Modeling of heat transfer attenuation by ablative gases during the Stardust re-entry

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Flowfield
- Reacting flow, thermal non-equilibrium, radiation, strong shocks, boundary layer, transition, etc.
- CFD, DSMC, simplistic relations (Fay-Riddel, Newton, etc.)

Surface chemistry
- Ablation (diffusion, oxidation, sublimation), catalysis, melting
- Tables, chemistry model in the flow, chemistry model in the material response

Material response
- Heat conduction, internal chemical reactions (pyrolysis), radiative emission, gas flow through porous media, etc.
- Thermal response code, simplistic assumptions (steady state conduction, radiative emission), etc.

TPS modeling
Goal

Using a novel carbon/phenolic in air chemistry model, assess the effects of blowing gases in reducing heat fluxes on a capsule during re-entry.
Chemistry model

The flow field chemistry model accounts for the chemical species formed during ablation of a charring carbon/phenolic ablator in air

• Ablation species are obtained through a loose coupling of CFD and material response codes, and a chemical equilibrium calculation at the wall

• The process was used on the Stardust trajectory and the projected CEV lunar return trajectory

• Using the GRI-MECH chemical database, all reactions that contain those species are selected
Chemistry model

- Air species and reactions are replaced by the 11 species air model from Park
- Using SENKIN (of the CHEMKIN package), a sensitivity analysis is performed on temperature and the rate of production of CN, CO, OH and H$_2$O
- The reduced model has 38 species and 158 reactions

C$_2$H, C$_2$H$_2$, C$_3$, CH$_3$, CH$_4$, CO, CO$_2$, H, H$_2$, H$_2$O, HCN, N, N$_2$, NO, O, O$_2$, OH

N$_2^+$, N$^+$, O$^+$, NO$^+$, O$_2^+$, CO$^+$, C$^+$, H$^+$ e$^-$

CH, CH$_2$, C, C$_2$, NCO, NH, HNO, HCO, H$_2$O$_2$, HO$_2$, CN, CN$^+$
LeMANS

- A multi-dimensional, massively parallel CFD code for the simulation of weakly ionized hypersonic flows in thermo-chemical non-equilibrium
- Uses METIS for domain decomposition and MPI for inter-processor communications
- Solves the Navier-Stokes equations with finite-rate chemistry and internal energy relaxation
- Solves the equations over a mixed unstructured grid
- Uses an Arbitrary Lagrangian-Eulerian approach for mesh deformation
- Calculates the inviscid fluxes using a modified form of the Steger-Warming Flux Vector Splitting scheme
- Computes steady state solutions by integrating over time with a point implicit or line implicit method
- Uses a blowing wall boundary condition (mass balance and momentum conservation) and can be coupled to a material response code for energy balance.
Stardust test-case

- Stardust return capsule (fastest re-entry for a man made object)
- PICA heat shield
- Conditions in the *Echelle* period (where spectroscopic measurements were made)

<table>
<thead>
<tr>
<th>Time [s]</th>
<th>Altitude [km]</th>
<th>$U_\infty$ [km/s]</th>
<th>$T_\infty$ [K]</th>
<th>$\rho_\infty$ [kg/m$^3$]</th>
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<td>224.</td>
<td>$7.72 \times 10^{-4}$</td>
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</table>
Stardust: blowing boundary conditions

- Valid for Stardust calculations, since almost no surface recession was observed
- Heat fluxes are first obtained with a CFD code
- Blowing rate, surface temperature and blowing species mass fractions are obtained using an uncoupled material response (MR) code
- Using the pressure (CFD), temperature (MR) and elemental mass fractions (MR), the blowing species mass fractions at equilibrium are obtained using a chemistry code

<table>
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<tr>
<th>Time [s]</th>
<th>$Y_{N_2}$</th>
<th>$Y_{CO}$</th>
<th>$Y_{H_2}$</th>
<th>$Y_{H_2O}$</th>
<th>$Y_{OH}$</th>
<th>$Y_O$</th>
<th>$Y_{CO_2}$</th>
<th>$Y_{NO}$</th>
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Stardust: surface properties

Surface temperature and blowing rate
Stardust 76 km

Stagnation line temperatures

Individual heat flux components
Species concentrations along the stagnation line for the Stardust re-entry vehicle at an altitude of 76 km.

Figure 5. Species concentrations along the stagnation line for the Stardust re-entry vehicle at an altitude of 76 km.
Species concentrations along the stagnation line at 76 km: blowing species

Stardust: gas composition

Figure 5. Species concentrations along the stagnation line for the Stardust re-entry vehicle at an altitude of 76 km (38 s in t or e - e n t r y )
Species concentrations along the stagnation line at 71 km: important species.
Species concentrations along the stagnation line at 71 km: other species

Figure 5. Species concentrations along the stagnation line for the Stardust re-entry vehicle at an altitude of 76 km (38 m/s at entry).

Species compositions:
- CH$_3$
- CH$_2$
- NCO
- C$_2$
- C$_3$
- HCO
- C$_2$H
- C$_2$H$_2$
- CO$^+$
- H$^+$
Stardust: comments (1)

• Most blowing species are immediately destroyed as soon as they enter the flow (CO and OH tend to stay longer, depending on the re-entry points)

• Two atomic species, H and C, are created in high concentration near the boundary, as is CN

• CN eventually decreases as it enters the high temperature region, and is ionized into CN$^+$

• HNO and NH appear in the shock region; these species were neglected in past models

• Species that are not created in high concentration remain important as they appear at lower altitudes, or on other trajectories
Stardust: heat reduction

Blowing effects on the stagnation line
translational-rotational temperature at 76 km
Stardust: heat reduction

Heat reduction by blowing effects at 76 km

Translational-Rotational heat flux

Vib.-Elec-Elec heat flux

Heat flux [W/cm²]

Axial distance [m]
Stardust: heat reduction

Mass diffusion heat flux

Relative heat fluxes

Heat reduction by blowing effects at 76 km
The shock is significantly moved away from the surface of the vehicle.

This changes the shape of the curves, and therefore affects the gradient at the wall.

However, there is no direct correlation with the change in steepness of the gradient and the heat flux reduction.

The most important effect that contributes to heat flux reduction is the composition of the gas in the boundary layer by way of modifying the gas phase conductivity.
Stardust: heat reduction

Relative contribution of individual components of the heat flux with the blowing effects

(a) Re-entry altitude of 81 km
(b) Re-entry altitude of 78.5 km
(c) Re-entry altitude of 76 km
(d) Re-entry altitude of 73.5 km
(e) Re-entry altitude of 71.2 km
(f) Re-entry altitude of 68.9 km
• The translational-rotational component always contributes the most

• The amount of blowing has a direct and linear influence on the translational-rotational heat flux

• An increase in blowing rates has a major impact on the overall heat flux

• The mass diffusion heat flux increases but does not become the dominant component
Stardust: radiative emission

- Performed using the NASA code NEQAIR
- Non-equilibrium radiative transport (tangent slab method)

Temperatures and radiating species concentrations along the stagnation line at 71 km (42 s)
Stardust: spectra comparison

- CN emission has a close match for 81 km and is over-evaluated by a factor of 2 for 71 km, which is remarkably good.

- CN calculation are run independently of the air calculations, and in the latter case, the N2+ system was omitted because of known issues with the software.
Conclusion

- A comprehensive chemistry model for computing the flow around a re-entry vehicle using an ablative heat shield is used in a CFD code to evaluate the mechanisms of heat reduction.

- As expected, the convective heat flux predicted using the new model was significantly reduced when compared to a fixed temperature boundary condition, whether a non-catalytic or a super-catalytic wall is used.

- At chemical equilibrium injection conditions, most species blown from the surface immediately react in the flowfield and are transformed.

- These results indicate the need to use an appropriate chemistry model in the flow field, and that the chemistry model should be significantly different than that used to model pyrolysis gas behavior inside the TPS.

- Also, it was observed that the blowing rates were directly proportional to the mass diffusion heat flux, which in turn was directly proportional to the reduction of the translational-rotational conduction heat flux.
Conclusion

• The main source of heat flux reduction is by the translational-rotational conduction component, for all trajectory points.

• This clearly indicates that the chemical composition of the boundary layer is of great importance, and that the diffusion coefficients of each species, as well as the mixing rules, must be calculated with great care.

• Flow field results were used to perform a radiative spectral emission analysis for CN, using NEQAIR, which was then compared to the Echelle experimental data with a good agreement.
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Questions?