Advanced Modeling and Simulation (AMS) Seminar Series
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Validation of a Fully Coupled Fluid-Ablation Interaction Solver for Low and High Temperature Ablators

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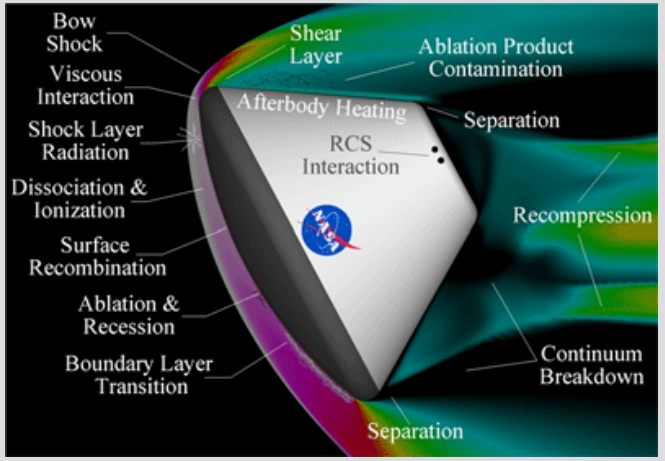


Financial support. NASA Kentucky EPSCoR RA Award no. 80NSSC19M0144 and NASA EPSCoR R3 Award no. 80NSSC19M0084

Hypersonic Flight

- Extreme aerothermal conditions at hypersonic speeds (Mach > 5):
  - Thermochemical non-equilibrium behind the shock layer
  - Radiation
  - Dissociation/recombination
  - Ionization
  - Flow transition/turbulence
  - Material ablation
- Ground testing in arc-jet environment.
- Computational modeling of aerothermal environment and material thermal response.

Schematics of hypersonic flow over a protection material[1]



Arc-jet testing of TPS material. Credit NASA

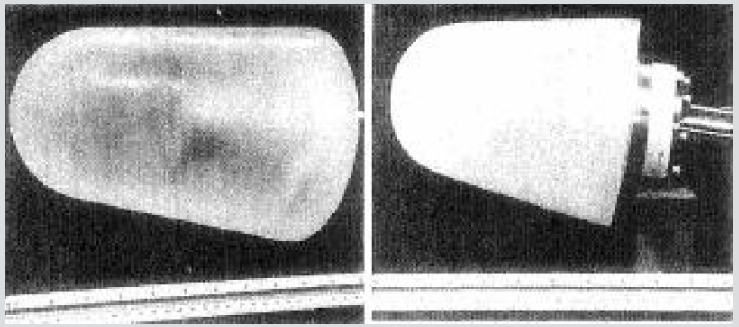


[1]Adapted from http://class.tamu. edu/projects/pecos

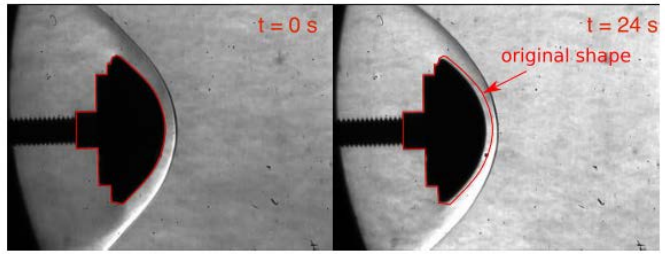
Low – temperature Ablators

- Low-temperature ablators: camphor, wax, naphthalene, dry ice.
- Testing in low-enthalpy facilities (hypersonic tunnels).
- Cheaper testing for prototyping and study of physical phenomena:
  - Shape change study and similarity to real flight.[1]
  - Flow transition research in 70s.
- Easier to model flow environment and ablation process (sublimation).

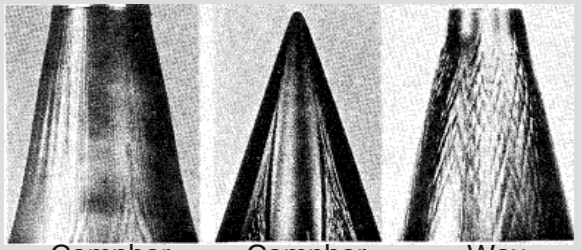
Camphor nosetip ablation at angle of attack (Baker1972)



Phoebus at Mach 6 flow (Turchi 2019)



Ablation surface patterns on cones.(Stock1975)

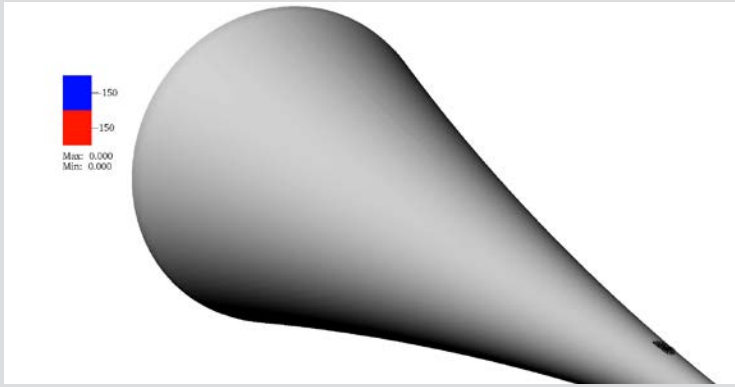


[1]Rotondi, M., Migliorino, M.T., Bianchi, D., Pagani, P. and Turchi, A., 2022. Numerical Assessment of Camphor Ablation Flight Relevance in Hypersonic Wind-Tunnel Testing. *Journal of Spacecraft and Rockets*, pp.1-18.

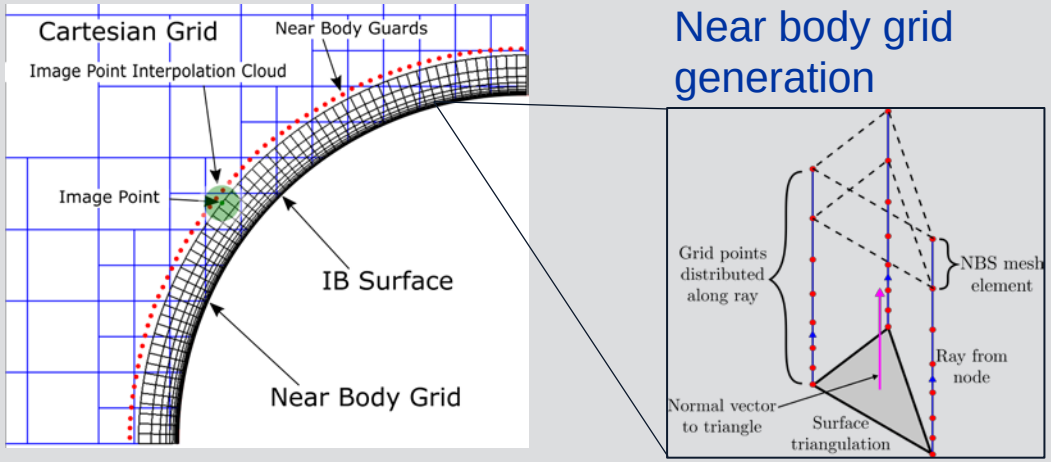
Computational Modeling
Flow solver

- Near Body Solver within Cartesian Higher-Order Adaptive Multi-Physics Solver Framework (CHAMPS NBS-Cart).
- Overset approach between near body curvilinear grid and off-body Cartesian grid.
- Near body solver resolves the boundary layer and the Cartesian solver resolves the shock and wake with adaptive mesh refinement.
- Automatic mesh generation and regeneration to follow the recessing surface.

Particle-induced transition, Browne2020

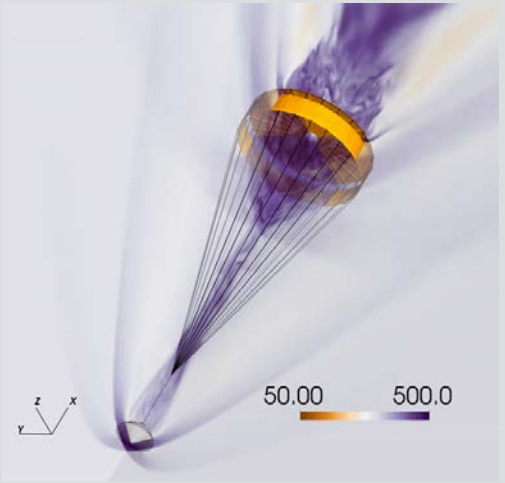


Cartesian – near body grid framework



Near body grid generation

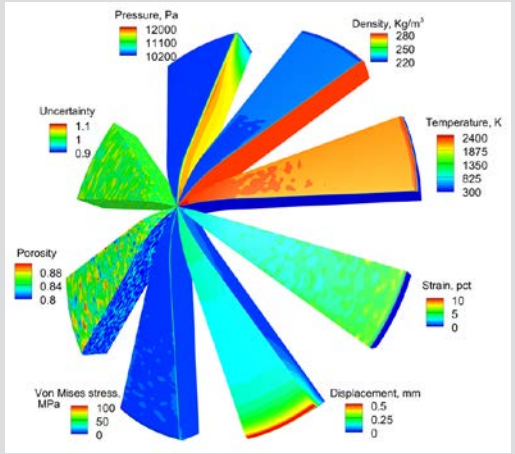
Fluid – structure interaction, Boustani2021



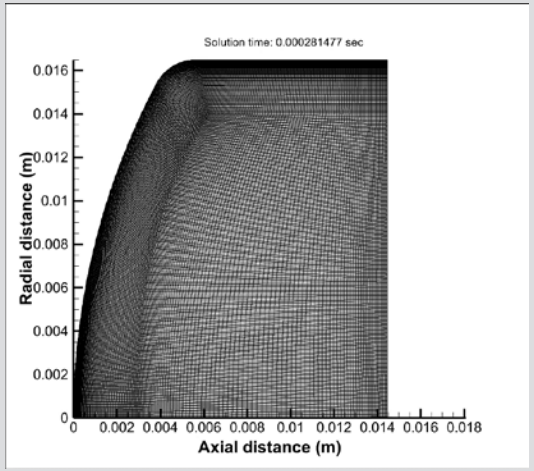
Computational Modeling
Material Response Solver

- Kentucky Aerothermodynamics and Thermal response System (KATS - MR).
- Applications:
  - Thermo – chemical models for charring and surface ablators
  - Thermo-structural
  - Incorporation of uncertainty into material properties
  - Large scale simulations (Stardust capsule)
  - Mesh motion problems
- Interface for coupling flow boundary conditions.

KATS modules[1]



Mesh motion in KATS



[1]Fu, R., Weng, H., Wenk, J.F. and Martin, A., 2018. Thermomechanical coupling for charring ablators. *Journal of Thermophysics and Heat Transfer*, *32*(2), pp.369-379.

Outline

1. Governing equations:
    1. CHAMPS NBS-Cart.
    2. KATS + mesh motion + surface balance equations for coupling.
2. Chemical models and thermophysical properties.
3. Coupling framework and setup of the simulations.
4. Validation study and discussion:
    1. Camphor ablation at Mach 6 flow (low-enthalpy conditions).
    2. Graphite ablation at arc-jet conditions.
5. Summary.

CHAMPS Governing Equations

- Compressible N-S equations.
- Camphor ablation – low-enthalpy environment:
  - Thermal and chemical equilibrium (non – reactive flow).
  - 3-species: $[N_2, O_2, C_{10}H_{16}O]$.
- Graphite ablation – high-enthalpy environment:
  - Thermo-chemical non-equilibrium 2-temperature air model.
  - 11-species: $[N_2, O_2, NO, N, O, CO, CO_2, CN, C, C_2, C_3]$.

Convective

$$\boldsymbol{F^1} = \begin{bmatrix} \rho_1 u \\ \vdots \\ \rho_s u \\ \rho u^2 + p \\ \rho uv \\ \rho uw \\ (E+p)u \\ E_{ve} u \end{bmatrix} \quad \boldsymbol{F^2} = \begin{bmatrix} \rho_1 v \\ \vdots \\ \rho_s v \\ \rho vu \\ \rho v^2 + p \\ \rho vw \\ (E+p)v \\ E_{ve} v \end{bmatrix} \quad \boldsymbol{F^3} = \begin{bmatrix} \rho_1 w \\ \vdots \\ \rho_s w \\ \rho wu \\ \rho wv \\ \rho w^2 + p \\ (E+p)w \\ E_{ve} w \end{bmatrix}$$

Viscous

$$\boldsymbol{F_v^1} = \begin{bmatrix} -J_{1,x} \\ \vdots \\ -J_{s,x} \\ \tau_{xx} \\ \tau_{xy} \\ \tau_{xz} \\ f_v^1 \\ f_v^4 \end{bmatrix} \quad \boldsymbol{F_v^2} = \begin{bmatrix} -J_{1,y} \\ \vdots \\ -J_{s,y} \\ \tau_{yx} \\ \tau_{yy} \\ \tau_{yz} \\ f_v^2 \\ f_v^5 \end{bmatrix} \quad \boldsymbol{F_v^3} = \begin{bmatrix} -J_{1,z} \\ \vdots \\ -J_{s,z} \\ \tau_{zx} \\ \tau_{zy} \\ \tau_{zz} \\ f_v^3 \\ f_v^6 \end{bmatrix}$$

Source

$$W = \begin{bmatrix} \dot{w}_1 \\ \vdots \\ \dot{w}_s \\ 0 \\ 0 \\ 0 \\ 0 \\ Q_{t2v} + Q_{c2v} \end{bmatrix}$$

KATS Governing Equations

- Governing equation for solid energy:

$$\frac{\partial E_s}{\partial t} - \nabla \cdot \left(F_d + F_g\right) = 0$$

Grid flux: $F_g = E_s \bar{\omega}$

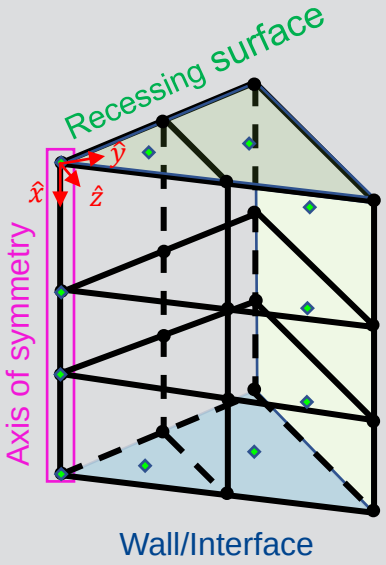
Face averaged velocity: $\bar{\omega}_j = \frac{\Delta \bar{V}_j}{A_j \Delta t}$

- Mesh motion:

Radial Basis Function interpolation of surface displacement to the nodes

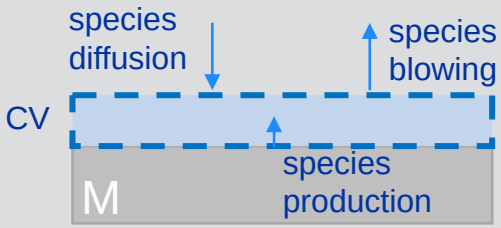
Approximation function: $s(\boldsymbol{r}_j) = \sum_{i=1}^{N_n} \alpha_i \phi(|\boldsymbol{r}_j - \boldsymbol{r}_i|)$

Basis function: $\phi(\xi) = \begin{cases} \phi(\xi), \text{if } 0 \le \xi \le 1 \\ 0, \quad \xi > 1 \end{cases}$



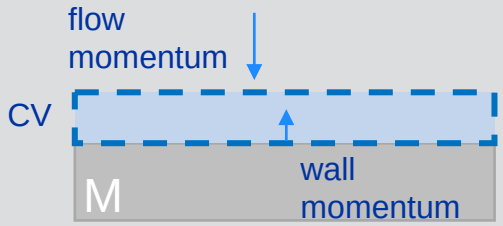
- Surface balance equations:
  - Mass balance

$$-\rho_w D_w \frac{\partial Y_s}{\partial \eta} + m_s'' = m_w'' Y_{s,w}$$



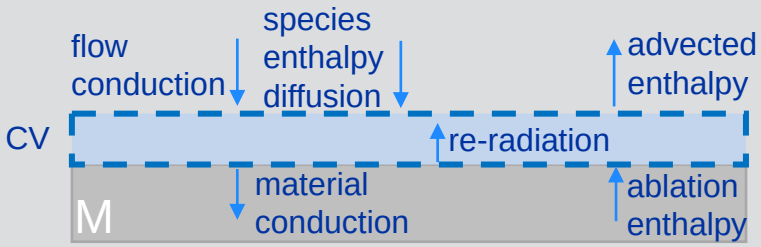
  - Momentum balance

$$p_f + \rho_f u_f^2 = p_w + \rho_w u_w^2$$



  - Energy balance

$$-\kappa_{tr} \nabla T \cdot \hat{\boldsymbol{n}} - \kappa_{ve} \nabla T_v \cdot \hat{\boldsymbol{n}} - \sum_{k=1}^{ns} \rho h_k D \nabla Y_k \cdot \hat{\boldsymbol{n}}$$
$$= -\kappa_s \nabla T \cdot \hat{\boldsymbol{n}} + \epsilon \sigma (T_w^4 - T_\infty^4) + m_w'' (h_w - h_{s,w})$$



Chemical Models

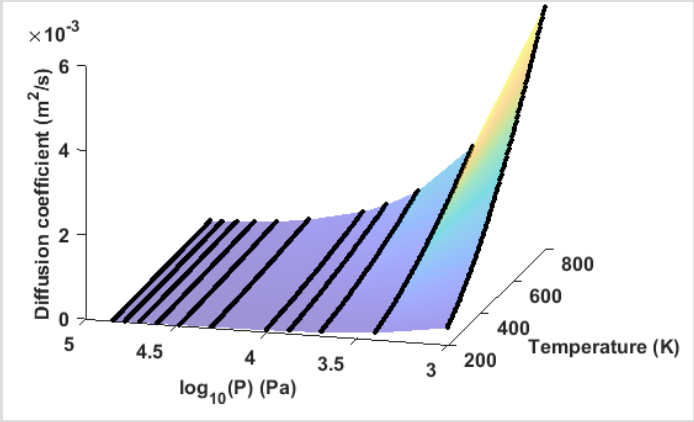
- Camphor:
  - Gas phase contains 3 non-reactive species.
  - Surface reactions – single sublimation species.
- Graphite:
  - Gas phase contains 11-species and solves 24 reactions, accounting for dissociation and exchange reactions[1].
  - Gas-surface reactions are modeled with recently developed ACA[2] model based on molecular beam experiments:
    - ACA model: continuous beam of O, O_2, N and N_2 at nominal velocity of 2000 m/s at resistively heated vitreous carbon surface at temperature 800 – 1873 K.
  - Knudsen-Langmuir model for sublimation reactions: C, C_2, C_3 species.

[1]McQuaid, J.A., Zibitsker, A.L., Martin, A. and Brehm, C., 2022. Simulation of Graphite Ablation using an Overset Near Body Solver on an Adaptive Block-Structured Cartesian Off-Body Grid. In *AIAA AVIATION 2022 Forum* (p. 4088).
[2]Prata, K.S., Schwartzentruber, T.E. and Minton, T.K., 2022. Air–carbon ablation model for hypersonic flight from molecular-beam data. *AIAA journal*, *60*(2), pp.627-640.

Thermal and transport properties

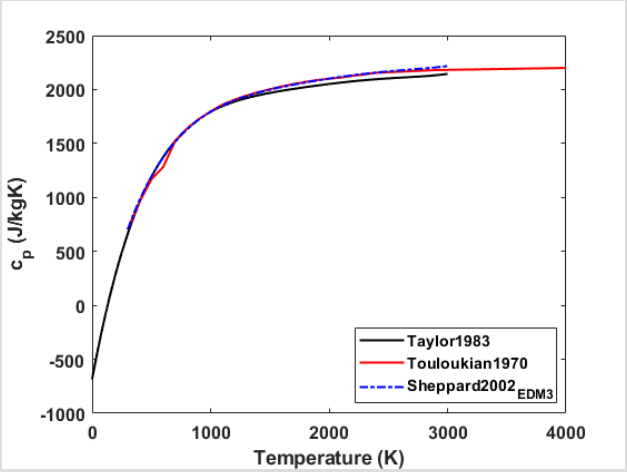
- Camphor:
  - Solid properties - constant.
  - Camphor gas properties - obtained from quantum-chemical simulation by J. Haskins at NASA Ames. Reasonable agreement to literature.
- Graphite:
  - Solid properties - POCO graphite from Sheppard EDM3.
  - Gas properties – kinetic theory, Blottner curves and Eucken relations.

Camphor diffusion in air[1]

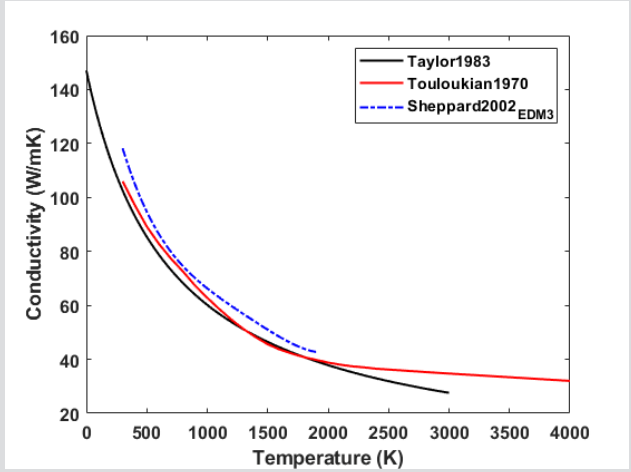


Solid properties

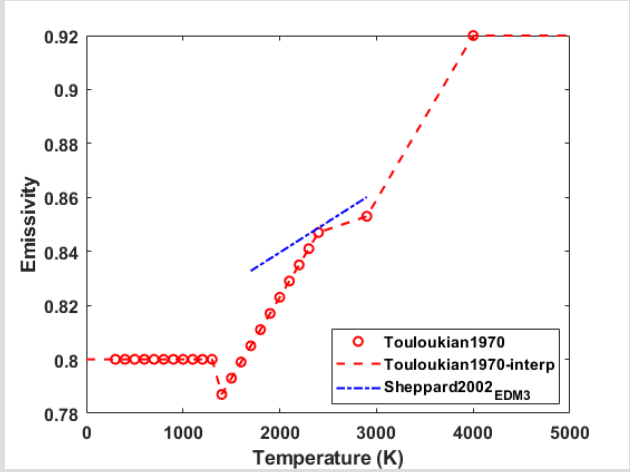
Specific heat



Conductivity



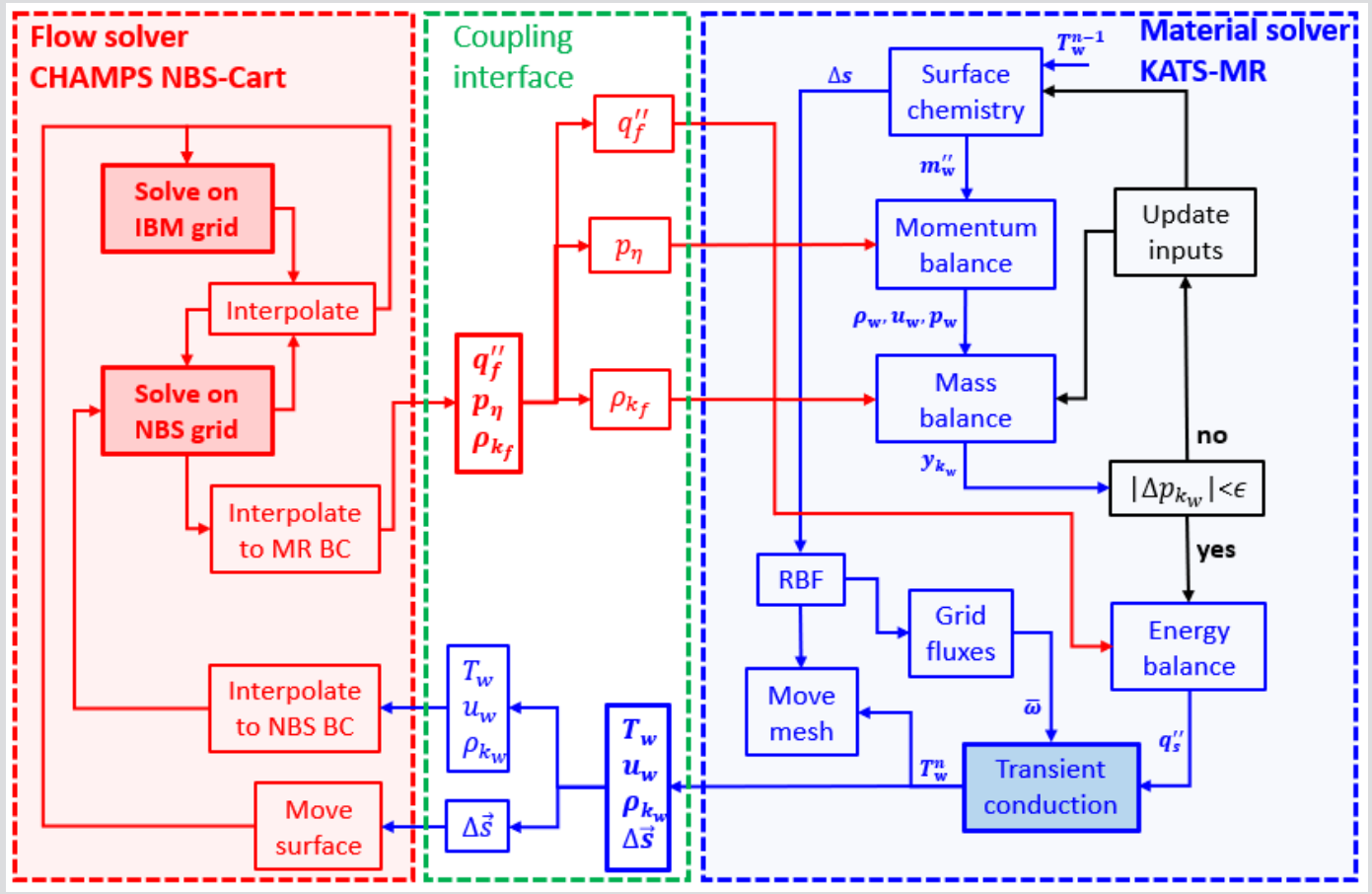
Emissivity



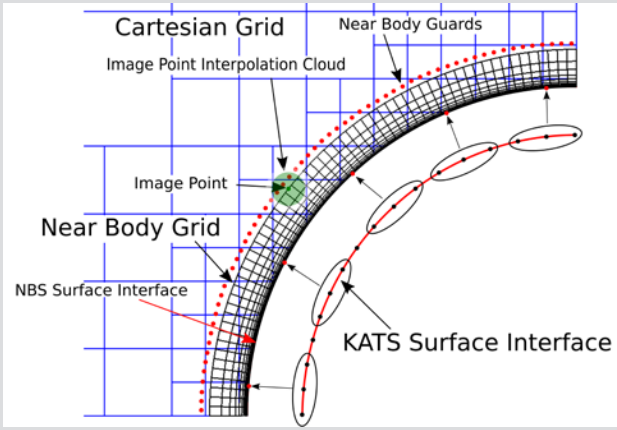
[1]J. Haskins2021. NASA Ames.

Coupling Framework

Coupling scheme



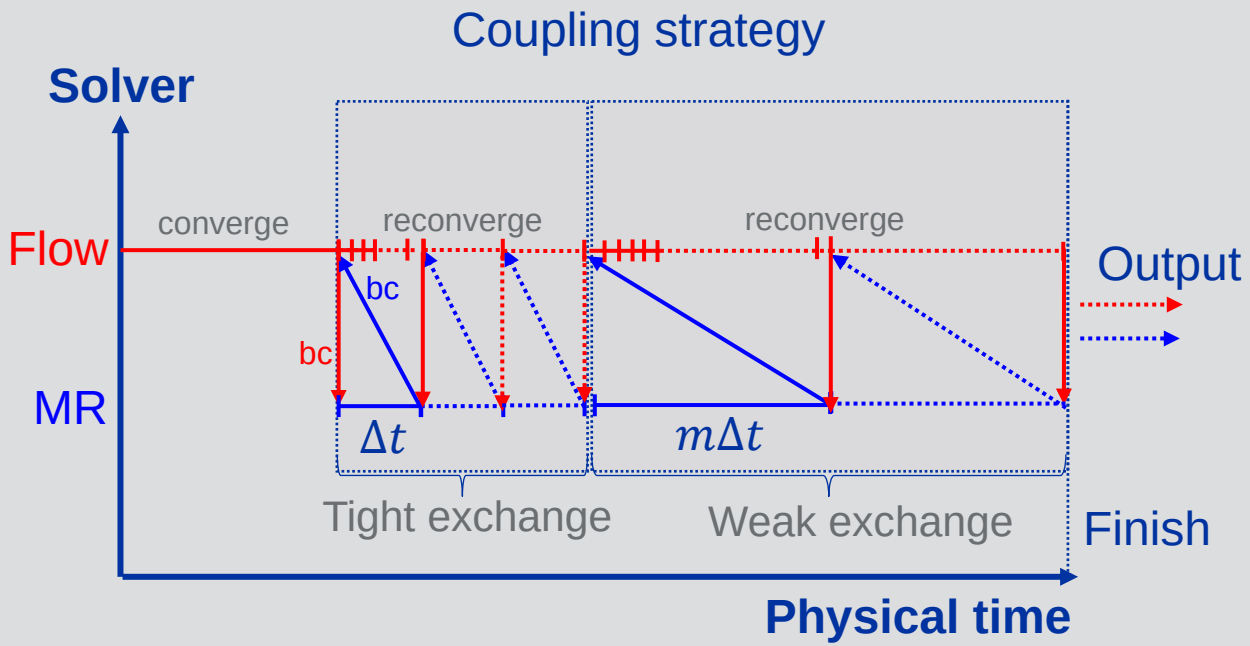
flow ↔ material interpolation



MR to fluid

Simulation Setup

- Converge the baseflow solution.
- Tight exchange of BC, followed by weak exchange with $\Delta t_{\mathrm{MR}} = m\Delta t_{\mathrm{flow}}$.
- Flow solver dictates the time step, implicit with CFL=10,000.
- Flow solver performs sub-steps to reconverge after every exchange of BC.



Simulation Studies



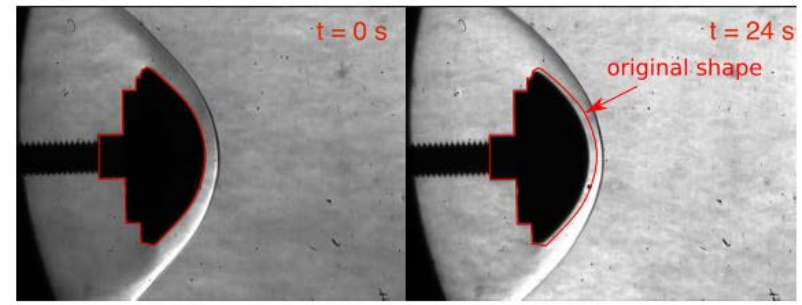
Camphor Ablation

- Experiment in hypersonic H3 facility at VKI:
  - Mach 6, low-enthalpy flow (~0.5 MJ/kg).
  - 30 sec duration until complete ablation of camphor.
  - Three total pressure conditions.

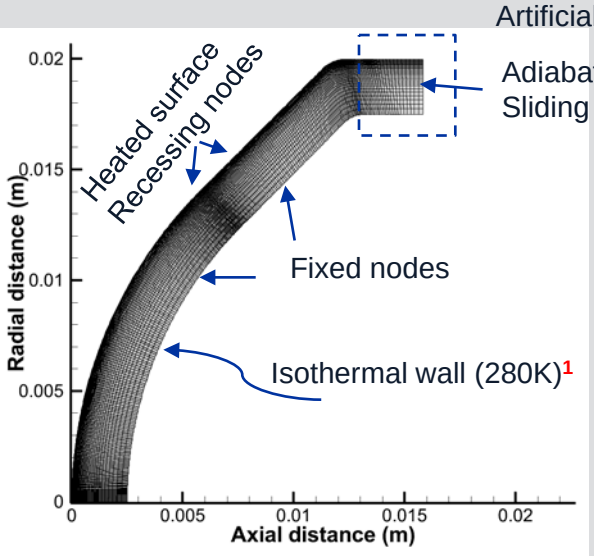
Phoebus capsule with layer of camphor



Experiment at Mach 6 flow (Turchi 2019)



Material discretization



Experimental conditions

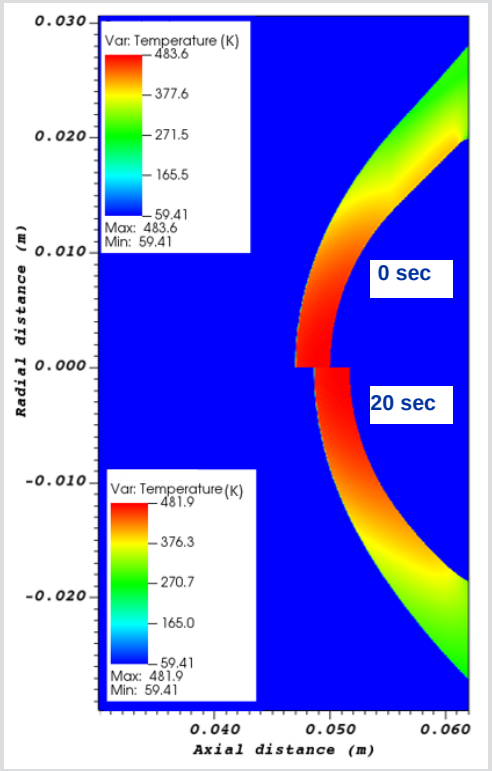
Test	Total Pressure [bar]	Total Temperature [K]	Mach no.
P15	15.647 ± 0.093	524.78 ± 2.31	6
P20	20.569 ± 0.126	487.18 ± 3.91	6
P25	25.660 ± 0.039	511.01 ± 7.04	6

[1]Zibitsker, A.L., McQuaid, J., Brehm, C. and Martin, A., 2022. Fully-Coupled Simulation of Low Temperature Ablator and Hypersonic Flow Solver. In *AIAA SCITECH 2022 Forum* (p. 0676).

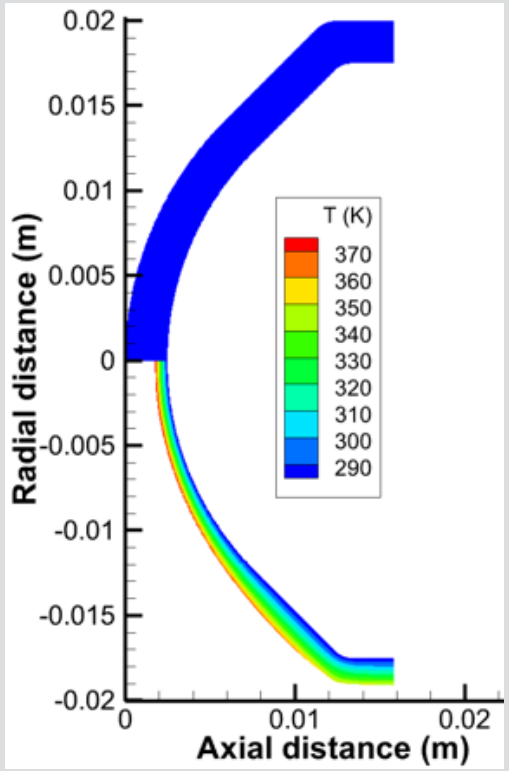
Validation Results

Temperature contours

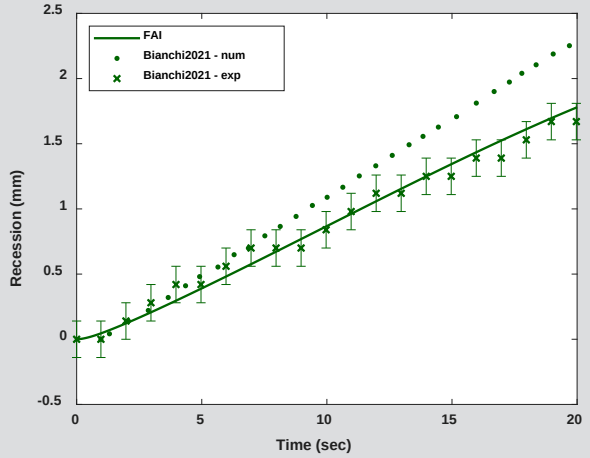
Flow



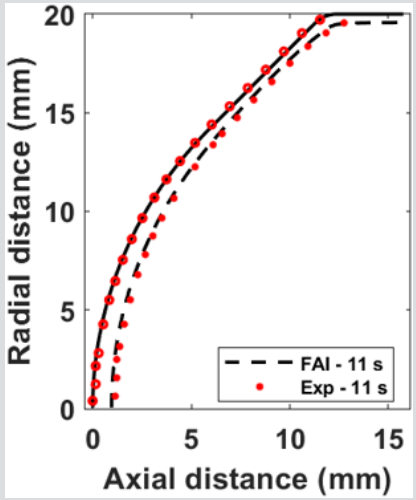
Material



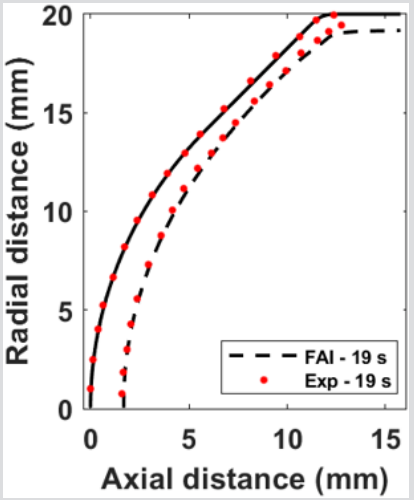
Stagnation point recession comparison



Shape at 11 sec



Shape at 19 sec

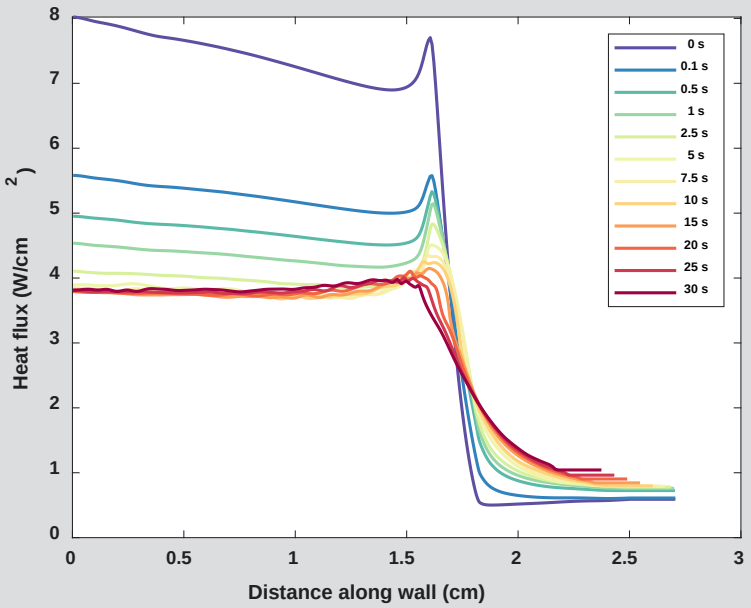


Zibitsker, A., McQuaid, J., Brehm, C. and Martin, A. Study of a Two-Dimensional Shape Change of Blunt-Body Geometries at Hypersonic Conditions Using Fully-Coupled Simulation. In *AIAA Aviation Forum, 2022*.

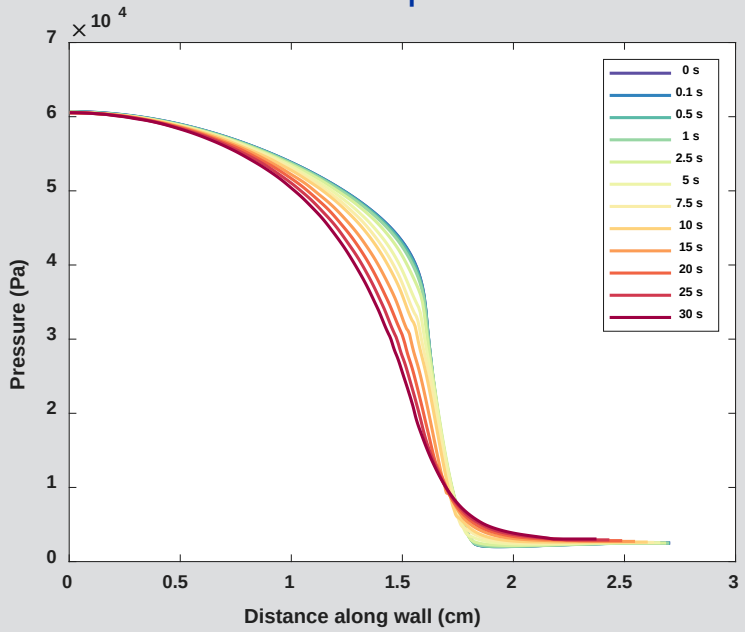
Shape Change Study of iso-q Geometry

- Simulating ablation of 1.3" iso-q camphor model at Mach 6 flow (20 bar case).

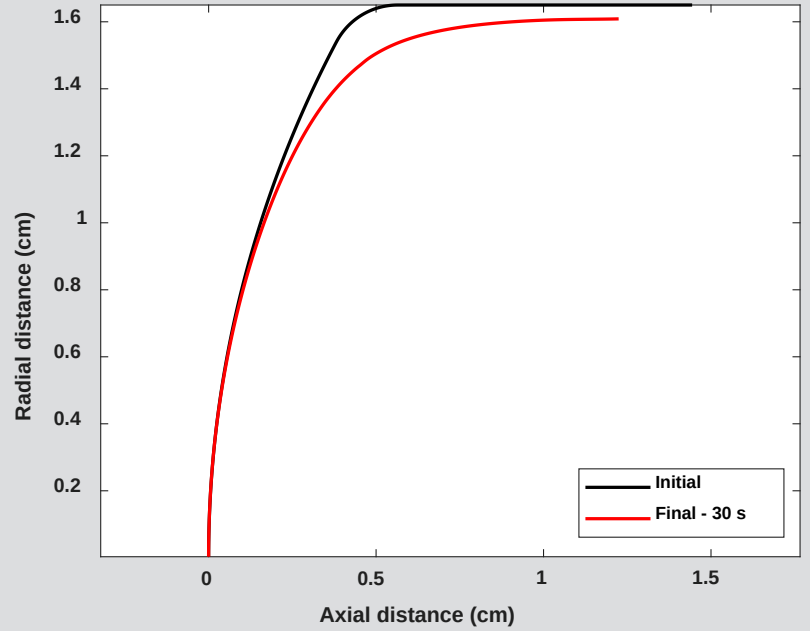
Heat flux profiles



Pressure profiles



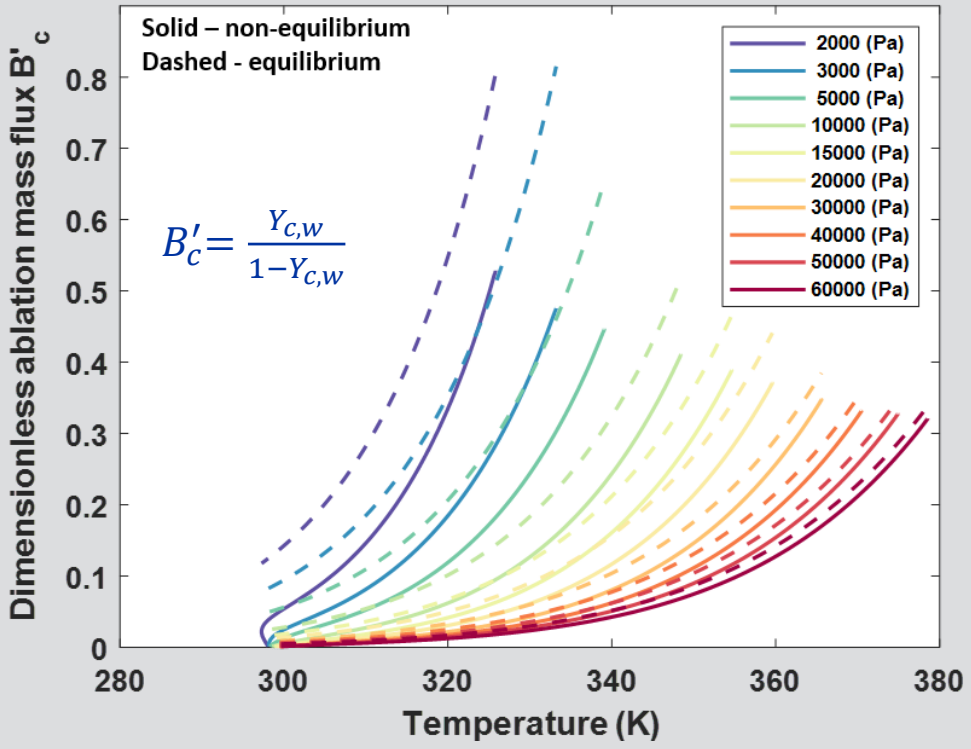
Relative shape change



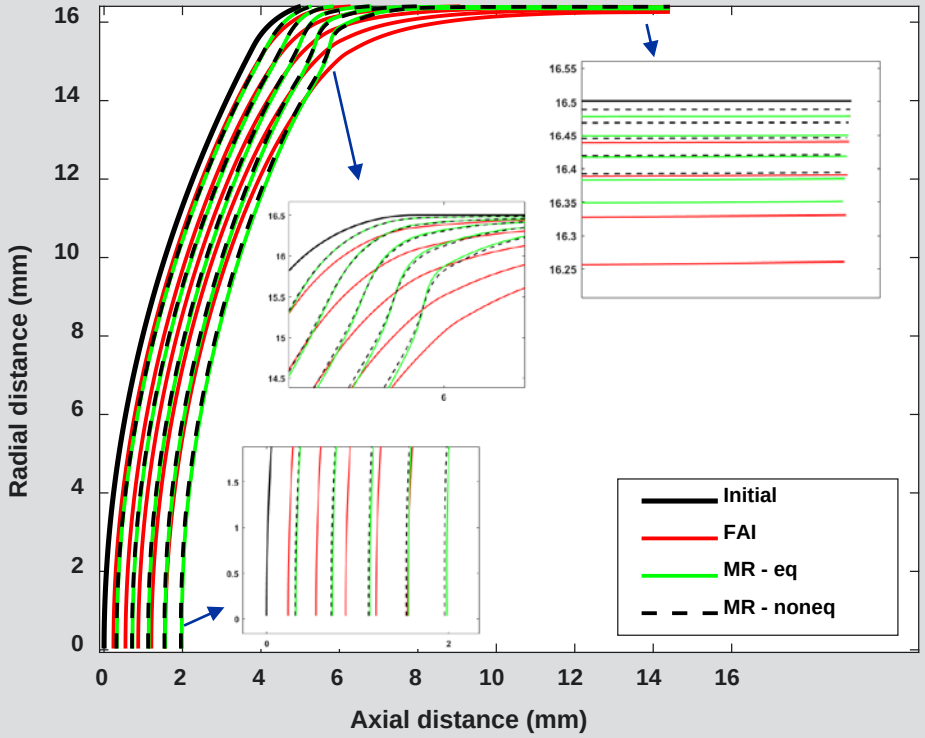
Shape Change Study

- Comparison of fully coupled and uncoupled (MR only) solutions.

Non-dimensional ablation rate (Bprime)



Recession profiles comparison
Time: 0 to 20 s in 4 s intervals



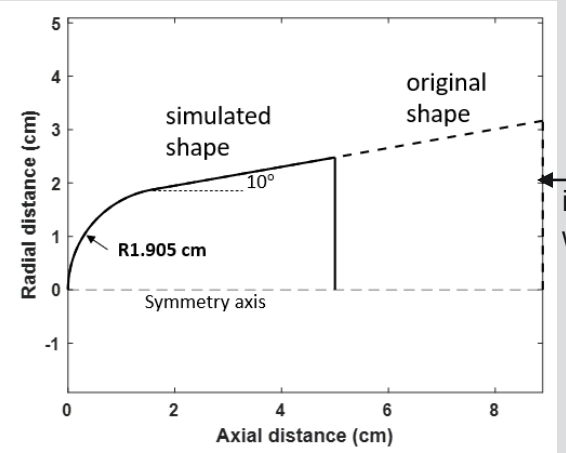
Ablation flux

$$m''_c = C_{m,0}\Omega_{blw}B'_c$$

Graphite Ablation – Case 1

- High-enthalpy (27 MJ/kg), 30 sec duration experiment conducted in IHF arc-jet facility at NASA Ames.[1]
- 10° half-angle sphere-cone with nose radius of 1.905 cm (0.75 in) and length of 8.89 cm (3.5 in).
- POCO graphite.
- Instrumentation:
  - Pyrometer at 45° and IR camera
  - Recession over time at 0° and 45°
- Studied by several groups: Chen2003, Chen2005, Bianchi2010, Bersbach2022 with various levels of fidelity:
  - Equilibrium conditions and heat conduction.
  - Finite-rate chemistry and steady state surface heating.

Schematics of the simulated geometry



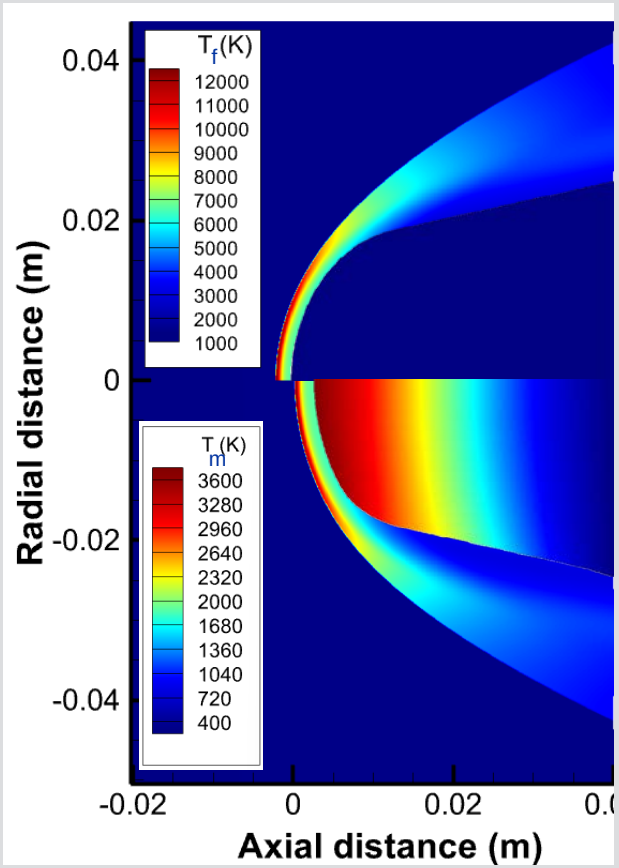
Free-stream conditions

Condition	Value
V (m/s)	5354
ρ (kg/m^3)	3x10^{-3}
T_{tr} and T_v (K)	1428
Y_k (%): N_2,O2, NO, N, O, Ar	61.69, 0, 0.46, 12.12, 25.73, 0
Duration (s)	30
T_{wall} (K)	312

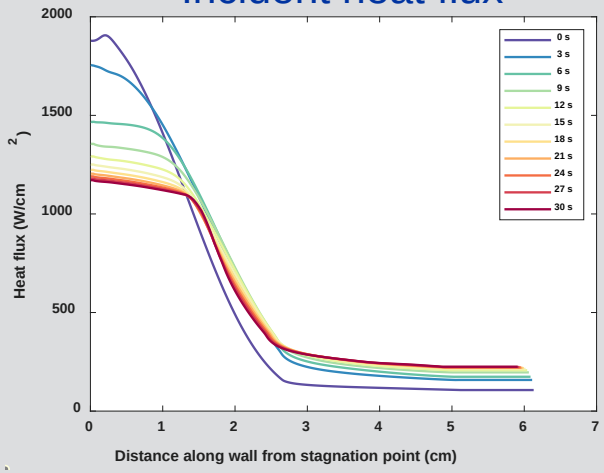
[1]Chen, Y.K., Milos, F., Reda, D. and Stewart, D., 2003, June. Graphite ablation and thermal response simulation under arc-jet flow conditions. In *36th AIAA Thermophysics Conference* (p. 4042).

Case 1 - Results

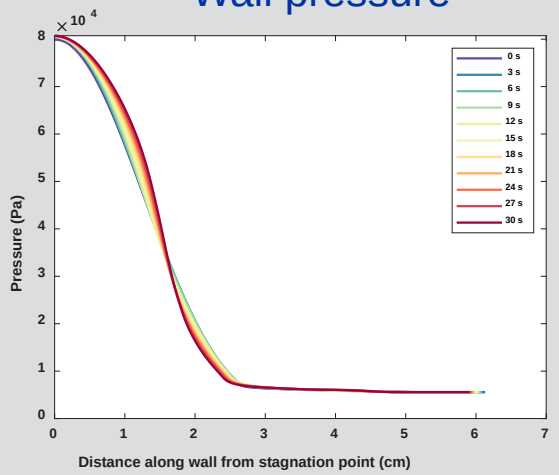
Flow and material temperature at 0 and 30 s



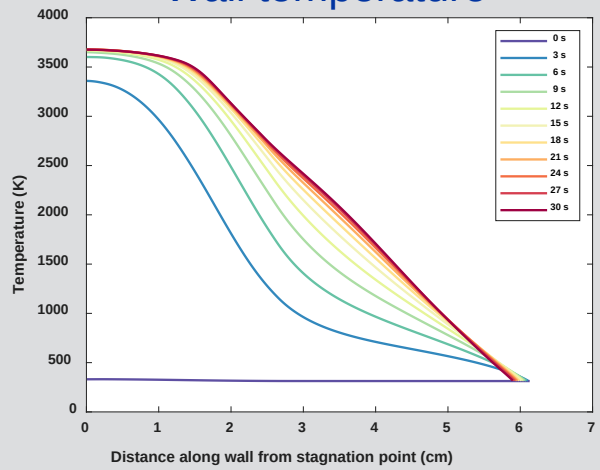
Incident heat flux



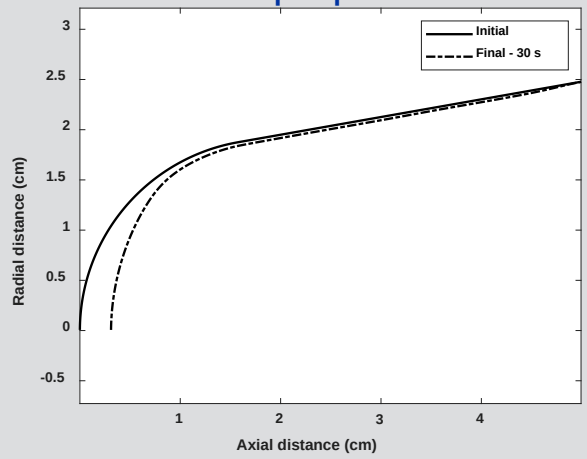
Wall pressure



Wall temperature



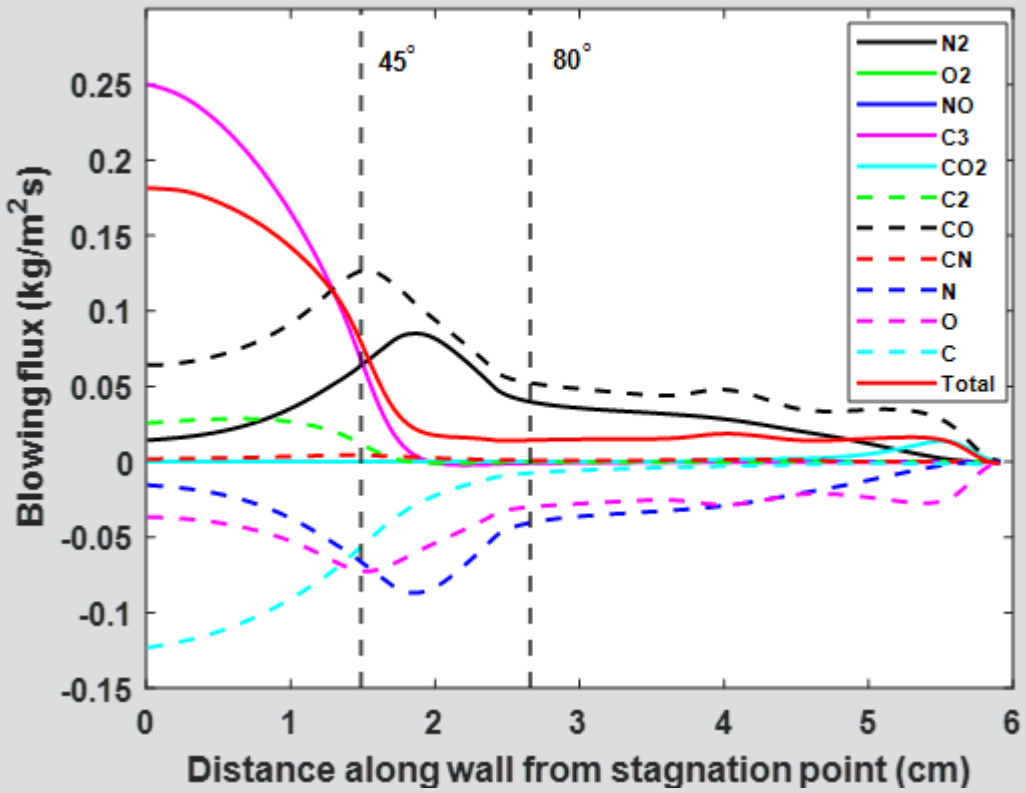
Shape profiles



Zibitsker A., Martin A., McQuaid J., Brehm C., Palmer G., Libben B., Stern E. Study of Graphite Ablation at Arc-Jet Conditions using Finite-Rate and Equilibrium Chemistry Models.. In *ICCFD11, Maui, HI, USA, 2022*.

Case 1 - Results

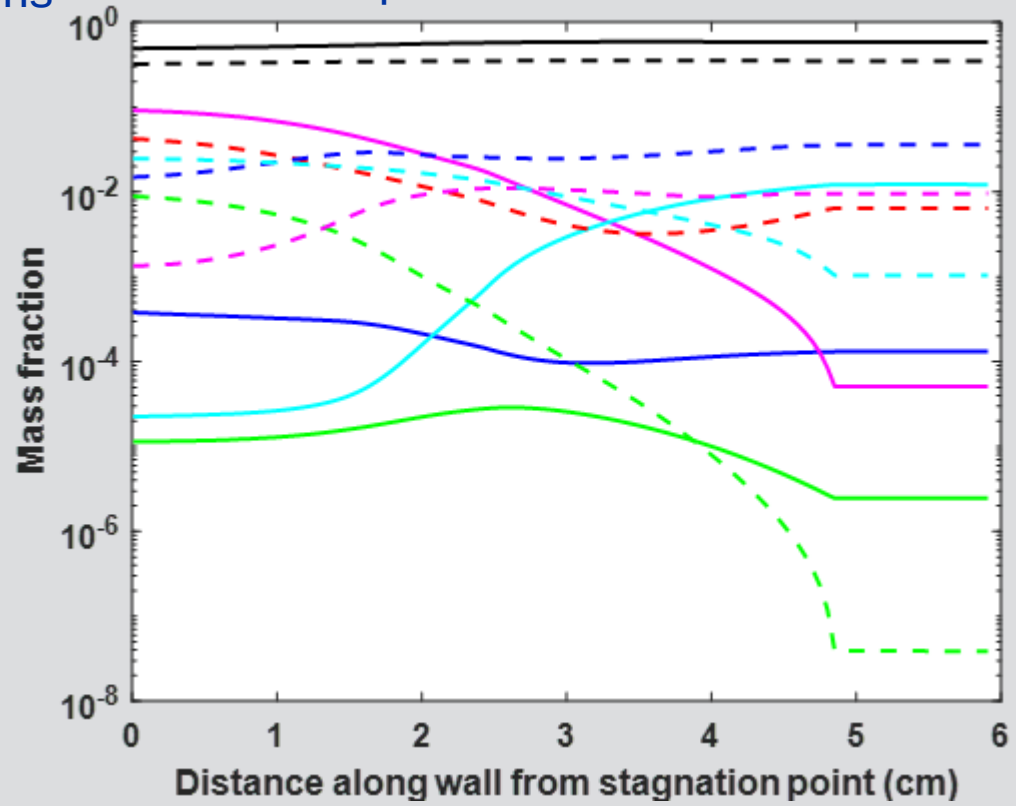
Species blowing fluxes



Stagnation point mass fractions

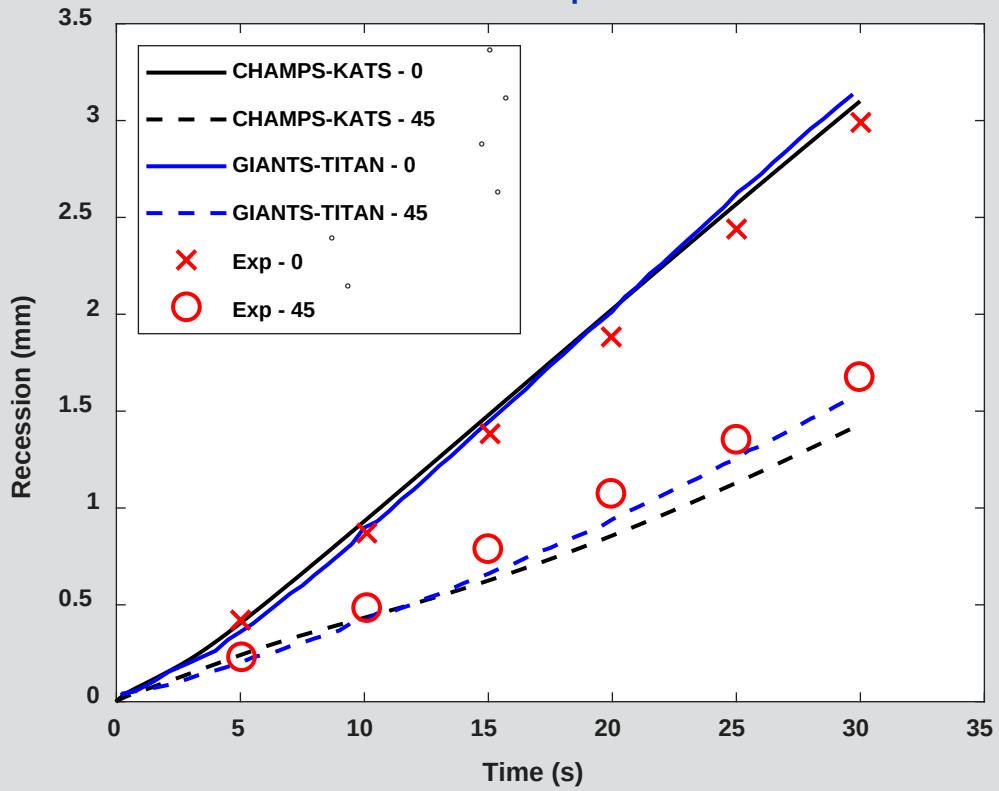
50%	-	N_2
0%	-	O_2
0.03%	-	NO
8%	-	C_3
0%	-	CO_2
0.7%	-	C_2
33%	-	CO
4%	-	CN
2%	-	N
0.2%	-	O
3%	-	C

Species mass fractions

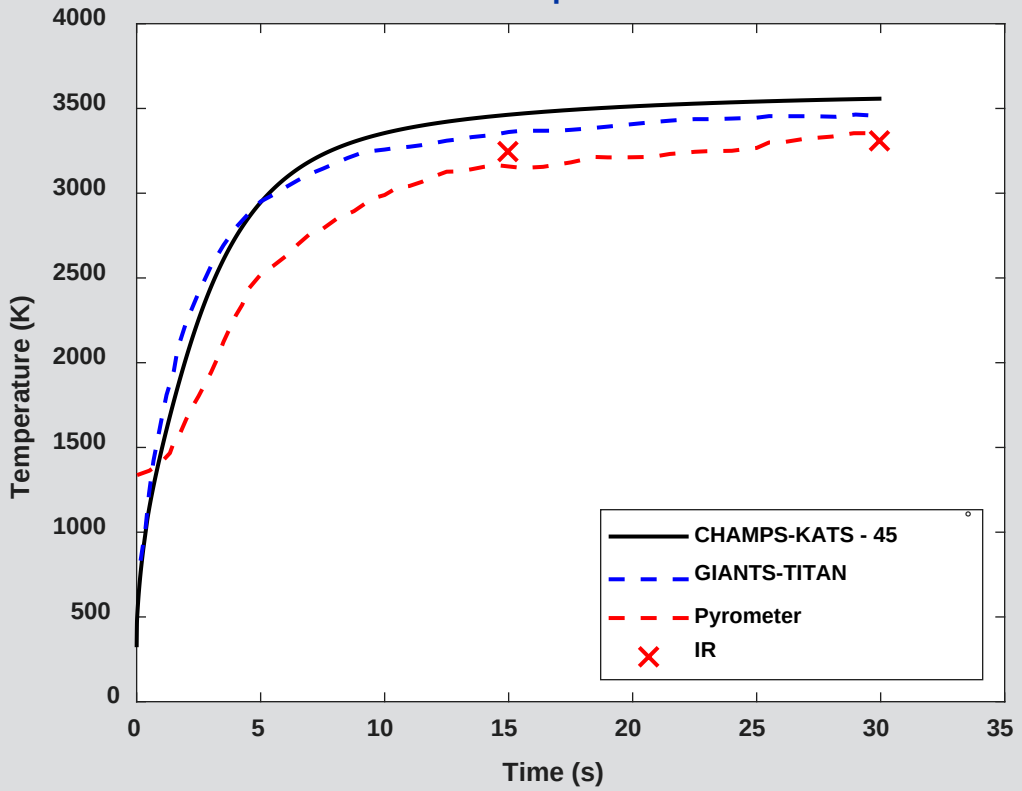


Case 1 - Comparisons

Recession profiles



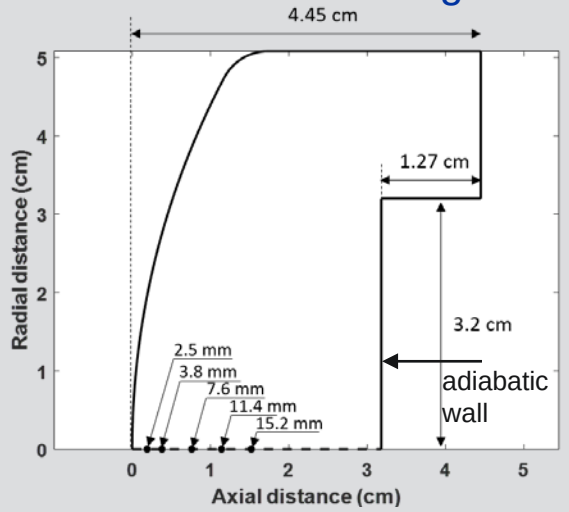
Surface temperature at 45°



Graphite Ablation - Case 2

- Lower-enthalpy (20.7 MJ/kg), 5.5 and 10.5 sec duration experiment conducted in IHF arc-jet facility at NASA. Ames in 2022
- 10.16 cm (4″) iso-q model.
- Poco graphite.
- Instrumentation:
  - Pyrometers at 0°
  - 5 thermocouples on stagnation line
  - Negligible recession of 0.1 mm and 0.7
- Arc-jet simulation with DPLR code and extraction of free-stream conditions on centerline before the shock.

Schematics of simulated geometry

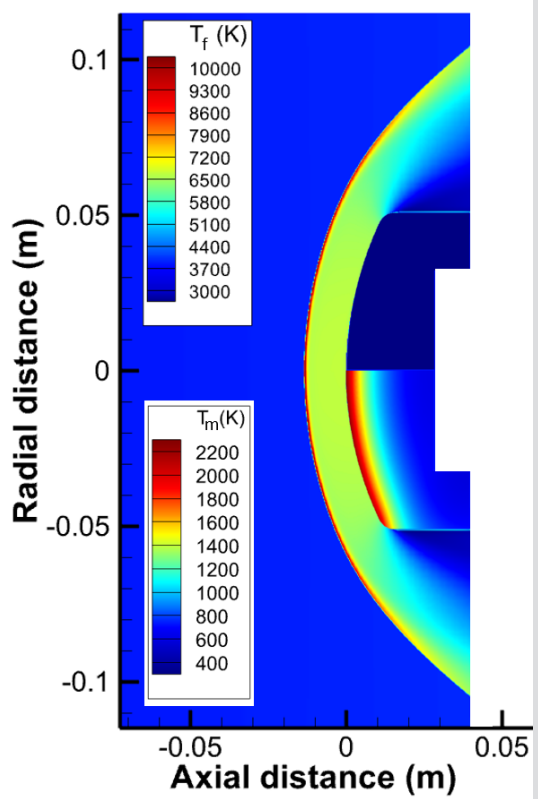


Free-stream conditions

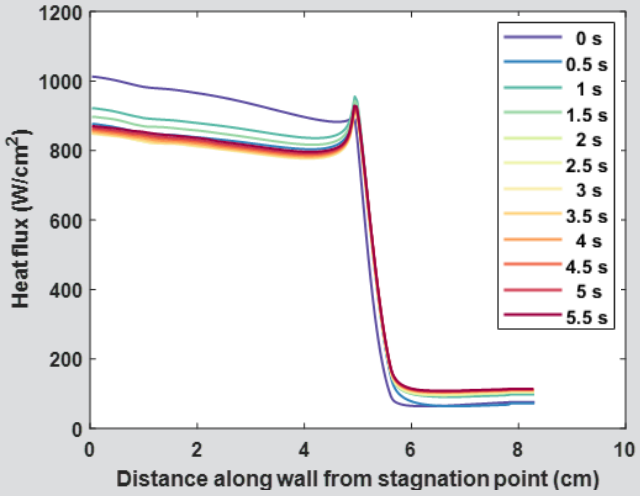
Condition	Value	Modified
V (m/s)	4327.4	Same
ρ (kg/m^3)	7.63x10^{-3}	Same
T_{tr}/T_v (K)	3812/4035	Same
Y_k (%) : N_2, O2,NO, N, O, Ar	63.17, ~0, 0.044, 7.6, 21.7, 7.5	68.28, ~0, 0.047, 8.23, 23.42, 0
Duration (s)	5.5	Same
T_{wall} (K)	Insulated	Same
Gas enthalpy (MJ/kg)	7.33	7.76

Case 2 - Results

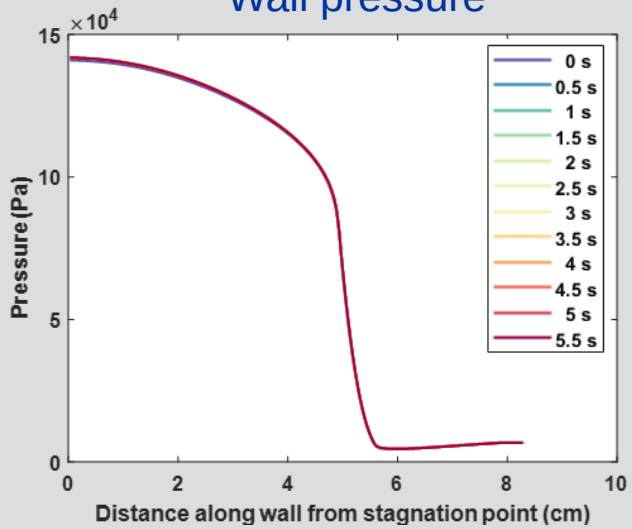
Flow and material temperature at 0 and 5.5 s



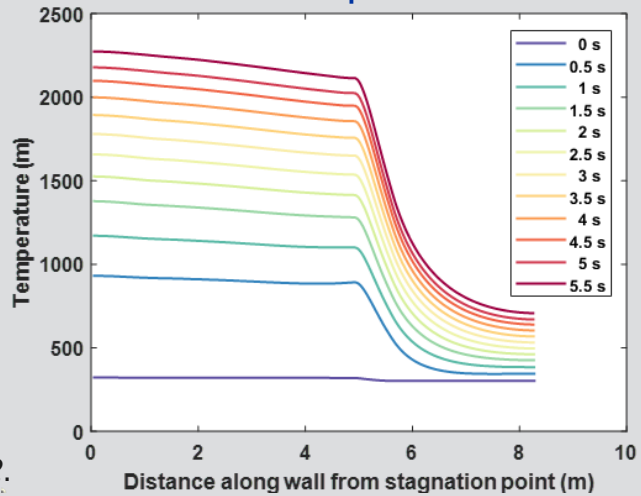
Incident heat flux



Wall pressure



Wall temperature

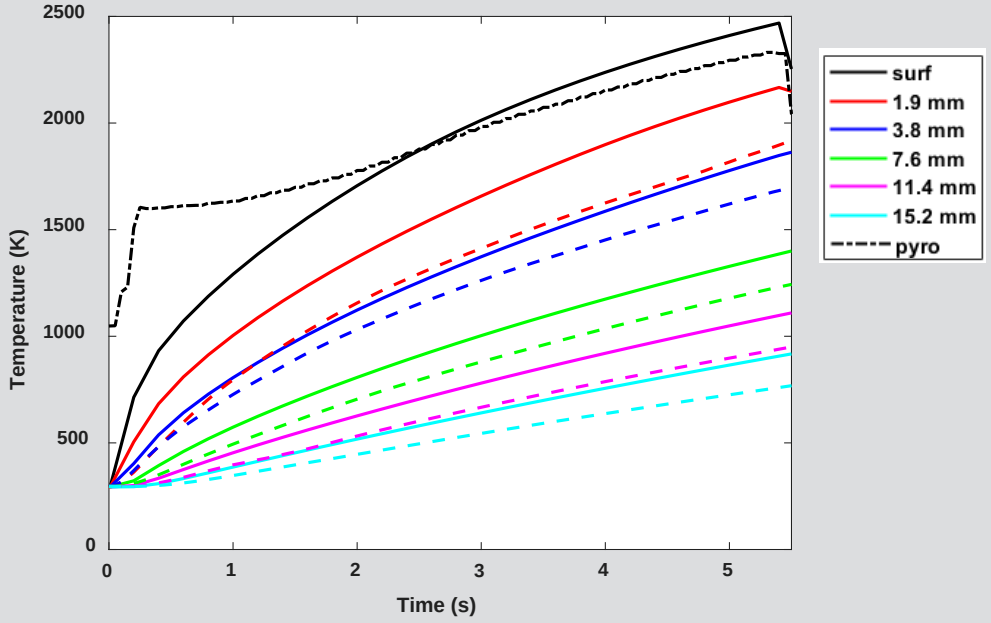


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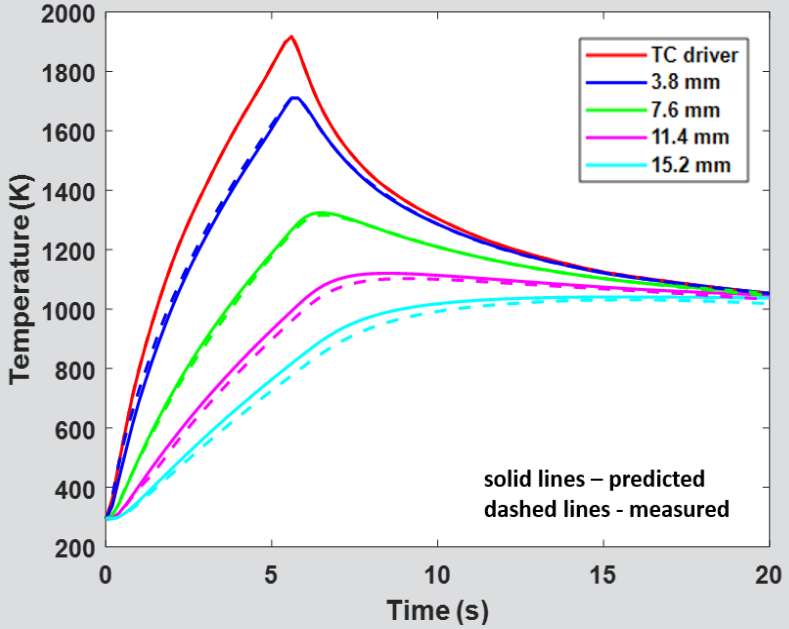
Case 2 – Uncoupled Results

- Measurements:
  - Negligible recession (0.1 mm) – no affect of shape change on the boundary conditions.
  - Measured surface and thermocouple data (5 locations).
- Uncoupled simulation uses fully-catalytic heat flux predicted by DPLR.
- TC-driver approach for verification of material properties.

Uncoupled - equilibrium ablation



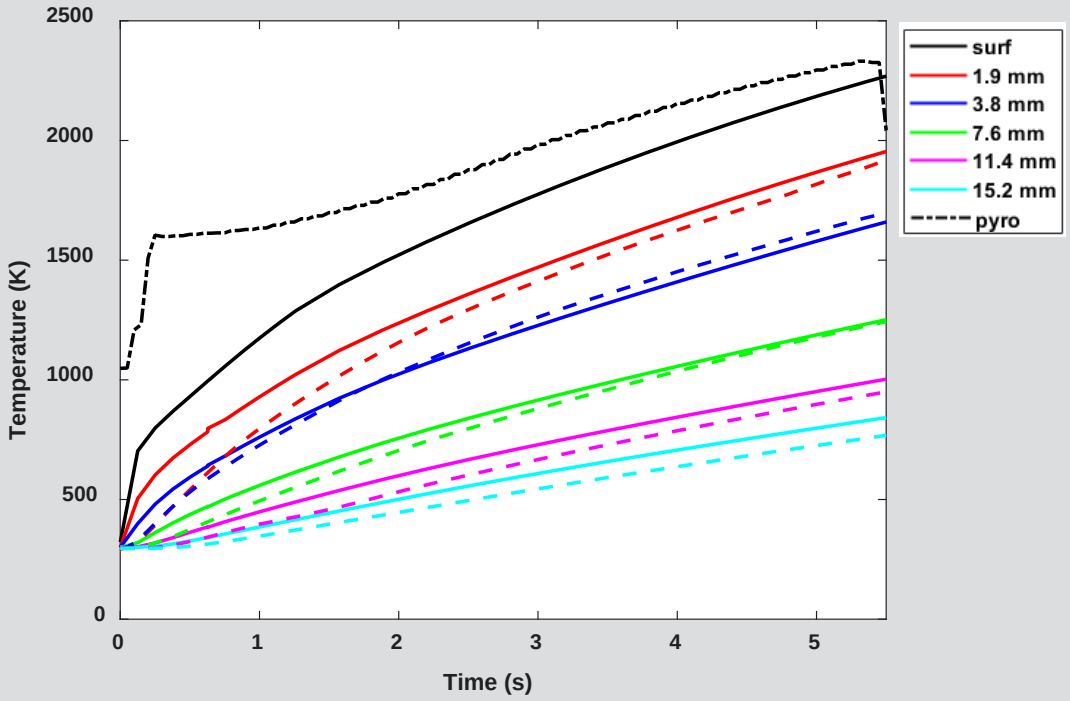
TC-driver approach



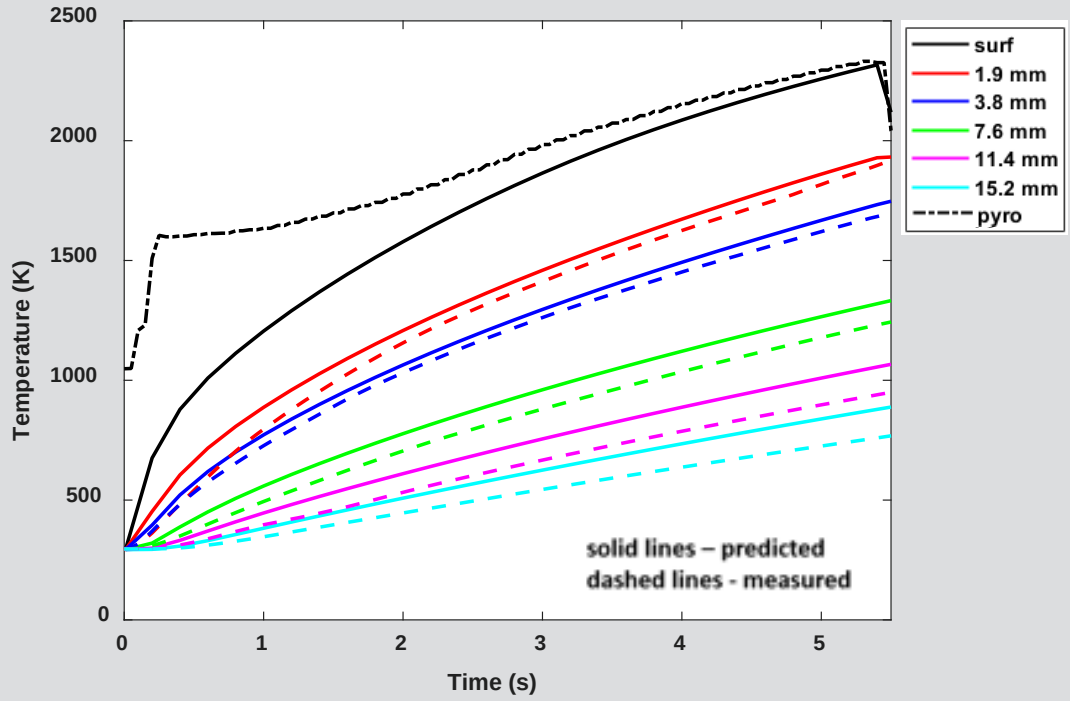
Case 2 - Comparison

- Comparison of fully coupled and uncoupled simulations:
  - Uncoupled simulation uses non-catalytic heat flux.

Fully coupled - finite-rate ablation



Uncoupled – non-catalytic heat flux



Summary

- Presented fully coupled framework between CHAMPS and KATS solvers for simulation of non-reactive flows and flows in thermochemical non-equilibrium interacting with ablative material.
- Validation with experimental data for low and high temperature ablators (camphor and graphite).
- Camphor case:
  - Validation of recession against Phoebus capsule experiment at Mach 6 flow.
  - Study of the iso-q model ablation indicated smoothing of the shoulder spike and flattening of the heat flux profile.
  - Uncoupled simulation overpredicts stagnation region recession and incorrectly predicts ablation of the shoulder.
- Graphite case:
  - Validation of recession and temperature against experimental data from IHF facility (sphere-cone and iso-q models).
  - Case 1 – sphere-cone:
    - Comparable agreement of recession and surface temperature with numerical and experimental data.
    - Strong sublimation regime with decent amount of oxidation.
  - Case 2 – iso-q:
    - Significant overestimation of in-depth temperature with fully-catalytic heat flux in uncoupled simulation.
    - Comparable agreement of in-depth temperatures in fully-coupled simulation.
    - Comparable agreement of in-depth temperatures with non-catalytic heat flux in uncoupled simulation.
    - Validated material properties, negligible material recession and measured temperatures provide a way for validation of the simulated flow environment on ablative material surface.

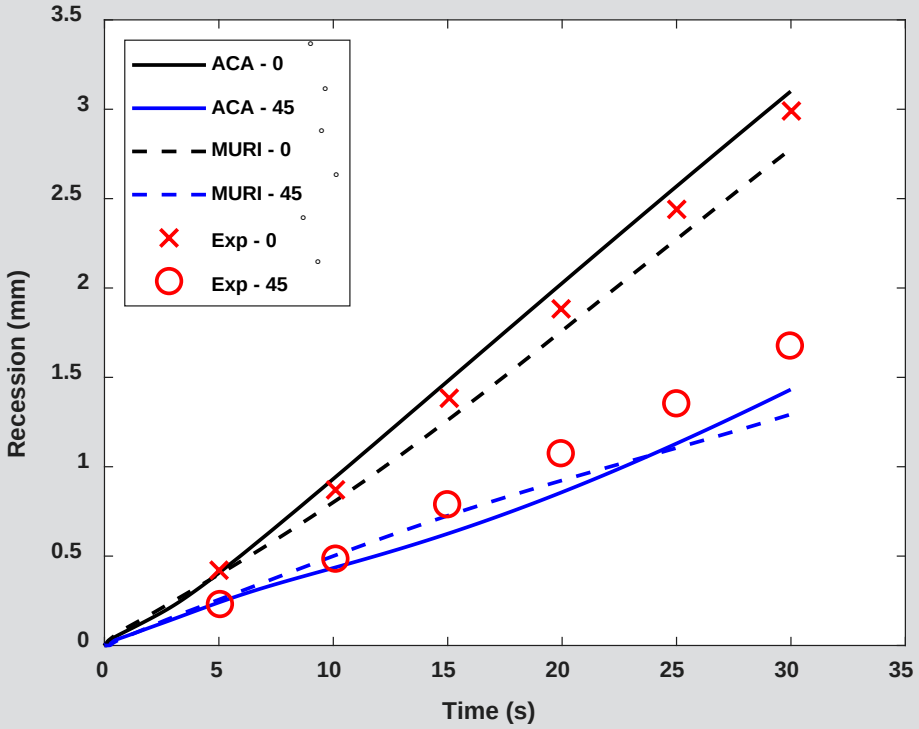
Thank you!

Questions?

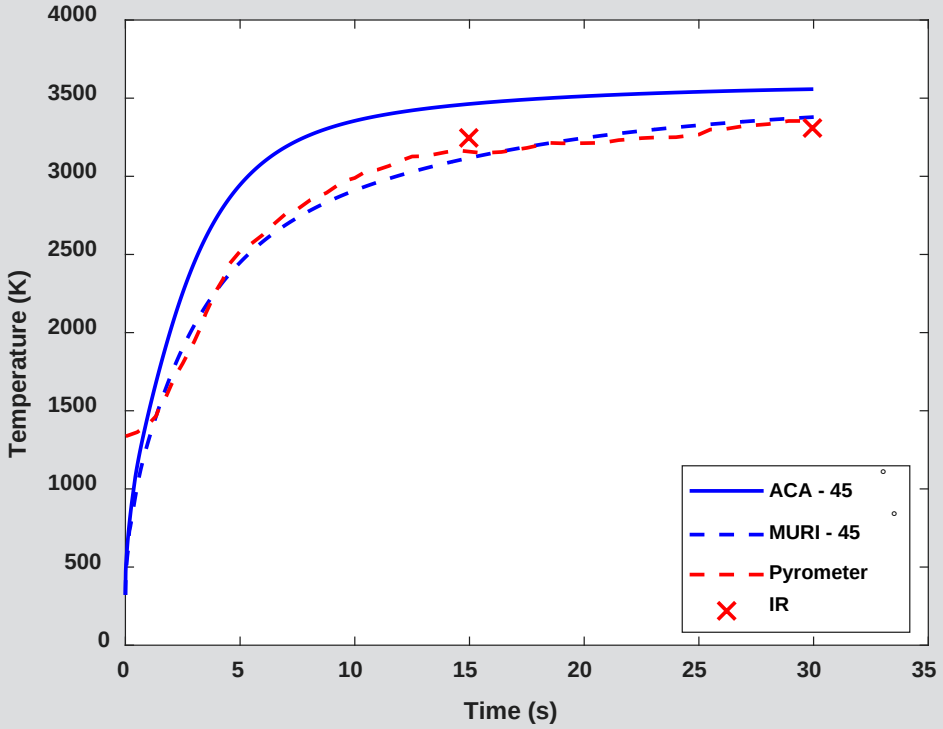
Case 1 - Comparisons

- ACA and MURI gas-surface reaction models.

Recession profiles



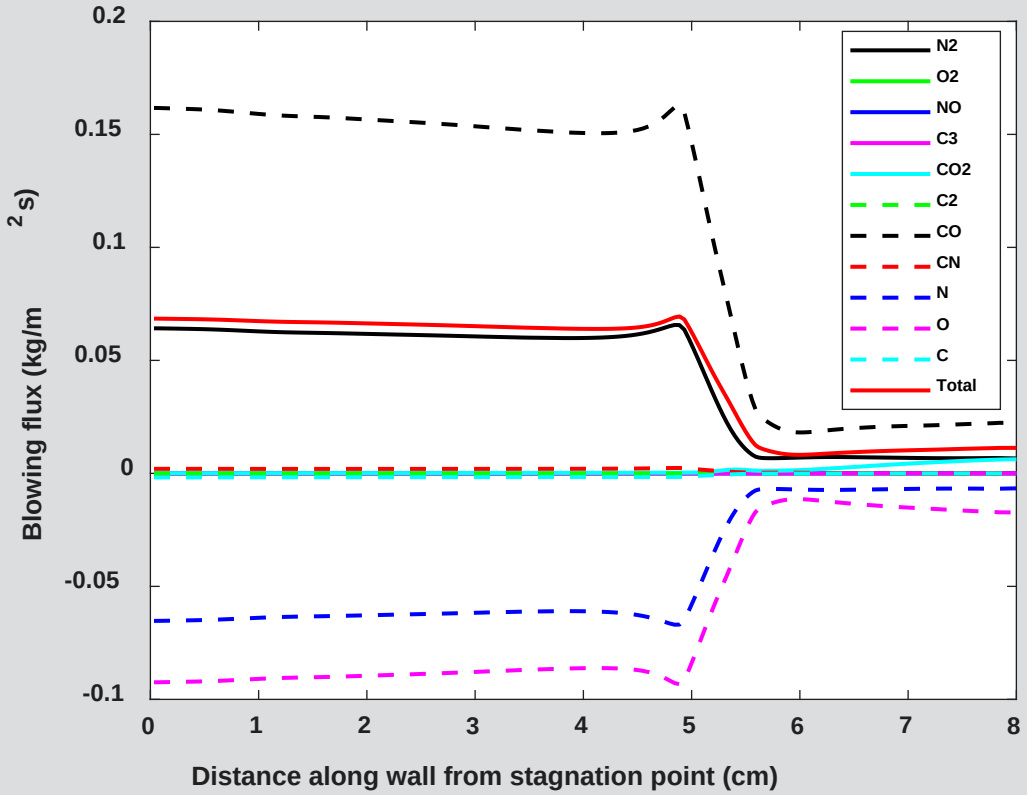
Surface temperature at 45°



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Case 2 - Results

Species blowing fluxes



Stagnation point mass fractions

65% - N_2
0.00% - O_2
0.00% - NO
0.00% - C_3
0.02% - CO_2
0.00% - C_2
35% - CO
0.03% - CN
0.1% - N
0.1% - O
0.01% - C

Species mass fractions

