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

...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:
  \[
  \dot{q}_{cw} = \dot{q}_{cw} \left( T_{cw}, \gamma_{ref}, h_e, \frac{\partial u_e}{\partial x}, \frac{\partial}{\partial y} \left( \frac{\partial u_e}{\partial x} \right) \right)
  \]

**Pros & Cons**
- Limited computational cost
- Ablative boundary condition not yet implemented

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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

**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**

\[ k \left. \frac{\partial T}{\partial \eta} \right|_w + \sum_{i=1}^{N_c} h_{iw} \rho D_{im} \left. \frac{\partial y_i}{\partial \eta} \right|_w + \dot{m}_c h_{cw} + \dot{q}_{radnet} = (\rho v)_w h_w + \dot{q}_{cond}^{ss} \]
**Player #3: Stagnation-Line Code**

The thermochemical ablation model considers the following reactions:

**Oxidation**
- \( C_s + O \rightarrow CO \)
- \( 2C_s + O_2 \rightarrow 2CO \)

**Nitridation**
- \( C_s + N \rightarrow CN \)

**Sublimation**
- \( 3C_s \rightarrow C_3 \)

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

PLASMATRON

Experimental conditions

Geometry

Measurements

Rebuilding Code (boundary layer)

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

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THE PLAYERS

29%
PUT THE PLAYERS TOGETHER

- Experimental conditions
- Geometry
- Measurements

ICP code

Rebuilding Code (boundary layer)

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

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

Yes

\( m_e, T_e, y_{i,e} \)

No

\( Y_{ref,Cu} \)

\( T_{cw} \)

\( P_{sta} \)

\( R_{sample} \)

\( P_{dyn} \)

\( q_{cw} \)

\( y_{k,e} \)
STEP 1: BOUNDARY-LAYER CODE

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

STEP 2: STAGNATION-LINE CODE

- \( \text{CS} + \text{O} \rightarrow \text{CO} \)
- \( 2\text{CS} + \text{O}_2 \rightarrow 2\text{CO} \)
- \( \text{CS} + \text{N} \rightarrow \text{CN} \)
- \( 3\text{CS} \rightarrow \text{C}_3 \)
- \( \text{N} + \text{N} \rightarrow \text{N}_2 \)
- TPS wall emissivity
UNCERTAINTIES WON’T MAGICALLY DISAPPEAR

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
- $\{\psi_{\alpha}\}_{\alpha=0,...,P}$ polynomial functions orthogonal w.r.t $p_\xi$ (input PDF)
- correspondence between $p_\xi$ and $\{\psi_{\alpha}\}$
- $\{u_{\alpha}\}_{\alpha=0,...,P}$: 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 $\rightarrow$ 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
**LET’S START…FROM THE END**

**STEP 1: BOUNDARY-LAYER CODE**
- Dynamic Pressure
- Static Pressure
- Cold Wall Heat Flux
- Cold Wall Temperature
- Catalycity
- Nitrogen/Oxygen ratio

**STEP 2: STAGNATION-LINE CODE**

<table>
<thead>
<tr>
<th>VARIABLE</th>
<th>DISTRIBUTION</th>
<th>RANGE</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_S + O \rightarrow CO$</td>
<td>?</td>
<td>?</td>
</tr>
<tr>
<td>$2C_S + O_2 \rightarrow 2CO$</td>
<td>?</td>
<td>?</td>
</tr>
<tr>
<td>$C_S + N \rightarrow CN$</td>
<td>?</td>
<td>?</td>
</tr>
<tr>
<td>$3C_S \rightarrow C_3$</td>
<td>?</td>
<td>?</td>
</tr>
<tr>
<td>$N + N \rightarrow N_2$</td>
<td>?</td>
<td>?</td>
</tr>
<tr>
<td>TPS wall emissivity</td>
<td>?</td>
<td>?</td>
</tr>
</tbody>
</table>
**REACTION PROBABILITY UNCERTAINTIES ASSESSMENT**

**Atomic oxygen**

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

**Molecular oxygen**

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

$2C_s + O_2 \rightarrow 2CO$
**DEFINE THE INPUT UNCERTAINTIES**

**STEP 1: BOUNDARY-LAYER CODE**
- Dynamic Pressure
- Static Pressure
- Cold Wall Heat Flux
- Cold Wall Temperature
- Catalycity
- Nitrogen/Oxygen ratio

**STEP 2: STAGNATION-LINE CODE**

<table>
<thead>
<tr>
<th>VARIABLE</th>
<th>DISTRIBUTION</th>
<th>RANGE</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_S + O \rightarrow CO$</td>
<td>Uniform</td>
<td>0.37–1</td>
</tr>
<tr>
<td>$2C_S + O_2 \rightarrow 2CO$</td>
<td>LogUniform</td>
<td>0.00001–0.1</td>
</tr>
<tr>
<td>$C_S + N \rightarrow CN$</td>
<td>Uniform</td>
<td>0–0.3</td>
</tr>
<tr>
<td>$3C_S \rightarrow C_3$</td>
<td>LogUniform</td>
<td>0.01–1</td>
</tr>
<tr>
<td>$N + N \rightarrow N_2$</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>
STAGNATION-LINE CODE NOMINAL OUTPUTS

ABLATION QOI

<table>
<thead>
<tr>
<th>VARIABLE</th>
<th>MEAN</th>
</tr>
</thead>
<tbody>
<tr>
<td>w/ nitridation</td>
<td></td>
</tr>
<tr>
<td>mass blowing rate</td>
<td>0.041[kg / m²s]</td>
</tr>
<tr>
<td>temperature</td>
<td>2534 [K]</td>
</tr>
<tr>
<td>w/o nitridation</td>
<td></td>
</tr>
<tr>
<td>mass blowing rate</td>
<td>0.021[kg / m²s]</td>
</tr>
<tr>
<td>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>

**OXYGEN DIFFUSION LIMITS THE ABLATION RATE!**
**Define the Input Uncertainties**

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**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>
</tbody>
</table>

**STEP 2: STAGNATION-LINE CODE**

<table>
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<tr>
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<td>TPS wall emissivity</td>
<td>Uniform</td>
<td>0.8–0.95</td>
</tr>
</tbody>
</table>

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BOUNDARY-LAYER CODE ANALYSIS

EXPERIMENTAL UNCERTAINTIES ARE AFFECTING THE QOI THE MOST!
## Boundary-Layer Code Analysis

### Mean Edge Mass Fractions

<table>
<thead>
<tr>
<th>Species</th>
<th>Mass Fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>O₂</td>
<td>1.24e-05</td>
</tr>
<tr>
<td>N₂</td>
<td>1.79e-01</td>
</tr>
<tr>
<td>NO</td>
<td>1.29e-03</td>
</tr>
<tr>
<td>O⁺</td>
<td>2.42e-04</td>
</tr>
<tr>
<td>N⁺</td>
<td>6.95e-04</td>
</tr>
<tr>
<td>O</td>
<td>2.32e-01</td>
</tr>
<tr>
<td>N</td>
<td>5.87e-01</td>
</tr>
<tr>
<td>e⁻</td>
<td>3.55e-08</td>
</tr>
</tbody>
</table>

**Oxygen practically unaffected by the uncertainties!**
COUPLED ANALYSIS: INPUT UNCERTAINTY DISTRIBUTIONS

COUPLED RESULTS

83%

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83%

Alessandro Turchi
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/m²s]</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>

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

<table>
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<tr>
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<th>$\Delta_{stoch - nom}$</th>
<th>$\varepsilon_{old}(\pm)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>mass blowing rate</td>
<td>0.020 [kg $/m^2s$]</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**

- error: ±6.79%

**Wall temperature**

- error: ±4.18%

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**
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