

Efficient Parametric Uncertainty Analysis of an Earth Entry Vehicle Concept using Least Angle Regression

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The objective of this work was to outline and apply an efficient and accurate parametric uncertainty propagation approach to the analysis of convective heating on an Earth entry vehicle concept. The described approach was based on Least Angle Regression used to solve a sparse and underdetermined linear system in the point-collocation non-intrusive polynomial chaos surrogate method. This approach involved an iterative process to computing the non-zero terms of the underlying polynomial chaos model using only enough samples to converge uncertainty interval predictions and Sobol index values based global nonlinear sensitivity estimates. The Earth entry vehicle was analyzed at three points along a representative trajectory for a Mars return mission. 329 sources of uncertainty were identified in the computational fluid dynamics model used to predict the forebody convective heating. These included uncertainty in flow field chemical rates, collision integrals, heats of formation, surface finite rate char model reaction rates, wall roughness height, and the turbulent Schmidt number. Results from this study showed that convective heating uncertainty as high as $\pm 50\%$ of the nominal was predicted with only about 50 evaluations of the computational model. This was far fewer than would be required for a sampling-based approach or a full basis polynomial chaos model, which would have required over 50,000 samples. Additionally, results showed that over 90% of the total convective heating uncertainty was due to uncertainty in the N_2 catalytic rate on the surface, while the remainder of the uncertainty was attributed to the turbulent Schmidt number and the wall roughness uncertainties.

Nomenclature

$\mathcal{A}$	Active Set	S	Sobol Index
$\mathcal{A}^c$	Active Set Complement	Sc_T	Turbulent Schmidt Number
C	Absolute Maximum Correlation	$\mathbf{u}$	Equiangular Vector
c	Correlation	x	Deterministic Variables
D	Total Variance	$\mathbf{y}$	Training Data Vector
N_t	Number of Terms	α	Polynomial Chaos Expansion Coefficient
n	Number of Random Dimensions	γ	Update Magnitude
p	Polynomial Order	ϵ	Truncation Error
R	Stochastic Response	Ψ	Random Basis Function
r	Least Angle Regression Predicted Response	ξ	Standard Input Random Variable

I. Introduction

As NASA begins the development of a Mars sample return mission, uncertainty quantification (UQ) will serve as a key capability for estimating risk and identifying key sources of uncertainty that drive margins. While an Earth entry vehicle (EEV) system as a whole is subject to significant uncertainty, the thermal protection system (TPS) is one subsystem that is plagued by numerous sources of uncertainty due to the complex physics associated with both the aerothermodynamics modeling and the material response. A reliable TPS design is absolutely critical to ensuring not only the survival of the collected samples but also to avoid potentially contaminating the Earth due to the uncontrolled release of the samples by a compromised entry vehicle.

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Previous work by Johnston et al. [1] investigated the impact of uncertainty on stagnation point convective and radiative heating predictions during hyperbolic Earth entry, similar to that of a Mars sample return mission. Their UQ approach was to assume the impact of uncertainty sources were independent from one another and that heating was monotonic with the uncertainty. This approach significantly reduced the number of simulations needed to obtain an overall heating uncertainty prediction but required assumptions with unknown impact. Additionally, Johnston and Kleb [2] performed a detailed uncertainty analysis of forebody radiative heating during lunar-return Earth entry using fuzzy set logic. This approach used a Cauchy deviates method, which required approximately 10,000 evaluations of the computational model.

Following these previous works on UQ of planetary entry vehicle heating, West et al. [3] leveraged a technique based on compressed sensing [4] and polynomial chaos. This optimization-based approach was shown to drastically reduce the computational cost of propagating numerous sources of uncertainty through an expensive computational model. West et al. [5] applied the compressed sensing-based polynomial chaos approach to the analysis of radiative heating uncertainty on the Stardust sample return capsule backshell. While these past works both investigated the impact of uncertainty on heating predictions and reduced the computational cost of doing so, there is a need for less computationally complex techniques and additional computational savings.

The overall objective of this work is to outline a methodology for propagating numerous sources of uncertainty through a computationally expensive model. A technique termed least angle regression (LAR) [6] is used in conjunction with point-collocation based non-intrusive polynomial chaos (NIPC) [7] to construct a sparse polynomial chaos representation of the uncertainty. Previous work by Blatman and Sudret [8] explored using LAR in conjunction with NIPC. They showed that the technique was viable for the problems considered, demonstrating accurate statistical moment predictions when compared to Monte Carlo sampling. The LAR-NIPC iterative approach enables potentially significant computational savings over both traditional sampling-based approaches and full basis regression models. In addition to outlining this approach and proposed convergence techniques, this paper provides comparisons between other uncertainty propagation methods, such as compressed sensing, to highlight LAR-NIPC accuracy and computational savings.

The LAR-NIPC approach is applied to a computational fluid dynamics (CFD) model of convective heating on the surface of an EEV returning from Mars. Hundreds of parametric uncertainty sources are considered in this study. In the flow field, these include uncertainties in the chemical rate model for each reaction and species heats of formation. Uncertainty in binary collision integrals used to approximate transport properties, the turbulent Schmidt number, and wall roughness height are also considered, as well as uncertainties associated with the finite rate char process used to model the TPS surface chemistry. Key uncertainty sources are identified that may serve as indicators for prioritizing future investments to reduce overall parametric uncertainty.

In the next section, the UQ approach used in this study is described in detail. Section III then outlines the CFD model used to simulate the EEV during entry into Earth's atmosphere. Section IV presents the results of this study including a description of the baseline forebody heating predictions, followed by details of the uncertainty analysis study. The last section highlights key findings from this work.

II. Uncertainty Quantification Approach

In this section the uncertainty quantification approach is described in detail. First, an overview of polynomial chaos is given, followed by an description of the least angle regression technique. Lastly, a discussion of convergence measures is given along with details of performing variance deposition algebraically with a polynomial chaos expansion.

A. Generalized Polynomial Chaos

Polynomial chaos is a surrogate modeling technique based on a spectral representation of the uncertainty. An important aspect of spectral representations is the decomposition of a response value or random function, R , into a linear combination of separable deterministic and stochastic components, as shown in Eq. (1) for a polynomial of order p and dimension n .

$$R(\mathbf{x}, \boldsymbol{\xi}) \approx \sum_{i=0}^{N_i-1} \alpha_i(\mathbf{x}) \Psi_i(\boldsymbol{\xi}) + \epsilon \quad (1)$$

Here, α_i is the deterministic component, and Ψ_i is the random variable basis functions corresponding to the i^{th} mode. The basis functions, Ψ_i , of each random variable are determined using the Askey key [9] and are dependent on the distribution of each random variable. The response, R , is a function of independent, deterministic variables, $\mathbf{x}$, and n

independent, standard random variables, ξ . Note that this series is, by definition, an infinite series; however, in practice, it is truncated, and a sum is taken over a discrete number of output modes, leaving a finite truncation error, ϵ . To form a complete basis or a total order expansion, N_t terms are required, which can be computed from Eq. (2) for a polynomial chaos expansion (PCE) of order p and a number of random dimensions or variables, n .

$$N_t = \frac{(n+p)!}{n!p!} \quad (2)$$

Special consideration is needed when epistemic variables are present, which is the case in the present study. For epistemic variables with a bounded domain (i.e., intervals), the Legendre polynomials can serve as an appropriate basis, as they too have a bounded domain. Then, the second-order probability approach described by Eldred and Swiler [10] can be applied to propagate mixed uncertainty through the PCE and obtain intervals at select probability levels of interest. Further details on polynomial chaos theory is given by Ghanem and Spanos [11]. A description of more recent developments, including the analysis of mixed uncertainty with stochastic expansions is given by Eldred [12].

B. Point-Collocation, Non-Intrusive Polynomial Chaos

The objective with any PCE method is to determine the expansion coefficients, α_i . To do this, polynomial chaos methods can be implemented using an intrusive or a non-intrusive approach. While an intrusive method may appear straightforward in theory, for complex problems this process may be computationally expensive and difficult to implement as changing the deterministic model is required [13]. In contrast, the non-intrusive approach can be easily implemented to construct a surrogate model that represents a complex computational simulation because no modification to the deterministic model is required. The non-intrusive methods require only the response (or sensitivity [14–16]) values at selected sample points to approximate the stochastic response surface.

Several methods have been developed for NIPC. Of these, the point-collocation NIPC method has been used extensively in many aerospace simulation and CFD problems [7, 14, 17, 18] for improved computational efficiency and tractability for high-dimension problems over other spectral-projection-based approaches. The point-collocation method starts with replacing a stochastic response or random function with its PCE by using Eq. (1). N_s sample vectors are chosen in random space, and the deterministic code is evaluated at these points, which is the left hand side of Eq. (1). Following this, a linear system of N_s equations can be formulated and solved for the expansion coefficients of the PCE. This system is shown in Eq. (3).

$$\begin{pmatrix} R(\mathbf{x}, \xi_1) \\ R(\mathbf{x}, \xi_2) \\ \vdots \\ R(\mathbf{x}, \xi_{N_s}) \end{pmatrix} = \begin{pmatrix} \Psi_0(\xi_1) & \Psi_1(\xi_1) & \cdots & \Psi_{N_t-1}(\xi_1) \\ \Psi_0(\xi_2) & \Psi_1(\xi_2) & \cdots & \Psi_{N_t-1}(\xi_2) \\ \vdots & \vdots & \ddots & \vdots \\ \Psi_0(\xi_{N_s}) & \Psi_1(\xi_{N_s}) & \cdots & \Psi_{N_t-1}(\xi_{N_s}) \end{pmatrix} \begin{pmatrix} \alpha_0 \\ \alpha_1 \\ \vdots \\ \alpha_{N_t-1} \end{pmatrix} \quad (3)$$

Note that for this linear system, N_t is equal to the minimum number of deterministic samples, N_s , required to obtain an exact solution. If more linearly independent samples are available, the system is considered overdetermined and can be solved using a least squares approach. On the contrary, if the number of samples is less than the number of terms in the PCE, N_t , then the linear system in Eq. (3) has infinitely many solutions. West et al. [3] proposed using compressed sensing [4] to seek out a solution with a minimum number of nonzero PCE coefficients. This approach, while highly effective and efficient, requires the solution of an L_1 -minimization problem. A desired approach may be to obtain the same level of (or better) efficiency without relying on solving an optimization problem, which may induce error in the solution and subsequent uncertainty estimation.

C. Sparse Approximation via Least Angle Regression

One approach to obtaining a unique solution to an underdetermined linear system of equations is to use a technique called LAR. LAR was proposed by Efron et al. [6] as a means of efficiently obtaining the solution of a linear system with the minimum number of nonzero terms, similar to compressed sensing [3, 4]. However, the LAR approach does not require the solution of an optimization problem, which may reduce complexity and minimize potential error.

LAR is an iterative or stagewise procedure that incrementally adds terms to a polynomial model of the response. Here, that model is the polynomial chaos expansion. The number of terms added is based on the number of samples, N_s , available for the regression. LAR begins by setting a prediction vector, $\mathbf{r}$, to zero. The correlations, c_i , between the

polynomial terms and the current residual between the training data, $\mathbf{y}$, and the current LAR predicted responses is given by (4).

$$\mathbf{c} = \Psi'(\mathbf{y} - \mathbf{r}) \quad (4)$$

At each step in the iterative procedure, the set of active terms (or covariates), $\mathcal{A}$, contains the indices of PCE terms included in the current model (i.e., the columns of Ψ). At each iteration, the term with the absolute maximum correlation, defined by Eq. (5), to the training data is added to the active set.

$$C = \max_i \{|c_i|\} \quad (5)$$

After updating the active set with a new term, the next step is to update the prediction vector, $\mathbf{r}$. To do this, LAR uses an equiangular step direction. The equiangular vector is defined by Eq. (6).

$$\mathbf{u}_{\mathcal{A}} = \Psi_{\mathcal{A}} \left(\mathbf{1}_{\mathcal{A}}' (\Psi_{\mathcal{A}}' \Psi_{\mathcal{A}})^{-1} \mathbf{1}_{\mathcal{A}} \right)^{-1/2} (\Psi_{\mathcal{A}}' \Psi_{\mathcal{A}})^{-1} \mathbf{1}_{\mathcal{A}} \quad (6)$$

Here, the vector of ones, $\mathbf{1}_{\mathcal{A}}$, has length equal to that of the active set (i.e., the number of terms in the current prediction). The prediction vector update is then given by Eq. (7).

$$\mathbf{r}_{\mathcal{A}_+} = \mathbf{r}_{\mathcal{A}} + \gamma \mathbf{u}_{\mathcal{A}} \quad (7)$$

The prediction update magnitude, γ , is defined by Eq. (8).

$$\gamma = \min_{i \in \mathcal{A}^c} + \left\{ \frac{C - c_i}{A_{\mathcal{A}} - a_i}, \frac{C + c_i}{A_{\mathcal{A}} + a_i} \right\} \quad (8)$$

Here, $A_{\mathcal{A}}$ and a_i are given by Eq. (9) and Eq. (10), respectively. Also, the $+$ indicates only positive components for each i , and $\mathcal{A}^c$ is the complement set to $\mathcal{A}$.

$$A_{\mathcal{A}} = \left(\mathbf{1}_{\mathcal{A}}' (\Psi_{\mathcal{A}}' \Psi_{\mathcal{A}})^{-1} \mathbf{1}_{\mathcal{A}} \right)^{-1/2} \quad (9)$$

$$\mathbf{a} = \Psi' \mathbf{u}_{\mathcal{A}} \quad (10)$$

Starting with the active set $\mathcal{A}$ empty, the stagewise process outlined in Eqs. (6) through (10) is repeated, adding one term to the active set at each iteration. This is done until convergence of the predicted responses is observed, or all of the available training data are included in the active set. Note that the active set length is limited by the number of available training data. As the active set length approaches that of a full polynomial model, the LAR procedure tends to a least squares result, and no additional error is incurred by including more data. The final LAR predicted response, $\mathbf{r}$, can then be used to estimate the PCE coefficients, $\boldsymbol{\alpha}$, by solving the linear system in Eq. (3) with only the terms in the active set.

For computationally expensive problems, monitoring convergence of the PCE model as the LAR approach progresses is the key to reducing computational cost. Stopping the procedure when an acceptable level of error is achieved may limit the number of times a computational model needs to be executed. With the LAR approach, even one training point will return a result. However, enough data should be included to reach a desired level of polynomial chaos model convergence. Note that adaptive sampling approaches are the subject of future work. In this study, a large sample set of points are chosen from a Latin hypercube design, and points are randomly added to the set of training data.

D. Least Angle Regression Convergence

While monitoring the coefficients individually would be ideal, this may be unrealistic for large problems with hundreds or thousands of terms. Test points and cross validation approaches may be feasible but are often subject to significant error, particularly for small sample sizes. In this work, the approach was to track convergence of the total Sobol index [19] values for each uncertain variable. Because these values are based on the polynomial model terms directly, they are ideal for monitoring convergence, as well as determining a relative ranking of each uncertainty source in terms of their contribution to the total uncertainty. Sobol indices can be derived via *Sobol Decomposition*, which is a variance-based global sensitivity analysis method. First, the total variance, D , can be written in terms of the PCE, as shown in Eq. (11).

$$D = \sum_{j=1}^P \alpha_j^2(t, \vec{x}) \left\langle \Psi_j^2(\vec{\xi}) \right\rangle \quad (11)$$

Then, as shown by Sudret [19], the total variance can be decomposed as:

$$D = \sum_{i=1}^{i=n} D_i + \sum_{1 \leq i < j \leq n}^{i=n-1} D_{i,j} + \sum_{1 \leq i < j < k \leq n}^{i=n-2} D_{i,j,k} + \cdots + D_{1,2,\dots,n} \quad (12)$$

where the partial variances ($D_{i_1,\dots,i_s}$) are given by:

$$D_{i_1,\dots,i_s} = \sum_{\beta \in \{i_1,\dots,i_s\}} \alpha_\beta^2 \left\langle \Psi_\beta^2(\vec{\xi}) \right\rangle, \quad 1 \leq i_1 < \dots < i_s \leq n \quad (13)$$

Then the Sobol indices ($S_{i_1,\dots,i_s}$) are defined as,

$$S_{i_1,\dots,i_s} = \frac{D_{i_1,\dots,i_s}}{D} \quad (14)$$

which satisfy the following equation:

$$\sum_{i=1}^{i=n} S_i + \sum_{1 \leq i < j \leq n}^{i=n-1} S_{i,j} + \sum_{1 \leq i < j < k \leq n}^{i=n-2} S_{i,j,k} + \cdots + S_{1,2,\dots,n} = 1.0 \quad (15)$$

The Sobol indices provide a sensitivity measure due to individual contribution from each input uncertain variable, S_i , as well as the mixed contributions ($\{S_{i,j}\}, \{S_{i,j,k}\}, \dots$). As shown by Sudret [19], the total (combined) effect, S_{T_i} , of an input parameter i is defined as the summation of the partial Sobol indices that include the particular parameter:

$$S_{T_i} = \sum_{L_i} \frac{D_{i_1,\dots,i_s}}{D}; \quad L_i = \{(i_1, \dots, i_s) : \exists k, 1 \leq k \leq s, i_k = i\} \quad (16)$$

For example, with $n = 3$, the total contribution to the overall variance from the first uncertain variable ($i = 1$) can be written as:

$$S_{T_1} = S_1 + S_{1,2} + S_{1,3} + S_{1,2,3} \quad (17)$$

The accuracy of the Sobol indices depends highly on the PCE coefficients, making them an ideal measure of PCE convergence. Also, because the number of total Sobol indices is the same as the number of uncertain parameters, n , there are less parameters to track, as $n < N_t$ for a total order expansion. Tracking Sobol indices also enables a global ranking of each uncertain variable in terms of relative contribution to the total predicted uncertainty. This may be particularly useful for dimension reduction strategies [3, 14] and to help guide investments into effectively reducing uncertainty with future efforts.

An additional approach to tracking convergence of the LAR-NIPC approach is to track statistics of interest to a given analysis. This may include statistical moments or a desired uncertainty interval. Tracking convergence based on the first moment alone should be cautiously considered as the mean is known to converge rapidly, while other moments, such as the variance, often require much more information. Convergence of the variance, defined back in Eq. (11), is part of the Sobol indices approach described above. Convergence of an uncertainty interval may be useful as it is generally a desired output from an uncertainty analysis. However, uncertainty measures are determined after propagating uncertainty sources through the NIPC model, which makes them subject to sampling error. Enough samples are needed to minimize this error.

III. Computational Modeling Approach and Sources of Uncertainty

This section describes the CFD model used to predict the convective heating on the forebody of an EEV concept of interest. The first section details the geometry and computational domain used in this study. The next section describes the CFD model, followed by a detailed description of the uncertainty sources considered in this study.

A. Geometry and Computational Domain

The aeroshell geometry was a 45 deg. sphere-cone with a 0.3 meter nose radius and a base diameter of 1.3 meters. Images of the geometry used in this study are given in Fig. 1. The computational domain was axisymmetric about the centerline with 106 nodes in the streamwise direction, up to the shoulder, and 141 nodes normal to the wall. The grid for the final solution is shock-aligned with 80% of the grid normal to the wall lying inside the shock layer. Wall normal grid spacing was achieved via grid adaption with a target cell Reynolds number of 1.0.

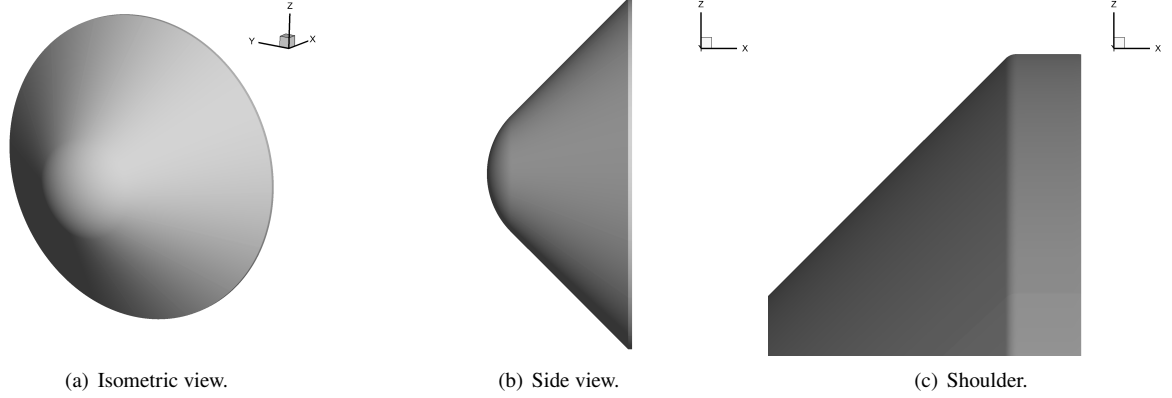


Fig. 1 Earth entry vehicle conceptual geometry.

B. Computational Fluid Dynamics Model

The flow field was modeled using the Langley Aerothermodynamic Upwind Relaxation Algorithm (LAURA) software, which is a finite-volume, Navier-Stokes flow solver [20]. LAURA uses a second-order, upwind, discretization scheme with Roe's flux-difference splitting and Yee's Symmetric Total Variation Diminishing (STVD) formulation of the inviscid flux. The flow field was assumed to be steady state, and the boundary layer was modeled as fully-turbulent employing the Baldwin-Lomax algebraic turbulence model [21]. Additionally, a roughness augmentation model described by Krogstad [22] was used to model a mean wall roughness height of 0.7 millimeters. A coupled ablation wall boundary condition is modeled on the vehicle forebody surface.

The gas properties were modeled with a thermochemical nonequilibrium assumption using the two temperature model [23, 24]. Freestream mass fractions were assumed to be 76% N_2 and 24% O_2 by mass. The coupled ablation flowfield was modeled using the following 30 species: N_2 , O_2 , N , N^+ , NO , NO^+ , N_2^+ , O_2^+ , O , O^+ , e^- , C , C^+ , CO , CO^+ , CO_2 , C_2 , C_3 , C_2H , CN , CN^+ , H , H^+ , H_2 , C_2H_2 , HCN , CH , CH_4 , CH_3 , and CH_2 . The rate model used in this study is presented in Tables 4, 5, and 6 in the appendix. Note that the parameters in these tables are those of an Arrhenius form. The forward reaction rate for each mechanism was computed with Eq. (18), where U_i is the rate uncertainty factor.

$$k_{f,i} = U_i A_{f,i} T_{f,i}^{n_{f,i}} \exp(-D_{f,i}/T_{f,i}) \quad (18)$$

In the ablation model, the surface char rate was determined assuming the finite rate chemistry model described by Johnston [25]. The pyrolysis rate and wall temperatures are fixed at values based on a material response at the nominal conditions of each trajectory point studied. Additional details of the material model are left out of this paper due to the sensitive nature of the information. Quantifying the impact of uncertainty in the material response model that would ultimately affect the pyrolysis rate wall temperature is the subject of future work. However, the UQ process described in the previous section would accommodate this additional level of modeling fidelity without alteration.

Shock-layer radiation was modeled using the High-Temperature Aerothermodynamic Radiation (HARA) code [26, 27]. HARA uses atomic levels and lines obtained from the National Institute of Standards and Technology (NIST) database [28], Opacity Project databases [29], and atomic bound-free (photoionization) cross-sections from TOPbase [30]. Molecular radiation mechanisms modeled include CO , CN , H_2 , N_2 , N_2^+ , and NO . Capturing uncertainty in the radiative heating predictions is the subject of future work. Spectral line and continuum radiation from excited N and O are also modeled. Collisional Radiative (CR) or non-Boltzmann modeling was used for all atomic and molecular electronic states. The non-Boltzmann approach used in this study is described by Johnston et al. [31]. Coupled radiation

was modeled in the flowfield energy equations. A ray-tracing approach [32] was applied for computing the radiative heating at the wall, while the tangent-slab approach was used to compute the divergence of the radiative flux.

C. Parametric Sources of Uncertainty

Numerous parametric uncertainty sources were considered in this study. In the flow field, uncertainties in the chemical rate model for each reaction (see Tables 4, 5, and 6 for uncertainty ranges and references) were considered. Transport properties (diffusion, thermal conductivity, and viscosity) were approximated using binary collision integrals given by Gupta et al. [33]. Available higher order curve fits provided by Wright et al. [34, 35], who also estimated collision pair specific uncertainties, were used when possible. Uncertainty for all collision pairs not identified by Wright et al. was assumed to be $\pm 30\%$. In total, 210 collision pair uncertainties were considered.

The heats of formation of many ablation products have uncertainty that may impact surface chemistry. Specifically, heat of formation uncertainty in C_2 , C_3 , and C_2H have been previously investigated in detail as these are common products produced from sublimation of primarily carbon ablators [36–38]. These uncertainties are listed in Table 1. This uncertainty may impact the species compositions within the ablation layer, which in turn impacts the heat flux on the surface, as shown by Moss and Simmonds [39]. The uncertainties used for these three species were given by Gurvich et al. [36]. These are also in agreement with uncertainties identified more recently by Sharma et al. [38]. Johnston et al. [1] used these same uncertainties for a Mars return Earth entry scenario but did not find significant impact due to relatively low ablation rates. Heats of formation for the other species modeled in the flowfield were assumed to be $\pm 3\%$.

Table 1 Heat of formation uncertainty for C_2 , C_3 , and C_2H .

Species	$\Delta_f H(0)$, (kJ/mol)	Uncertainty
C_2	822.4	$\pm 1.22\%$
C_3	831.0	$\pm 1.56\%$
C_2H	565.0	$\pm 1.10\%$

The exact value of the turbulent Schmidt number, Sc_T , especially for high enthalpy flows, is a subject of debate. The turbulent Schmidt number is effectively the diffusion rate of mass to the wall. Edquist et al. [40] found that published values of the turbulent Schmidt number typically fall in the range of $0.5 \leq Sc_T \leq 1.0$. Recent work by Erb et al. [41] on Galileo probe forebody recession reconstruction suggested that the lower bound on the turbulent Schmidt number should be 0.8. However, the massive blowing by the Galileo probe TPS makes it unique and may not be representative of the Mars return environments considered in this study. While the current baseline solution employs a value of $Sc_T = 0.9$, the full range of $0.5 \leq Sc_T \leq 1.0$ is considered in this study. Additionally, a $\pm 30\%$ roughness height uncertainty was assumed in this study.

Because the current work considers a nonequilibrium char ablation model on the vehicle surface, uncertainties associated with the surface chemistry model were also considered. These uncertainties are given in Table 2, along with references for each uncertainty magnitude. Finite rate surface model uncertainty sources considered included surface oxidation rates, carbonous sublimation rates, the surface nitridation rate, and the N_2 catalytic recombination rate.

Table 2 Coupled ablation uncertainties.

Parameter	Uncertainty	Reference
$O + C(s) \rightarrow CO$ Oxidation Rate	[0.5, 10.0]	[42]
$O_2 + 2C(s) \rightarrow 2CO$ Oxidation Rate	[0.5, 1.5]	[42]
C Sublimation Rate	[0.1, 10.0]	[43]
C_2 Sublimation Rate	[0.1, 10.0]	[43]
C_3 Sublimation Rate	[0.1, 10.0]	[43]
$N + C(s) \rightarrow CN$ Nitridation Rate	[0.2, 5.0]	[44]
$N + N(s) \rightarrow N_2$ Recombination Rate	[0.1, 10.0]	[44]

IV. Results and Discussion

In this section, results of the current study are presented, along with discussion of key findings. First, the baseline or nominal solution of the EEV forebody flow field is described. Then, the parametric uncertainty in the predicted convective heating is given, based on the LAR-NIPC approach outlined in section II. Key sources of uncertainty are identified, and a comparison with alternative uncertainty propagation approaches is provided.

A. Baseline Solutions

Three freestream conditions of interest were considered in this study and are listed in Table 3. These conditions are representative of a plausible entry trajectory for a Mars sample return vehicle.

Table 3 Freestream conditions studied.

Case	Velocity (m/s)	Density (kg/m ³)	Temperature (K)
1	11152.0	3.372e-04	244.4
2	10183.0	8.550e-04	260.0
3	6844.5	3.327e-03	249.1

Convective and radiative heating rates and wall temperatures for the three conditions are shown in Fig. 2. Peak total heating occurs at the conditions for case 2 where total convective and radiative heating is about 830 W/cm². Peak radiative heating occurs earlier in the trajectory at case 1 conditions with the stagnation point being subject to about 243 W/cm² of radiative heating versus only about 210 W/cm² at case 2 conditions. At case 3 conditions, radiative heating has diminished to near zero, while convective heating is only slightly decreased from case 2. This is primarily due to diffusion limited oxidation remaining high at conditions past those of peak heating (i.e., case 2). The decrease in convective heating is more pronounced along the flank or cone portion of the vehicle for case 3.

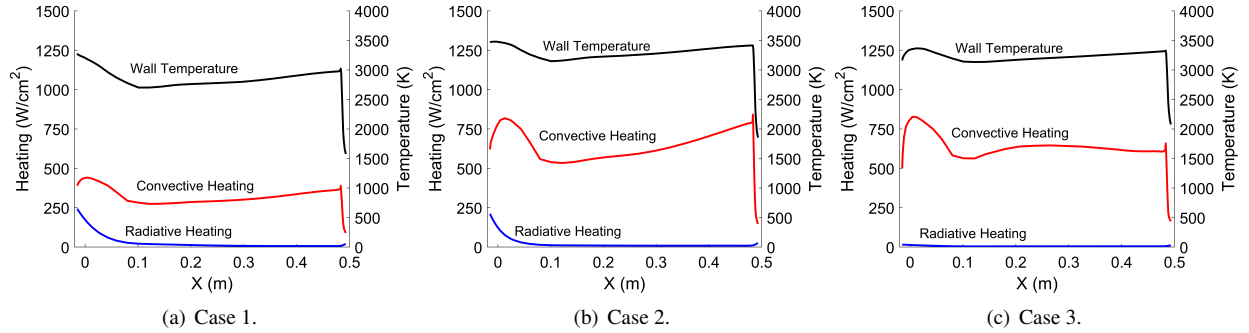


Fig. 2 Baseline heating and wall temperatures.

B. Uncertainty Analysis

To assess the impact of the 329 uncertainty sources identified above, the LAR-NIPC approach was applied directly to the full dimension problem. A second order PCE with 329 uncertainty sources has nearly 55,000 terms, determined using Eq. (2). Construction of a full order expansion would require at least 55,000 CFD model evaluations, which is not feasible. Using the LAR-NIPC iterative approach, a sample size of only 50 was determined to be sufficient for accurate prediction of both the uncertainty bounds and the Sobol sensitivity indices. The resulting convective heating uncertainty bounds along the surface of the EEV forebody are shown in Fig. 3 for each of the three freestream conditions. For case 1, the uncertainty ranges from about ± 30 -35% along the entire surface. At case 2 conditions, the uncertainty can range from nearly ± 40 % on the spherical portion of the vehicle to about $[+50\%, -40\%]$ near the shoulder. These percentages are similar for case 3. Recall that these results do not include the impact of uncertainty in the material response, which is the subject of future work. This would likely push the uncertainty intervals wider, particularly at the stagnation point where blowing is the highest.

Convergence of the above convective heating uncertainty bounds is shown in Fig. 4 as a function of the number of samples used in the LAR-NIPC routine. This figure shows the convergence for three points on the surface: the

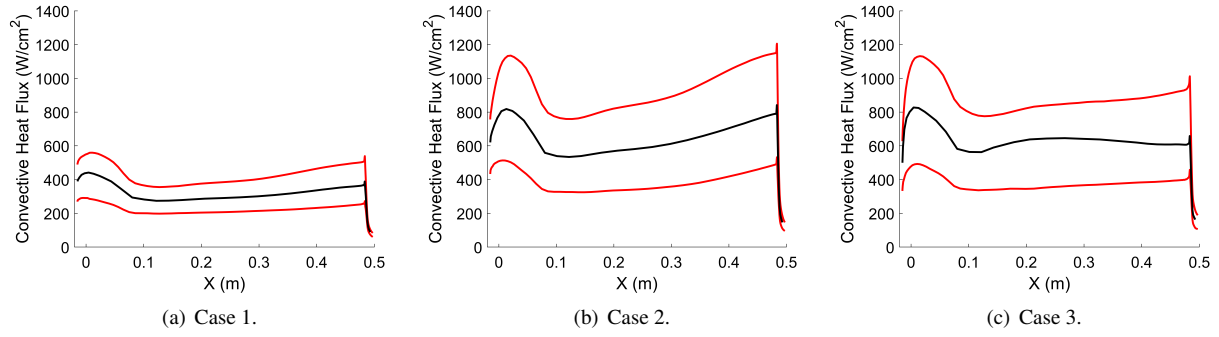


Fig. 3 Maximum and minimum uncertainty bounds.

stagnation point ($X = -0.02$ m), $X = 0.10$ m, and $X = 0.40$ m). Notice that for all three cases and at all three points on the body, the maximum and minimum uncertainty bounds converge rapidly, requiring less than 20-30 samples to reach near asymptotic heating values. This rapid convergence is a function of the polynomial chaos model sparsity. With three parameters accounting for over 90% of the total variance in the convective heating output, only about four of the nearly 55,000 terms in the second order polynomial have values of significant magnitude. This problem highlights the applicability of the LAR-NIPC approach to very high dimension stochastic problems.

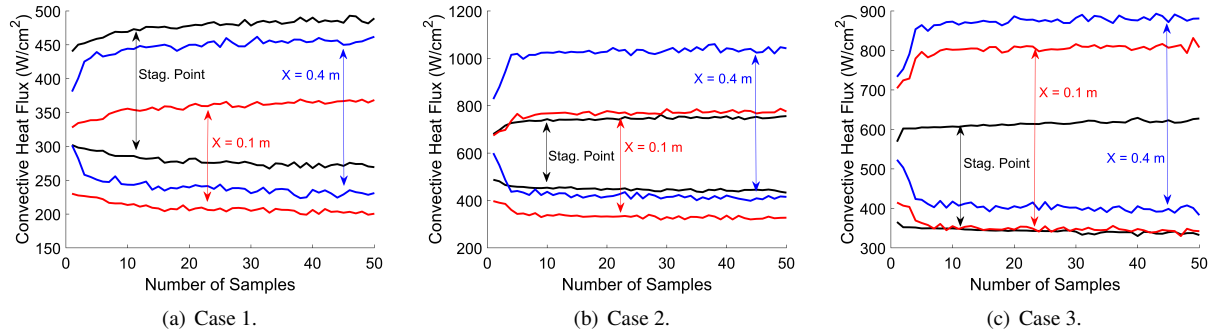


Fig. 4 Convective heating convergence as a function of LAR samples.

The top contributors to the total uncertainty along the surface are shown in Fig. 5. For each of the three cases, the N_2 catalytic rate uncertainty constitutes over 90% of the convective heating uncertainty at the stagnation point. This percentage decreases to between 70-75% approaching the shoulder where the turbulent Schmidt number and roughness height uncertainties begin to contribute more significantly due to the impact of turbulent augmentation. Near the shoulder, the turbulent Schmidt number contributes about 15% of the total uncertainty with the roughness reaching between 5-10% of the uncertainty. All together these three parameters make up 92-98% of the total uncertainty on the surface, at each of the three trajectory points investigated. The other 326 uncertainty sources are found to each contribute less than 1% to the convective heating uncertainty.

Similar to the uncertainty intervals, convergence of the above total Sobol indices can also be used to verify sample independence and convergence of PCE. Plots of total Sobol index convergence for case 4 are shown in Fig. 6 for the stagnation point and a point near the shoulder. Each of these convergence plots contains 329 lines for each of the uncertain parameters, yet only one parameter at the stagnation point and three parameters near the shoulder are distinguishable. Notice that convergence of the percent parameter contributions is achieved rapidly for both locations. The low level of samples required to rank the key parameters is attributed to the sparse nature of EEV convective heating uncertainty problem.

To assess how well the LAR approach compares to other techniques, case 2 was analyzed using the compressed sensing approach [3, 4], which has previously been shown to accurately predict heating uncertainty magnitudes on planetary entry vehicles. A comparison of the uncertainty bounds for the same 50 samples is shown in Fig. 7. Notice

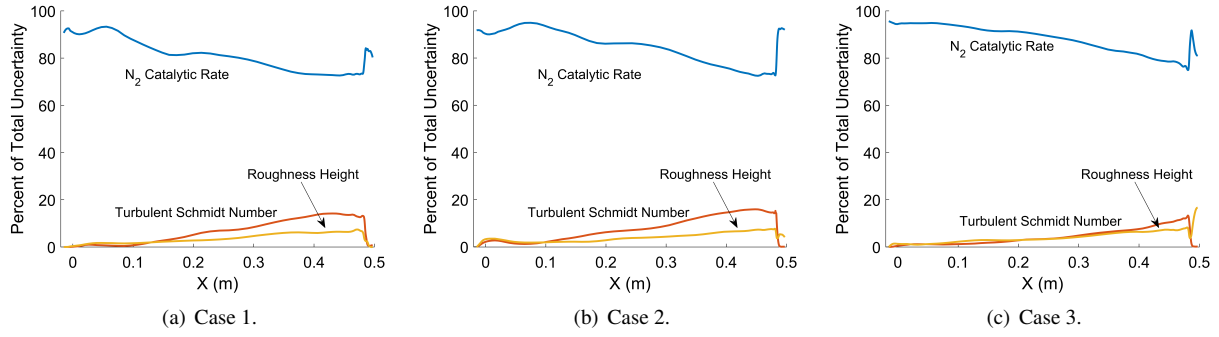


Fig. 5 Top uncertain parameters along the surface.

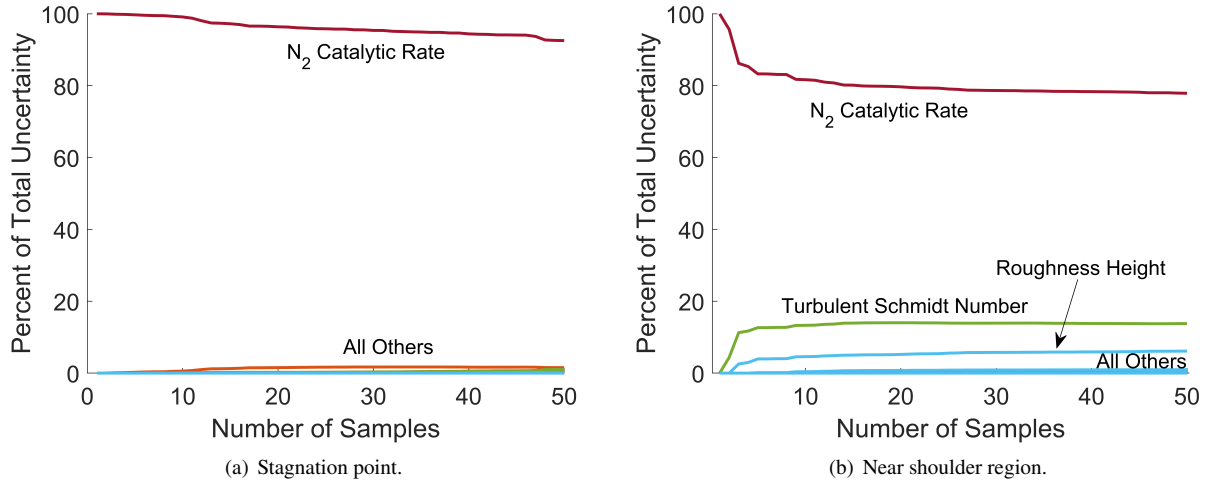


Fig. 6 Sobol indices convergence for case 4.

that both approaches yield nearly the same convective heating along the surface, with the largest difference of about ± 2.5 W/cm² (or about 0.3% of the nominal convective heating) being near the shoulder. The compressed sensing approach also identifies the same top three uncertainty sources with similar contributions to the total uncertainty. For example, LAR-NIPC estimated that 92% of the uncertainty at the stagnation point came from the the N₂ recombination rate while compressed sensing estimated a contribution of 93%. Overall, this illustrates that the LAR-NIPC approach is adequate for problems of this nature, but this approach involves much less complexity than optimization-based approaches, such as compressed sensing.

V. Conclusions

Efficient parametric uncertainty analysis for planetary entry systems is critical for informing vehicle design and assessing thermal protection system margins. The large number of uncertainty sources and associated computational expense of the modeling can make obtaining accurate heating uncertainty predictions challenging. The least angle regression based non-intrusive polynomial chaos expansion (LAR-NIPC) described in this work was shown to provide accurate heating uncertainty estimates and global nonlinear sensitivities at significantly less computational cost when compared to sampling or other surrogate-based approaches. Key uncertainties found to impact convective heating included N₂ surface catalysis, the turbulent Schmidt number, and the surface roughness height. Future investments could be made to further understand and perhaps reduce these uncertainties. Results from the LAR-NIPC approach were compared to those produced by a compressed sensing technique, which is generally accepted as the benchmark

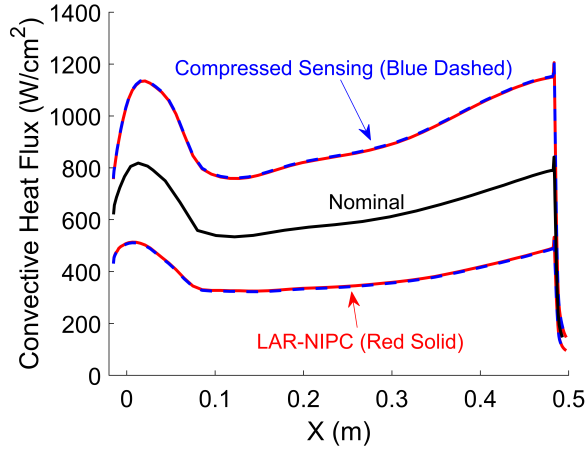


Fig. 7 Comparison of LAR-NIPC and compressed sensing based uncertainty bound predictions.

for sparse, high-dimension problems. This work showed that similar results could be obtained using this LAR-NIPC approach, which is much easier to implement than compressed sensing due to the optimization requirement.

References

- [1] Johnston, C. O., Mazaheri, A., Gnoffo, P., Kleb, B., and Bose, D., “Radiative Heating Uncertainty for Hyperbolic Earth Entry, Part 1: Flight Simulation Modeling and Uncertainty,” *Journal of Spacecraft and Rockets*, Vol. 50, No. 1, 2013, pp. 19–38. doi:10.2514/1.A32254.
- [2] Johnston, C. O., and Kleb, B., “Uncertainty Analysis of Air Radiation for Lunar-Return Shock Layers,” *Journal of Spacecraft and Rockets*, Vol. 49, No. 3, 2012, pp. 425–434.
- [3] West, T. K., and Hosder, S., “Uncertainty Quantification of Hypersonic Reentry Flows with Sparse Sampling and Stochastic Expansions,” *Journal of Spacecraft and Rockets*, Vol. 52, No. 1, 2015, pp. 120–133. doi:10.2514/1.A32947.
- [4] Donoho, D. L., “Compressed Sensing,” *IEEE Transactions on Information Theory*, Vol. 52, No. 4, 2006, pp. 1289–1306. doi:10.1109/TIT.2006.871582.
- [5] West, T. K., Johnston, C. O., and Hosder, S., “Uncertainty and Sensitivity Analysis of Afterbody Radiative Heating Predictions for Earth Entry,” *Journal of Thermophysics and Heat Transfer*, Vol. 31, No. 2, 2017, pp. 294–306. doi:10.2514/1.T4948.
- [6] Efron, B., Hastie, T., Johnstone, I., and Tibshirani, R., “Least angle regression,” *The Annals of Statistics*, Vol. 32, No. 2, 2004, pp. 407 – 499. doi:10.1214/009053604000000067.
- [7] Hosder, S., Walters, R. W., and Balch, M., “Point-Collocation Nonintrusive Polynomial Chaos Method for Stochastic Computational Fluid Dynamics,” *AIAA Journal*, Vol. 48, No. 12, 2010, pp. 2721–2730. doi:10.2514/1.39389.
- [8] Blatman, G., and Sudret, B., “Adaptive sparse polynomial chaos expansion based on least angle regression,” *Journal of Computational Physics*, Vol. 230, No. 6, 2011, pp. 2345–2367. doi:https://doi.org/10.1016/j.jcp.2010.12.021.
- [9] Xiu, D., and Karniadakis, G., “The Wiener–Askey Polynomial Chaos for Stochastic Differential Equations,” *SIAM Journal on Scientific Computing*, Vol. 24, No. 2, 2002, pp. 619–644. doi:10.1137/S1064827501387826.
- [10] Swiler, L. P., and Eldred, M. S., “Efficient algorithms for mixed aleatory-epistemic uncertainty quantification with application to radiation-hardened electronics. Part I, algorithms and benchmark results.”, September 2009. doi:10.2172/972887.
- [11] Ghanem, R. G., and Spanos, P. D., *Stochastic Finite Elements: A Spectral Approach*, Springer-Verlag, New York, 1991. doi:10.1007/978-1-4612-3094-6.
- [12] Eldred, M. S., “Recent Advances in Non-Intrusive Polynomial Chaos and Stochastic Collocation Methods for Uncertainty Analysis and Design,” AIAA Paper 2009-2274, 2009. doi:10.2514/6.2009-2274.

- [13] Hosder, S., and Bettis, B., “Uncertainty and Sensitivity Analysis for Reentry Flows with Inherent and Model-Form Uncertainties,” *Journal of Spacecraft and Rockets*, Vol. 49, No. 2, 2012, pp. 193–206. doi:10.2514/1.A32102.
- [14] West, T. K., Hosder, S., and Johnston, C. O., “Multistep Uncertainty Quantification Approach Applied to Hypersonic Reentry Flows,” *Journal of Spacecraft and Rockets*, Vol. 51, No. 1, 2014, pp. 296–310. doi:10.2514/1.A32592.
- [15] Lockwood, B., and Mavriplis, D., “Gradient-based methods for uncertainty quantification in hypersonic flows,” *Computers and Fluids*, Vol. 85, 2013, pp. 27 – 38. doi:10.1016/j.compfluid.2012.09.003.
- [16] Roderick, O., Anitescu, M., and Fischer, P., “Polynomial Regression Approaches Using Derivative Information for Uncertainty Quantification,” *Nuclear Science and Engineering*, Vol. 164, No. 2, 2010, pp. 122–139. doi:10.13182/NSE08-79.
- [17] Bettis, B., Hosder, S., and Winter, T., “Efficient Uncertainty Quantification in Multidisciplinary Analysis of a Reusable Launch Vehicle,” AIAA Paper 2011-2393, 2011. doi:10.2514/6.2011-2393.
- [18] Han, D., and Hosder, S., “Inherent and Model-Form Uncertainty Analysis for CFD Simulation of Synthetic Jet Actuators,” AIAA Paper 2012-0082, 2012. doi:10.2514/6.2012-82.
- [19] Sudret, B., “Global sensitivity analysis using polynomial chaos expansions,” *Reliability Engineering & System Safety*, Vol. 93, No. 7, 2008, pp. 964 – 979. doi:10.1016/j.res.2007.04.002.
- [20] Thompson, K. B., Hollis, B. R., Johnston, C. O., Kleb, B., Lessard, V. R., and Mazaheri, A., “LAURA Users Manual: 5.6,” Tech. rep., NASA/TM-2020-2220566, Feb. 2020.
- [21] Baldwin, B., and Lomax, H., “Thin-layer approximation and algebraic model for separated turbulentflows,” AIAA Paper 1978-257, 1978. doi:10.2514/6.1978-257.
- [22] Krogstad, P.-A., “Modification of the van Driest damping function to include the effects of surface roughness,” *AIAA Journal*, Vol. 29, No. 6, 1991, pp. 888–894. doi:10.2514/3.10675.
- [23] Gnoffo, P. A., Gupta, R. N., and Shinn, J. L., “Conservation Equations and Physical Models for Hypersonic Air Flows in Thermal and Chemical Nonequilibrium,” Tech. rep., NASA TP 2867, Feb. 1989.
- [24] Park, C., Howe, J. T., Jaffe, R. L., and Candle, G. V., “Review of Chemical-Kinetic Problems for Future NASA Missions, II: Mars Entries,” *Journal of Thermophysics and Heat Transfer*, Vol. 8, No. 1, 1994, pp. 9–23.
- [25] Johnston, C. O., “Study of Aerothermodynamic Modeling Issues Relevantto High-Speed Sample Return Vehicles,” VKI Lecture STO-AVT-218, 2014.
- [26] Johnson, C. O., Hollis, B. R., and Sutton, K., “Spectrum Modeling for Air Shock-layer Radiation at Lunar-Return Conditions,” *Journal of Spacecraft and Rockets*, Vol. 45, No. 5, 2008, pp. 865–878.
- [27] Johnson, C. O., Hollis, B. R., and Sutton, K., “Non-Boltzman Modeling for Air Shock Layers at Lunar Return Conditions,” *Journal of Spacecraft and Rockets*, Vol. 45, No. 5, 2008, pp. 879–890.
- [28] Ralchenko, Y., “NIST Atomic Spectra Database, Version 3.1.0,” 2006. URL physics.nist.gov/PhysRefData/ASD/.
- [29] The Opacity Project Team, *The Opacity Project*, Vol. 1, 1995.
- [30] Cunto, W., Mendoza, C., Ochsenbein, F., and Zeippen, C., “TOPbase at the CDS,” *Astronomy and Astrophysics*, Vol. 275, 1993, pp. L5–L8.
- [31] Johnston, C. O., Brandis, A. M., , and Sutton, K., “Shock Layer Radiation Modeling and Uncertainty for Mars Entry, AIAA 2012-2866,” 43rd AIAA Thermophysics Conference, New Orleans, LA, 2012.
- [32] Mazaheri, A., Johnston, C. O., and Sefidbakht, S., “Three-Dimensional Radiation Ray-Tracing for Shock-Layer Radiative Heating Simulations,” *Journal of Spacecraft and Rockets*, Vol. 50, No. 3, 2013, pp. 485–493.
- [33] Gupta, R., Yos, J., Thompson, R. A., and Lee, K., “A Review of Reaction Rates and Thermodynamic and Transport Properties for an 11-Species Air Model for Chemical and Thermal Nonequilibrium Calculations to 30,000 K,” NASA RP 1232, Aug. 1990.
- [34] Wright, M., “Recommended Collision Integrals for Transport Property Computations Part 1: Air Species,” *AIAA Journal*, Vol. 43, No. 12, 2005, pp. 2558–2564.
- [35] Wright, M., “Recommended Collision Integrals for Transport Property Computations Part 2: Mars and Venus Entries,” *AIAA Journal*, Vol. 45, No. 1, 2005, pp. 281–288.

- [36] Gurvich, L. V., Veyts, I. V., and Alcock, C. B., *Thermodynamic Properties of Individual Substances*, Hemisphere Publishing Corp., New York, 1989.
- [37] Jones, J. J., “The Optical Absorption of Triatomic Carbon C₃ for the Wavelength Range 260 to 560 nm,” Tech. rep., NASA TP-1141, 1978.
- [38] Sharma, M. P., Jaffe, R. L., Munafò, A., and Panesi, M., “Calculation of Thermochemical Properties of Carbon-cluster Ablation Species,” AIAA paper 2018-4179, 2018. doi:10.2514/6.2018-4179.
- [39] Moss, J. N., and Simmonds, A. L., “Galileo Probe Forebody Flowfield Predictions,” AIAA paper 82-0874, 1982.
- [40] K, T. E., Dyakonov, A. A., Wright, M. J., and Tang, C. Y., “Aerothermodynamic Design of the Mars Science Laboratory Heatshield,” AIAA paper 2009-4075, 2009.
- [41] Erb, A. J., West, T. K., and Johnston, C. O., “Investigation of Galileo Probe Entry Heating with Coupled Radiation and Ablation,” *Journal of Spacecraft and Rockets*, Vol. 57, No. 4, 2020, pp. 692–706. doi:10.2514/1.A34751.
- [42] Park, C., “Effects of atomic oxygen on graphite ablation,” *AIAA Journal*, Vol. 14, No. 11, 1976, pp. 1640–1642. doi:10.2514/3.7267.
- [43] Palmer, H. B., and Shelef, M., *Vaporization of Carbon*, Marcel Dekker, Inc., New York, 1968, Vol. Chemistry and Physics of Carbon 4, pp. 85–135.
- [44] Driver, D., and MacLean, M., “Improved Predictions of PICA Recession in Arc Jet Shear Tests,” AIAA paper 2011-141, 2011. doi:10.2514/6.2011-141.
- [45] Johnston, C. O., and Brandis, A. M., “Modeling of nonequilibrium CO Fourth-Positive and CN Violet emission in CO₂ — N₂ gases,” *Journal of Quantitative Spectroscopy and Radiative Transfer*, Vol. 149, No. 1, 2014, pp. 303–317. doi:10.1016/j.jqsrt.2014.08.025.
- [46] Fujita, K., Yamada, T., and Ishii, N., “Impact of Ablation Gas Kinetics on Hyperbolic Entry Radiative Heating,” AIAA paper 2006-1185, 2006. doi:10.2514/6.2006-1185.
- [47] Gokcen, T., “N₂-CH₄-Ar Chemical Kinetic Model for Simulations of Atmospheric Entry to Titan,” *Journal of Thermophysics and Heat Transfer*, Vol. 21, No. 1, 2007, pp. 9–18. doi:10.2514/1.22095.
- [48] Johnston, C. O., West, T. K., and Brandis, A. M., “Features of Afterbody Radiative Heating for Titan Entry,” AIAA paper 2019-3010, 2019. doi:10.2514/6.2019-3010.
- [49] Park, C., *Nonequilibrium Hypersonic Aerothermodynamics*, 1st ed., Wiley, New York, 1990.
- [50] Grover, M. S., Suchyta, C. J., and Josyula, E., “Ab Initio Based Rate Coefficients For Two-Temperature Nonequilibrium Models In Hypersonic Blunt Body Flow,” AIAA paper 2019-0790, 2019. doi:10.2514/6.2019-0790.
- [51] Hanson, R. K., and Baganoff, D., “Shock-Tube Study of Nitrogen Dissociation Rates Using Pressure Measurements,” *AIAA Journal*, Vol. 10, No. 2, 1972, pp. 211–215. doi:10.2514/3.50082.
- [52] Jaffe, R., Schwenke, D., and Chaban, G., “Theoretical Analysis of N₂ Collisional Dissociation and Rotation-Vibration Energy Transfer,” AIAA paper 2009-1569, 2019. doi:10.2514/6.2009-1569.
- [53] Koshi, M., Bando, S., Saito, M., and Asaba, T., “Dissociation of nitric oxide in shock waves,” *Symposium (International) on Combustion*, Vol. 17, No. 1, 1979, pp. 553–562. doi:10.1016/S0082-0784(79)80056-9.
- [54] Wray, K. L., and Teare, J. D., “Shock-Tube Study of the Kinetics of Nitric Oxide at High Temperatures,” *The Journal of Chemical Physics*, Vol. 36, No. 10, 1962, pp. 2582–2596. doi:10.1063/1.1732338.
- [55] Gorelov, V. A., Gladyshev, M. K., Kireev, A. Y., Yegorov, I. V., Plastinin, Y. A., and Karabadzha, G. F., “Experimental and Numerical Study of Nonequilibrium Ultraviolet NO and N Emission in Shock Layer,” *Journal of Thermophysics and Heat Transfer*, Vol. 12, No. 2, 1998, pp. 172–179. doi:10.2514/2.6342.
- [56] Kim, J. G., and Park, G., “Thermochemical nonequilibrium parameter modification of oxygen for a two-temperature model,” *Physics of Fluids*, Vol. 30, No. 1, 2018, p. 016101. doi:10.1063/1.4996799.
- [57] Kulakhmetov, M., Gallis, M., and Alexeenko, A., “Ab initio-informed maximum entropy modeling of rovibrational relaxation and state-specific dissociation with application to the O₂ + O system,” *The Journal of Chemical Physics*, Vol. 144, No. 17, 2016, p. 174302. doi:10.1063/1.4947590.

- [58] Park, C., Jaffe, R. L., and Partridge, H., “Chemical-Kinetic Parameters of Hyperbolic Earth Entry,” *Journal of Thermophysics and Heat Transfer*, Vol. 15, No. 1, 2001, pp. 76–90. doi:10.2514/2.6582.
- [59] Ibragimova, L., “Recommended rate constants of CO + O₂ - reversible - CO₂ + O reactions,” *Khim. Fiz.*, Vol. 10, 1991, pp. 307–310.
- [60] Cruden, B. A., and Brandis, A. M., “Measurements and Prediction of Radiative Non-equilibrium for Air Shocks Between 7-9 km/s,” AIAA paper 2017-4535, 2017. doi:10.2514/6.2017-4535.
- [61] Nelson, H. F., Park, C., and Whiting, E. E., “Titan atmospheric composition by hypervelocity shock-layer analysis,” *Journal of Thermophysics and Heat Transfer*, Vol. 5, No. 2, 1991, pp. 157–165. doi:10.2514/3.243.
- [62] Park, C., “Effects of Lyman Radiation on Nonequilibrium Ionization of Atomic Hydrogen,” AIAA Paper 2004–2277, 2004.
- [63] Leibowitz, L. P., and Kuo, T., “Ionizational Nonequilibrium Heating During Outer Planetary Entries,” *AIAA Journal*, Vol. 14, No. 9, 1976, pp. 1324–1329.
- [64] Park, C., “Assessment of a two-temperature kinetic model for dissociating and weakly ionizing nitrogen,” *Journal of Thermophysics and Heat Transfer*, Vol. 2, No. 1, 1988, pp. 8–16. doi:10.2514/3.55.
- [65] Dunn, M. G., and Kang, S., “Theoretical and experimental studies of reentry plasmas,” NASA CR 2232, Apr. 1973.
- [66] Dunn, M. G., and Lordi, J. A., “Measurement of O₂⁺ plus e[−] dissociative recombination in expanding oxygen flows,” *AIAA Journal*, Vol. 8, No. 4, 1970, pp. 614–618. doi:10.2514/3.5730.
- [67] Park, C., “Review of chemical-kinetic problems of future NASA missions. I - Earth entries,” *Journal of Thermophysics and Heat Transfer*, Vol. 7, No. 3, 1993, pp. 385–398. doi:10.2514/3.431.
- [68] Annaloro, J., Morel, V., Bultel, A., and Omaly, P., “Global rate coefficients for ionization and recombination of carbon, nitrogen, oxygen, and argon,” *Physics of Plasmas*, Vol. 19, No. 7, 2012, p. 073515. doi:10.1063/1.4737147.
- [69] Losev, S. A., Makarov, V. N., and Pogosbekyan, M. Y., “Model of the physico-chemical kinetics behind the front of a very intense shock wave in air,” *Fluid Dynamics*, Vol. 30, 1995, pp. 299–309.
- [70] Carlson, L. A., and Gally, T. A., “Effect of electron temperature and impact ionization on Martian return AOTV flowfields,” *Journal of Thermophysics and Heat Transfer*, Vol. 5, No. 1, 1991, pp. 9–20. doi:10.2514/3.220.
- [71] Bourdon, A., and Vervisch, P., “Study of a low-pressure nitrogen plasma boundary layer over a metallic plate,” *Physics of Plasmas*, Vol. 4, No. 11, 1997, pp. 4144–4157. doi:10.1063/1.872535.
- [72] Teulet, P., Gonzalez, J. J., Mercado-Cabrera, A., Cressault, Y., and Gleizes, A., “One-dimensional hydro-kinetic modelling of the decaying arc in AIR–PA66–copper mixtures: I. Chemical kinetics, thermodynamics, transport and radiative properties,” *Journal of Physics D: Applied Physics*, Vol. 42, No. 17, 2009, p. 175201. doi:10.1088/0022-3727/42/17/175201.
- [73] Kang, S., Jones, W. L., and Dunn, M. G., “Theoretical and Measured Electron-Density Distributions at High Altitudes,” *AIAA Journal*, Vol. 11, No. 2, 1973, pp. 141–149. doi:10.2514/3.50446.

VI. Appendix

The following appendix gives tables of the four groups of uncertain parameters for the convective heat transfer model used in this study. Note that the parameters of Tables 4, 5, and 6 are those of an Arrhenius form.

Table 4 Flow Field Dissociation Reactions

Reaction	$A_{f,i} \left(\frac{\text{cm}^3}{\text{mol-s}} \right)$	$n_{f,i}$	$D_{f,i} (K)$	$T_{f,i}$	Third Body, M	U_i	Reference
$\text{C}_2 + \text{M} \leftrightarrow 2\text{C} + \text{M}$	4.50e+18	-1.00	7.15e+04	$T_{tr}^{0.5} T_{ve}^{0.5}$	All	0.1, 10.0	[45]
$\text{C}_2\text{H} + \text{M} \leftrightarrow \text{C}_2 + \text{H} + \text{M}$	1.70e+35	-5.16	5.74e+04	$T_{tr}^{0.5} T_{ve}^{0.5}$	All	0.1, 10.0	[46]
$\text{C}_2\text{H}_2 + \text{M} \leftrightarrow \text{C}_2\text{H} + \text{H} + \text{M}$	4.00e+16	0.00	5.40e+04	$T_{tr}^{0.5} T_{ve}^{0.5}$	All	0.1, 10.0	[46]
$\text{C}_3 + \text{M} \leftrightarrow \text{C}_2 + \text{C} + \text{M}$	1.68e+21	-1.50	8.77e+04	$T_{tr}^{0.7} T_{ve}^{0.3}$	H, C, N, O	0.1, 10.0	[46]
	8.40e+20	-1.50	8.77e+04	$T_{tr}^{0.7} T_{ve}^{0.3}$	others	0.1, 10.0	[46]
$\text{CH} + \text{M} \leftrightarrow \text{C} + \text{H} + \text{M}$	1.90e+14	0.00	3.37e+04	$T_{tr}^{0.5} T_{ve}^{0.5}$	All	0.5, 2.0	[47]
$\text{CH}_2 + \text{M} \leftrightarrow \text{CH} + \text{H} + \text{M}$	4.00E+15	0.00	4.18e+04	$T_{tr}^{0.5} T_{ve}^{0.5}$	All	0.1, 10.0	[47]
$\text{CH}_2 + \text{M} \leftrightarrow \text{C} + \text{H}_2 + \text{M}$	1.30E+14	0.00	2.97e+04	$T_{tr}^{0.5} T_{ve}^{0.5}$	All	0.1, 10.0	[47]
$\text{CH}_3 + \text{M} \leftrightarrow \text{CH} + \text{H}_2 + \text{M}$	5.00E+15	0.00	4.28e+04	$T_{tr}^{0.5} T_{ve}^{0.5}$	All	0.1, 10.0	[47]
$\text{CH}_3 + \text{M} \leftrightarrow \text{CH}_2 + \text{H} + \text{M}$	1.02E+16	0.00	4.56e+04	$T_{tr}^{0.5} T_{ve}^{0.5}$	All	0.1, 10.0	[47]
$\text{CH}_4 + \text{M} \leftrightarrow \text{CH}_3 + \text{H} + \text{M}$	2.25E+27	-1.87	5.29e+04	$T_{tr}^{0.5} T_{ve}^{0.5}$	All	0.1, 10.0	
$\text{CN} + \text{M} \leftrightarrow \text{C} + \text{N} + \text{M}$	6.00e+15	-0.40	7.10e+04	$T_{tr}^{0.5} T_{ve}^{0.5}$	All	0.3, 1.9	[48]
$\text{CO} + \text{M} \leftrightarrow \text{C} + \text{O} + \text{M}$	2.70e+21	-1.00	1.29e+05	$T_{tr}^{0.5} T_{ve}^{0.5}$	H, C, N, O	0.25, 1.5	[45]
	1.20e+21	-1.00	1.29e+05	$T_{tr}^{0.5} T_{ve}^{0.5}$	others	0.25, 1.5	[45]
$\text{CO}_2 + \text{M} \leftrightarrow \text{CO} + \text{O} + \text{M}$	1.38e+22	-1.50	6.33e+04	$T_{tr}^{0.5} T_{ve}^{0.5}$	H, C, N, O	0.1, 1.0	[45]
	6.90e+21	-1.50	6.33e+04	$T_{tr}^{0.5} T_{ve}^{0.5}$	others	0.1, 1.0	[45]
$\text{H}_2 + \text{M} \leftrightarrow 2\text{H} + \text{M}$	0.00e+00	0.00	4.84e+04	$T_{tr}^{0.5} T_{ve}^{0.5}$	H	0.25, 1.5	[46, 47]
	9.00e+14	0.00	4.84e+04	$T_{tr}^{0.5} T_{ve}^{0.5}$	others	0.25, 1.5	[46, 47]
$\text{HCN} + \text{M} \leftrightarrow \text{CN} + \text{H} + \text{M}$	3.57e+26	-2.60	6.28e+04	$T_{tr}^{0.7} T_{ve}^{0.3}$	All	0.15, 3.0	[48]
$\text{N}_2 + \text{M} \leftrightarrow 2\text{N} + \text{M}$	3.00e+22	-1.60	1.13e+05	$T_{tr}^{0.7} T_{ve}^{0.3}$	C, N, O	0.2, 3.0	[48–52]
	3.00e+22	-1.60	1.13e+05	$T_{tr}^{0.7} T_{ve}^{0.3}$	H	0.1, 0.8	[48]
	7.00e+21	-1.60	1.13e+05	$T_{tr}^{0.7} T_{ve}^{0.3}$	others	0.5, 4.0	[48–51]
$\text{NO} + \text{M} \leftrightarrow \text{N} + \text{O} + \text{M}$	4.57e+17	0.00	7.55e+04	$T_{tr}^{0.7} T_{ve}^{0.3}$	H, C, N, O, NO, CO2	0.2, 2.5	[45, 49, 53–55]
	2.08e+16	0.00	7.55e+04	$T_{tr}^{0.7} T_{ve}^{0.3}$	others	0.2, 2.5	[45, 49, 53–55]
$\text{O}_2 + \text{M} \leftrightarrow 2\text{O} + \text{M}$	1.00e+22	-1.50	5.94e+04	$T_{tr}^{0.7} T_{ve}^{0.3}$	H, C, O, N	0.3, 1.3	[49, 50, 56, 57]
	2.00e+21	-1.50	5.94e+04	$T_{tr}^{0.7} T_{ve}^{0.3}$	others	0.3, 1.3	[49, 50, 56, 57]

Table 5 Flow Field Exchange Reactions

Reaction	$A_{f,i} \left(\frac{\text{cm}^3}{\text{mol-s}} \right)$	$n_{f,i}$	$D_{f,i} (K)$	$T_{f,i}$	U_i	Reference
$\text{C}_2 + \text{C}_2\text{H}_2 \leftrightarrow 2\text{C}_2\text{H}$	1.10e+14	-0.38	6.87e+03	T_{tr}	0.1, 10.0	[46]
$\text{C}_2 + \text{N}_2 \leftrightarrow \text{CN} + \text{CN}$	1.50e+13	0.00	2.10e+04	T_{tr}	0.5, 150.0	[48]
$\text{C}_2\text{H} + \text{H} \leftrightarrow \text{C}_2 + \text{H}_2$	1.60e+13	0.15	1.46e+04	T_{tr}	0.1, 10.0	[46]
$\text{C}_3 + \text{C} \leftrightarrow \text{C}_2 + \text{C}_2$	6.00e+11	1.07	1.65e+04	T_{tr}	0.1, 10.0	[46]
$\text{C}_3 + \text{N} \leftrightarrow \text{CN} + \text{C}_2$	1.00e+12	0.00	3.42e+04	T_{tr}	0.1, 10.0	[58]
$\text{CH} + \text{C} \leftrightarrow \text{C}_2 + \text{H}$	2.00e+14	0.00	0.00e+04	T_{tr}	0.1, 10.0	[47]
$\text{CH} + \text{CO} \leftrightarrow \text{C}_2\text{H} + \text{O}$	2.50e+10	0.67	3.90e+04	T_{tr}	0.1, 10.0	[46]
$\text{CH} + \text{N}_2 \leftrightarrow \text{HCN} + \text{N}$	4.40e+12	0.0	1.11e+04	T_{tr}	0.1, 10.0	[47]
$\text{CH}_2 + \text{H} \leftrightarrow \text{CH} + \text{H}_2$	6.03e+12	0.00	-9.00e+02	$T_{tr}^{0.5} T_{ve}^{0.5}$	0.1, 10.0	[47]
$\text{CH}_2 + \text{N} \leftrightarrow \text{HCN} + \text{H}$	5.00e+13	0.00	0.00e+00	$T_{tr}^{0.5} T_{ve}^{0.5}$	0.1, 10.0	[47]
$\text{CH}_3 + \text{H} \leftrightarrow \text{CH}_2 + \text{H}_2$	6.03e+12	0.00	7.60e+03	$T_{tr}^{0.5} T_{ve}^{0.5}$	0.1, 10.0	[47]
$\text{CH}_3 + \text{N} \leftrightarrow \text{HCN} + 2\text{H}$	7.00e+13	0.00	0.00e+00	$T_{tr}^{0.5} T_{ve}^{0.5}$	0.1, 10.0	[47]
$\text{CN} + \text{C} \leftrightarrow \text{C}_2 + \text{N}$	3.00e+14	0.00	1.81e+04	T_{tr}	0.5, 3.0	[48]
$\text{CN} + \text{H}_2 \leftrightarrow \text{HCN} + \text{H}$	2.95e+05	0.00	1.13e+03	T_{tr}	0.5, 1.5	[48]
$\text{CN} + \text{O} \leftrightarrow \text{NO} + \text{C}$	1.60e+12	0.10	1.46e+04	T_{tr}	1.0, 10.0	[45]
$\text{CO} + \text{C} \leftrightarrow \text{C}_2 + \text{O}$	2.40e+17	-1.00	5.80e+04	T_{tr}	0.1, 10.0	[24]
$\text{CO} + \text{C}_2 \leftrightarrow \text{C}_3 + \text{O}$	1.00e+12	0.00	4.12e+04	T_{tr}	0.1, 10.0	[58]
$\text{CO} + \text{N} \leftrightarrow \text{CN} + \text{O}$	1.00e+14	0.00	3.86e+04	T_{tr}	0.1, 10.0	[45]
$\text{CO} + \text{NO} \leftrightarrow \text{CO}_2 + \text{N}$	8.00e+06	0.88	1.33e+04	T_{tr}	0.1, 10.0	[46]
$\text{CO} + \text{O} \leftrightarrow \text{O}_2 + \text{C}$	3.90e+13	-0.18	6.92e+04	T_{tr}	1.0, 10.0	[45]
$\text{CO}_2 + \text{O} \leftrightarrow \text{O}_2 + \text{CO}$	2.71e+14	0.00	3.38e+04	T_{tr}	0.1, 10.0	[59]
$\text{H} + \text{C}_2\text{H}_2 \leftrightarrow \text{C}_2\text{H} + \text{H}_2$	1.00e+16	-0.50	1.55e+04	T_{tr}	0.1, 10.0	[46]
$\text{H} + \text{CH}_4 \leftrightarrow \text{CH}_3 + \text{H}_2$	1.32e+04	3.00	4.05e+03	T_{tr}	0.1, 10.0	[47]
$\text{H} + \text{CN} \leftrightarrow \text{CH} + \text{N}$	1.50e+15	-0.12	4.978e+04	T_{tr}	0.1, 10.0	[46]
$\text{H} + \text{CO} \leftrightarrow \text{CH} + \text{O}$	6.70e+14	0.15	8.85e+04	T_{tr}	0.1, 10.0	[46]
$\text{H}_2 + \text{C} \leftrightarrow \text{CH} + \text{H}$	4.00e+14	0.00	1.17e+04	T_{tr}	0.1, 10.0	[47]
$\text{H}_2 + \text{H} \leftrightarrow 2\text{H} + \text{H}$	8.50e+19	-1.10	5.23e+04	$T_{tr}^{0.5} T_{ve}^{0.5}$	0.1, 10.0	[46]
$\text{N} + \text{CO} \leftrightarrow \text{NO} + \text{C}$	1.10e+14	0.07	5.35e+04	T_{tr}	0.1, 10.0	[46]
$\text{N}_2 + \text{C} \leftrightarrow \text{CN} + \text{N}$	5.24e+13	0.0	2.26e+04	T_{tr}	0.5, 1.5	[48]
$\text{N}_2 + \text{CO} \leftrightarrow \text{CN} + \text{NO}$	1.20e+16	-1.23	7.70e+04	T_{tr}	0.1, 10.0	[46]
$\text{N}_2 + \text{O} \leftrightarrow \text{NO} + \text{N}$	6.00e+13	0.10	3.80e+04	T_{tr}	0.4, 1.3	[46, 49, 58, 60],
$\text{O}_2 + \text{N} \leftrightarrow \text{NO} + \text{O}$	2.49e+09	1.18	4.01e+03	T_{tr}	0.1, 10.0	[46]

Table 6 Flow Field Ionization Reactions

Reaction	$A_{f,i} \left(\frac{cm^3}{mol-s} \right)$	$n_{f,i}$	$D_{f,i} (K)$	$T_{f,i}$	U_i	Reference
$C + e^- \leftrightarrow C^+ + e^- + e^-$	3.90e+33	-3.78	1.31e+05	T_{ve}	0.1, 10.0	[24, 58]
$C + N \leftrightarrow CN^+ + e^-$	1.00e+15	1.50	1.64e+05	T_{ve}	0.1, 10.0	[61]
$C + O \leftrightarrow CO^+ + e^-$	8.80e+08	1.00	3.31e+04	T_{ve}	0.1, 10.0	[24]
$C^+ + CO \leftrightarrow CO^+ + C$	1.00e+13	0.00	3.14e+04	T_{lr}	0.1, 10.0	[24]
$C^+ + N_2 \leftrightarrow N_2^+ + C$	1.11e+14	-0.11	5.00e+04	T_{lr}	0.1, 10.0	[61]
$CN^+ + N \leftrightarrow CN + N^+$	9.80e+12	0.00	4.07e+04	T_{el}	0.1, 10.0	[61]
$H + e^- \leftrightarrow H^+ + e^- + e^-$	2.20e+30	-2.80	1.58e+05	T_{ve}	0.1, 10.0	[58, 62, 63]
$N + N \leftrightarrow N_2^+ + e^-$	4.40e+07	1.50	6.75e+04	T_{ve}	0.3, 1.3	[49, 64–66]
$N + O \leftrightarrow NO^+ + e^-$	5.30e+12	0.00	3.19e+04	T_{ve}	0.1, 10.0	[67]
$N + e^- \leftrightarrow N^+ + e^- + e^-$	2.50e+34	-3.82	1.68e+05	T_{ve}	0.5, 2.0	[49, 68–70]
$N^+ + N_2 \leftrightarrow N_2^+ + N$	1.00e+12	0.50	1.22e+04	T_{ve}	0.05, 1.7	[60, 65–67, 71, 72]
$N_2 + O^+ \leftrightarrow N_2^+ + O$	9.10e+11	0.36	2.28e+04	T_{lr}	0.1, 10.0	
$N_2 + e^- \leftrightarrow 2N + e^-$	6.00e+3	2.60	1.13e+05	T_{ve}	0.1, 10.0	[49, 60, 71]
$NO + O^+ \leftrightarrow N^+ + O_2$	1.40e+05	1.90	2.66e+04	T_{lr}	0.1, 10.0	[49]
$NO^+ + C \leftrightarrow C^+ + NO$	1.0e+13	0.00	2.32e+04	T_{lr}	0.1, 10.0	[24]
$NO^+ + N \leftrightarrow N_2^+ + O$	7.20e+13	0.00	3.55e+04	T_{lr}	0.1, 10.0	[49]
$NO^+ + N \leftrightarrow O^+ + N_2$	3.40e+13	-1.08	1.28e+04	T_{lr}	0.1, 10.0	[49]
$NO^+ + O \leftrightarrow N^+ + O_2$	1.00e+12	0.50	7.72e+04	T_{lr}	0.1, 10.0	[49]
$NO^+ + O \leftrightarrow O_2^+ + N$	7.20e+12	0.29	4.86e+04	T_{lr}	0.1, 10.0	[49]
$NO^+ + O_2 \leftrightarrow NO + O_2^+$	2.40e+13	0.41	3.26e+04	T_{lr}	0.1, 10.0	[49]
$O + O \leftrightarrow O_2^+ + e^-$	7.10e+02	2.70	8.06e+04	T_{ve}	0.1, 10.0	[67]
$O + e^- \leftrightarrow O^+ + e^- + e^-$	3.90e+33	-3.78	1.59e+05	T_{ve}	0.4, 3.0	[49, 68–70, 73]
$O_2 + C^+ \leftrightarrow O_2^+ + C$	1.00e+13	0.00	9.40e+03	T_{lr}	0.1, 10.0	
$O_2^+ + N \leftrightarrow O_2 + N^+$	8.700e+13	0.14	2.86e+04	T_{lr}	0.1, 10.0	[49]
$O_2^+ + N_2 \leftrightarrow N_2^+ + O_2$	9.90e+12	0.00	4.07e+04	T_{lr}	0.1, 10.0	[49]
$O_2^+ + O \leftrightarrow O^+ + O_2$	4.00e+12	-0.09	1.80e+04	T_{lr}	0.1, 10.0	[67]