Predictive Uncertainty Quantification of An Ablating Entry Vehicle Heatshield

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1. Entry Vehicle Physics

2. Mathematical Models and Formulations

3. Model Calibrations

4. Results
Entry Vehicle Physics

Full System, Uncertainties

- High enthalpy aerothermochemistry, hypersonic flow

- Submodel uncertainties (turbulence, nitridation, kinetics)
- Numerical limitations (discretization, UQ error)
- Modeling unknowns (missing/wrong physics?)
Calibrated Uncertainty Quantification
1 Entry Vehicle Physics

2 Mathematical Models and Formulations

3 Model Calibrations

4 Results
Introduction

Physics of Full System Simulation (FSS)

- Compressible Navier-Stokes

Conservation Equations

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \, u) = 0
\]
\[
\frac{\partial \rho u}{\partial t} + \nabla \cdot (\rho uu) = -\nabla P + \nabla \cdot \tau
\]
\[
\frac{\partial \rho E}{\partial t} + \nabla \cdot (\rho Hu) = -\nabla \cdot \dot{q} + \nabla \cdot (\tau u)
\]
Mathematical Models and Formulations

Introduction

Physics of Full System Simulation (FSS)

- Compressible Navier-Stokes, in chemical non-equilibrium

Conservation Equations

\[
\frac{\partial \rho_s}{\partial t} + \nabla \cdot (\rho_s \mathbf{u}) = \nabla \cdot (\rho D_s \nabla c_s) + \dot{\omega}_s
\]

\[
\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla P + \nabla \cdot \mathbf{\tau}
\]

\[
\frac{\partial \rho E}{\partial t} + \nabla \cdot (\rho H \mathbf{u}) = -\nabla \cdot \dot{\mathbf{q}} + \nabla \cdot (\mathbf{\tau} \mathbf{u}) + \nabla \cdot \left( \rho \sum_{s=1}^{n_s} h_s D_s \nabla c_s \right)
\]
Introduction

Physics of Full System Simulation (FSS)

- Compressible Navier-Stokes, in chemical non-equilibrium, in thermal non-equilibrium

Conservation Equations

\[
\frac{\partial \rho_s}{\partial t} + \nabla \cdot (\rho_s \mathbf{u}) = \nabla \cdot (\rho \mathbf{D}_s \nabla c_s) + \dot{\omega}_s
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\]

\[
\frac{\partial \rho e_V}{\partial t} + \nabla \cdot (\rho e_V \mathbf{u}) = -\nabla \cdot \dot{\mathbf{q}}_V + \nabla \cdot \left( \rho \sum_{s=1}^{n_s} e_{V_s} \mathbf{D}_s \nabla c_s \right) + \dot{\omega}_V
\]
Introduction

Physics of Full System Simulation (FSS)

- Compressible Navier-Stokes, in chemical non-equilibrium, in thermal non-equilibrium
- + turbulence/transition, surface ablation + radiation

Conservation Equations

\[
\frac{\partial \rho_s}{\partial t} + \nabla \cdot (\rho_s \mathbf{u}) = \nabla \cdot (\rho \mathbf{D}_s \nabla c_s) + \dot{\omega}_s
\]

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\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla P + \nabla \cdot \mathbf{\tau}
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\]

\[
\frac{\partial \rho e_V}{\partial t} + \nabla \cdot (\rho e_V \mathbf{u}) = -\nabla \cdot \dot{\mathbf{q}}_V + \nabla \cdot \left( \rho \sum_{s=1}^{n_s} e_{V_s} \mathbf{D}_s \nabla c_s \right) + \dot{\omega}_V
\]
Stabilized Navier-Stokes

\[ \frac{\partial U}{\partial t} + A_i \frac{\partial U}{\partial x_i} = \frac{\partial}{\partial x_i} \left( K_{ij} \frac{\partial U}{\partial x_j} \right) + \dot{S} \]

Conservation variables \( U \) are chosen to satisfy

\[ \int_{\Omega} \left[ W \cdot \left( \frac{\partial U}{\partial t} - \dot{S} \right) + \frac{\partial W}{\partial x_i} \cdot \left( K_{ij} \frac{\partial U}{\partial x_j} - A_i U \right) \right] \, d\Omega \]

\[ + \sum_{e=1}^{n_{el}} \int_{\Omega_e} \tau_{\text{SUPG}} \frac{\partial W}{\partial x_k} \cdot A_k \left( \frac{\partial U}{\partial t} + A_i \frac{\partial U}{\partial x_i} - \frac{\partial G_i}{\partial x_i} - \dot{S} \right) \, d\Omega \]

\[ + \sum_{e=1}^{n_{el}} \int_{\Omega_e} \nu_{\text{DCO}} \left( \frac{\partial W}{\partial x_i} \cdot g_{ij} \frac{\partial U}{\partial x_j} \right) \, d\Omega - \oint_{\Gamma} W \cdot (g - f) \, d\Gamma = 0 \]

for all \( W \) in the discretized function space.
Ablation Processes

- Ablation is a multi-scale, multi-physics process
- Inherently transient, moving domain

Mathematical Models and Formulations

\[ q_{\text{rad}} - q_{\text{cond}} + \sum_{i=1}^{N_s} J_i h_i = \dot{m}_{\text{ch}} \rho_{\text{ch}} \]

Substrate
Virgin Material
C\(_{100}\)H\(_{89.4}\)O\(_{17.8}\)N\(_8\)(SiO\(_2\))\(_{64.2}\)

Shock Layer
Boundary Layer

\[ M_a = 31 \]

Pyrolysis Zone
Pyrolysis Gas Flow
Char
Virgin Material
Substrate

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Quasi-steady Ablation

- Simulation ablation timescale $\ll$ trajectory timescale
- 1-D ablation in surface reference frame is steady
Fully Implicit Ablation Coupling

Quasi-Steady Ablation

- Boundary conditions:
  - Nonlinear Robin BC for masses, energies
  - Nonlinear Dirichlet BC for momentum
- Standard FEM weak source term for Robin BC
- Penalty formulation for nonlinear Dirichlet BC

Mathematical Formulations

\[ J_i + \rho v_w C_i = \tilde{N}_i(C_i, T) \]

\[ k \frac{\partial T}{\partial n} - \sum h_i(T) = \frac{\partial}{\partial n} \left( J_i + \rho v_w C_i \right) \]

\[ + \dot{m}_{ch} h_{ch}(T) - \rho v_w h(T) + \alpha \dot{q}_r'' - \sigma \epsilon T^4 \]

\[ + \rho v_w h_{f,v}^o(T_{ref}) = 0 \]

\[ \rho v_w = \sum \tilde{N}_i(C_i, T_w) = \dot{m}_{ch}'' \]
Not all uncertain parameters are equal

- \( \sim 300 \) parameters
- \(< 30\) parameters account for 95\%+ uncertainty
- \(> 150\) parameters negligible to within numerical error
Primary Model Calibrations

Ablator Nitridation Uncertainty
- Probability of C(s) + N(g) → CN(g) at surface
- 4 OOM Prior Uncertainty range in literature
- $\beta_N$ sensitivity enormous in prior, negligible after calibration

Air Reaction Chemistry Uncertainty
- Strong output sensitivities to $N_2 + O$, NO + O reactions
- Calibration via shock tube spectroscopy

Turbulence Model Uncertainty
- Prior “Turbulence augmentation” uncertainty: 0 – 150% range
- Posterior: 8-parameter Spalart-Allmaras with momentum-thickness transition, calibrated against supersonic boundary layer data, DNS
Ablator Nitridation Uncertainty

\[ \dot{m}_{N,c}'' = -\sqrt{\frac{k_b T}{2\pi m_N}} \rho y_N \beta_N(T) \]

Nitridation coefficient \( \beta_N \)
- Probability of surface CN formation upon free nitrogen impact
- Becomes more significant at higher reentry speeds
Ablator Nitridation Uncertainty

Nitridation coefficient $\beta_N$

- “Safe” value from initial expert opinion: 0.3
- Literature disagreement, uncertainty range: $(0.00003, 0.4)$
- Highest predicted submodel uncertainty contribution
Carbon Reaction Chemistry

\[
k = A T^n e^{-\frac{T_r}{T}}
\]

- \(C_2 + M \leftrightarrow 2C + M\)
- \(CN + M \leftrightarrow C + N + M\)
- \(CO + M \leftrightarrow C + O + M\)
- \(CO + C \leftrightarrow C_2 + O\)
- \(CO + O \leftrightarrow O_2 + C\)
- \(CO + N \leftrightarrow CN + O\)
- \(N_2 + C \leftrightarrow CN + N\)
- \(CN + O \leftrightarrow NO + C\)
- \(CN + C \leftrightarrow C_2 + N\)
- \(CO + C_2 \leftrightarrow C_3 + O\)

Uncertain Reaction Rates

- Arrhenius pre-exponential uncertainty: +/- 1 OOM
- Strong ablation sensitivities to \(N_2 + C, CO + N, CO + C_2\)
- Joint calibration
Carbon Reaction Chemistry

Experimental Data

- Spectroscopy as part of Mars test campaign, Electric Arc Shock Tube (EAST) facility, NASA Ames
- 96%CO₂ + 4%N₂ test gas
- 6-7 km/s shock speeds
Turbulence Model Uncertainty

A Priori Uncertainty
- Algebraic (Baldwin-Lomax) model, no transition
- Scalar “Turbulence augmentation” factor $\in (0, 1.5)$
- Second greatest contribution to output uncertainty

Calibrated Uncertainty
- Spalart-Allmaras PDE
- Joint calibration, 8 uncertain parameters
- Multi-model Bayesian validation
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Baseline, Transition

ISS return trajectory, peak heating, Mach 21

- Order of magnitude wall clock speedup over lagged ablation coupling
- Transition downstream of peak heating
- Shock radiation negligible (for this trajectory)
Latin Hypercube and Calibration

LHS
- Quantile bins in each parameter
- 1 sample per bin
- Reduce variance from additive response components
- Calibrated joint PDFs are not separable tensor products!

LHS+MCMC
- LHS for uncalibrated variables
- SRS from each calibrated+filtered joint distribution
Off-Baseline Convergence

Convergence

- Aggressive + paranoid adaptive time stepping
  - Orders of magnitude higher time steps
  - Ought to be replaced with estimator-based adaptivity
- Secondary transient spike well captured
- 8 OOM convergence
  - Transition smoothing needed?
Ablation Rate PDFs

UQ Output

- Dramatic prediction changes
  - Priors: $\approx 2.0 \times 10^{-5} m/s$
  - First calibrations: $\approx 4.4 \times 10^{-6} m/s$
  - Second calibrations: $\approx 7.8 \times 10^{-6} m/s$
- $100\times$ lower nitridation
- Faster C kinetics?
Conclusions

Forward Uncertainty Propagation

- Wide priors require fat, well-resolved tails
  - Adaptive importance sampling?
- Model inadequacy should be propagated too!
  - “Unknown unknowns” can exceed “known unknowns”

Rapid Application Development

- Rapid application development and testing is practical:
  - FIN-S at PSAAP inception: “toy” perfect gas problems
  - FIN-S 4 years later: high-enthalpy reacting multiphysics
  - 5 part-time contributors, 0 full-time FIN-S developers
- Critical factors:
  - Avoid “Not invented here” where practical
  - Modularity first, physics second
  - Multidisciplinary expertise
  - Collaborative, open source development
## Open Source Tools

- **libMesh** - [http://libmesh.github.io/](http://libmesh.github.io/)
  - FEM discretizations, interfaces
- **GRINS** - [https://github.com/GRINSfem/GRINS](https://github.com/GRINSfem/GRINS)
  - Subsonic flow, other subsystem physics
- **ANTIOCH** - [https://github.com/libantioch/antioch](https://github.com/libantioch/antioch)
  - Thermochemistry and transport
- **MASA** - [https://github.com/manufactured-solutions/MASA](https://github.com/manufactured-solutions/MASA)
  - Solution verification via MMS
- **QUESO** - [http://libqueso.com/](http://libqueso.com/)
  - Model calibration, validation
- **DAKOTA** - [https://dakota.sandia.gov](https://dakota.sandia.gov)
  - Forward uncertainty propagation, analysis