Numerical investigation of three-dimensional effects within a charring ablator

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Introduction and Motivation

Atmospheric entry/re-entry of vehicle takes place in the hypersonic flow regime where flow field is extremely complex. High temperature gradients occurring in the shock-layer region ionizes and dissociates the air. Even if a large portion of heat generated during this process is convected away in the surrounding air, a fraction of it is still transferred to the vehicle. Therefore, efficient design of the Thermal Protection System (TPS) is necessary in order to reduce the heat conducted into the body surface, optimized the heat shield and avoid structural failure of the vehicle.

In the case of using ablative material, which has been proven an efficient way to reduce the rate of heat transfer into the vehicle, ablation modeling is a challenging task, as it involves simulating complex processes of mass loss and energy absorption through complex chemical reactions. Moreover, in case of decomposing (charring) ablators, inner pyrolysis takes place. This results in the formation of porous material as well as inner gas, further increasing the complexity of the numerical model. Available literature indicates that most of the past investigations either do not consider the actual physical processes occurred during ablation, or are limited to one and two-dimensional models.

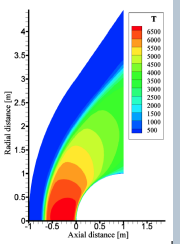
In present investigation an attempt has been made to simulate the actual physics of thermal ablation phenomenon by considering anisotropic, multilayer, variable material properties model in three-dimensions. The newly developed model is verified using closed form analytical solutions and validated with the available data. This effort consists of the first steps of an ongoing project to develop a comprehensive multiscale, multi-physics and multi-dimensional material response code aimed at modeling charring and surface ablators. Preliminary results will show the successful development of a numerical model for simulating the multidimensional heat transfer phenomena that occurred in a typical ablative TPS.

FreeCFD [1]

-A second order finite volume approach for spatial variables and uses a fully implicit first-order backward Euler time integration.

-Performs three-dimensional simulation of a typical problem, uses the popular CGNS format for computational grids and takes advantage of parallel computing through domain decomposition (ParMETIS) and MPI.

-Linked to the PETSc library, which provides efficient methods for solving solving large and sparse linear systems.



Temperature isocontours for the Mach 10 Argon flow over cylinder

-Convective fluxes are solved by a variety of available methods, which allows the code to solve problems ranging from Mach 0.001 to more than Mach 10.

-Uses numerical Jacobians, which provides a simple and versatile approach.

Proposed Model

The governing equation solved in FreeCFD takes the form of

$$\frac{\partial \mathbf{Q}}{\partial t} + \nabla \cdot (\mathbf{F} - \mathbf{F_d}) = \mathbf{S}$$

And the time-implicit control volume approach is given by

$$\left[\frac{V}{\Delta t}\frac{\partial \mathbf{Q}}{\partial \mathbf{P}} - \frac{\partial \mathbf{R}}{\partial \mathbf{P}}\right]\Delta \mathbf{P} = \mathbf{R}$$

In this equation, V is the volume of the cell, t the time step, $\mathbf{Q}$ is the conservative variables vector and $\mathbf{P}$ the primitive variables vector. The right side of the equation, represented by $\mathbf{R}$, is defined as:

$$\sum_{\text{faces}} -\mathbf{F_n} A + \mathbf{S} V$$

where A is the area of each face of the cell, and $\mathbf{F_n}$ is the normal component of the $\mathbf{F}$-$\mathbf{F_d}$ flux across that face. $\mathbf{S}$ represents the source term. The primitive formulation on the left hand side of the equations allows to directly update the physical variables, and therefore compute them while preserving a conservative formulation.

Governing Fluid Dynamics Equations

The conserved variables, source terms, and primitive variables are given by

$$\mathbf{Q} = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ E \end{pmatrix}, \quad \mathbf{S} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad \mathbf{P} = \begin{pmatrix} \rho \\ u \\ v \\ w \\ T \end{pmatrix}, \quad \mathbf{F} = \begin{pmatrix} \rho u & \rho v & \rho w \\ \rho u^2 + p & \rho uv & \rho uw \\ \rho uv & \rho v^2 + p & \rho vw \\ \rho uw & \rho vw & \rho w^2 + p \\ (E+p)u & (E+p)v & (E+p)w \end{pmatrix}, \quad \mathbf{F_d} = \begin{pmatrix} 0 & 0 & 0 \\ \tau_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \tau_{yy} & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \tau_{zz} \\ \mathbf{u\tau - q} \end{pmatrix}$$

where $\boldsymbol{\tau}$ is the viscous tensor and $\mathbf{q}$ is the directional heat flux vector.

Governing Equations for Material Response Code

The governing equations for the proposed material response model include energy, momentum and mass conservation equations for solid and gas medium. The conservative variables, source terms, and primitive variables are given by

$$\mathbf{Q} = \begin{pmatrix} E_s + E_v \\ \phi\rho_g \\ \rho_{s_1} \\ \cdots \\ \rho_{s_{ns}} \\ \phi\rho_g u \\ \phi\rho_g v \\ \phi\rho_g w \end{pmatrix}, \quad \mathbf{S} = \begin{pmatrix} 0 \\ \omega_{g} \\ \omega_{s_1} \\ \cdots \\ \omega_{s_{ns}} \\ -\phi\frac{\partial}{\partial x}p \\ -\phi\frac{\partial}{\partial y}p \\ -\phi\frac{\partial}{\partial z}p \end{pmatrix}, \quad \mathbf{P} = \begin{pmatrix} T \\ \phi\rho_g \\ \rho_{s_1} \\ \cdots \\ \rho_{s_{ns}} \\ u \\ v \\ w \end{pmatrix}, \quad \mathbf{F} = \begin{pmatrix} \phi(E_g + p)u & \phi(E_g + p)v & \phi(E_g + p)w \\ 0 & 0 & 0 \\ \phi\rho u^2 + \phi p & \phi\rho uv & \phi\rho uw \\ \phi\rho uv & \phi\rho v^2 + \phi p & \phi\rho vw \\ \phi\rho uw & \phi\rho vw & \phi\rho w^2 + \phi p \end{pmatrix}, \quad \mathbf{F_d} = \begin{pmatrix} \kappa\frac{\partial T}{\partial x} & \kappa\frac{\partial T}{\partial y} & \kappa\frac{\partial T}{\partial z} \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

Variable ϕ represent the porosity of the material, and subscript g and s are the gas and solid phase, respectively. As for the parameters μ and K, used to define flow through a porous media, they are respectively the viscosity and the permeability, and they are used to integrate Darcy's Law in the momentum equation. The solid material model includes multiple species. Then total density of the material is therefore computed with

$$\rho_s = -\sum_{i=1}^{ns} \Gamma_i \rho_i$$

where Γ_i is the volume fraction of species i in the virgin composite. The solid decomposition rate in terms of component decomposition rates can be evaluated by performing temporal derivative of above equation.

$$\frac{\partial \rho_s}{\partial t} = -\sum_{i=1}^{ns} \Gamma_i \frac{\partial \rho_i}{\partial t}$$

Decomposition of each component is assumed to follow a modified Arrhenius relation given by

$$\omega_{s_i} = \frac{\partial \rho_i}{\partial t} = -k_i \rho_{v_i} \left(\frac{\rho_{s_i} - \rho_{c_i}}{\rho_{v_i}}\right)^{\psi_i} \exp\left(\frac{-E_i}{RT}\right)$$

Where subscript v and c are respectively for the virgin and charred state of the solid material. The source terms for the solid and mass equations balance themselves, thus ensuring total mass conservation

$$\omega_g = -\sum_{i=1}^{ns} \Gamma_i \omega_{s_i}$$

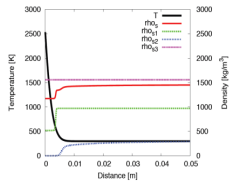
Material Response: 3D carbon-phenolic cube

-A 0.05 meter carbon-phenolic cube, on which a constant heat flux $1\times10^6 \mathrm{W/m^2}$ for 2 seconds is applied.

-The material properties used for the simulation are the one presented in Ref.[2].

-The mesh is composed of roughly 6000 cells, with clustering on the face where the heat flux is applied.

-Results are presented in the following figure. The solid densities demonstrate the behavior of the material under intense thermal inner decomposition, as the temperature rises. It provides a good indication that the code performs as expected.



Temperature, total and partial densities for the 3D carbon-phenolic cube: results are presented in 1D, in the x direction.

Material Response: IRV-2 test vehicle

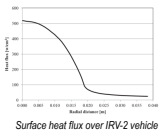
-The carbon-carbon properties (non-charring) defined in Ref.[2] are used.

-Total heat flux is externally computed and is applied at the vehicle surface; whereas, insulated wall boundary conditions have been imposed at the remaining boundaries.

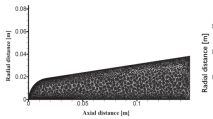
-Test condition, computational grid and heat flux distribution are shown as following. Figure (a) illustrates the computed temperature distribution for the IRV-2 vehicle after 4 seconds of constant exposure. As expected, maximum levels of temperature is observed at the blunted nose section of the body. A gradual decrease in temperature values is also apparent as one move towards the base section. Figure (b) to (c) illustrates the same results while using different values of an anisotropic thermal conductivity. As can be seen, the results are significantly different.

Temperature	Density
220.0 K	1878.96 kg/m^3

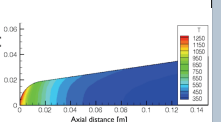
Initial condition for the material response test case



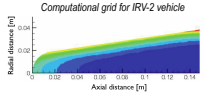
Surface heat flux over IRV-2 vehicle



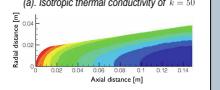
Computational grid for IRV-2 vehicle



(a). Isotropic thermal conductivity of $k = 50$



(b). Isotropic thermal conductivity of $k_{xx} = 5$ and $k_{yy} = 50$



(c). Isotropic thermal conductivity of $k_{xx} = 50$ and $k_{yy} = 5$

Conclusion

The first steps of an anisotropic multilayer and multidimensional material response code for charring ablators have been presented. The code, part of an integrated CFD framework that allows the simulation of hypersonic flow, allows to model the complex physical processes that occur during a typical atmospheric re-entry. Preliminary results have been presented, both from the flow solver and the material response modules. Those results are encouraging, and shows that the integrated solvers is an efficient and robust method to solve this class of problems. The final version of this work will include an extensive set of verifications and validations, and results will be compared to existing numerical and experimental data.

Future Plans

-Spallation prediction capability
-Integrated coupling with the fluid part of the code
-Internal chemical decomposition modeling
-Spalled particle tracking
-Surface chemistry

References

[1] Sozer, E., "freeCFD," http://www.freecfd.com, August 2010.
[2] Amar, A. J., Modeling of One-Dimensional Ablation with porous Flow Using Finite Control Volume Procedure, Master's thesis, North Carolina State University, Raleigh, NC, 2006.

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