RECENT ADVANCEMENTS IN THE PATO MATERIAL RESPONSE CODE.

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Brief Presenter Biography: John Thornton is a Materials Scientist with AMA, Inc., an on-site contractor at NASA Ames Research Center working in the Thermal Protection Materials Branch. He has been at Ames for five years working on modeling heatshield material response at the macro and microscales.

Introduction: Predicting the complicated multiphysics phenomena during atmospheric entry requires high-fidelity modeling tools to refine estimates of mission risks during entry. To this end, new capabilities are being added to the Porous-material Analysis Toolbox based on OpenFOAM (PATO) [1,2,3]. PATO is an open-source software for Computational Material Response (CMR) of reactive porous materials submitted to high-temperature environments.

The objective of this work is to highlight current efforts to add to and improve upon the modeling capabilities of PATO. These include efforts to loosely couple PATO with other discipline specialized codes including hypersonic Computational Fluid Dynamics (CFD), to assess the interaction effects between pyrolysis gas blowing and the boundary layer, and Computational Solid Mechanics (CSM), to address modeling of mechanical erosion. Other refinements include surface phenomena modeling capabilities to address the effects of silicone-based coatings applied to the TPS during flight preparation, and a unified multiphase solver for a mixed porous-material and plain-fluid domain.

Coupling CMR with CFD (CMR/CFD): A loose coupling between PATO and the Data Parallel Line Relaxation (DPLR) [4] CFD code has been achieved by making use of a blowing boundary condition at the heatshield surface available in DPLR. Starting with heat flux estimates with no pyrolysis gas blowing at the surface, blowing gases are computed by the CMR and passed to the CFD such that aerothermal properties of the environment can be recomputed for a new CMR computation. This leads to an iterative process which is supplemented with an estimate of the radiative heat flux using the Nonequilibrium air radiation (NEQAIR) [5] program. The entire iterative process is illustrated in Figure 1. This coupling strategy has been utilized in computing the MSL material response. The goal is to compare the

coupled CMR/CFD results with material response results obtained using traditional blowing corrections.

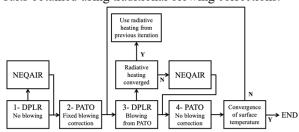


Fig. 1. Coupling process between CFD and material response.

Coupling CMS with CMR: A mechanical erosion model is currently being implemented in PATO to account for the additional mass removal induced by high shear conditions. The modeling process at each timestep consists of updating the mechanical properties as a function of temperature and computing the stress tensor and displacement fields of the material. Then, a failure criteria model determines the regions in which the stress exceeds the ultimate strength values resulting in mesh movement to account for mass removal. This model allows the material response simulation to compute the recession due to both oxidation and shear-induced erosion. The model is demonstrated by computing material response of sphere-cone are jet samples.

Surface Modeling Capabilities: NuSil, a silicone-based coating, was sprayed onto the MSL and Mars 2020 heatshields to mitigate shedding of phenolic dust. To better understand the effects of the NuSil coating on the material response, a novel model has been implemented in PATO. In this model, the equilibrium of the charred NuSil surface is modeled as pure silica, and a constant offset, inspired by the classical spallation model, is added to the the char blowing rate and wall enthalpy to reproduce HyMETS experimental results. The model has also been used to estimate the 3D material response of the MSL heatshield [6].

Unified Solver: In addition to the iterative loose coupling approach mentioned above, a multiphase unified solver is being developed to couple the environment (plain-fluid phase) and the porous-material phase.

The solver is based on the volume averaged conservation of mass, momentum, and energy for the macroscale with closure models which include microscale effects through effective physicochemical properties. The unified solver has been used to compute flow through a porous plug and solve the Beavers and Joseph problem [7]. Since the strong coupling between phases is inherent to this solver, modeling assumptions present in other coupling methods of material response are mitigated. This strategy also makes it feasible to capture the competition between surface and volume ablation in the same computational domain, which is usually not possible with other coupling approaches.

References:

- [1] J. Lachaud et al. (2014), *J Thermophys Heat Tran*, 28, 191–202.
- [2] J. Lachaud et al. (2017), Int J Heat Mass Tran, 108, 1406–1417.
- [3] J. B.E. Meurisse et al. (2018), *Aerosp Sci Technol*, 76, 497-511.
- [4] M.J. Wright et al. (2009), DPLR Code User Manual: Acadia-Version 4.01.1.
- [5] E. Whiting et al. (1996) NASA RP-1389.
- [6] J.B.E Meurisse et al. (2021), IPPW.
- [7] G.S. Beavers and D.D. Joseph (1967) *J Fluid Mechanics*, 30, 197-207.