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Loose-Coupling Algorithm for Simulating Hypersonic Flows with Radiation and Ablation

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A procedure has been developed to couple a hypersonic reacting flow model, a radiative heat transfer model, and a surface ablation model to study the surface heat transfer and surface ablation rate of atmospheric reentry vehicles. The two-way loose-coupling algorithm is described for each of the models, as is the solution procedure to achieve convergence. Observations on the challenges of the loose-coupling strategy are given. Representative results are presented for two-dimensional benchmark examples and for three-dimensional flow at an angle of attack past a symmetric capsule based on the Crew Exploration Vehicle reentry vehicle. Effects due to the interaction with radiation and ablation are shown for two quantities of interest: the predicted peak surface heat flux and the ablation rate on the vehicle heat shield. Uncertain parameters are identified in each of the submodels, and a preliminary parameter sensitivity study is carried out by varying these values to examine their effects on the heat transfer and ablation rates in the coupled problem.

Nomenclature

A	=	generic operator representing the ablation update
a_λ	=	spectral absorption coefficient, 1/m
C_i	=	species mass fraction
$C_{i,g}$	=	pyrolysis gas species mass fractions
e	=	specific internal energy, J/kg
$F(U)$	=	all terms in energy equation except radiation
h_i	=	species enthalpy, J/kg
$h^o_{f,v}$	=	heat of formation of the virgin material at reference temperature T_{ref}, J/kg
$I_{b,\lambda}$	=	Planck distribution, W/m²-sr
I_{sp}	=	integrated intensity, W/m²
I_λ	=	radiative intensity, W/m²-sr
J_i	=	mass flux, kg/m²-s
k	=	gas thermal conductivity, W/m²-K
$\tilde{N}_i$	=	mass production
N_s	=	number of gas species
n	=	unit normal vector
P	=	Pressure, Pa
$\mathbf{q}_{\text{rad}}$	=	heat flux vector, W/m²
$R(U)$	=	generic operator whereby the radiative heat flux is computed given the current value of the primitive variables
T	=	Temperature, K
T_V	=	vibrational temperature, k
T_w	=	wall temperature, k
U	=	primitive flow variables
v_w	=	wall velocity, m/s
z	=	distance from surface, m
$\dot{m}''_c$	=	mass loss of char, kg/m²-s
$\dot{m}''_g$	=	mass loss of pyrolysis gas species, kg/m²-s
$\dot{q}''_r$	=	incident radiative heat flux, W/m²
α	=	absorptivity of wall
Γ	=	ablating surface
Δt	=	time step, s
δs	=	shock standoff distance
ϵ	=	emissivity
θ, ϕ	=	azimuth and inclination relative to tangent plane
ρ	=	gas density, kg/m³
σ	=	Stefan–Boltzmann constant, W/m²-K⁴

I. Introduction

THE aerothermodynamic processes encountered by atmospheric entry vehicles involve a wide variety of physical phenomena. In addition to the strong shocks generated in a hypersonic flow environment, the combined heating and pressurizing of multicomponent atmospheric gases initiates complex chemical reactions between gas species, ionization, and emission and absorption of radiation. The inclusion of an ablative heat-shield material, which serves to protect a vehicle from the harsh environment, also introduces a multicomponent outgassing process at the vehicle surface that further complicates the external flow, particularly within the boundary layer. Hence, it is crucial for the design and analysis of such vehicles to be able to identify and accurately model hypersonic flow, radiation, and ablation. However, these processes are clearly not independent of one another: they are *coupled*, through overlapping domains for the radiative transport and interfacial coupling for ablation. Furthermore, the goal of the vehicle analyst is not only to determine a single solution to this coupled flow and transport problem, but more important, to study the uncertainty of particular functionals of the solution, known as *quantities of interest*. In the current work, we focus on the peak convective heat flux and peak ablation rate of an entry vehicle as the quantities of interest.

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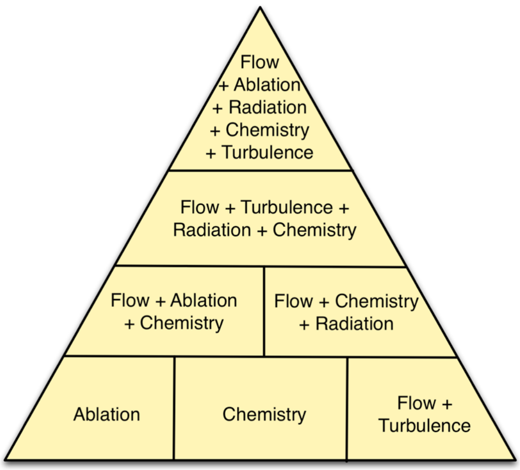

Fig. 1 Representative validation pyramid for hypersonic reentry physics.

This work is part of a broader investigation by the Center for Predictive Engineering and Computational Sciences[††] (PECOS) involving verification, validation, and uncertainty quantification. One of the central tenets within the validation efforts of the center is the notion of a *validation pyramid*, illustrated conceptually in Fig. 1. The figure illustrates a hierarchical framework for which we begin by first validating component models at the lower level of the pyramid. Then, as we ascend the pyramid, we validate more complete representations of the physics of interest, and finally, we reach the complete complex problem of interest at the peak of the pyramid. Note that as we ascend the pyramid, the various component models from the base of the pyramid must be coupled. Thus, it is a PECOS goal as part of the overall validation process to enable the simulation of multiphysics phenomena. Accordingly, our purpose here is to investigate multiphysics coupling aspects of the simulation problem for a representative model class at the top of the pyramid. Hence, we do not focus on aspects of validation as this is well beyond the scope of this paper. It is, however, a topic of ongoing research within the PECOS center. In the present case, the models considered include important topics of compressible fluid flow, finite rate chemistry, turbulence, shock-layer radiation, and surface ablation. In what follows, we consider the compressible flow, turbulence, and chemistry models together as flow models for convenience of notation.

A number of studies have analyzed coupling of radiation and/or ablation models with flow models using various schemes. For example, Hassan et al. [1] used a loose-coupling approach in which the steady-state Navier–Stokes equations were solved at specific points in the reentry trajectory. Once the flow was computed, it was held fixed and then an unsteady material response model was used to compute the time-dependent changes within the ablator between two trajectory points. The resulting blowing rate was then fixed for flow calculations at the next trajectory point. In a subsequent paper [2], stability was improved by linearly interpolating between different trajectory points. In both works, an equilibrium surface chemistry was used for the ablating surface and finite rate reactions were used for the boundary layer. Chen and Milos [3] used a steady ablation model coupled to a steady Navier–Stokes solver. The flow and ablation models were coupled one way. Instead of determining the ablator wall temperature by an energy balance at the surface, an experimentally measured temperature profile was imposed on the ablator. A coupled flow–ablation scheme studied by Gosse and Candler [4] accounts for both material that is ablated away and in-depth heat conduction. Here, the flow was assumed to be in thermochemical nonequilibrium and was computed over a trajectory. The temperature at the fluid–solid interface was computed using mass and energy balances, a manner very similar to the approach used in this work. The surface recession rate was integrated over the trajectory and the mesh was adjusted according to this rate. Sakai and Sawada [5] studied the effects of radiation in air with carbonaceous species present using an implicit coupling scheme. No ablation coupling was present. The radiation model used a tangent-slab approximation with a multiband spectral model, and the flow neglected viscous effects.

In another loosely coupled model, Suzuki et al. [6] studied the MUSES-C reentry capsule using a one-way coupled radiation model and a Charring Material Thermal Response and Ablation (CMA) ablation model. The flow in thermochemical nonequilibrium provided data to a radiation model using a multiband spectral representation and tangent-slab approximation. The material response of the ablator was computed from the input of the radiation model and a loose-coupling iteration between the flowfield and the ablator, which acted as a boundary condition on the flowfield. In this manner, the material response was computed over a trajectory such that the intermediate response could be interpolated. Interestingly, the authors noted that the convergence of the loose-coupling scheme was achieved in a few iterations. A different approach was taken by Matsuyama et al. [7] to study the Galileo probe. Here, the viscous shock-layer equations were used to model the flow as a hydrogen–helium gas mixture and an ablation gas mixture. The gases were assumed to be in thermochemical equilibrium. The radiation model was implicit using a tangent-slab approximation and a multiband spectral model. The ablation model was a quasi-steady boundary condition and was loosely coupled with the flowfield calculation. The authors noted the strong effect of the turbulence model on the simulated recession. Coupled radiation, ablation, and hypersonic flow simulations were conducted by Gnoffo et al. [8]. They assumed local chemical equilibrium for the gas-phase flow as well as for the ablator. The local chemical compositions were completely determined using the Gibbs free-energy minimization for the entire domain (gas and solid surfaces). Johnston et al. [9] used this coupling scheme to study the effects of ablation on radiative heating. Hence, we have several exploratory studies leading, in spirit, toward the current work.

In the current work, we focus on *two-way* coupling of an existing steady-state, chemically reacting, compressible Navier–Stokes code with new simulations of shock-layer radiation and surface ablation. Finite rate chemistry is used both for the flow solution and the ablation model. The focus here is the numerical behavior of the coupling algorithm, as there appears to be a dearth of discussion in the literature on this topic for this class of problems and this type of coupling strategy. The overall coupling strategy is introduced in Sec. II. In Sec. III, the radiation model and overlapping subdomain coupling to the underlying flow model are described. Some example calculations in two and three dimensions are also presented. The interfacial coupling to the ablation model is given in Sec. IV, and preliminary results for test cases in two and three dimensions are shown. Finally, preliminary results for the sensitivity of the peak ablation rate are obtained by varying several parameters in the flow, radiation, and ablation models; this is summarized in Sec. V. Concluding remarks concerning simulation results and the coupled approach are given in Sec. VI.

II. Coupling Strategy

Our primary aim is to study the behavior of the coupling scheme. Of particular interest are convergence properties, efficiency, and to a limited extent, accuracy of the coupling scheme. In the present work, reacting hypersonic flow is coupled with shock-layer radiation on an overlapping radiation subdomain and with surface ablation models via interfacial coupling. Based on the flow temperature and pressure at a given time step as well as on the temperature of the reradiating wall, the radiation model performs a discrete-transfer integration to determine what sources or sinks appear in the flow energy equation due to radiative heat flux. For the ablation model, the conservation equations for the mass of each chemically reacting element and for the energy of the mixture are satisfied across the ablating wall interface.

[††]Data available online at http://pecos.ices.utexas.edu.

These models couple to the flow equations as follows:

$$\nabla \cdot \mathbf{q}_{\mathrm{rad}} = R(U, U|_\Gamma) \qquad \frac{\mathrm{d}\rho e}{\mathrm{d}t} = F(U) + R(U, U|_\Gamma)$$
$$U|_\Gamma = A\left(U|_\Gamma, \frac{\partial U}{\partial n}\bigg|_\Gamma, \mathbf{q}_{\mathrm{rad}}\right) \tag{1}$$

Figure 2 illustrates the coupling schematically. For brevity, we do not explicitly reproduce the compressible real-gas Navier–Stokes equations, but focus on the coupling scheme and the radiation and ablation submodels.

The radiation equations are included in the flow approximation explicitly. At each time step, the divergence of the radiative heat flux is calculated in each cell. This divergence is then used as an explicit source or sink term to be integrated in time through that step. A modified Dirichlet–Neumann nonoverlapping Schwarz method is introduced to solve the ablation interface equations, as follows: the flow solver supplies initial values and fluxes to the ablation model, and following an update by the ablation solver, the ablation model will supply Dirichlet boundary conditions for the flow. These procedures are iterated as the flow solver time steps until convergence is reached.

This loose-coupling update strategy can be generally viewed as an operator-splitting approach with implicit quasi-steady updates on the flow variables and explicit updates via the coupling terms computed from the radiation and ablation physics models:

$$M(U^{(\mathrm{new})}, U^{(\mathrm{old})}, \Delta t) = F(U^{(\mathrm{new})}) + R(U^{(\mathrm{old})}, U^{(\mathrm{old})}|_\Gamma)$$
$$U^{(\mathrm{new})}|_\Gamma = A\left(U^{(\mathrm{old})}|_\Gamma, \frac{\partial U^{(\mathrm{old})}}{\partial n}\bigg|_\Gamma, \mathbf{q}_{\mathrm{rad}}\right) \tag{2}$$

Although algorithms of this type are notoriously challenging for obtaining robust convergence, the implementation requires relatively simple changes to existing software infrastructures. In this case, using a loose-coupling strategy provided a way to leverage existing hypersonic flow solver software to obtain solutions to very challenging physical problems, providing a test bed for doing simple parameter studies on the *coupled* problem. The NASA code DPLR (Data Parallel Line Relaxation [10]) provides the analysis for the hypersonic flow problem, and coupling methodology and software were developed to incorporate iteratively coupled radiation and ablation models as described next.

We note that other coupling schemes are possible, in that different combinations of explicit and implicit terms are possible for each of the physics models. The current strategy was chosen for ease of implementation with the existing DPLR code. In particular, it allows for independent development of radiation and ablation models, once an application programming interface is agreed upon for the software. Furthermore, the operator-splitting approach introduces the possibility of lagging terms in time. Indeed, we studied lagging both the radiation and ablation models for multiple time steps with the flow update. However, we found the destabilizing effect of time lagging updates in the radiation case to be too great, whereas in the ablation case, convergence was prolonged.

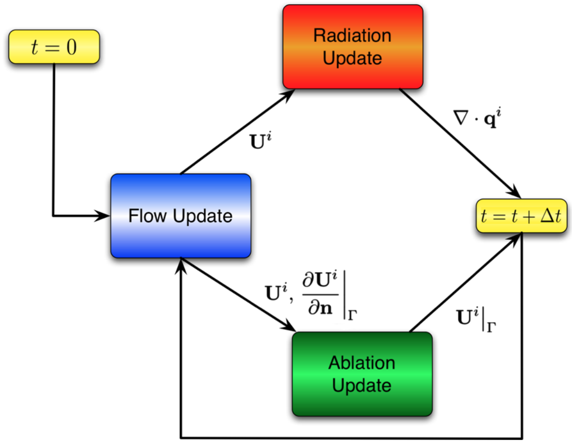

Fig. 2 Schematic of loose-coupling scheme.

III. Radiation Model and Results

From a coupling perspective, the operator splitting allows us to integrate any radiation code that takes the flow state variable field $U^{(\mathrm{old})}$ as input and that produces the radiative heat flux divergence $\nabla \cdot \mathbf{q}_{\mathrm{rad}}$ as output. This interface belies the great underlying complexity of radiation modeling, however. Radiative intensity I can be viewed as a field that is dependent not only on three spatial dimensions but also on two directional dimensions and on radiation wavelength. Our initial simulations simplify the problem, by assuming local thermodynamic equilibrium when calculating absorption and emission coefficients, using the discrete-transfer method with a tangent-slab approximation to integrate radiative fluxes through the domain and using a gray-gas model to integrate over wavelength.

For local thermodynamic equilibrium, the Planck distribution and spectral absorption coefficient describe emission of radiation, in which case the radiative heat transfer equation along a ray parameterized by s takes the form [11,12]

$$\frac{\mathrm{d}I_\lambda(s)}{\mathrm{d}s} = a_\lambda(U) I_{b,\lambda}(U) - a_\lambda(U) I_\lambda(s) \tag{3}$$

The dimensionality of the radiation transfer is reduced by the tangent-slab approximation. Consider a line normal to the surface. For radiation in layered flow structures such as our shock layer, where state variables can depend strongly on z but vary only gradually in the tangent directions x and y, we can simplify the problem by assuming no variation in the tangent directions. Conceptually, the problem being solved on each line is the same as it would be on a domain of tangent slabs. The radiative transfer problem reduces to a set of 1-D problems, decoupling each line from others and allowing an "embarrassingly parallel" simultaneous solution of multiple lines. On each line, the problem also becomes 1-D instead of 2-D in direction, because symmetry implies that the radiative intensity solution is independent of ϕ. Each radiation update requires temperature and pressure data along lines normal to the radiating surface. The line of cells in a structured mesh in the surface-normal direction are used to approximate the true surface-normal line. For the meshes we use, it is expected that this will have minimal impact on solution fidelity in regions where the surface is flat, and this technique both simplifies the implementation of and accelerates the execution of mesh data transfer between the flow solver and the external radiation model. Although sharing the spatial discretization of the flow solver, our radiation solver uses its own discretization of θ. Experimentation has shown a uniform discretization in 25 directions to give accurate results at reasonable computational expense.

Examination of our current results at International Space Station (ISS) return reentry conditions appears to show excellent support for the tangent-slab approximation for capsule geometries, even at modest angles of attack. The shock layer is locally relatively flat, and property variations in the tangent directions are relatively insignificant compared with property variations in the normal direction. At high angles of attack, or at higher velocities where gas radiation has greater influence, the curvature of the leading lip of the capsule may be an issue.

The dependence of radiative intensity on wavelength is avoided via the gray-gas approximation [11,12]. This simplifies the evaluation of the multiphysics problem by removing expensive line-by-line calculations from the coupling loop. We use high-fidelity computationally expensive spectroscopic solves from SPECAIR [13] only to precalculate curve fits $a(T_v, P)$, which approximate the (vibrational/electronic) temperature- and pressure-dependent absorptivity coefficient to be used in the coupled simulations. For an approximate shock standoff distance δs and for homogenous flow properties U, SPECAIR is used to compute an integrated intensity I_{sp} along a path, which is converted into an equivalent mean gray-gas absorption coefficient via the formula

$$a(\phi) = \frac{-1}{\delta s} \ell n \left(1 - \frac{I_{sp}(U)}{I_b(U)}\right) \tag{4}$$

where the calculated intensity I_{sp} depends on the solution of Eq. (3) for all wavelengths, integrated along the entire path length and spectrum for a path with uniform state U.

Examination of our capsule results has shown that the validity of the gray-gas approximation is limited, at best. For lunar return reentry conditions, most of the radiation within the shock layer appears to be generated by gas at local thermochemical equilibrium, and spectroscopic solves that assume local equilibrium can be used to produce a curve fit to T_v and P alone, which gives useful results for the gas radiation. For ISS return reentry conditions, the strongest component of the radiation appears to be generated immediately postshock, as the flow reaches thermodynamic equilibrium, but before the molecules in the gas are completely dissociated. In this layer of the flow, the absorption coefficient is still strongly dependent on the changing chemistry, and attempting to approximate the absorptivity with T_v and P data alone does not appear to be robust. Fortunately, for ISS return reentry conditions, the effects of gas radiation as a whole are not dominant, and the high model error in our radiation model has a limited influence on our quantities of interest. However, the chemistry dependence of radiation is an issue that will need to be addressed in future work.

Given that the radiation model is updated explicitly, it is no surprise that the stability and robustness of the method depend strongly on the strength of the radiative source term and the time-step size used in the simulation. Results of our numerical experiments demonstrate two common failure modes when running coupled flow and radiation simulations. The first occurs when the flow is being cooled by the effects of the radiation. Specifically, as the flow cools, the shock will recede toward the surface of the blunt body. If the time-step size is too large, or if the radiation model is not updated frequently enough with the flow solution, then the shock will recede past the area of strong radiation emission and the freestream gases will begin emitting. This causes a sudden drop in temperature to nonphysical values, leading to sudden divergence of the numerical solution. A more subtle failure mode occurs in the case of a transient advancing shock. Here, using excessively large time steps causes the radiative heat flux to overshoot the value that would have been obtained by an implicit solve; in subsequent time steps, this causes the shock to oscillate. Over several time steps, this instability can grow and eventually cause numerical solution divergence when the temperature drops to nonphysical values. In both cases, the instability can be controlled by using a sufficiently small time step. Experience has shown that the time-step size depends strongly on the Mach number. The higher the Mach number, the stronger the effects of radiation and the tighter the time step required.

Some example 2-D calculations comparing flow solutions, without and with the shock-layer radiation model enabled, are given in Fig. 3 for reacting air. In both cases, the peak temperature is near 13,000 K. The shock contracts approximately 10% toward the surface of the cylinder with the radiation model enabled. Figure 4 shows a comparison of the convective heat flux with a perfect gas model with no radiation, a 5-species air model with radiation excluded, and a 5-species air model with radiation enabled for a 3-D symmetric capsule at an angle of attack. Not surprisingly, we see that radiation has little effect at these (ISS) flow conditions.

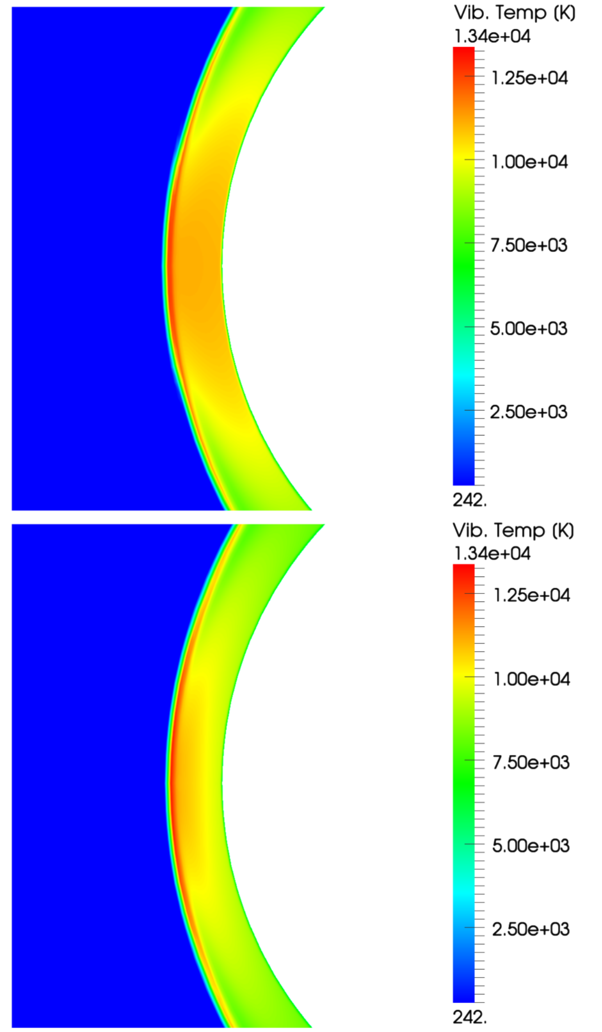

Fig. 3 Close-up of subregion near 1 m cylinder with a 5-species air model at Mach 31; without shock-layer radiation (top) and with shock-layer radiation (bottom).

IV. Ablation Model and Results

Unlike the *overlapping* domain problem for the radiation coupling, the ablation model coupling is actually an *interfacial* domain problem. Our current model [14] uses an assumption of quasi-steady ablation, combined with a locally 1-D control-volume analysis, which reduces the ablation problem to a nonlinear Robin-type boundary condition on the ablating interface. At an interface between the ablating material and the gas flow, with normal vector **n**, the following system of equations is to be satisfied:

$$J_i|_{gas,w} + \rho v_w C_i = \tilde{N}_i(C_i, T_w) + \dot{m}''_g C_{i,g}; (i{:}\ 1, \ldots, N_s) \tag{5}$$

$$k \frac{\partial T}{\partial y}\bigg|_{gas,w} - \sum_{i=1}^{N_s} h_i(T_w)[\tilde{N}_i + \dot{m}''_g C_{i,g}] + \alpha \dot{q}''_r - \sigma\epsilon T_w^4 + \rho v_w h^o_{f,v}(T_{ref}) = 0 \tag{6}$$

$$\rho v_w = \dot{m}''_c + \dot{m}''_g \tag{7}$$

Equation (5) represents the conservation of mass of each of the N_s gas species across the interface; fluxes from the flow and blowing gas are balanced by production terms for sublimation, oxidation, nitridation, and/or catalysis reactions at the wall. Pyrolyzing ablators also include production terms for the mass loss of pyrolysis gas species. Equation (6) represents the conservation of energy at the surface: convective heat flux from the gas, enthalpy flux from species diffusion, enthalpy outflow from blowing gases, absorbed radiative heat flux, emitted radiation, enthalpy inflow from pyrolysis gases, and conductive heat flux into the ablator material all balance. Equation (7) represents the relation of mass loss to recession (wall velocity). We include only the final form of these equations here; we refer the reader to [14] for the full derivation.

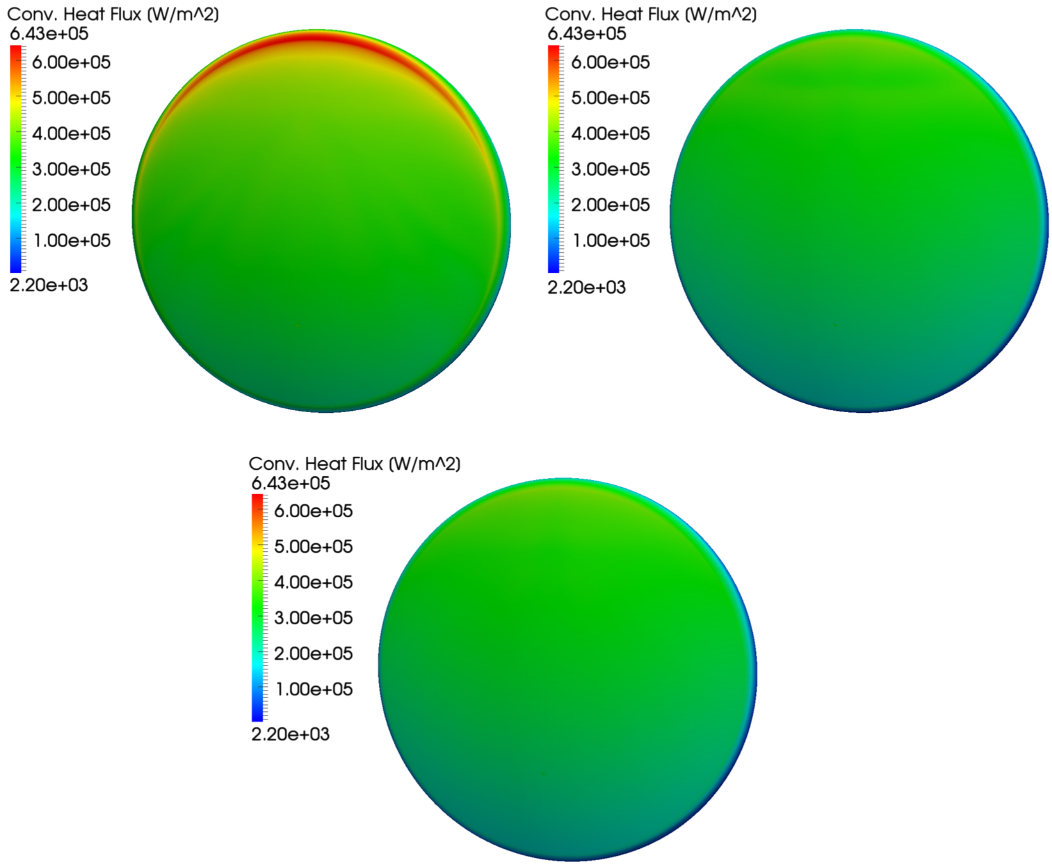

Fig. 4 Surface convective heat flux on a 3-D symmetric capsule; perfect gas with no radiation modeling (top left), 5-species air with no radiation modeling (top right), and 5-species with radiation modeling (bottom). All scales are the same.

We note here that although this model is not a complete description of the capsule ablation phenomena, the focus of the PECOS center is not primarily high-fidelity modeling of reentry physics, but rather the validation of the models used. In this case, we seek the simplest possible models in order to exercise validation (or perhaps invalidation) of the models used in future work. If it is found that the current model is invalid, then suitable enrichments to the current model will be made. Again, we note that the focus of this paper is on the coupling methodology and its behavior and not validation of the mathematical models.

We use a modified Dirichlet–Neumann nonoverlapping Schwarz method to solve these interface equations. At each ablation coupling step, the heat and mass flux are first extracted from the flow solution at the surface and used to construct Robin boundary conditions for the ablation model. Because of the complex nonlinear reaction terms in the ablation model, pure Neumann boundary conditions were found to produce unstable results, whereas adding Robin terms and allowing some modification of boundary fluxes led to more reliable convergence. In the output of the ablation model, the temperature T, mass flux $\dot{m}$, and species mass fractions $C_{i,w}$ are computed at the wall so as to satisfy these equations and are then used as Dirichlet data in the flow update. This procedure is iterated until convergence of the interface residual is achieved.

In the computations, each cell on a specified ablating surface is treated as an independent ablator, so we solve the above equations on every cell on the ablating surface. Therefore, even if the ablation model is 1-D, we can model variations in ablation rates at different locations at the surface. As with the radiation model, these explicit updates make the implementation into existing codes relatively simple, but at a price of reduced convergence rates, stability, and robustness.

Numerical studies conducted in this investigation show that in order to successfully activate flow coupling to the ablation model, a spinup procedure must be used. In particular, a reasonably converged flow solution with an isothermal or adiabatic wall for the soon-to-be ablating surface must be obtained. Then reasonable starting iterates for the wall temperature and mass flux are used to initialize some blowing in the wall boundary layer. Uniform blowing rate distributions have proven to be sufficient. Finally, the ablation model is enabled following several time steps of convergence from the initial iterate values of temperature and mass flux.

We study a 2-D geometry inspired by work done in [3] and a 3-D symmetric capsule at angle of attack. Our coupled simulation results for the 2-D calculations are given in Fig. 5. Figure 6 illustrates the convergence behavior of the flow and ablation residuals. The former is normalized by the density residual at initial flow startup; the latter is normalized by the initial ablation residual and the current Courant–Friedrichs–Lewy number to ensure comparability with the flow residual. Figure 7 presents results for surface ablation rate and net radiative heat flux for ablation and radiation coupling for the 3-D computations.

V. Effect of Parameter Variation

A key goal of the PECOS work is enabling technology for uncertainty quantification. The simulations that use each of the submodels integrated in this development depend on uncertain physical parameters. The hypersonic flow model is based on uncertainty in chemical reaction rates, coefficients in diffusive flux models, turbulence models, and other constitutive equations. Past investigations of flow uncertainty [15] for Crew Exploration Vehicle low-Earth-orbit reentry peak heating conditions found significant convective heat transfer sensitivity to the N_2-O, N_2-N, and N-O collision integrals; however, the flow quantities of interest were found to be insensitive to vibration–dissociation coupling, vibration–translation relaxation times, and chemical reaction rates. Our initial gas radiation model depends on uncertain mean absorption coefficient curve fits, and the reradiation depends on uncertain emissivity of the hot ablating

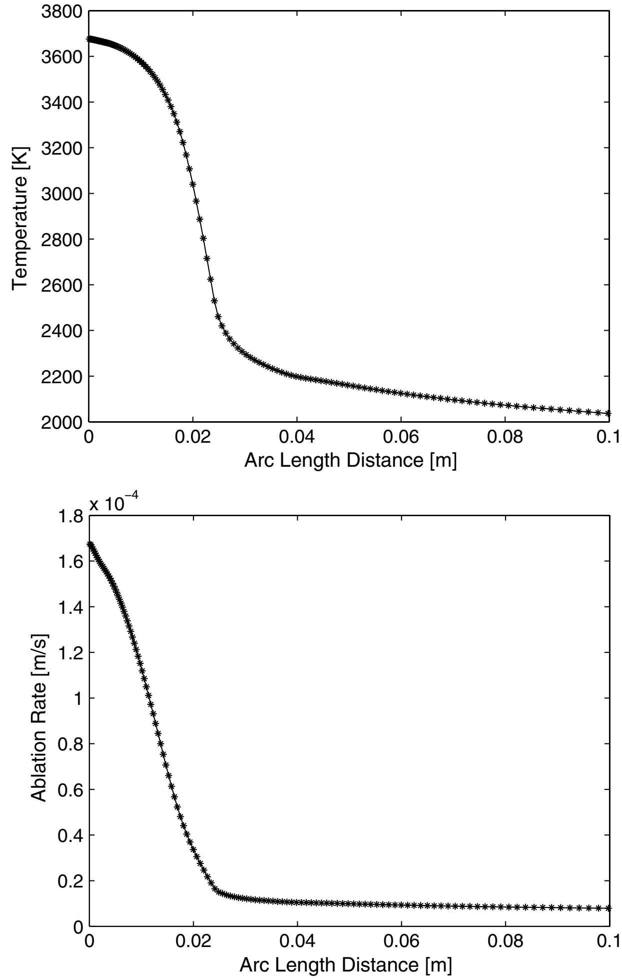

Fig. 5 Surface temperature (top) and surface ablation rate (bottom). Sphere-cone geometry and flow conditions are taken from [3].

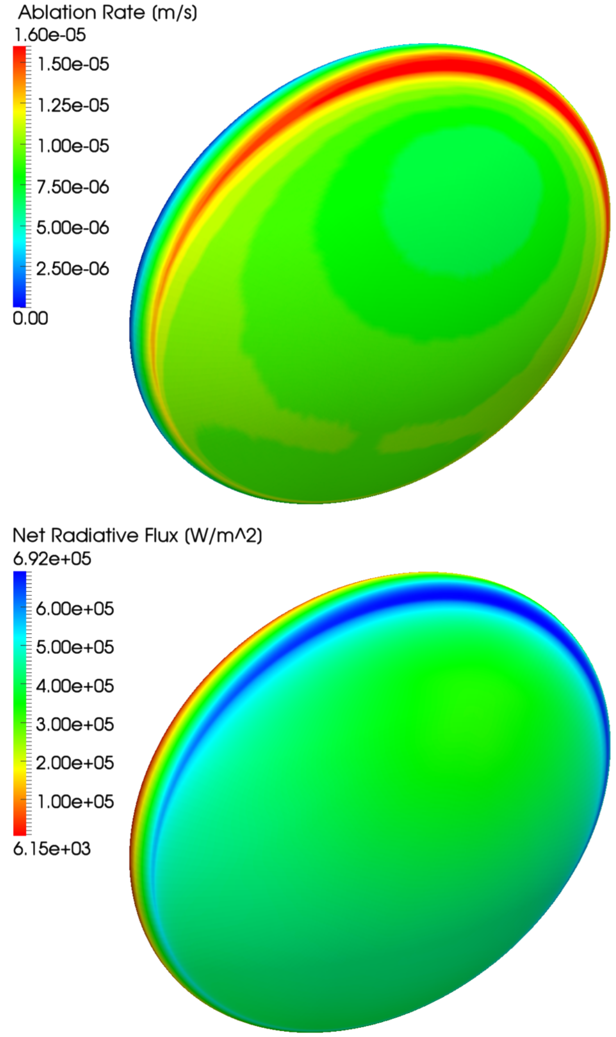

Fig. 7 Three-dimensional symmetric capsule with a 13-species air model at Mach 21 and 23° angle of attack with coupled radiation and ablation; surface ablation rate (top) and net surface radiative flux (bottom).

surface. Our ablation model depends on equilibrium and finite rate chemistry parameters, ablator chemical composition and enthalpy of formation, virgin and char densities, and pyrolysis gas chemistry and enthalpies. Parameter sensitivity studies of other ablators [16] show strong dependence on binary collision integrals for species related to the ablation chemistry, on wall catalycity, and on the conductivities, enthalpies, and densities involved in the pyrolyzing ablation.

The multiway coupling in our model is a necessity for analyzing sensitivities in a quantity of interest such as the ablation rate, which is directly influenced by each of the submodels. Feedback between submodels can greatly amplify or dampen sensitivities observed in

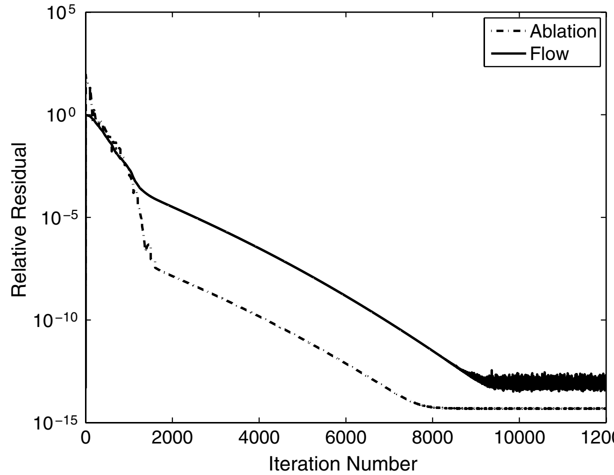

Fig. 6 Two curves illustrate l_2 norm convergence of the density residual in the flow domain and the total residual in the ablation equations over the ablating surface.

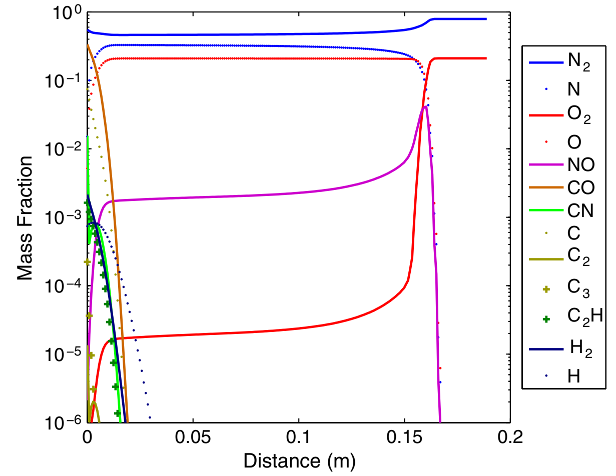

Fig. 8 Thirteen-species air model concentrations approaching the peak ablation point for a 3-D symmetric capsule at Mach 21 and 18° angle of attack.

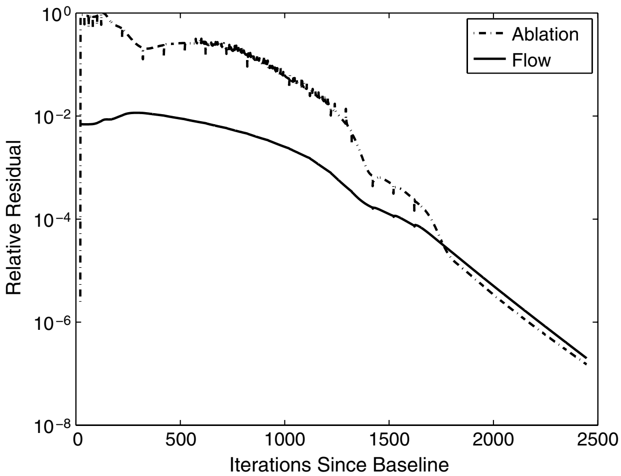

Fig. 9 Two curves illustrate l_2 norm convergence of the density residual in the flow domain and the total residual in the ablation equations over the heat-shield surface.

decoupled problems. Initial decoupled ablation sensitivity studies [14], for example, revealed the three strongest uncertain influences on recession rate to be the term appearing in the exponential function for the equilibrium C3 vapor pressure definition, the surface nitridation coefficient, and the surface emissivity. However, when the flow inputs are not held fixed, but are instead allowed to react in a coupled solve, the effects of the uncertain parameters change. Nitridation chemistry (especially, sublimation chemistry uncertainty) effects are dampened, and the importance of other parameters (such as char and virgin ablator densities) increases.

Additionally, multiway coupling adds new uncertain parameters that are not easily tested in a decoupled or one-way coupled setting. Carbon species chemistry in the ablating boundary layer becomes quite significant, as shown in Fig. 8, which is a plot of a cut line through the shock layer near the leading-edge capsule lip. Thermal diffusivity effects are still critical, and the contributions from N_2-N, N_2-O, and N-O collision integrals are still important, but collision integrals and chemical reaction rates with the various gaseous carbon species take similar significance.

Turning to the convergence behavior, we observe that although obtaining a solution for the baseline capsule simulation requires some care and many iterations, this solution serves as an excellent initial guess for cases at similar parameter values. Figure 9 illustrates convergence of flow and ablation residuals for a representative simulation from ISS reentry baseline initial conditions to a perturbed parameter solution. We see that we can achieve reasonable convergence to the perturbed case in far fewer iterations; the exact number of iterations does, however, depend on the sensitivity of the parameter and how much it is perturbed.

In ongoing work on this iteratively coupled model we undertake simple parameter sensitivity studies by varying model parameters

Table 1 Some classes of parameters that were varied in preliminary sensitivity analysis and the approximate variation of parameters in each class

Parameter/submodel name	Variation
Ablation	
Arrhenius coefficients	±10%
Nitridation coefficient	±50%
Oxidation coefficient	±50%
Char, virgin densities	±10%
Flow	
Arrhenius coefficients	± order of magnitude
Collision integral curve fits	±10%
Turbulence terms	±50%
Radiation	
Gas absorption coefficient	±50%
Reradiation emissivity	±20%

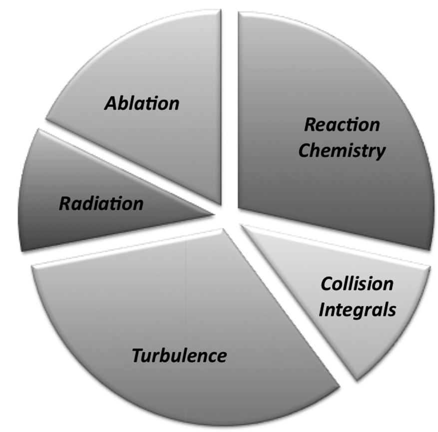

Fig. 10 Relative variation of the peak ablation rate with respect to several parameters.

within a priori uncertain ranges to assess their influence on the peak convective heat flux and peak ablation rate on the capsule surface. Table 1 lists the parameters varied in our initial study. Figure 10 shows the relative sensitivity of the quantity of interest to each of the uncertainties in the various submodels. Each pie chart slice shows the total change in the peak ablation rate from variation of parameters within a single submodel, normalized by the total change over all parameters within every submodel.

Of particular interest for future PECOS efforts is the concept of parameter triage. The high-dimensional space of uncertain variables (e.g., 91 collision pairings for a 13-species air model, with 2–3 collision integral parameters each) limits the utility of many sophisticated uncertainty quantification techniques. Fortunately, our simulations imply that the uncertainty in the ablation quantity of interest is independent of many of these parameters. Over 150 have effects only on the order of numerical error, and 95% of the total output uncertainty is due to less than 30 input parameters. A future paper with detailed sensitivity results is in preparation.

VI. Conclusions

In this work, we have described a multiway coupling strategy using an established hypersonic flow code, a shock-layer radiation model, and a finite rate surface chemistry ablation model. Several two- and three-dimensional examples were shown illustrating the effects of the coupling. With respect to radiation coupling, we were able to achieve reasonably robust convergence with explicit updates for ISS return conditions when using sufficiently small time steps. Our study illustrated that the tangent-slab approximation was adequate for capsule-type geometries at modest angles of attack using ISS return conditions, whereas the validity of the gray-gas approximation is limited, at best. Note that an advantage of the explicit loose-coupling strategy used in the present work is that it allows for the addition of radiation/ablation multiphysics coupling with only relatively minor changes to an existing hypersonic flow code. However, a disadvantage is that the explicit coupling nature does come at the price of reduced convergence rates, stability, and robustness when compared with an implicitly coupled system. As an example, numerical studies conducted in this investigation show that in order to successfully activate flow coupling with the developed ablation model, a spinup procedure was required to initialize the mass blowing from the surface into the boundary layer. Furthermore, due to the complex nonlinear reaction terms in the ablation model, pure Neumann boundary conditions were found to produce unstable results, whereas adding Robin terms and allowing some modification of boundary fluxes led to more reliable convergence. A preliminary sensitivity analysis on the peak ablation rate of a 3-D symmetric capsule was performed by varying several uncertain model parameters in the flow, radiation, and ablation models. Interestingly, although parameter sensitivity analyses for component models are valuable, the results may be quite different when coupled. For example, we observed that when flow inputs are not held fixed, but are instead allowed to react in a coupled solve, the effects of the uncertain parameters change. Nitridation chemistry (especially, sublimation chemistry uncertainty) effects are dampened, and the importance of other parameters (such as char and virgin ablator densities) increases. Although the coupling strategy presented represents a strong step in the direction of multiphysics analysis for this problem, much work remains to be done. In particular, the stability and convergence behavior of the coupling algorithm needs to be improved. Thousands of iterations are required to obtain a reasonably converged solution. Although this may be acceptable for a single analysis requiring only a few simulations, the cost becomes prohibitive when one intends to use such methods for design cycles or quantification of uncertainty. One such improvement may come in the form of tightly coupled algorithms where the radiation and ablation models are solved simultaneously and implicitly with the flow variables. Efforts in this direction are underway under the umbrella of the Fully Implicit Navier–Stokes (FIN-S) [17] solver. Of course, convergence of coupled multiphysics algorithms for a specified model class will vary with the degree of difficulty of the application case and with the models applied, as well as their mode of coupling. The present study provides some insight into the computational complexity and degree of difficulty of some coupling forms, as well as an indication of associated model sensitivity.

We recognize that some models, such as capsule transport, are less detailed than others and reiterate that the model complexity in applications should depend on the quantity of interest. Clearly, coupling to more complex capsule models will be warranted in reentry survival simulations and based on the work presented herein, we anticipate the radiation model to require enrichment, particularly for flows related to lunar reentry.

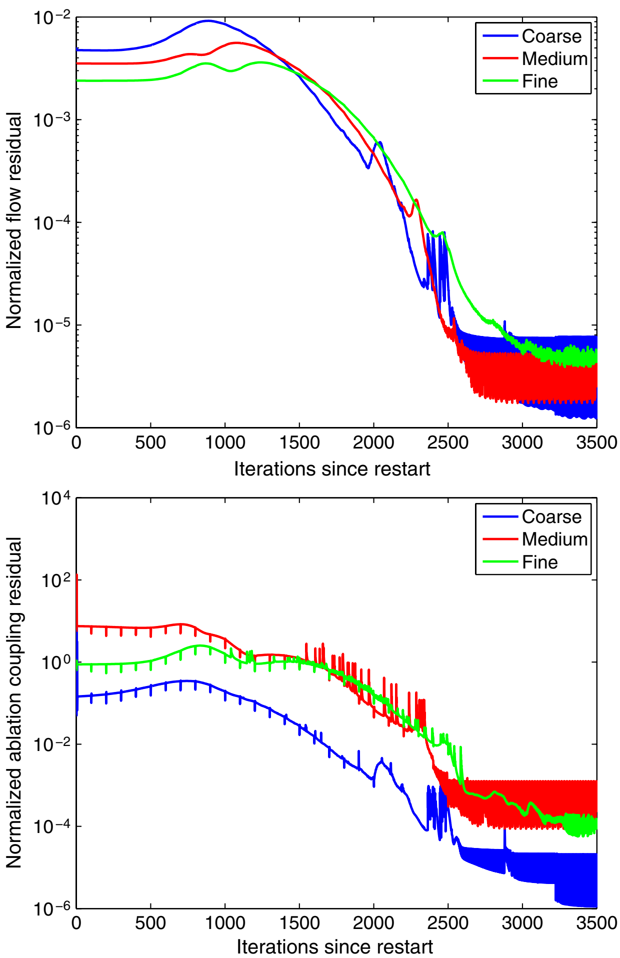

Fig. A1 Flow and ablation residual convergence histories for offbaseline simulations.

Appendix A: Grid Convergence

To the best of our knowledge, there are no known analytical solutions for three-dimensional problems of the problem class discussed in this paper for which we can compute exact error values in quantities of interest, nor are methods such as manufactured solutions feasible within the current software infrastructure used. We are working toward enriching these methods related to work stemming from [17], but the present nonlinear complex models still remain beyond this scope. In keeping with the theme of the paper, we have investigated the convergence behavior for three different mesh resolutions for an offbaseline simulation. In this case, we chose one of the turbulence parameters because it was a strong source of sensitivity to the quantity of interest. To generate the three grids used, we started with the finest grid and uniformly coarsened the grid to produce the coarser grids. This was done because it was observed that the coarse-grid solutions exhibit strong sensitivity to the grid alignment in the quantity of interest. The coarsening strategy used then guarantees a consistent alignment between the three grids, as opposed to three independent aligned grids that may be quite different. The three grids contained approximately 10,000, 100,000 and 1,000,000 elements for the coarse, medium, and fine grids, respectively. Figure A1 shows the flow and ablation residual histories (normalized as before) for the three different grids. We see no strong deviations in the convergence behavior between the three grids for either flow or ablation coupling convergence.

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