Uncertainty Analysis of Carbon Ablation in the VKI Plasmatron

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JOINT EXP/NUM WORK IS MANDATORY

Motivations

- **To understand** the operational behavior of the TPS materials
- **To study** the gas/surface interaction physics occurring during reentry
- **To improve** the prediction capacity and *reduce* the design margins

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**GALILEO MISSION**

Destination: Jupiter  
Date: 1989–2003

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*...THE BEST RACE CAR IS THE ONE THAT FALLS APART RIGHT AFTER THE FINISH LINE...*
LET’S INTRODUCE OUR PLAYERS

Player 1
"the oven"

Player 2
"the recipe"

Test conditions
\[ T_e = 8000 \text{ K} \]
\[ P_e = 1500 \text{ Pa} \]
\[ v_e = 1500 \text{ m/s} \]

Player 3
"the customer"
Let’s Introduce Our Players

Player 1

"the oven"

PLASMATRON

Player 2

"the recipe"

Test conditions
\[ T_e = 8000 \text{ K} \]
\[ P_e = 1500 \text{ Pa} \]
\[ v_e = 1500 \text{ m/s} \]

Rebuilding Code
(boundary layer)

Player 3

"the customer"

Stagnation-line code
(w/ ablative b.c.)
PLAYER #1: PLASMATRON FACILITY

Role: performing reusable/ablative TPS tests

- Gas: Air, N₂, CO₂, Ar
- Power: 1.2 MW – most powerful ICP in the world –
- Heat-flux: up to 16 MW/m² (superorbital re-entry)
- Pressure: 10 – 800 mbar
PLAYER #1: PLASMATRON FACILITY

TPS MATERIAL OPERATIONAL TESTING IS ACHIEVABLE!!
PLAYER #2: BOUNDARY-LAYER CODE*

Role: rebuilding of enthalpy (calorimeter)

Description

- Solves the reacting boundary layer equations along the stagnation line
- Assumes catalytic surface ($N + N \rightarrow N_2$ and $O + O \rightarrow O_2$)
- Rebuilds the boundary layer edge conditions to match the measured wall heat flux:

$$\dot{q}_{cw} = \dot{q}_{cw} \left( T_{cw}, \gamma_{ref}, h_e, p_e, \delta, \frac{\partial u_e}{\partial x}, v_e \frac{\partial}{\partial y} \left( \frac{\partial u_e}{\partial x} \right) \right)$$

Pros & Cons

- Limited computational cost
- Ablative boundary condition not yet implemented

**PLAYER #3: STAGNATION-LINE CODE**

*Role: rebuilding of the ablation test (test sample)*

**Description**

- Solves a reduced form of the Navier–Stokes equations along the stagnation line
- Applicable to both sub- and supersonic flow over spheres and cylinders
- Chemistry solved via the Mutation++ Library. Up-to-date thermodynamic and transport properties dataset

**Pros & Cons**

- Ablative boundary condition implemented
- Medium computational cost

**PLAYER #3: STAGNATION-LINE CODE**

### Surface Mass Balance

\[
\rho D_{im} \left. \frac{\partial y_i}{\partial \eta} \right|_w + \dot{m}_{i,c} = (\rho v)_w y_{iw}
\]

### Surface Energy Balance

\[
k \left. \frac{\partial T}{\partial \eta} \right|_w + \sum_{i=1}^{N_C} h_{iw} \rho D_{im} \left. \frac{\partial y_i}{\partial \eta} \right|_w + \dot{m}_c h_{cw} + \dot{q}_{\text{rad,net}} = (\rho v)_w h_w + \dot{q}_{\text{cond}}^{ss}
\]
The thermochemical ablation model considers the following reactions:

**Oxidation**
- $Cs + O \rightarrow CO$
- $2Cs + O_2 \rightarrow 2CO$

**Nitridation**
- $Cs + N \rightarrow CN$

**Sublimation**
- $3Cs \rightarrow C_3$

Surface source terms are given in the form:

$$\dot{m}_i = \beta_{0i} \left( m_i n_i \sqrt{\frac{kT_w}{2\pi m_i}} \right)$$

Reaction probabilities evaluated experimentally

PUT THE PLAYERS TOGETHER

Experimental conditions
Geometry
Measurements
Rebuilding Code (boundary layer)
Stagnation-line code (w/ ablative b.c.)

PLASMATRON

THE PLAYERS

29%
PUT THE PLAYERS TOGETHER

**Experimental conditions**

**Geometry**

**Measurements**

**Rebuilding Code (boundary layer)**

**ICP code**

**Stagnation-line code (w/ ablative b.c.)**

\[ q_{cw}^{(n)} = q_{cw}^{(exp)} \]

Yes

No

\[ Y_{ref,Cu} \]

\[ T_{cw} \]

\[ m_{e}, T_{e}, y_{i,e} \]
Uncertain inputs generate...uncertain outputs!!!
Objectives

1. **Evaluate** the ablative model uncertainty impact on the final QOIs

2. **Quantify** the influence of the free-stream condition uncertainties on the final QOIs
POLYNOMIAL CHAOS (PC) EXPANSIONS

1. The QOI \( u \) is expanded in a convergent series

\[
u(\xi) \approx u^{PC}(\xi) = \sum_{\alpha=0}^{P} u_{\alpha} \psi_{\alpha}(\xi),
\]

- \( P = (n_\xi + N_0)!/n_\xi!N_0! \), \( N_0 \): expansion degree
- \( \{\psi_{\alpha}\}_{\alpha=0,\ldots,P} \) polynomial functions orthogonal w.r.t \( p_\xi \) (input PDF)
- correspondence between \( p_\xi \) and \( \{\psi_{\alpha}\} \)
- \( \{u_{\alpha}\}_{\alpha=0,\ldots,P} \): deterministic spectral coefficients

2. A non-intrusive spectral method is used to determine \( \{u_{\alpha}\} \)

\[
u_{\alpha} = ||\psi_{\alpha}||^{-2} \int u(\xi)\psi_{\alpha}(\xi) \approx ||\psi_{\alpha}||^{-2} \sum_{i=1}^{n} u(x, t, \xi_i)\psi_{\alpha}(\xi_i)\omega_i
\]

- \( (\xi_i, \omega_i) \) quadrature formulae points and weights → deterministic code used as a black box

* Wiener 38; Cameron & Martin 47; Ghanem & Spanos 91
SENSITIVITY ANALYSIS

From PC expansions of QOIs

1. MEANS AND VARIANCES ARE OBTAINED

\[ E(u_{PC}) = u_0, \quad \text{Var}(u_{PC}) = \sum_{\alpha=1}^{P} u_\alpha^2(x) \langle \psi_i^2 \rangle \]

2. SENSITIVITY ANALYSIS BY ANOVA DECOMPOSITION

- **Sobol first order indices** \( \{S_i\}_{i=1,\ldots,n_\xi} \)
  
  Quantifies the contribution to the QOI variance of the \( i^{th} \) random parameter

- **Sobol total order indices** \( \{S_T,i\}_{i=1,\ldots,n_\xi} \)
  
  Quantifies the contribution to the QOI variance of the \( i^{th} \) random parameter including interactions with other parameter \( j \in \{1, \ldots, n_\xi\}, j \neq i \)

* Crestaux, Le Maitre & Martinez 09

ASCIENTIST ANALYSIS

Alessandro Turchi
STEP 1: BOUNDARY-LAYER CODE

VARIABLE
- Dynamic Pressure
- Static Pressure
- Cold Wall Heat Flux
- Cold Wall Temperature
- Catalycity
- Nitrogen/Oxygen ratio

STEP 2: STAGNATION-LINE CODE

VARIABLE | DISTRIBUTION | RANGE
--- | --- | ---
$C_S + O \rightarrow CO$ | ? | ?
$2C_S + O_2 \rightarrow 2CO$ | ? | ?
$C_S + N \rightarrow CN$ | ? | ?
$3C_S \rightarrow C_3$ | ? | ?
$N + N \rightarrow N_2$ | ? | ?
TPS wall emissivity | ? | ?
REACTION PROBABILITY UNCERTAINTIES ASSESSMENT

Atomic oxygen

\[ \text{Cs} + \text{O} \rightarrow \text{CO} \]

Molecular oxygen

\[ 2\text{Cs} + \text{O}_2 \rightarrow 2\text{CO} \]

S-L CODE INPUT CHARACTERIZATION
**Reaction Probability Uncertainties Assessment**

Atomic oxygen

\[ C_s + O \rightarrow CO \]

Molecular oxygen

\[ 2C_s + O_2 \rightarrow 2CO \]
DEFINE THE INPUT UNCERTAINTIES

STEP 1: BOUNDARY-LAYER CODE

VARIABLE
Dynamic Pressure
Static Pressure
Cold Wall Heat Flux
Cold Wall Temperature
Catalycity
Nitrogen/Oxygen ratio

STEP 2: STAGNATION-LINE CODE

VARIABLE
\( C_S + O \rightarrow CO \)
\( 2C_S + O_2 \rightarrow 2CO \)
\( C_S + N \rightarrow CN \)
\( 3C_S \rightarrow C_3 \)
\( N + N \rightarrow N_2 \)
TPS wall emissivity

DISTRIBUTION
Uniform
LogUniform
Uniform
LogUniform
Uniform
Uniform

RANGE
0.37–1
0.00001–0.1
0–0.3
0.01–1
0–0.5
0.8–0.95
STAGNATION-LINE CODE NOMINAL OUTPUTS

ABLATION QOI

<table>
<thead>
<tr>
<th>VARIABLE</th>
<th>MEAN</th>
</tr>
</thead>
<tbody>
<tr>
<td>w/ nitridation mass blowing rate</td>
<td>0.041 [kg / m^2 s]</td>
</tr>
<tr>
<td>w/ nitridation temperature</td>
<td>2534 [K]</td>
</tr>
<tr>
<td>w/o nitridation mass blowing rate</td>
<td>0.021 [kg / m^2 s]</td>
</tr>
<tr>
<td>w/o nitridation temperature</td>
<td>2840 [K]</td>
</tr>
</tbody>
</table>
STAGNATION-LINE CODE W/ NITRIDATION

### ABLATION QOI

<table>
<thead>
<tr>
<th>VARIABLE</th>
<th>MEAN</th>
<th>VARIANCE</th>
<th>$\Delta_{stoch - nom}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>mass blowing rate</td>
<td>0.031 [kg/m$^2$s]</td>
<td>2.69e-05</td>
<td>-24.4%</td>
</tr>
<tr>
<td>temperature</td>
<td>2722 [K]</td>
<td>1.54e+04</td>
<td>+7.4%</td>
</tr>
</tbody>
</table>

### Wall mass blowing rate

- Error: ±16.72%

### Wall temperature

- Error: ±4.56%

NITRIDATION AND RECOMBINATION ARE STRONGLY RELATED!
### Stagnation-Line Code W/O Nitridation

#### Ablation QoI

<table>
<thead>
<tr>
<th>VARIABLE</th>
<th>MEAN</th>
<th>VARIANCE</th>
<th>$\Delta_{\text{stoch} - \text{nom}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>mass blowing rate</td>
<td>0.021 [kg/m²s]</td>
<td>2.63e-10</td>
<td>-0.6%</td>
</tr>
<tr>
<td>temperature</td>
<td>2903 [K]</td>
<td>2.74e+03</td>
<td>2.2%</td>
</tr>
</tbody>
</table>

#### Wall Mass Blowing Rate

- **Oxidation**: Error ±1.15%
- **O₂ Oxidation**: Error ±1.15%
- **Sublimation**: Error ±1.15%
- **Recombination**: Error ±1.15%
- **Wall Emissivity**: Error ±1.15%

#### Wall Temperature

- **Oxidation**: Error ±1.80%
- **O₂ Oxidation**: Error ±1.80%
- **Sublimation**: Error ±1.80%
- **Recombination**: Error ±1.80%
- **Wall Emissivity**: Error ±1.80%

**Oxygen Diffusion Limits the Ablation Rate!**
DEFINE THE INPUT UNCERTAINTIES

**STEP 1: BOUNDARY-LAYER CODE**

<table>
<thead>
<tr>
<th>VARIABLE</th>
<th>DISTRIBUTION</th>
<th>MEAN</th>
<th>ERROR (±)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dynamic Pressure</td>
<td>Normal</td>
<td>48 Pa</td>
<td>8.0%</td>
</tr>
<tr>
<td>Static Pressure</td>
<td>Normal</td>
<td>20000 Pa</td>
<td>0.3%</td>
</tr>
<tr>
<td>Cold Wall Heat Flux</td>
<td>Normal</td>
<td>2962 kW/m²</td>
<td>10.0%</td>
</tr>
<tr>
<td>Cold Wall Temperature</td>
<td>Normal</td>
<td>350 K</td>
<td>10.0%</td>
</tr>
<tr>
<td>Catalycity</td>
<td>Uniform</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Nitrogen/Oxygen ratio</td>
<td>Uniform</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Range</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.001–1</td>
<td>(79/21) ± 2%</td>
</tr>
</tbody>
</table>

**STEP 2: STAGNATION-LINE CODE**

<table>
<thead>
<tr>
<th>VARIABLE</th>
<th>DISTRIBUTION</th>
<th>RANGE</th>
</tr>
</thead>
<tbody>
<tr>
<td>CS + O → CO</td>
<td>Uniform</td>
<td>0.37–1</td>
</tr>
<tr>
<td>2CS + O₂ → 2CO</td>
<td>LogUniform</td>
<td>0.00001–0.1</td>
</tr>
<tr>
<td>CS + N → CN</td>
<td>Uniform</td>
<td>0–0.3</td>
</tr>
<tr>
<td>3CS → C₃</td>
<td>LogUniform</td>
<td>0.01–1</td>
</tr>
<tr>
<td>N + N → N₂</td>
<td>Uniform</td>
<td>0–0.5</td>
</tr>
<tr>
<td>TPS wall emissivity</td>
<td>Uniform</td>
<td>0.8–0.95</td>
</tr>
</tbody>
</table>
**Boundary-Layer Code Analysis**

**Edge mass flow rate**
- Error: ±8.00%

**Edge temperature**
- Error: ±9.41%

**Edge velocity gradient**
- Error: ±7.64%

**Experimental Uncertainties Are Affecting the QoI the Most!**

Alessandro Turchi

B-L Code Results

79%
OXYGEN PRACTICALLY UNAFFECTED BY THE UNCERTAINTIES!
COUPLED ANALYSIS: INPUT UNCERTAINTY DISTRIBUTIONS

Mean=2.540e−01 σ =2.467e−02
10 bins
Scott's bin width
Kernel density

0.16 0.18 0.2 0.22 0.24 0.26 0.28 0.3 0.32
Samples

Mean=7.494e+03 σ =8.522e+02
10 bins
Scott's bin width
Kernel density

6000 7000 8000 9000 10000 11000
Samples

COUPLED RESULTS
COUPLED ANALYSIS W/ NITRIDATION

<table>
<thead>
<tr>
<th>VARIABLE</th>
<th>MEAN</th>
<th>VARIANCE</th>
<th>$\Delta_{stoch-nom}$</th>
<th>$\varepsilon_{old}(\pm)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>mass blowing rate</td>
<td>0.029 [kg/m$^2$s]</td>
<td>3.48e-5</td>
<td>-28.4%</td>
<td>16.72%</td>
</tr>
<tr>
<td>temperature</td>
<td>2661 [K]</td>
<td>2.17e+4</td>
<td>+5.0%</td>
<td>4.56%</td>
</tr>
</tbody>
</table>

Wall mass blowing rate
error: ±20.17%

Wall temperature
error: ±5.53%

CONSIDERING ALL THE UNCERTAINTIES SLIGHTLY AFFECT THE ERROR!
COUPLED ANALYSIS W/O NITRIDATION

<table>
<thead>
<tr>
<th>VARIABLE</th>
<th>MEAN</th>
<th>VARIANCE</th>
<th>$\Delta_{stoch - nom}$</th>
<th>$\varepsilon_{old}(\pm)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>mass blowing rate</td>
<td>0.020 [kg /m$^2$/s]</td>
<td>1.94e-6</td>
<td>-2.9%</td>
<td>1.15%</td>
</tr>
<tr>
<td>temperature</td>
<td>2818 [K]</td>
<td>1.39e+4</td>
<td>+0.8%</td>
<td>1.80%</td>
</tr>
</tbody>
</table>

**Wall mass blowing rate**

**Wall temperature**

REBUILDING UNCERTAINTIES AFFECT THE MASS BLOWING RATE!
CONCLUDING REMARKS

CONCLUSIONS

• DECOUPLED ANALYSIS
  • STRONG IMPACT ON THE QOIs OF A QUESTIONABLE PHENOMENON SUCH AS THE SURFACE NITRIDATION WHEN CONSIDERED
  • SMALL VARIATIONS OF THE QOIs UNCERTAINTIES WHEN NITRIDATION IS NEGLECTED: CONSEQUENCE OF THE ANALYZED ABLATION REGIME

• COUPLED ANALYSIS
  • THE INFLUENCE OF THE NITRIDATION UNCERTAINTIES REMAINS THE BIGGER
  • MEASUREMENT AND MODEL UNCERTAINTIES FROM THE REBUILDING PROCEDURE CAUSE THE ERROR TO GROW WHEN NITRIDATION IS NEGLECTED

PERSPECTIVES

• ASSESS MORE PLAUSIBLE RANGES FOR THE MOST INFLUENTIAL PARAMETERS
• ANALYZE DIFFERENT ABLATION REGIMES
• COMPARE THE OBTAINED RESULTS WITH THE EXPERIMENTAL MEASUREMENTS
Uncertainty Analysis of Carbon Ablation in the VKI Plasmatron