

# Determination of Uncertainties for Analytically Derived Material Properties to be used in Monte Carlo Based Orion Heatshield Sizing

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**Ablative materials are often used for spacecraft heatshields to protect underlying structures from the extreme environments associated with atmospheric reentry. NASA's Orion EM-1 capsule has been designed to use a molded Avcoat material system. In order to determine the required heatshield thickness, a Monte Carlo approach to the sizing process was proposed. To perform the Monte Carlo simulation, statistical uncertainties on all material property input parameters were required. Obtaining these values for measured properties is straightforward, however input parameters that are derived analytically have historically used uncertainties based on engineering judgment. A MATLAB program was created to use laboratory generated thermogravimetric analysis (TGA) data to calculate uncertainties on the Arrhenius parameters for molded Avcoat. Uncertainties associated with the normalized ablation rate and pyrolysis gas enthalpy were also generated using a wrapper script and the ACE code. These uncertainties could then be tied directly to measured values of individual elemental constituents. The resulting uncertainty values will allow for a probabilistic sizing approach on molded Avcoat with a higher level of confidence in the input parameters.**

## Nomenclature

$B'_c$  = no dimensional char mass loss rate

$\rho$  = density

$\varphi$  = decomposition reaction order

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$k$	= decomposition pre-exponential coefficient
$\tilde{K}$	= elemental mass fraction
$r$	= residual char mass fraction
$\sigma$	= standard deviation
$u$	= uncertainty
$\mu$	= mean

## I. Introduction

Ablative thermal protection materials are often used for spacecraft heatshields to protect underlying structures from the extreme environments associated with atmospheric reentry. NASA's Orion capsule for Exploration Mission 1 (EM-1) has been designed to use a molded block version of the Avcoat ablative material. Based on extensive material property testing, a high fidelity thermal response model for molded Avcoat was developed for use in the CHarring Ablator Response (CHAR) code<sup>1</sup>. To determine the required heatshield thickness, the Orion program currently uses a four-branch, root-sum-squared (RSS) method to account individually for the effects of uncertainty on trajectory dispersions, aerothermal heating and material properties along with a nominal case. Those sizing results, combined in an RSS process, and further adjusted by either a recession margin or thermal factor of safety determine the final sized heatshield thickness for a given bodypoint. This process for Orion TPS<sup>2</sup> sizing was also used for the sizing of the Mars Science Laboratory TPS<sup>3</sup>.

The current method used to account for the material property uncertainties in the appropriate RSS sizing branch is to reduce the allowable bondline temperature limit by 60°C. This value has been used consistently since the early phases of the Orion program and is based on resulting two sigma values from earlier planetary mission studies using a number of different materials. Understandably, there is a desire to determine whether this value is appropriate for the case of molded Avcoat on Orion.

Additionally, in place of this existing sizing approach, it has been proposed that a probabilistic design approach be taken for future heatshield sizing that makes use of a Monte Carlo simulation<sup>4</sup>. This simulation would use the material property and modelling uncertainties, randomize these variables according to an appropriate probability distribution, size the TPS, and report the thermal sizing for each iteration. The output of a Monte Carlo based heatshield sizing would be a distribution of sizes that could be approximated as normal. As a final sizing of a heatshield, a  $3\sigma$  value from the simulation could be used as a replacement for a factor-of-safety based sizing. This methodology is explained in detail in multiple studies<sup>5, 6</sup>.

As part of the proposed Monte Carlo simulation, statistical uncertainties on all material property inputs to the CHAR model were required for the molded Avcoat material. The overall uncertainty in the TPS sizing and reliability results from the combined effect of all the uncertainties in the model input parameters. Therefore, without accurately determining these material property uncertainties that are inputs to the process, there cannot be a great deal of confidence in the resulting system reliability values. Fortunately, many of the required uncertainty values for this effort are obtained directly via statistical analysis of material property measurements. Multiple laboratory measured values for density or specific heat for example can be used to calculate a mean and standard deviation. The uncertainties associated with analytically derived input parameters, however, cannot be determined via traditional methods. These model inputs include the pyrolysis gas enthalpy, the non-dimensional mass loss rate ( $B'_c$ ), and parameters associated with the material decomposition.

Similar Monte Carlo based sensitivity studies have been performed in the past on numerous types of TPS materials<sup>6,7,8</sup> to investigate ablator model performance with respect to input parameters and to assess the reliability of the ablative thermal protection system design. None of these studies, however, attempt to calculate the uncertainties on analytically derived material property inputs and instead rely on estimates based on engineering judgment or on holdover values from earlier studies. This paper will present a method for calculating the uncertainties of analytically derived ablative material properties.

## II. Method

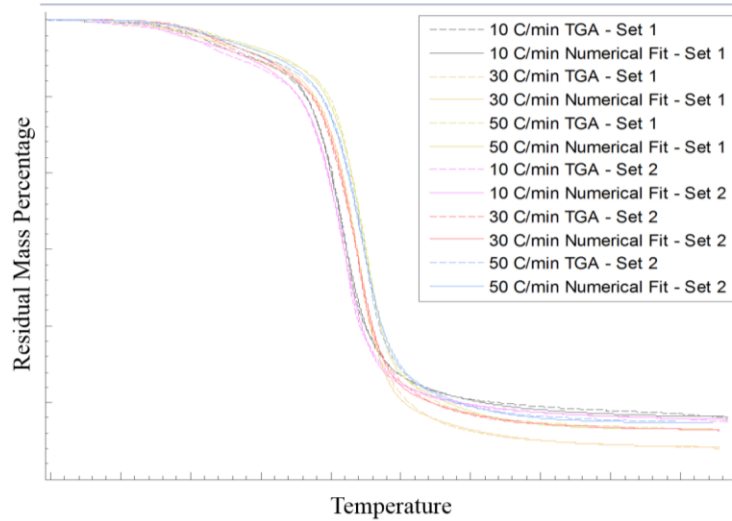
### A. Decomposition Parameters

Ablator decomposition, the transition from the virgin to char state and production of pyrolysis gas, is modelled in CHAR using the Arrhenius reaction equation. The complete molded Avcoat decomposition was modelled using three Arrhenius equations of the form show in equation 1.

$$\frac{\partial \rho_i}{\partial t} = -k_i \rho_{v,i} \left( \frac{\rho_i(t) - \rho_{c,i}}{\rho_{v,i}} \right)^{\varphi_i} e^{-\frac{T_{a,i}}{T(t)}} \quad (1)$$

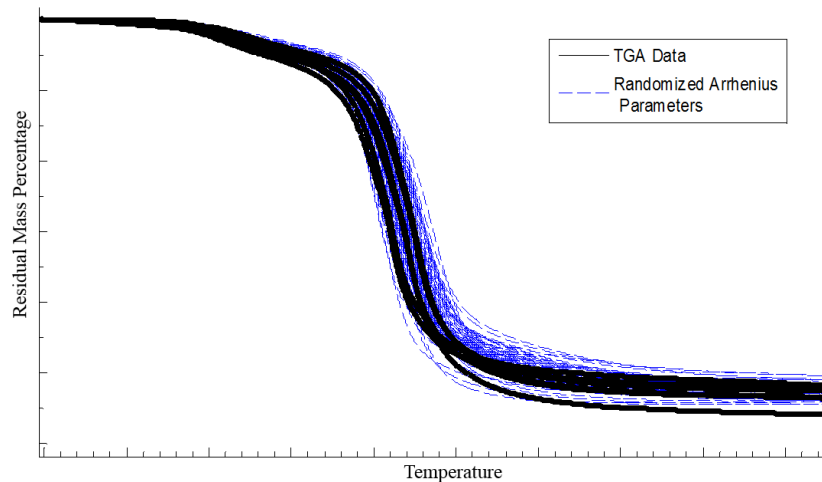
The virgin material density  $\rho_v$  and the char density  $\rho_c$  are determined from initial volume and mass measurements and from thermogravimetric analysis (TGA) residual char yield. The remaining parameters must be determined from TGA data: the pre-exponential factor  $k$ , the reaction order  $\varphi_i$ , and the activation temperature  $T_a$ .

Common Arrhenius curve fitting techniques were not able to be directly applied to the TGA data available. Avcoat cannot be accurately modelled as a single Arrhenius reaction and constant-temperature reaction data was not available. For these reasons, a general curve-fitting approach was used to fit Arrhenius equations to TGA data. A MATLAB program was written to optimize Arrhenius parameters from the TGA data. For each of the six laboratory measurements available, an initial guess for the parameters was provided, and the Arrhenius equation was solved using MATLAB's differential equation solver. The goodness-of-fit was evaluated by residual sum-of-squares calculation between the computed result and the test data. The parameters were randomized and iterated using a multivariable derivative-free optimization algorithm to minimize the residual sum-of-squares. MATLAB optimized the nine independent Arrhenius parameters to produce the fitted curves shown in Figure 1.



**Figure 1. Curve fits to TGA data.**

The mean, standard deviation, and uncertainty were calculated for each of the nine parameters using the six sets of TGA data. As a check on the calculated mean values and uncertainties for each equation, the Arrhenius parameters and char density were randomized according to a normal distribution as they would be in the full Monte Carlo simulation. The resulting randomized curves were then shown to bound the available TGA data as seen in Figure 2 for all but one outlier.



**Figure 2. Randomized Parameter Curves.**

## B. Pyrolysis Gas Enthalpy

The enthalpy of the pyrolysis gas was calculated using the Aerotherm Chemical Equilibrium code (ACE)<sup>9</sup>, as a function of temperature and pressure. The strategy to generate uncertainties was to run selected

conditions rather than the full enthalpy table for a large number of pyrolysis gas elemental fraction possibilities. The elemental composition of the pyrolysis gas is derived as follows:

$$\tilde{K}_{pgi} = \frac{\tilde{K}_{vi} - r\tilde{K}_{ci}}{1-r} \quad (2)$$

Where  $\tilde{K}_{pgi}$ ,  $\tilde{K}_{vi}$ , and  $\tilde{K}_{ci}$  are the elemental mass fractions in the pyrolysis gas, virgin material and char material, respectively. The residual mass fraction is represented by  $r$ . So the average elemental composition of the pyrolysis gas is derived from the compositions of the virgin and char materials and knowledge of the ratio of char to virgin density.

Elemental analysis was performed on four virgin molded Avcoat material samples, four char samples and the residual char yields from six TGA runs were used to calculate the uncertainties going into the analysis. The pyrolysis gas composition calculated for each run and an ACE wrapper script varied the elemental constituents and residual mass fraction on a random normal distribution.

The wrapper script performing the Monte Carlo ACE analysis was run at varying temperatures and pressures across the nominal pyrolysis gas enthalpy table to determine the pyrolysis gas uncertainties. The resulting distributions for a number of pressure, temperature combinations are shown in Figure 3.

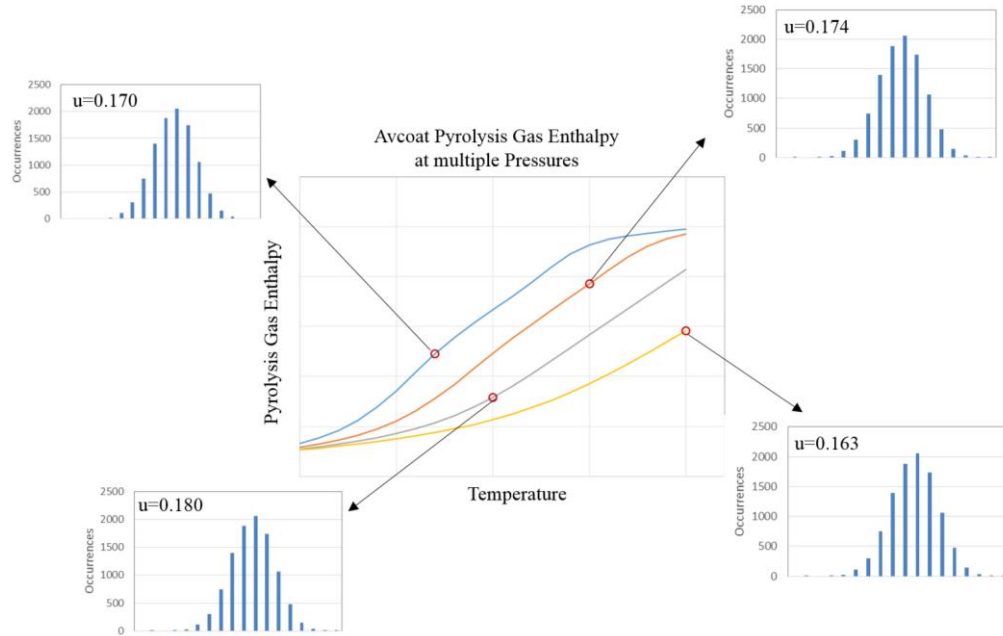
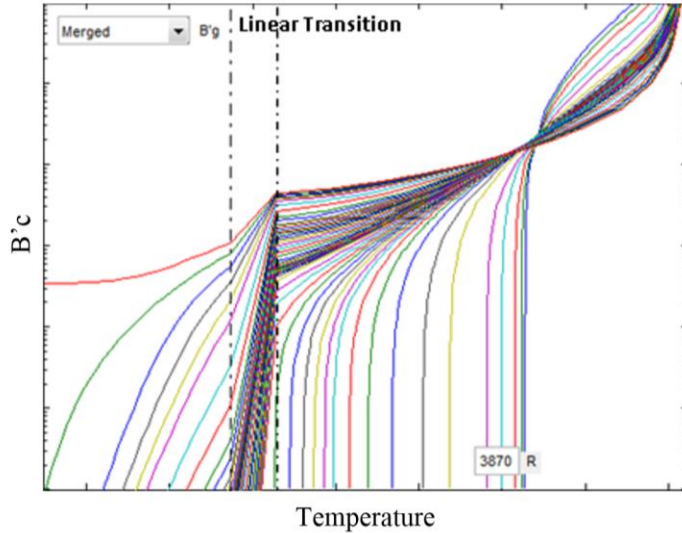


Figure 3. Pyrolysis Gas Enthalpy Uncertainties

### C. Normalized Ablation Rate, $B'_c$

The  $B'$  tables are likely the most influential of inputs to an ablation model in terms of recession. Much like the pyrolysis gas enthalpy, these tables are typically generated with the use of a thermochemical equilibrium code. Fixed mass molecular compositions are evaluated from relative elemental quantities, species thermochemical data and two-state properties (temperature and pressure). The environment gas

composition, pyrolysis gas composition, and char composition are required inputs. In addition, the allowed resultant chemical species are required in the form of JANAF thermochemical tables. A representative set of  $B'_c$  curves for a single pressure is shown in Figure 3.



**Figure 3. Normalized Ablation Rate Curves for molded Avcoat at a Single Pressure**

For this analysis multiple laboratory measurements were made for both virgin and char elemental composition which allowed the calculation of mean mass percentages of carbon, silicon, hydrogen, etc. Variability in the elemental composition of Avcoat char and char yield percentage was determined and a series of Monte Carlo runs were made using an ACE wrapper script at a number of different flight-relevant B' table combinations of pressure, temperature and pyrolysis blowing rates. The distribution of the resulting  $B'_c$  values from these runs were assumed to be normal and uncertainty values were calculated.

### III. Results

For the purposes of ease-of-comparison between parameters, the standard deviation was normalized to an uncertainty calculated as twice the coefficient of variance.

$$u = 2 \cdot \frac{\sigma}{\mu} \quad (3)$$

The resulting uncertainties from this study are given in Table 1. Values assumed in earlier studies<sup>3,6,7,8</sup> are also given for comparison. The Arrhenius parameter uncertainties calculated from the test data and computed best-fit curves are reported in Table 2. Notably, the best-fit reaction orders varied greatly and produced a high uncertainty, while the best-fit activation temperatures were grouped closely together.

	<b>Current Study</b>	<sup>7</sup> Chen et al. 2006	<sup>6</sup> Wright et al. 2007	<sup>8</sup> Sepka et al. 2009	<sup>3</sup> Wright et al. 2014
Ablative Material	<b>Molded Avcoat</b>	PICA, SLA-561v	SLA-561v	PICA	SLA-561v
Decomposition	<b>Table 2</b>	0.20	0.20	0.15	0.16
Char Recession Rate, $B'_c$	<b>.15</b>	1.0	n/a	0.15	n/a
Pyrolysis gas Enthalpy	<b>.18</b>	0.75	0.50	0.15	n/a

**Table 1. Resulting uncertainty values compared with past studies.**

Equation 1	Pre-exponential factor	0.109
	Reaction Order	0.263
	Activation Temperature	0.060
Equation 2	Pre-exponential factor	0.179
	Reaction Order	0.388
	Activation Temperature	0.061
Equation 3	Pre-exponential factor	0.188
	Reaction Order	0.263
	Activation Temperature	0.033

**Table 2. Decomposition Parameter Uncertainties**

#### IV. Conclusion

In previous Monte Carlo based sensitivity studies, there was no uncertainty applied to the individual decomposition parameters. Uncertainties on pyrolysis gas enthalpy and normalized ablation rate tables were estimated based on engineering judgment or in some cases not used at all. A MATLAB program was developed to allow for faster, more accurate and automated computation of Arrhenius reaction parameters. This MATLAB program, along with TGA data, was used to generate uncertainties on the Arrhenius parameters for molded Avcoat. Uncertainties associated with the normalized ablation rate and pyrolysis gas enthalpy were also generated with the use of the ACE code wrapper script, using the uncertainties in individual elemental constituents based on a number of laboratory measurements. The resulting calculated uncertainty values allow for new TPS sensitivity studies and sizing efforts on molded Avcoat using values having a higher level of confidence and a better tie to measured data.

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