vapors" mass fraction at volume i
X_{k,i}: Actual burned mass fraction of the chemical constituent k at volume i
X_{k_eq,i}: Equilibrium mass fraction of chemical k at volume i
X_{bu,i}: Burned gases mass fraction at volume i
(X_{bu,i} = 1 - X_{sp,i} - X_{oxy,i})

For the first chamber volume, the upstream convective term of the oxidizer conservation equation is replaced by the corresponding flow of the injected vapor. For any chamber volume, the vapors production is represented by the terms m_{vap_sp}, m_{vap_oxy} (vaporization models, see before) and consumed proportionally to the formation of burned gases (terms x_{sp}m_{bu}, x_{oxy}m_{bu}), previously calculated according to a characteristic burning time.

Combustion gases properties calculation

This section provides the formulation for the variables (pressure, temperature, composition, and combusted gases properties) needed to establish the previously mentioned conservation equations. It is supposed that any molar fraction follows a global reaction rate in accordance with the previously mentioned burning time:

$$y'_{\text{bu},k,i} = (y_{k_eq,i} - y_{\text{bu},k,i}) / \tau_{\text{bu}}$$

- y_{k_eq,i}: Equilibrium molar fraction of the chemical constituent k at volume i
y_{bu,k,i}: Actual burned molar fraction of the chemical constituent k at volume i

For each chamber volume i, equilibrium composition of the combustion gases is calculated using the Minimum Gibbs energy method as a function of the gas mixture molar fractions, the pressure and the enthalpy. The gas mixture molar fractions are calculated as follows:

Oxidizer vapor contributions:

$$N_{\text{oxy},k,i} = x_{\text{oxy},i} \frac{y_{\text{oxy},k}}{MW_{\text{mix,oxy}}}; \quad MW_{\text{mix,oxy}} = \sum_{k=1, N_{\text{chem}}} y_{\text{oxy},k} MW_k$$

Solid propellant gas contribution:

$$N_{\text{sp},k,i} = x_{\text{sp},i} \frac{y_{\text{sp},k}}{MW_{\text{mix,sp}}}; \quad MW_{\text{mix,sp}} = \sum_{k=1, N_{\text{chem}}} y_{\text{sp},k} MW_k$$

Burned gas contribution:

$$N_{\text{bu},k,i} = x_{\text{bu},i} \frac{y_{\text{bu},k,i}}{MW_{\text{mix,bu}}}; \quad MW_{\text{mix,bu}} = \sum_{k=1, N_{\text{chem}}} y_{\text{bu},k,i} MW_k$$

Gas mixture:

$$N_{k,i} = N_{\text{oxy},k,i} + N_{\text{sp},k,i} + N_{\text{bu},k,i}$$

Where:

- N_{chem}: extended to any chemical treated by the FLUID_PROPERTIES library
MW_k: Molecular weight of the chemical constituent k
X_{xxx,i}: Mass fractions of oxidizer vapor, solid propellant vapor and burned gases (see conservation equations)
y_{oxy,k}: Molar fraction of chemical k of the oxidizer mixture
y_{sp,k}: Molar fraction of chemical k of the solid propellant vapor
y_{bu,k,i}: Molar fraction of chemical k of the burned gas mixture at volume i
N_{k,i}: Number of moles of the chemical constituent k of the reactant mixture at volume i

Once the number of moles of the solid propellant gases, oxidizer and burned gases mixture has been evaluated, and using the enthalpy value obtained from the conservation equations, it is possible to call the Minimum Gibbs energy method to obtain the equilibrium combustion gases composition:

$$(y_{k_eq}, T_{\text{eq}})_i = f_{\text{minGibbs}}(N_{k,i}, h_{\text{T}} - V_i^2/2, P_i)$$

Two possibilities are foreseen calling the previous function: a/ Equilibrium and b/ frozen flow. In the latter case (no ignition) the molar fractions remain constant: y_{k_eq,i} = N_{k,i}.

The effective combustion gas constants (R_i, Cp_i, cond_i, visc_i) are derived using the 'mixture properties'

equations as a function of $y_{bu,k,i}$. The pressure is obtained from the perfect gas equation: $P_i = \rho_i \cdot R_i \cdot T_i$

The molar fractions of the products of the last volume are transmitted to the outlet port to be used by the Nozzle component or in another possible ESPSS component.

Liquid (oxidizer) propellant consumption:

The mass of liquid contained at each volume ($M_{liq_oxy,i}$) and its temperature ($T_{liq_oxy,i}$) are calculated assuming that $Vel_gas = Vel_liq$ and neglecting Cp_liq derivatives:

$$M'_{liq_oxy,i} = M_{liq_oxy,i-1} vel_{i-1} / L_{i-1} - M_{liq_oxy,i} vel_i / L_i - m_{vap_oxy,i}$$

$$(M \cdot T)'_{liq_oxy,i} = (M \cdot T)_{liq_oxy,i-1} vel_{i-1} / L_{i-1} - (M \cdot T)_{liq_oxy,i} vel_i / L_i - m_{vap_oxy,i} T_{oxy,i} + hk_i (T_{sat_oxy} - T_{liq_oxy,i}) / Cp_{liq_oxy,i}$$

where L_i is the length of volume i . Note that these equations account for the residence time of the droplets inside the chamber, so the amount of vaporized liquid will depend on the chamber geometry.

Solid propellant consumption

The solid propellant consumption (grain mass and thickness evolution) is simply determined by the amount of released vapors:

$$M'_{sp,i} = -m_{vap_sp,i}$$

$$D_{sp,i} = (D_i^2 - 4M_{sp,i} / (\rho_{sp} \pi L_i))^{1/2}$$

$$th_{sp,i} = (D_i - D_{sp,i}) / 2$$

The derivative of volume i is calculated as follows:

$$V'_i = M'_{sp,i} / \rho_{sp}$$

The grain temperature $T_{sp,i}$ is calculated accounting for heat exchanges at the wall and at the gas core:

$$(M \cdot T)'_{sp,i} = -m_{vap_sp,i} T_{sp,i} + (hk_i (T_{sat_sp} - T_{sp,i}) - q_{wall,i}) / Cp_{sp}$$

- $th_{sp,i}$: Equivalent grain thickness at volume i
- $D_{sp,i}$: Equivalent grain port diameter at volume i
- D_i : Grain external diameter
- $M_{sp,i}$: Grain mass at volume i
- CP_{sp} : Grain heat capacity
- q_{wall} : Heat exchanged between the wall and the grain

Heat exchanged with the walls

The term q_{wall} appearing in the grain temperature equation permits the thermal interaction (conduction) between the grain and the external connected thermal components (e.g: a lateral wall, through the so-called THERMAL port)

$$th_{sp} > 10^{-6} \quad q_{wall,i} = 2 \frac{\lambda_{sp}}{th_{sp}} A_{wet,i} (T_{sp,i} - tp.T(i))$$

$tp.T(i)$ is the wall temperature, to be determined in the connected wall component.

C) Equilibrium approach

The user can force a simplified formulation assuming instantaneous equilibrium thanks to the simulation

parameter "rateOption". Two options are available for choosing equilibrium or reaction delay method:

- $rateOption = TRUE$: Mathematical model will just follow the above formulation based on a time-delay between the equilibrium and the actual burned gases composition.
- $rateOption = FALSE$: Vapors will react instantaneously as long as they are released from the grain or the droplets (oxidizer).

Component input data description

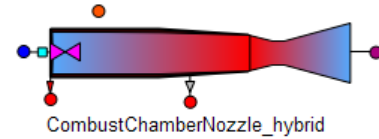


Figure 2 Solid / Hybrid component in ESPSS

To give an idea of the simulation scope, the table below shows some of the input data which this component depends on:

Name	Description	Units
Nsub	Number subsonic nodes	-
Nsup	Number supersonic nodes	-
Dt	Chamber throat diameter	m
Lc	Chamber length of subsonic part. To normalize axial position	m
Ld	Axial length from throat to exit	m
Dc_vs_L	Normalized chamber/nozzle diameters vs. normalized axial position (see note 1)	-
Dd_vs_L		-
Eta	Nozzle efficiency	-
frozen_th	Flag forcing frozen conditions in throat	-
Frozen_nz	Flag forcing frozen conditions in nozzle	-
P_ch	Initial Chamber pressure	Pa
T_ch	Initial Chamber temperature	K
x_nco	Initial non-condensable mass fraction	-
A_inj_oxy	Effective injection area for oxidizer	m ²
V_cav_oxy	Oxidizer cavity volume	m ³
capa	Chamber to Cavities heat capacity	J/K
cond	Chamber to Cavities conductance	W/K
emiss	Emissivity of the combustion gases	-
eta	Combustor efficiency	-
tau_b	Burning characteristic time	s
tau_c	Ignition time delay	s
D_dr_ox	Oxidizer droplets nominal size	m
rug	Equivalent grain rugosity	m
k_f	Multiplier of the friction factor	-
GasSolOption	Solid propellant "evaporation" model, either based on "a_sp, b_sp" constants or on the gas/grain heat exchange coefficient	-
a_sp	Solid propellant regression rate constant	m ³ /kg
b_sp	Solid propellant regression rate exponent	-
f_sp[3]	Adjustment coefficients of the real to cylindrical solid propellant wetted area (see note 3)	-
LH_sp	Enthalpy of formation of UsrDef rubber	J/kg
Tsat_sp	Solid propellant evaporation temperature	K
k_sp	Solid propellant thermal conductivity	W/m·K

Name	Description	Units
rho_sp	Solid propellant density	Kg/m ³
rubComp[]	Mass fractions of solid propellant <i>constituents</i> (see note 2)	-
rubUsrForm[]	RubUsr's formula according to the following atoms list -H, O, S, N, C, Ar, He, Al, K, Cl-	-
th_sp_ini	Solid propellant initial thickness	m
th_vs_L	Array of dimensionless grain thickness vs. node number.	-
dxc_vs_L	Array of dimensionless solid propellant lengths vs. node number. Assign the corresponding length ratios to each node. By default, elements of this array are set to 0 (equidistance nodes)	-

Notes:

1. *Dc_vs_L* and *Dd_vs_L* tables allow variable geometry in the chamber and in the nozzle respectively. The complete set of input data will also allow simulating non-uniform mesh size.
2. The mass fractions of the of the solid propellant *constituents* are input data (**rubComp[]** variable) within a predefined set of constituents {HTPB, IPDI, RubUsr, KNO3_a, Al_cr, S_a, NH4NO3_IV, NH4CLO4_}.
Two predefined rubbers are considered: HTPB (C10H15.4O0.07) and IPDI (C12H18O20.07N2). For a user-defined rubber, select a mass fraction for "RubUsr" type, introduce its formula within the "rubUsrForm" input data array and set "LH_sp" as the enthalpy of formation of the UsrDef rubber, normally low with respect to the reaction heat calculated by the code.
3. The adjustment coefficients of the real to cylindrical solid propellant wetted area are function of the grain thickness - $A_{wet}/A_{cyl} = f_{sp}[1] + f_{sp}[2] \cdot th + f_{sp}[3] \cdot th^2$
4. Using non-homogeneous grain thickness along the chamber allows to design particular thrust profiles, as it was the case using the adjustment coefficients of the real to cylindrical solid propellant wetted area, see note 3. Define as many nodes as different grain sections (with constant grain thickness) including one for the prechamber and one for the postchamber volumes, if any. For example, to define a combustor with a pre-chamber (no grain) along the 15% of the chamber, a grain zone with full grain thickness along the 80% of the chamber and a post-chamber with only 50% of the thickness along the last 5%, simply define the following data:
 $th_vs_L = \{0, 1, 0.5\}$
 $dxc_vs_L = \{0.15, 0.80, 0.05\}$
5. Lateral sections between the different grain zones will be automatically taken into account if parameter "latConsum" is set to TRUE.

APPLICATION EXAMPLES

A) Mass addition analytical validation case

The example below validates the Hybrid combustor capabilities concerning mass addition (related to the consumption of the solid propellant) by means of a

comparison with an analytical solution provided in Reference [5]. This analytical solution (for constant C_p , $\gamma = 1.4$) was coded under EcosimPro in a specific component.

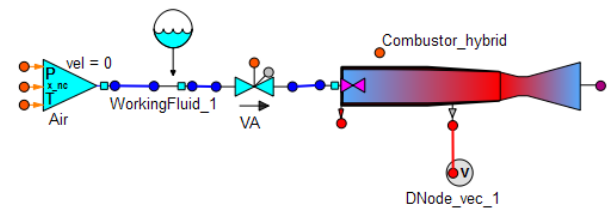


Figure 3 ESPSS Model used for validation

To be able to have a consistent comparison between the results of this model with the analytical solution, the following input data adaptation has to be performed:

- The VA valve has been closed because the mass injection only corresponds to the consumption of the solid propellant at the walls.
- The propellant composition and characteristics (user defined) are "artificially" set equal to those of the air at a gaseous state. Therefore, the solid propellant that is being injected in the chamber is in fact air as in the analytical solution.
- The thickness of the solid propellant keeps constant to maintain the same effective area at any simulation time (there is no consumption of the walls, only the mass flow is considered)

The combustor has a constant flow area (0.06 m effective diameter, 1.2 m length) and no wall friction (k_f input data = 0). The injected mass flow is supposed to be uniform in all the combustor nodes. The input values and the solid propellant characteristics are given in the experiment file:

...

BOUNDS

```

Combustor_hybrid.Combustor.IgnitFlag = 1 -- ignition
Combustor_hybrid.Combustor.f_v[50] = 1
Combustor_hybrid.np_out.P = 100000
...
FLUID_FLOW_1D.Damp = 1
FLUID_FLOW_1D.GRAV = 9.806
FLUID_PROPERTIES.VDW_option = 0
VA.s_pos.signal[1] = 0 -- inlet valve closed

```

BODY

```

Combustor_hybrid.Combustor.f_sp[01] = 1
-- Molar fractions of solid propellant constituents
Combustor_hybrid.rubComp[RubUsr] = 1.
-- actual composition of grain is AIR !!!
Combustor_hybrid.rubUsrForm[Elem_Ar] = 0.0092
Combustor_hybrid.rubUsrForm[Elem_O] = 0.2096
Combustor_hybrid.rubUsrForm[Elem_N] = 0.7812
...

```

Plot below has been automatically obtained using EXCEL files by inserting the reports generated with EcosimPro.

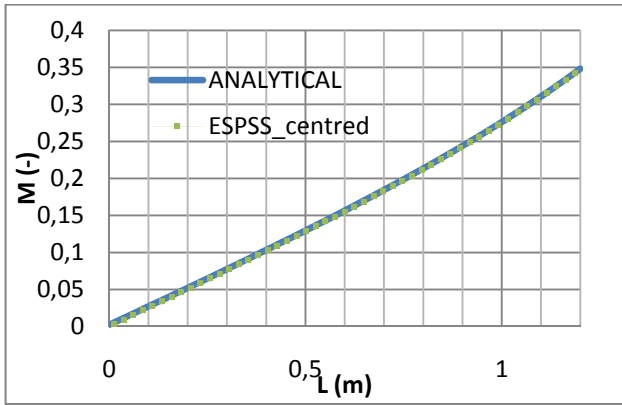


Figure 4 ESPSS versus analytical results

Main conclusions are:

- Present comparison validates the Hybrid 1D implementation of the governing equations in a combustor, that represent a more complex setup than in the Pipe component (it includes the mixture of the fluid propellants with the combustor products, the chemical equilibrium calculation according to CEA, etc.)
- It is pointed out that combustion was activated in this test case together with the injection of a mass flow along the chamber caused by the release of the solid propellant, being actually this propellant Air. The combustion does not insert any perturbation in the results since the equilibrium calculation does not change the composition.
- The mass added in the analytical case has the same conditions as the local fluid in the tube, while the hybrid combustor calculates the solid propellant consumption according to its saturation temperature and the local conditions of the fluid. To be able to compare, the hybrid combustor is modified imposing the saturation temperature of the solid propellant equal to the local temperature.
- There is nearly no differences between the results obtained with 50 and 200 nodes.

B) Basic Solid thruster test case

This model represents an example of a Solid rocket engine with a chamber containing a solid propellant. The valve is closed for avoiding the supply of the oxidizer. Input data are fictitious values, being the aim of this example only the demonstration of ESPSS Libraries capabilities in this type of engines.

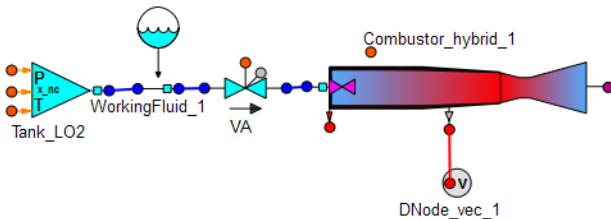


Figure 5 ESPSS model for simulating solid/hybrid thruster

The main dimensions are:

- Cylinder: $L = 1$ m; $D_{throat} = 0.06$ m. ($D/D_{th} = 2$, constant in 90% of the length; linearly decreasing until D_{throat})

- Grain propellant thickness = 0.03 m (Uniform in 90% of the length; linearly decreasing to 0 at throat)
- Nozzle D_{out}/D_{th} ratio = 2.4

In order to obtain a more neutral burning, grain factors $f_{sp}[1]$ and $f_{sp}[2]$ are respectively set to 3 and 65 (see “Component input data description”, Note 3). The boundaries (closed LOX valve), the time-dependant law to control the ignition, and some input data related to the combustion chamber and the solid propellant are given in the experiment file:

EXPERIMENT exp2 ON test_hybrid.default

...

BOUNDS

```
Combustor_hybrid_1.Combustor.IgnitFlag = step(TIME,0.1)
Combustor_hybrid_1.Combustor.start_m = 0
```

...

```
VA.s_pos.signal[1] = 0 -- LOX valve closed
```

```
Combustor_hybrid_1.np_out.P = 100000
```

BODY

-- Grain/gas exchange area factors :

```
Combustor_hybrid_1.Combustor.f_sp[1] = 3
```

```
Combustor_hybrid_1.Combustor.f_sp[2] = 65 ...
```

-- regression rate

```
Combustor_hybrid_1.a_sp = 1e-005
```

```
Combustor_hybrid_1.b_sp = 0.45
```

```
Combustor_hybrid_1.tau_c = 1e-3
```

```
Combustor_hybrid_1.tau_b = 1e-4
```

```
Combustor_hybrid_1.Tsat_sp = 400
```

-- Mass fractions of solid propellant constituents

```
Combustor_hybrid_1.rubComp[HTPB] = 0.14
```

```
Combustor_hybrid_1.rubComp[IPDI] = 0.
```

```
Combustor_hybrid_1.rubComp[RubUshr] = 0.
```

```
Combustor_hybrid_1.rubComp[KNO3_a] = 0
```

```
Combustor_hybrid_1.rubComp[Al_cr] = 0.16
```

```
Combustor_hybrid_1.rubComp[S_a] = 0
```

```
Combustor_hybrid_1.rubComp[NH4NO3_IV] = 0
```

```
Combustor_hybrid_1.rubComp[NH4CLO4_I] = 0.7
```

...

Some of the plots obtained are shown below:

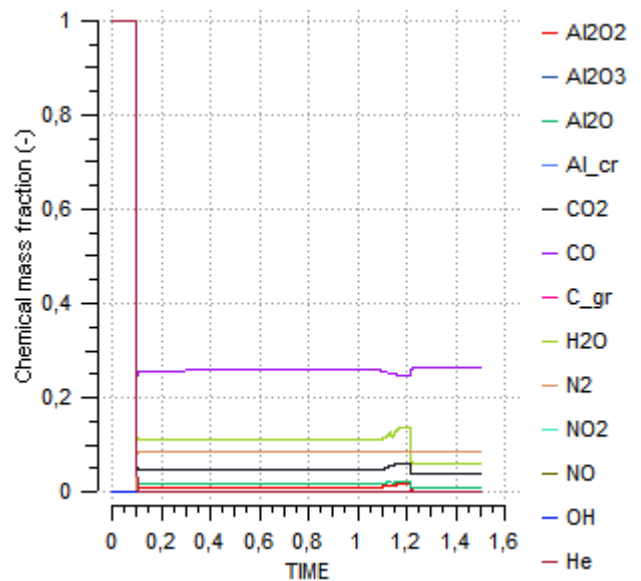


Figure 6 Chemical mass fraction at chamber outlet vs time

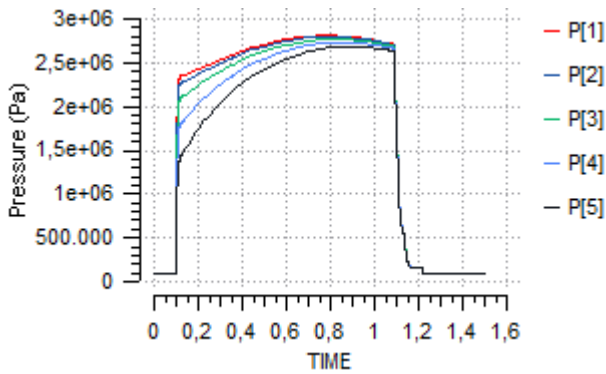


Figure 7 Chamber pressures vs time

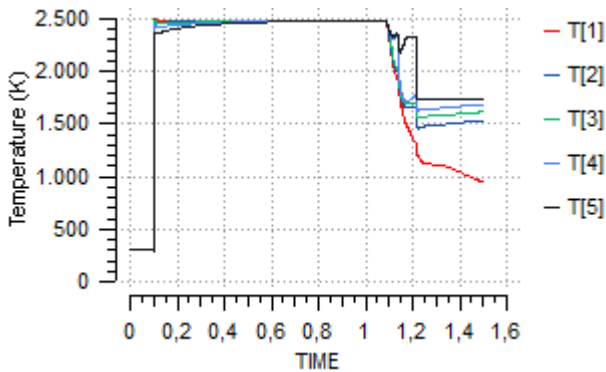


Figure 8 Chamber temperatures vs time

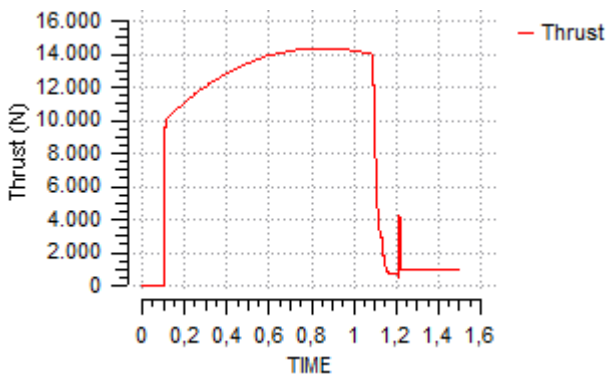


Figure 9 Thrust vs time

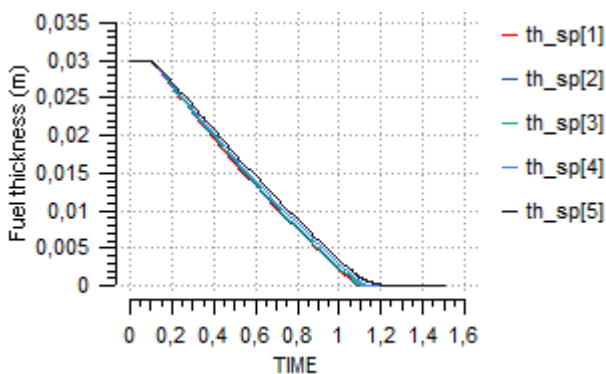


Figure 10 Fuel thickness vs time

The model calculates the chemical composition of the products at the equilibrium temperature and pressure in correspondence with the grain composition, the consumption of solid propellant and the

corresponding (choked) outlet mass flow for the given geometry:

- A fast pressure increase is detected at start-up; after that, the pressure and thrust increase slowly because the grain/gas effective area is increasing with the grain consumption. Note that in this case, the effective grain surface is corrected as a function of the grain thickness ($f_{sp}[2] = 65$, see "Component input data description"). A $f_{sp}[2] = 0$, would have produced an increasing pressure profile along the time because the effective grain surface area would also increase with the fuel consumption.
- The model is able to evaluate the influence of different grain compositions coupled with the shape of the grain and the combustor geometry.
- It is also observed that the extinction of the solid propellant is produced nearly at the same time for all the nodes along the chamber length.

C) Basic Hybrid thruster test case

This case uses the same model as the previous example but with different input values for regulating the time-dependant law to control the opening of the LOX valve and the ignition.

Other input data related to the combustion chamber and the solid propellant are given in the experiment file:

```

EXPERIMENT exp1 ON test_hybrid.default
DECLS
  TABLE_1D law_VAH = {{0., 0.1,0.2, 9.5, 10., 100} , {0, 1,
  1, 1, 0., 0. } }
...
BOUNDS
  Combustor_hybrid_1.Combustor.IgnitFlag =
  step(TIME,0.1)
...
-- Liquid oxygen injection conditions
Tank_LO2.s_pres.signal[1] = 100e5
Tank_LO2.s_temp.signal[1] = 90
Tank_LO2.s_xNonCond.signal[1] = 0
VA.s_pos.signal[1] = 0.5*timeTableInterp(TIME,law_VAH)
-- open LOX valve

BODY
-- Grain/gas exchange area factors :
Combustor_hybrid_1.Combustor.f_sp[01] = 5

Combustor_hybrid_1.Dt = 0.10 -- Greater throat
                             because LOX injection
VA.Ao = 1e-4                -- LOX injection area

--Solid propellant characteristics
Combustor_hybrid_1.GasSolOption = stdHybrid
Combustor_hybrid_1.a_sp = 1e-5
Combustor_hybrid_1.b_sp = 0.9
...
-- Molar fractions of solid propellant constituents
Combustor_hybrid_1.rubComp[HTPB] = 0.9
Combustor_hybrid_1.rubComp[IPDI] = 0.
Combustor_hybrid_1.rubComp[RubUsr] = 0.
Combustor_hybrid_1.rubComp[Al_cr] = 0.1
...

```

Below some plots obtained:

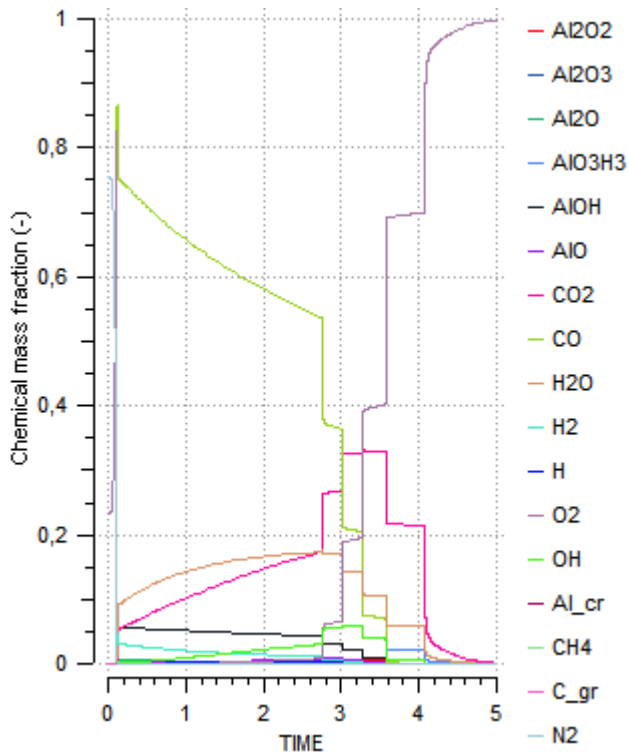


Figure 11 Chemical mass fraction (chamber outlet) vs time

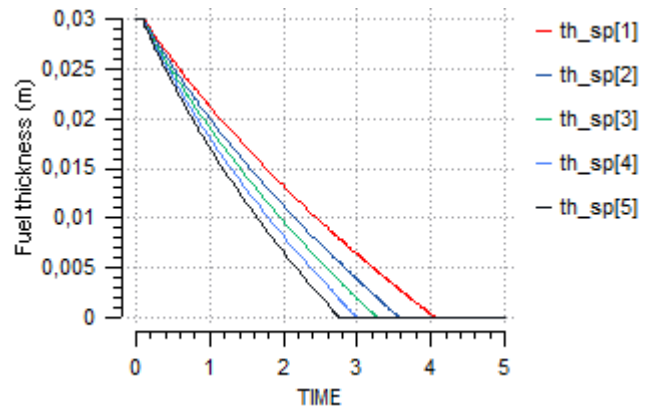


Figure 15 Fuel thickness vs time

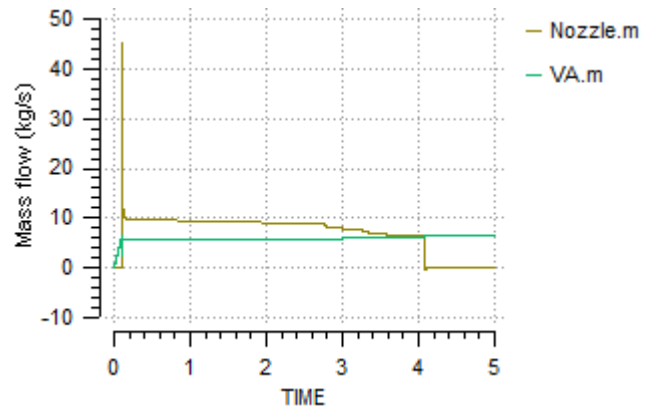


Figure 16 Mass flow vs time

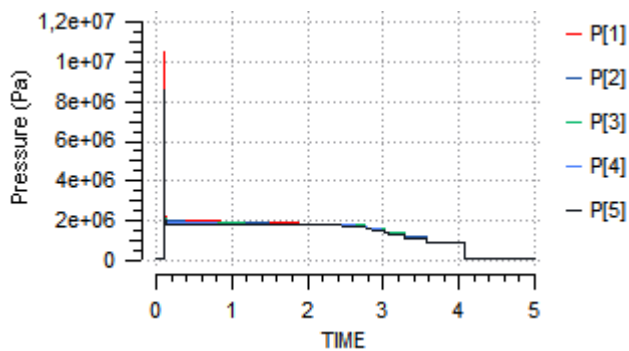


Figure 12 Chamber pressures vs time

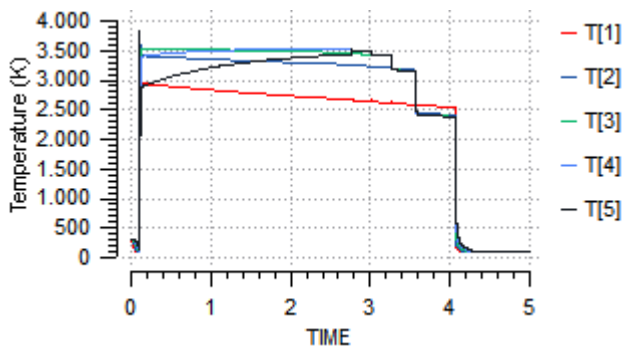


Figure 13 Chamber temperatures vs time

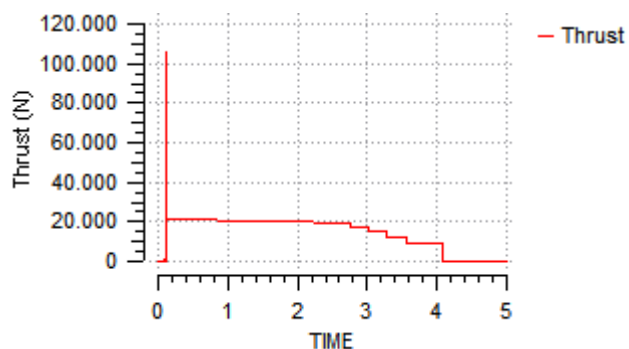


Figure 14 Thrust vs time

Following conclusions are extracted:

- The high pressure peak (nearly an explosion) during the startup is due to the fact that the rubber release regression law (proportional to the mass flow) is supposed to be valid during this first stage.
- The temperature evolution is different for each node because of the local mixture ratio depending on the LOX consumption and rubber “vapor” released calculated by the code along the chamber.
- The simulation results depend strongly on the oxidizer injection conditions (VA area and injection pressure) in this case, because the combusted gases compositions depends on the mixture of the evaporated LOX, also simulated in the ESPSS Combustor_hybrid component.
- It is also observed the extinction of the solid propellant at different stages along the chamber, being the final nodes the first ones in finishing the solid fuel because of their higher mass flow.

D) Sensitivity analysis of the solid combustor

This example analyses the sensitivity of the solid combustor performances to the variation of some of its parameters.

For all the parameters studied, the results obtained with the reference value are compared with an increment and decrement of the value. Besides, the equilibrium option is selected and the number of nodes inside the chamber is fixed to 1 to ease the comparison.

Sensitivity to throat diameter

Below the most representative results obtained with different throat diameters:

D _{th}	Thrust _{max}	P _{max}	m _{max}	T _{max}	t _{comb}
0.04 m	27630 N	117.7 bar	12 kg/s	2590 K	0.63 s
0.06 m	14220 N	27.0 bar	6.3 kg/s	2485 K	1.13 s
0.08 m	8670 N	9.2 bar	3.9 kg/s	2414 K	1.84 s

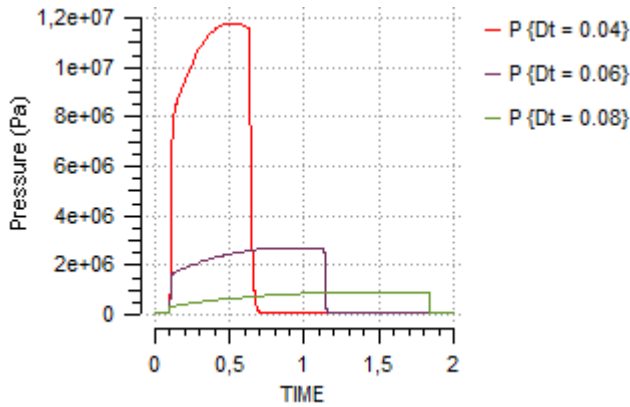


Figure 17 Influence of throat diameter on chamber pressure

As expected, the maximum pressure and thrust decrease when the throat diameter increase.

Sensitivity to initial fuel thickness

Below the most representative results obtained with different initial fuel thicknesses:

th _{ini}	Thrust _{max}	P _{max}	m _{max}	T _{max}	t _{comb}
0.02 m	14220 N	27 bar	6.28 kg/s	2487 K	0.82 s
0.03 m	14219 N	27 bar	6.28 kg/s	2487 K	1.13 s
0.04 m	14215 N	27 bar	6.28 kg/s	2487 K	1.56 s

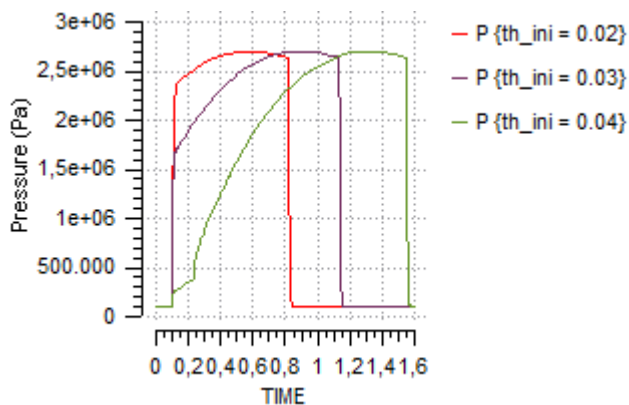


Figure 18 Influence of initial fuel thickness on chamber pressure

Sensitivity to fuel regression law (a_{sp} coefficient)

Below the most representative results obtained with different a_{sp} coefficients of the fuel regression law:

a _{sp}	Thrust _{max}	P _{max}	m _{max}	T _{max}	t _{comb}
9 · 10 ⁻⁶ m	11715 N	22.3 bar	5.2 kg/s	2473 K	1.35s

10 · 10 ⁻⁶ m	14220 N	27.0 bar	6.3 kg/s	2485 K	1.13s
11 · 10 ⁻⁶ m	16930 N	32.1 bar	7.5 kg/s	2499 K	0.97s

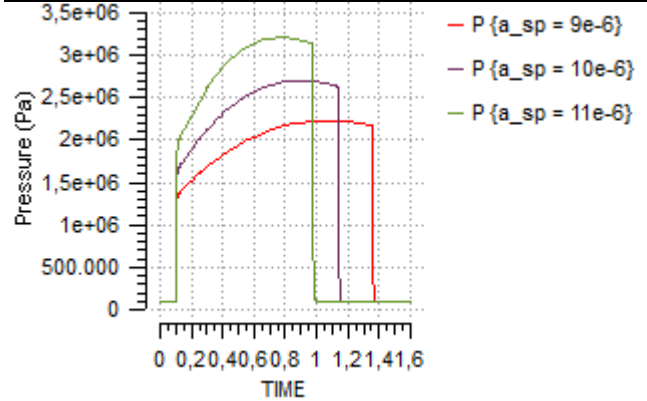


Figure 19 Influence of a_{sp} coefficient on pressure

As expected, higher burn rate coefficient values imply higher pressure values and lower combustion duration.

Sensitivity to equilibrium vs. rate combustion option

Below the differences in the results obtained using the two possible options to calculate the combustion: equilibrium and rate model with a burning characteristic time (intentionally large) of 10⁻³ seconds.

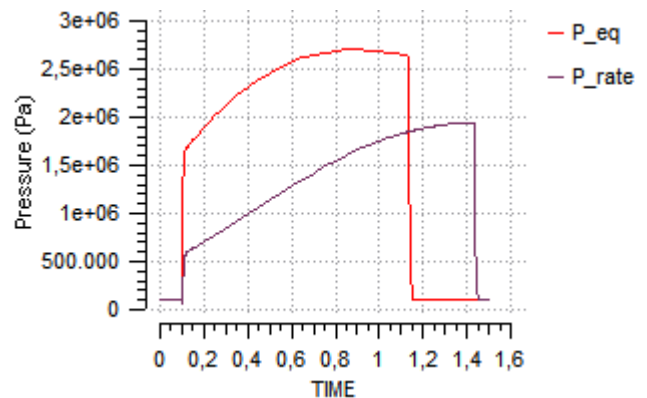


Figure 20 Influence of equilibrium on pressure

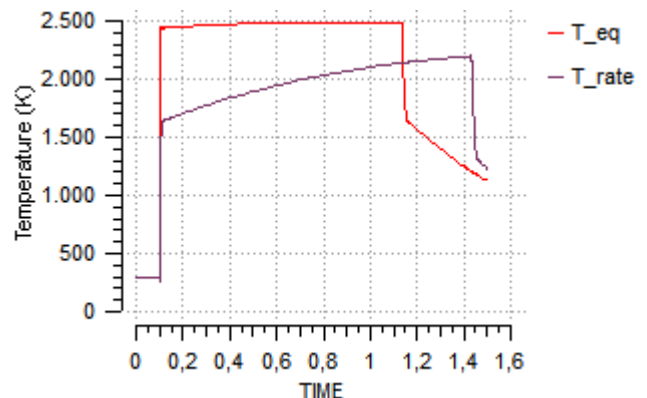


Figure 21 Influence of equilibrium on temperature

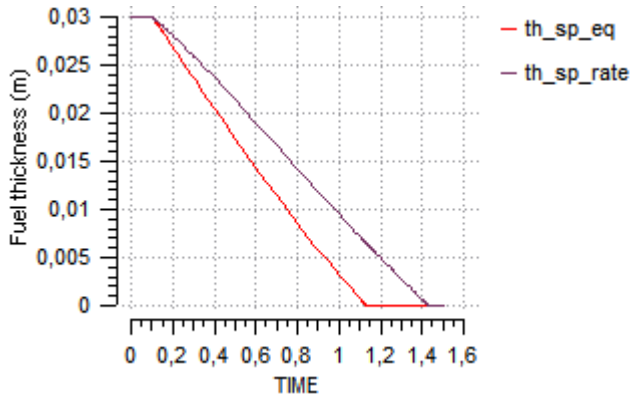


Figure 22 Influence of equilibrium on regression rate

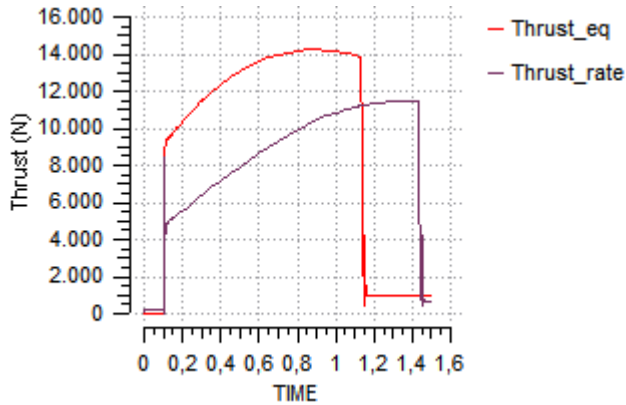


Figure 23 Influence of equilibrium on thrust

E) System case: solid combustor pressurizing a pressure fed engine

This case represents a complex model completely built with components of the ESPSS libraries. The model is just an example, which is able to simulate a solid combustor pressurizing a pressure fed engine:

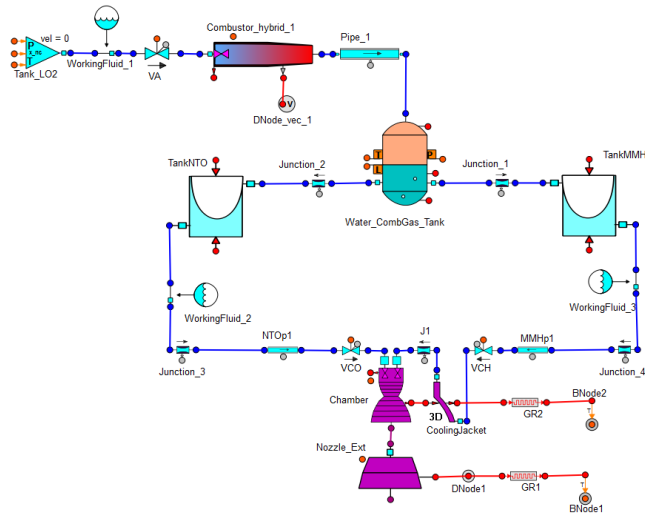


Figure 24 Complex model built with ESPSS

Some of the results obtained by simulating the model are shown in the images below. During the first second of simulation the solid engine pressurizes the water tank. The main chamber starts the first combustion phase at that time and finishes at 8 seconds, and at 10 seconds starts the second combustion phase.

In the figures below it is showed the evolution of the mass flow at different points of the system (combustion chamber injectors and water tank feeding branches), pressure at the fuel and oxidizer tanks and tanks level evolution during the simulation.

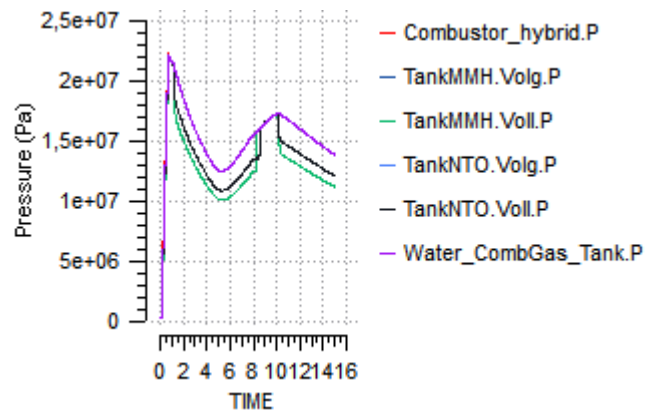
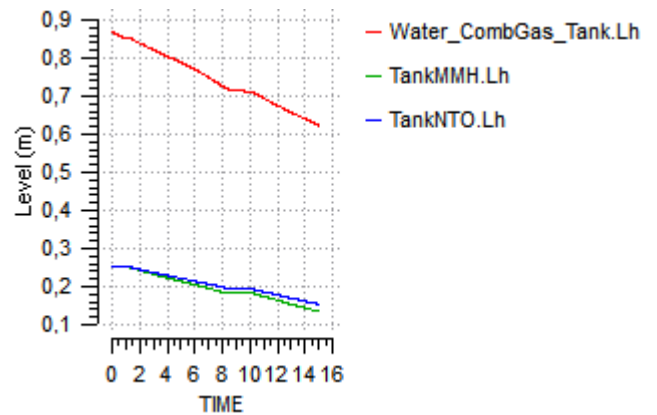
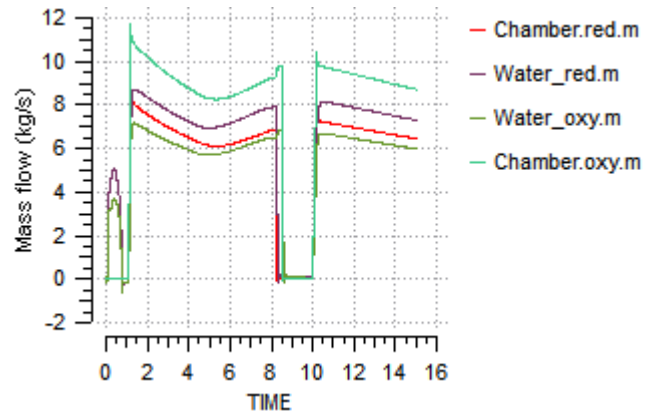


Figure 25 Results of the complex ESPSS system simulation

CONCLUSIONS

ESPSS V3 successfully includes new basic combustor models for hybrid and solid propellants. The corresponding components allow calculating a large variety of performances, between them:

1. The model is able to calculate the chemical composition of the products, solid propellant consumption, chamber pressure & temperature distribution, etc. in correspondence with the grain composition, oxidizer injection conditions, combustor and grain geometry.

2. Startup and shutdown processes can be also simulated, showing typical pressure picks at startups and the extinction of the solid propellant at different stages depending on the axial positions

An analytical comparison is also used for validating the implementation of the governing equations of the 1D hybrid combustor, which represents a more complex setup than a simple Pipe component.

Several application examples have been presented, in particular the possibility to connect a solid combustor to a Tank pressurization system supplying a pressure-fed engine.

REFERENCES

- 1 ESPSS: European Space Propulsion System Simulation- EcosimPro Libraries User Manual. ESA document 4000103800/11/NL/CP – TN4130. March, 2014
- 2 Gordon, S. and B.J. McBride: Computer Program for the Calculation of Complex Chemical Equilibrium Compositions with Applications. NASA Reference Publication 1311 (1994)
- 3 REFPROP V9.0. Thermodynamic & Transport Properties. National Institute of Standards & Technology. (NIST)
- 4 W. S. Winters. TOPAZ - The transient one-dimensional pipe flow analyser: user manual. SAND85-8215. Sandia National Laboratories, Livermore, CA, July 1985.
- 5 ACP7-GA-2008-21 1485 LAPCAT II. "Development of One-dimensional Propulsion Model"
- 6 Linda R. Petzold. A description of DASSL: a differential/algebraic system solver. SAND-82-8637; CONF-820810-21. Sandia National Labs., Livermore, CA (USA) (1982)