CFD Ablation Predictions with Coupled GSI Modeling for Charring and non-Charring Materials

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Outline

Flow Modeling and Surface Ablation Coupling

- The present state of the art is represented by loose coupling of high-fidelity CFD flow solvers with material thermal response codes
- Three major restrictions still present in these coupled models
  - surface chemical equilibrium assumption
  - non-ablating flow field prediction
  - simplified diffusion modeling based on transfer coefficient

Basic idea

To integrate CFD technology with Computational Surface Thermochemistry (CST) to model material erosion in solid rocket motor nozzle applications

Objectives

1. **To account** for the effect of **surface ablation** (charring and non-charring materials)
2. **To consider** the **pyrolysis gas injection** (charring materials)
3. **To determine** surface ablation and temperature as part of the CFD solution under **whatever ablation regime** (diffusion limited and kinetically limited)

LOOSE COUPLING: WHERE IT FAILS?

$$\underbrace{\rho_e u_e C_h (h_r - h_w)_e}_{q_{sen}} - \underbrace{\rho_e u_e C_m [(1 + B')h_w - h_{we}] + \dot{m}_c h_c + \dot{m}_g h_g}_{q_{chem}} = q_{rad_{out}} - q_{rad_{in}} + q_{cond}$$

1. Heat transfer coefficient (C_h)

- Evaluated from non-ablative calculation $\Longrightarrow$ **Blowing correction** required
- Depends on the wall temperature (and its profile)

2. Mass transfer coefficient (C_m)

- Evaluated from C_h $\Longrightarrow$ affected by C_h approximations
- Related to C_h throughout **semi-empirical relation**

3. Mass loss rate (B')

- Evaluated from equilibrium tables $\Longrightarrow$ kinetically-limited ablation regime?

Integration of CFD with GSI Modeling

The "ablative" boundary condition, based on surface mass and energy balances, is grounded on the following hypothesis:

- Steady-state ablation hypothesis:
  - **Closed solution** of the in-depth energy balance
  - Pyrolysis gas mass flow rate is a **known fraction** of the char mass flow rate
- Pyrolysis gas in chemical equilibrium at the wall temperature and pressure

The following **assumptions** are made in the analysis:

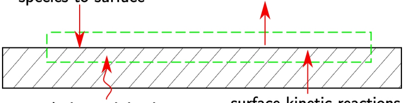
- Flow is axisymmetric and steady
- Radiation heat transfer is negligible
- Negligible effect of gas-phase reactions on ablation (due to small concentration of oxygen)

Code Specifications:

- RANS 2-D axisymmetric solver
- Finite difference method (λ scheme)
- Spalart-Allmaras turbulence model
- Multicomponent diffusion model
- Thermodynamic and transport properties described by curve fits (Gordon & McBride)

Surface Mass Balance (SMB)

- **SMB for the i^{th} species :**



$$\rho D_{im} \left.\frac{\partial y_i}{\partial \eta}\right|_w + \dot{m}_g y_{i,g} + \dot{m}_{i,c} = (\rho v)_w \, y_{i_w} \qquad i = 1, N_c$$

$\dot{m}_{i,c}$ is the mass flux of the i^{th} species produced or consumed by heterogeneous surface reactions between the solid char and the combustion gases

$y_{i,g}$ is the chemical composition (mass fractions) of the pyrolysis gas

Surface Mass Balance (SMB)

- **Overall SMB**:

$$(\rho v)_w = \dot{m}_g + \dot{m}_c = \dot{m}$$

$\dot{m}_c$ is the **char** mass flux
$\dot{m}_g$ is the **pyrolysis** gas mass flux
$\dot{m}$ is the **total** ablation mass flux

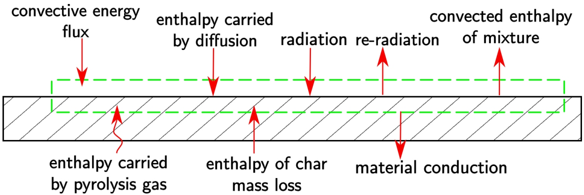
$$\rho D_{im} \left. \frac{\partial y_i}{\partial \eta} \right|_w + \dot{m}_g y_{i,g} + \dot{m}_{i,c} = (\rho v)_w \, y_{i_w} \qquad i = 1, N_c$$

$\dot{m}_{i,c}$ is the mass flux of the i^{th} species produced or consumed by heterogeneous surface reactions between the solid char and the combustion gases

$y_{i,g}$ is the chemical composition (mass fractions) of the pyrolysis gas

Surface energy balance (SEB)

- **Overall SEB**:



$$k \left. \frac{\partial T}{\partial \eta} \right|_w + \sum_{i=1}^{N_c} h_{i_w} \rho D_{im} \left. \frac{\partial y_i}{\partial \eta} \right|_w + \dot{m}_g h_{g_w} + \dot{m}_c h_{c_w} = \dot{m} h_w + \dot{q}_{cond}^{ss}$$

The conduction term $\dot{q}_{cond}^{ss}$ is represented by a closed expression available at steady state

Gas/solid interface governing equations

Surface energy balance (SEB)

- **Steady-state ablation approximation:**

By integrating the **in-depth energy equation** between the material back surface (virgin state) and the gas-solid interface and assuming the steady-state solution yields:

$$\dot{q}^{ss}_{cond} = \dot{m}_c h_{c_w} + \dot{m}_g h_{g_w} - (\dot{m}_c + \dot{m}_g) h_{v_{in}}$$

In the steady-state condition the pyrolysis gas mass flow rate becomes a **known fraction**, ϕ, of the char mass flow rate:

$$\phi = \frac{\dot{m}_g}{\dot{m}_c} = \left(\frac{\rho_v}{\rho_c} - 1\right) \qquad \rho_v = \text{"virgin" density} \qquad \rho_c = \text{"char" density}$$

ABLATION MODEL

Finite-rate ablation model for thermochemical erosion of carbon

Ablation model based on the multiple oxidizing species (MOS) reaction mechanisms

The rate of erosion (kg/m^2s) of carbon by an oxidizing species can be expressed as:

$$\dot{m}_i = {p_i}^n \cdot A_i {T_w}^b exp(-E_i/RT_w)$$

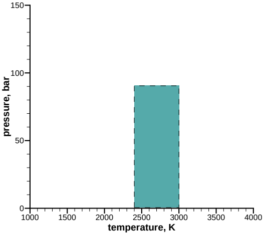
Surface reaction	A_i	E_i, kcal/mol	b	n
$C_s + H_2O \rightarrow CO + H_2$	4.8 x 10^5	68.8	0.0	0.5
$C_s + CO_2 \rightarrow 2CO$	9.0 x 10^3	68.1	0.0	0.5
$C_s + OH \rightarrow CO + H$	3.61 x 10^2	0.0	-0.5	1.0

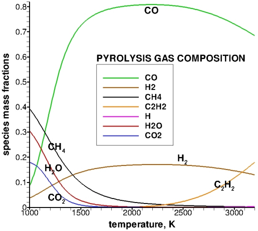
The total erosion rate of carbon due to the surface heterogeneous reactions is:

$$\dot{m}_c = \dot{m}_{H_2O} + \dot{m}_{CO_2} + \dot{m}_{OH} = \rho_c \dot{s} \quad (kg/m^2s)$$

The surface mass balance is solved for all the species without the need of any control procedure to switch from diffusion-limited to kinetic-limited erosion

Pyrolysis model



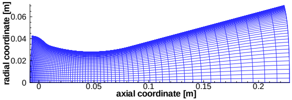


The pyrolysis gas composition injected into the main flow is considered to be in **chemical equilibrium** at the wall temperature and pressure

- Pyrolysis gas composition is calculated by a chemical equilibrium code at different values of pressure and temperature and stored in a database
- The elemental composition of the phenolic resin, to be used in the chemical equilibrium code, is calculated starting from a simple phenol molecule (C_6H_6O)

RSRM Subscale Nozzle Test Case: Input Data

Simulations address an experimental work carried out at the NASA JPL to study nozzle materials for the Space Shuttle Reusable SRM using the Ballistic Test and Evaluation System sub-scale motor (BATES)



Characteristics	RSRM subscale nozzle
Throat Diameter (cm)	5.588
TPS Material	carbon-phenolic (FM-5055)

- Orthogonal structured grid
- Grid stretched in axial and radial directions

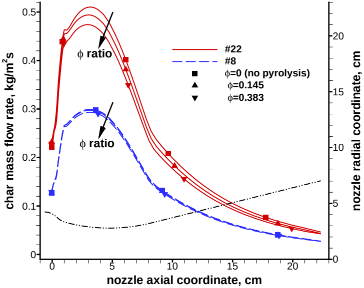
- Numerical investigation has addressed some of the tests that uses the FM-5055 carbon-phenolic material*:

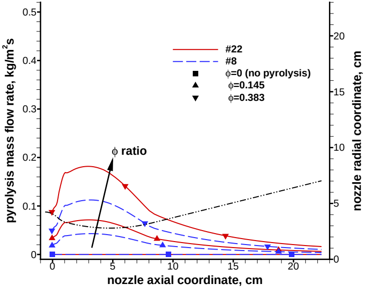
Test no	Prop.	t_b (s)	$\bar{p}_c$ (MPa)	$Al\%$	H_2O	CO_2	OH	ρ_v (g/cm^3)
#22	MOD. 8	11.52	4.73	16	0.1125	0.0298	0.0098	1.51
#1	MOD. 8	11.28	4.93	16	0.1125	0.0298	0.0098	1.50
#8	JPL-612	12.03	4.86	18	0.0643	0.0151	0.0035	1.50
#29	JPL-612	12.10	4.82	18	0.0643	0.0151	0.0035	1.51

* L. B. Powers, R. L. Bailey, B. H. Morrison, *Shuttle Solid Rocket Motor Nozzle Alternate Ablative Evaluation*, AIAA Paper 1981-1461

RSRM Subscale Nozzle Test Case: Results* (1/2)

- Steady-state simulations at mean chamber pressure have been conducted
- Different ϕ values have been used because of the **uncertainty of the char density** (highest and lowest ϕ values found in literature for the FM-5055)



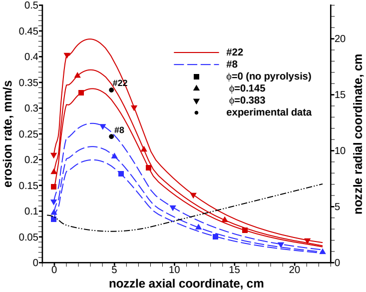


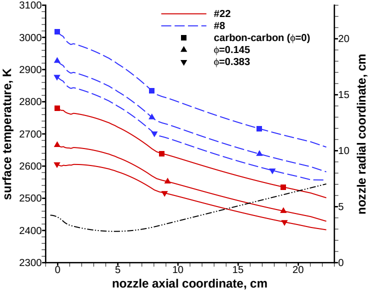
- Increasing the ϕ ratio produces an increase of the pyrolysis mass flow rate and a decrease of the char mass flow rate (due to the blowing effect of the pyrolysis gas injection)

* A. Turchi, D. Bianchi, F. Nasuti, *A Numerical Approach for the Study of the Gas–Surface Interaction in Carbon–Phenolic Solid Rocket* v Nozzles, submitted to Journal of Aerospace Science and Technology

RSRM Subscale Nozzle Test Case: Results* (2/2)

- A single steady-state simulation at mean chamber pressure provides the mean erosion rate





- Although the char mass flow rate is decreasing with ϕ, the erosion rate is yet increasing with increasing ϕ due to the decrease of the char density
- The growth of the erosion rate due to the increasing of the ϕ value produces a lowering in surface temperature

* A. Turchi, D. Bianchi, F. Nasuti, *A Numerical Approach for the Study of the Gas–Surface Interaction in Carbon–Phenolic Solid Rocket Nozzles*, submitted to Journal of Aerospace Science and Technology

ZEFIRO 23 & ZEFIRO 9A NOZZLES

Data provided by AVIO Group S.p.A. have been used to study the complete nozzle erosion of Zefiro 23 and 9A

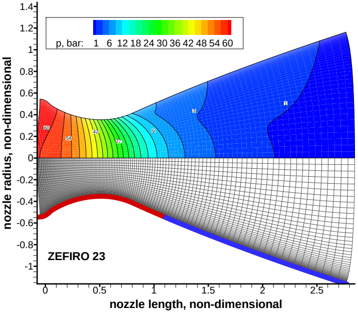
- The two motors share the **same architecture** for the nozzle thermal protection system:
  - CARBON-CARBON ablative liner for the throat/entrance and the after–throat divergent
  - CARBON-PHENOLIC ablative liner for the 1st forward divergent and 2nd forward divergent

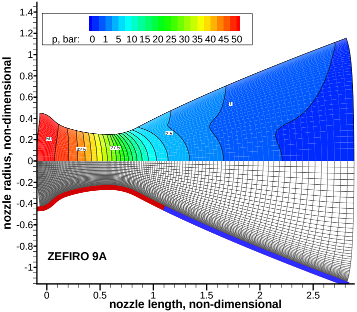
carbon-carbon

density $\rho \approx 1.9\,\mathrm{g/cm^3}$

carbon-phenolic

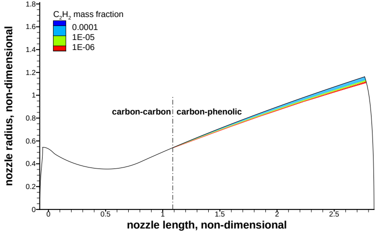
density $\rho \approx 1.5\,\mathrm{g/cm^3}$ ϕ ratio $= 0.12$

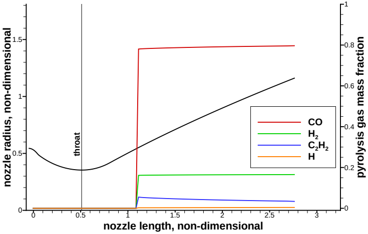




ZEFIRO 23 & ZEFIRO 9A: RESULTS*

Pyrolysis gas **injection** in the boundary layer for **Zefiro 23**



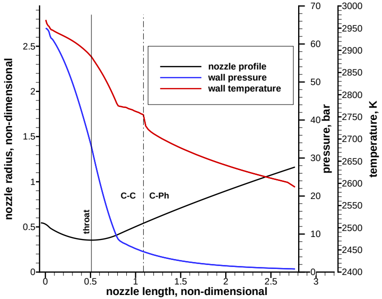


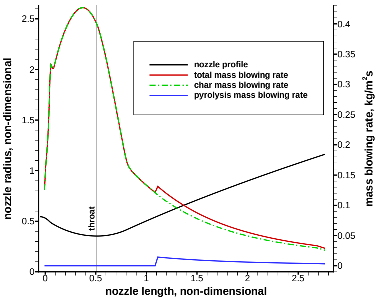
- The species C_2H_2 (acetylene) is only present in the pyrolysis gas, so it represents a **tracer species** which can be used to visualize the pyrolysis gas diffusion in the boundary layer
- The pyrolysis gas is mainly composed of CO and H_2, with a minor amount of C_2H_2 and H and its injection in the boundary layer blows the oxidizing species away from the surface (this effect, however, is minimal due to the small ϕ ratio)

* D. Bianchi, A. Turchi, F. Nasuti, *Numerical Analysis of Nozzle Flows with Finite–Rate Surface Ablation and Pyrolysis–Gas Injection*, AIAA 2011-6135

Zefiro 23 & Zefiro 9A: Results

Pressure, temperature and mass blowing rates (total, char, pyrolysis) distributions for **Zefiro 23**

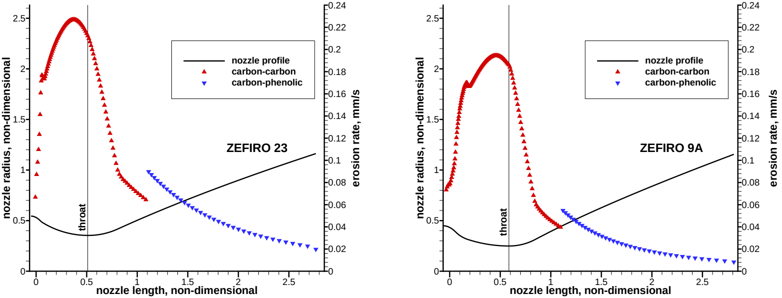




- Surface pressure is unaffected by the pyrolysis gas injection
- Surface temperature shows a drop corresponding to the material change
- Total mass blowing rate shows a step increase corresponding to the material change due to pyrolysis gas injection
- Char blowing rate is essentially unaffected by pyrolysis gas injection (pyrolysis blowing effect is minimal due to small ϕ ratio)

ZEFIRO 23 & ZEFIRO 9A: RESULTS

Erosion rate distribution for **Zefiro 23** and **Zefiro 9A**

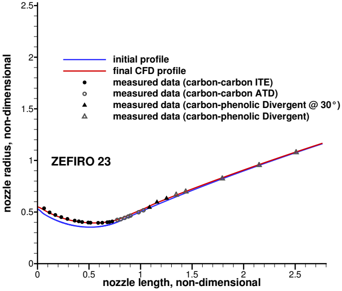


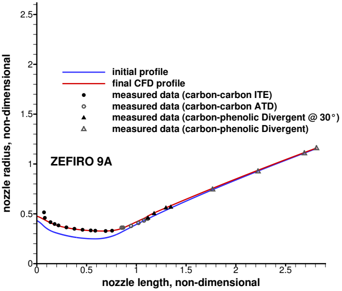
- Due to **different material densities** (higher for carbon-carbon and lower for carbon-phenolic), the step increase in terms of recession rate is larger than the one in terms of mass blowing rate
- The step is larger for Zefiro 23 because the material change occurs at a section with a lower expansion ratio than for Zefiro 9A
- The difference in recession rate corresponding to the material change is $\approx$ 0.025 mm/s for Zefiro 23 and $\approx$ 0.015 mm/s for Zefiro 9A. Such a difference can generate a step between the two materials of few millimeters at the end of the firing

ZEFIRO 23 & ZEFIRO 9A: RESULTS

Comparison between predicted and measured nozzle profile after motor firing

- Experimental measurements are available for each ablative liner
- Final nozzle shapes have been predicted considering the effect of **nozzle shape change** and of **variable chamber pressure**

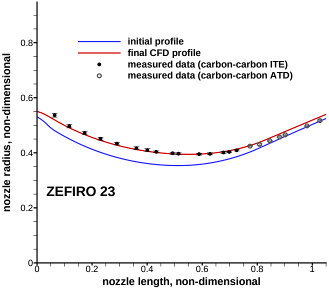


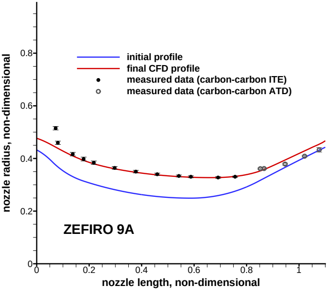


ZEFIRO 23 & ZEFIRO 9A: RESULTS

Comparison between predicted and measured nozzle profile after motor firing

- Experimental measurements are available for each ablative liner
- Erosion prediction shows a good agreement with the experimental data for the measuring points closer to the throat, but departs from the experimental profile for the remaining measuring points

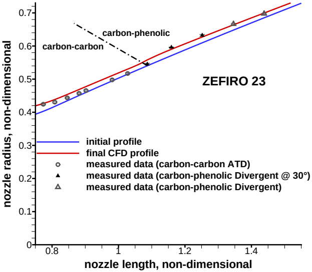


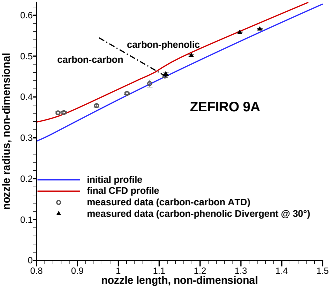


Zefiro 23 & Zefiro 9A: Results

Comparison between predicted and measured nozzle profile after motor firing

- Experimental measurements are available for each ablative liner
- Results show a good reproduction of the eroded profile for the **carbon-phenolic** forward divergent, provided that the measuring points are sufficiently far from the material change





CONCLUSIONS

- Integration of CST in CFD code permits to **bypass equilibrium thermochemical tables** and **semi-empirical coefficients** for the evaluation of the ablation rate in case of steady-state ablation
- Steady-state CFD simulation with **ablative boundary conditions** based on GSI modeling can be used for the evaluation of the erosion rate for carbon-based material
- A model able to describe the erosion behavior of **pyrolyzing and non-pyrolyzing carbon-based materials** for solid rocket nozzle applications has been developed and validated showing good results
- Time has come to **integrate more tightly** CFD and material thermal response code. We are looking forward to put aside the steady-state ablation approximation... Who is going to take the **challenge**?