The Quantification of Uncertainty in Mars Atmospheric Density Profiles Due to Dust

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This report documents the application of both probabilistic and probability bounding methods to quantify and propagate uncertainty in dust modeling parameters through a Mars atmosphere model. Overviews of Mars atmosphere uncertainty and Dempster-Shafer Evidence Theory are given. The data supporting mathematical representations of uncertainty in the dust parameters are then discussed. A polynomial response surface for atmospheric density at each altitude as a function of the dust parameters is then built based on the propagation of sample values of the dust parameters through a computational simulation of the Mars atmosphere. Uncertainty in the dust parameters is then propagated across that response surface. Using an appropriate Dempster-Shafer representation of probability bounds on the dust parameter uncertainty, it is found that uncertainty in the dust parameters alone leads to uncertainty in density on the scale of ±10%. Bayesian representations of uncertainty in the dust parameters are found to underestimate the uncertainty in atmospheric density by a factor of two.

I. Introduction

A. Mars atmosphere uncertainty overview

Uncertainty in the density profile of the Mars atmosphere greatly influences uncertainty in peak heating, peak loading, and final landing location during a Mars lander mission. Uncertainties in Mars atmosphere models stem from a myriad of sources. These uncertainty sources may be divided into a few main groups: initial/boundary condition uncertainty, discretization error, and physics sub-model uncertainty. At present, initial/boundary condition uncertainty and discretization error are not well-investigated in explorations of uncertainty in the Mars atmosphere. These uncertainty sources are not considered unimportant - simply practically indescribable. That will hopefully change in time. For this analysis and most contemporary analyses, physics sub-models are the prime target for uncertainty quantification.

Only one piece of the total uncertainty puzzle is examined in this report: uncertainty in the distribution of dust in the Mars atmosphere. This is one case of physics sub-model uncertainty. Examples of other uncertain physics sub-models include the planetary boundary layer model, the
surface layer model, top-level mixing parameterization, and the gas thermodynamic model. The dust model is selected for investigation due to its influence over the thermal structure of the atmosphere. The goal of pursuing dust uncertainty is to study a piece of the Mars atmosphere uncertainty puzzle that is both tractable and significant.

B. Quantifying epistemic uncertainty

Uncertainty in future Mars atmospheric dust levels is driven as much by lack of knowledge as by chaotic variability. Although data for describing the distribution of dust are available, these data are sparse in some parameters and highly imprecise in others. The prominence of epistemic uncertainty in the Mars dust problem throws the appropriateness of applying purely probabilistic methods into question.\textsuperscript{1-3} Under a Bayesian approach, all uncertainty is to be represented probabilistically, because Bayesian probability refers to a personal willingness to bet.\textsuperscript{4,5} However, the scientific community has long been ill at ease with Bayesian standards of truth.\textsuperscript{6-8}

In contrast, frequentist probability conforms to traditional scientific standards of truth. The frequentist probability of an event in a given situation is simply the frequency of occurrence of that event under similar situations.\textsuperscript{2,3} A scientist or engineer can validate a frequency of occurrence prediction in the same way that he or she can validate a temperature prediction: via observation and measurement. Under a frequentist approach, only aleatory uncertainty is represented probabilistically. A standard currently promulgated in the aerospace engineering community is that epistemic uncertainty in quantities of interest should be represented using intervals.\textsuperscript{9} When representing a mixture of aleatory and epistemic uncertainty in a frequentist context, it is necessary to utilize a mathematical framework that allows probabilistic and interval uncertainty to be propagated together.

This paper documents the application of both the Bayesian approach and the frequentist approach to the Mars atmosphere uncertainty problem. Given the data at hand, the frequentist approach admits a unique set of bounds on the frequentist probability distribution of the Mars atmosphere density profile. The Bayesian approach admits several different subjective probability assessments. Five possible Bayesian assessments are considered. The paper concludes by contrasting the results obtained using these two different approaches and considering the different actions to which they might lead a design engineer working on a Mars lander project.

C. Discrete Dempster-Shafer structures

Although the founders of Dempster-Shafer theory have advocated a subjective interpretation of their structures,\textsuperscript{10,11} belief and plausibility functions have been used to represent lower and upper bounds on frequentist probability.\textsuperscript{12-14} That approach proves both convenient and adequate in the representation and propagation of Mars atmospheric dust uncertainty.

In classic Dempster-Shafer Theory, basic belief assignment functions provide the basic method of representation for Dempster-Shafer structures. The basic belief assignment function plays the same role as the probability mass function in probability theory, except that basic belief may be assigned to sets rather than single points. A basic belief assignment, \( m_X (A) \), on an uncertain quantity, \( X \), must satisfy the following two conditions:

\[
m_X (A) \geq 0 \quad \forall A \subset \Omega_X \quad \text{and} \quad \sum_{A \subset \Omega_X} m_X (A) = 1.
\]

The sets for which \( m_X (A) > 0 \) are termed focal elements. Classic Dempster-Shafer Theory only considers uncertain quantities described using a finite number of focal elements, each having a finite basic belief assignment. Belief and plausibility may be calculated from the the basic belief assignment.
using the following formulas:

\[
\text{Bel}_X (A) = \sum_{B \subset A} m_X (B) \quad \text{and} \quad \text{Pl}_X (A) = \sum_{B \cap A \neq \emptyset} m_X (B).
\]

There are a number of special cases within Dempster-Shafer theory. If all of the focal elements in a discrete Dempster-Shafer structure are single points, that Dempster-Shafer structure’s basic belief assignment is a discrete probability mass function. Alternatively, if all of the focal elements in a discrete Dempster-Shafer structure are consonant (that is, if the focal elements form a set \( \{A_1, A_2, A_3, \ldots, A_n\} \) such that \( A_1 \subset A_2 \subset A_3 \subset \ldots \subset A_n \)), that Dempster-Shafer structure constitutes a fuzzy variable. Some examples of Dempster-Shafer structures are given in Figure 1.

**D. Propagation of discrete Dempster-Shafer structures**

Given a variable \( X \) described by a discrete Dempster-Shafer structure and a function of that variable \( Z = g(X) \), a Dempster-Shafer structure on \( Z \) based on \( X \) must satisfy

\[
\text{Bel}_Z (A_Z) = \text{Bel}_X (g^{-1}(A_Z)) \quad \forall A_Z \subset \Omega_Z
\]

where \( \Omega_Z \) is the universal set for \( Z \) and

\[
g^{-1}(A_Z) = \{x \in \Omega_X : g(x) \in A_Z\}
\]

i.e. \( g^{-1}(A_Z) \) is the complete set of all \( x \) such that \( g(x) \) is a member of \( A_Z \).

The Dempster-Shafer structure on \( Z \) satisfying the correctness condition given in Equation 1 is obtained by the following formula:

\[
m_Z (A_Z) = \sum_{B_X \subset \Omega_X : A_Z=g(B_X)} m_X (B_X) \quad \forall A_Z \subset \Omega_Z.
\]

The basic idea of Dempster-Shafer propagation is to take each focal element on \( X \), crank it through the function (by sampling or some other method), and carry the basic belief assignment to the resulting focal element on \( Z \). If two or more focal elements on \( X \) propagate to the same set on \( Z \), then their basic belief assignments are added together to give the basic belief assignment on that set on \( Z \). The process is simple, in principle, and can be generalized to the propagation of joint Dempster-Shafer structures on multiple variables through a function.
E. Random set theory

Since random and fuzzy variables can be continuous, it seems reasonable to expect that it should be possible to define a continuous Dempster-Shafer structure. Dempster-Shafer structures are generalized to the continuous case by random sets. A random set on a variable \( x \) consists of a seed variable, \( a \), with a fixed probability function and a function, \( M_X \), that maps individual values of \( a \) to sets of possible \( x \)-values. For all of the random sets used in this paper, the seed random variable is uniformly distributed on the unit interval. The belief and plausibility functions for a random set can be calculated as follows:

\[
\begin{align*}
\text{Bel}_X (A) &= \text{Pro}_a (\{ a : M_X (a) \subset A \}) \\
\text{Pl}_X (A) &= \text{Pro}_a (\{ a : M_X (a) \cap A \neq \emptyset \})
\end{align*}
\]

Belief functions supported by random sets all satisfy the same axioms as belief functions supported by Dempster-Shafer structures.\(^{15,16}\) The relationship between Dempster-Shafer structures and random set theory is analogous to the relationship between discrete probability distributions and general probability theory.

Specifically, continuous random sets can be approximated using discrete Dempster-Shafer structures in a Monte-Carlo fashion. In traditional Monte-Carlo sampling, an analyst takes a random sample of size \( N \) on the unit interval, maps that sample to the variable of interest using the inverse cumulative distribution function, and then approximates the random variable in question as a discrete random variable with a probability mass of \( \frac{1}{N} \) at each sampled point. This discrete random variable is used as an approximation for the continuous random variable. An analogous process may be performed for random sets using the map function as the inverse CDF. The result will be a discrete Dempster-Shafer structure with \( N \) focal elements each having a basic belief assignment of \( \frac{1}{N} \). Propagation of such a variable is then the same as for any Dempster-Shafer structure.

F. Representing Dempster-Shafer structures graphically

There are a number of ways to graphically represent a Dempster-Shafer structure on a real variable. One of the most natural is to display its map-function. This approach is taken in Figures 10, 12, and 13. In the course of this paper, it is necessary to graphically represent uncertainty in density at multiple altitudes all in the same plot. The approach taken is to simultaneously plot central belief intervals. To do so, it is necessary to define a canonical method for deriving central belief intervals from a Dempster-Shafer structure. First, one must define inverses of the cumulative belief and cumulative plausibility functions analogous to the inverse cumulative distribution function for a random variable. Those definitions are as follow:

\[
\begin{align*}
\text{CumBel}_X^{-1} (u) &= \inf \{ x \in \mathbb{R} : \text{Bel}_X ((-\infty, x]) \geq u \} \\
\text{CumPl}_X^{-1} (u) &= \sup \{ x \in \mathbb{R} : \text{Pl}_X ((-\infty, x]) \leq u \}
\end{align*}
\]

With these definitions it is possible to define, for a fixed level of belief \( \beta \), the critical offset \( \delta_\beta \) as

\[
\delta_\beta = \sup \left[ \left\{ u \in [0, 1] : \text{Bel}_X \left( \left[ \text{CumPl}_X^{-1} \left( \frac{u}{2} \right), \text{CumBel}_X^{-1} \left( 1 - \frac{u}{2} \right) \right] \right) \geq \beta \right\} \right].
\]

For belief of level \( \beta \), the canonical central belief interval \( A_\beta \) is given as

\[
A_\beta = \left[ \text{CumPl}_X^{-1} \left( \frac{\delta_\beta}{2} \right), \text{CumBel}_X^{-1} \left( 1 - \frac{\delta_\beta}{2} \right) \right].
\]

This is the method by which the confidence intervals of Figures 11 and 14 are derived from Dempster-Shafer structures on atmospheric density at various altitudes.
II. Thirty-day simulation at Holden crater

The specific problem investigated in this report is the quantification of uncertainty in dust sub-model parameters and the propagation of that uncertainty to atmospheric density at the end of a 30-day mesoscale simulation at Holden Crater. The Holden Crater simulation was chosen for its practical interest. Holden Crater remains a prospective landing location for the Mars Science Laboratory.

The atmospheric circulation model used is PRAMS (the Planetary Regional Atmospheric Modeling System). Initial conditions are loaded from the Ames MGCM (Mars Global Circulation Model). The simulation conducted is thirty days at Holden Crater starting in early Winter (a Solar Longitude of approximately 120°). The grid for this simulation is plotted in Figure 2. Initial conditions, boundary conditions, and parameters in all other physics sub-models are identical between different versions of the Holden Crater simulation used in the uncertainty analysis. Only dust parameters are perturbed in the runs of the PRAMS code used in the analysis presented in this report.

III. Uncertainty in dust parameters

A. Conrath dust model

The specific dust model used in this analysis is the Conrath dust model. The Conrath model is the simplest of all available dust models. It depends on only two parameters, total opacity and the Conrath parameter. Information for both of these parameters has been collected during Mars missions over the years. Measured vertical dust distributions never match the Conrath distribution exactly for any values of these two parameters, but its shape approximates real dust distributions adequately for the purposes of this analysis.

The Conrath dust model stipulates an exponential distribution of local dust loading, \( q(z) \), described by the following formula:

\[
q(z) = q_0 e^{\nu(1-e^{-z/H})}
\]

where \( z \) is altitude, \( H \) is the scale height (roughly 10 km), \( \nu \) is the Conrath parameter, and \( q_0 \) is the dust loading at ground level. The stipulated dust distribution results from an assumed balance between vertical mixing and gravitational settling.
There are no universal values for $q_0$ or $\nu$ that govern the Mars atmosphere for all time. The appropriate values for these two parameters are found to vary greatly on Mars with location, season, and transient weather. Usually, one does not measure $q_0$ directly but calculates it based on total opacity, $\tau_{\text{tot}}$, which is defined as

$$\tau_{\text{tot}} = \int_{0}^{\infty} q(z) \sigma \rho(z) \, dz$$

where $\sigma$ is the effective cross-section for radiative interaction (units of area) for the dust particles and $\rho(z)$ is atmospheric density. Measurements of $\tau_{\text{tot}}$ relevant to the analysis presented here are plentiful but imprecise. The Conrath parameter, on the other hand, is not observed directly but fitted to observed vertical dust profiles. In theory, the Conrath parameter has a physical meaning (see Conrath 1975, p. 40), but in practice it is adjusted to give the best fit to a given observed dust distribution curve.

B. Data on total opacity, $\tau_{\text{tot}}$

Mars Global Surveyor’s (MGS) Thermal Emission Spectrometer (TES) has been producing measurements of total opacity since 1998. These measurements cover all times of year and a wide range of longitude and latitude and can be accessed online. Dust behavior is generally consistent during early Southern Hemisphere winter. It is assumed in this analysis that the statistical distribution of total opacity measurements in the vicinity of Holden crater during the early winter season approximates the statistical distribution from which the total opacity will be realized during a future early-winter landing mission at Holden crater. This assumption is based, not upon a settled community standard (no such standard exists yet), but upon informed engineering judgment.

The statistical distribution of the available MGS total opacity data from 1998 to 2005 falling within the latitude range $[-30^\circ, -15^\circ]$, longitude range $[312^\circ, 340^\circ]$, and Solar Longitude range (i.e. time of year) $[110^\circ, 130^\circ]$ is described by the cumulative distribution function (CDF) plotted...
in left panel of Figure 3. This distribution is built on 59286 samples, which is adequate to justify neglecting uncertainty due to sample size.

However, each measurement is subject to substantial bias uncertainty generated in the data reduction process. The nominal value for the measurement uncertainty reported in the literature on TES results, \( \pm 0.05 \), is taken at face value as an interval uncertainty. Adding this interval onto the random variable in the left half of Figure 3 yields a conservative Dempster-Shafer representation of uncertainty in total opacity. Physically, total opacity cannot be negative. Therefore, one may clip off any part of the Dempster-Shafer structure for total opacity that dips below zero and still have a conservative estimate of uncertainty. Finally, the PRAMS code takes visible (rather than infrared) total opacity as its input to describe total dust level. Visible opacity may be extrapolated from infrared by multiplying the infrared opacity by a factor of two. The final Dempster-Shafer structure representing uncertainty in visible dust opacity is given in the right panel of Figure 3.

There is a caveat to this representation. Under the harshest frequentist standard, the 59286 samples are not all independent. The represented data were collected in roughly 112 orbits around the Mars atmosphere, split between two winters. It would be unreasonable to expect the data collected from neighboring points during an orbit to be stochastically independent, and upon inspection they do not appear to be. However, data from points at opposing edges of a given orbital sweep and collected on the same orbital sweep to appear stochastically independent. Since the presenters of this data claim to have all but eliminated random error in the data using some method of statistical control, it can only be concluded that the variability between these distant point reflects genuine variability in the dust levels. It is also found that day-to-day dust values at the same location also vary randomly, although there needs to be difference of roughly two days before the data values appear completely independent. Nevertheless, the assumption is made here that the bounds on the distribution represented by the Dempster-Shafer structure illustrated in Figure 3. Refining the estimate of the probability bounds would be a subject for future work.

C. Data on the Conrath parameter, \( \nu \)

As mentioned before, the Conrath parameter is adjusted to give the best possible fit to a given measured vertical dust profile. Vertical profiles of relative dust distribution are not readily available in the literature. The best-documented relative dust opacity profiles were found in a 1986 report by Jaquin et al on visual limb images from the Viking Orbiter. Plots were available in the \([-15^\circ, -25^\circ]\) Latitude range at Solar longitudes in the \([110^\circ, 130^\circ]\) range. The latitude range just barely misses the mark; Holden Crater is at a Latitude of \(-26^\circ\). No data are available in Jaquin’s paper for the appropriate Solar longitudes in the latitude band spanning \([-25^\circ, -35^\circ]\]. Vertical dust distributions at the appropriate Solar longitude are available in the latitude range of \([-35^\circ, -45^\circ]\) are available. In consideration of these two sets of data, it was decided that perturbing the Conrath parameter across the interval \([0.003, 0.17]\) more than adequately captured the uncertainty in the relative dust distribution. The lower bound may, in fact, be excessive. It is the \([-35^\circ, -45^\circ]\) latitude data that necessitates the lower bound of 0.003 on Conrath-\( \nu \), and the relevance of those profiles to the conditions at Holden Crater is questionable. The more immediately relateable data set in the \([-15^\circ, -25^\circ]\) latitude range can be covered with a lower bound of 0.03. Data from a later paper by Smith based on MGS observations supports the hypothesis that 0.03 may be an adequate lower bound for the Conrath parameter for the early-winter Holden crater simulation.

For the analysis in this report, the Conrath parameter is treated as being interval-uncertain on \([0.003, 0.17]\). The range of vertical relative opacity profiles generated by this interval is illustrated in the left half of Figure 4. For comparison, the right half of Figure 4 shows the range of vertical relative opacity profiles generated using the less conservative interval \([0.03, 0.17]\).
D. Conservative joint Dempster-Shafer structure for the Conrath parameter and total opacity

It cannot be reasonably argued that the two dust parameters are stochastically independent, nor is there an adequate scientific model or joint sampling information with which to describe the dependency between the two variables. Previous work has established that the Cartesian product provides tightest possible probability bounds for the joint Dempster-Shafer structure on two variables with unknown dependence when one of those variables is interval-uncertain. The joint structure for total opacity and the Conrath parameter is therefore described by,

\[ M_{\tau_{\text{tot}}} (u) = M_{\tau_{\text{tot}}} (u) \times [0.003, 0.17] \ \forall u \in [0, 1] \] (5)

where \( M_{\tau_{\text{tot}}} \) is the map-function illustrated in Figure 3.

IV. Dust-to-density response surface

The form of the relationship modeled by PRAMS between atmospheric density and the dust parameters lacks a clean analytic description. Therefore, in principle, the most reliable way to propagate the focal elements through PRAMS is brute force sampling. However, each thirty-day simulation of the PRAMS model requires roughly seven days of computing time to run to completion using the computing resources available. Although sample runs may be conducted in parallel, there were only four dozen processors available for use in this analysis. Each sample run requires one processor. To properly propagate the dust parameter focal elements requires the use of thousands of sample points. Thus, the direct approach to propagating the focal elements is practically untenable.

The next most direct approach is to use a response surface as a computationally inexpensive surrogate model. Constructing the response surface required a substantial amount of trial and error.
and personal judgment. The response surface serves only one purpose: to imitate the response of PRAMS-predicted density to perturbation in dust parameters. Any means to this end is deemed acceptable. Wild mathematical assumptions unacceptable in representing uncertainty may be granted in the construction of the response surface, so long as the resulting response surface passes inspection.

The response surface linking density to the dust parameters took the form of a piecewise cubic Hermite interpolating polynomial (PCHIP) using twenty-five sample values of total opacity and the Conrath parameter. These twenty-five input values for $\tau_{\text{tot}}$ and $\nu$ are plotted in Figure 5 along with the corresponding density profiles output by PRAMS for the grid-location closest to Holden Crater. The PCHIP response surface is then illustrated at four different altitudes in Figure 6.

A. Importance functions, weight functions, and sample choice

All sample-generation methods depend on a weight function assigned to the space being sampled. The normalized weight function used in sample generation plays a critical role in determining the accuracy of a response surface. As a general rule, traditional sample generation and response surface methods lead to response surfaces whose accuracy in a region of the domain varies positively with the weight assigned to that region of the domain. More weight means more accuracy. The normalized weight function, therefore, may be seen as assigning relative importance to different regions in the sampling space. In purely probabilistic methods, the probability density function appropriately serves as the weight function. However, in the absence of a defensible probability density function, the assignment of importance becomes (at least partly) a matter of subjective judgment.

Given interval uncertainty in some quantity, each point on that interval is equally important. Following this logic, it might make sense to build a weight function by evenly distributing a focal element’s basic belief assignment across all of its constituent points. Mathematically, the importance function, $\text{Imp}_X(x)$, for a variable defined using a Dempster-Shafer structure described by map $M_X$ is defined as

$$\text{Imp}_X(x) = \int_0^1 \frac{\text{bool} \left( \langle x \in M_X(u) \rangle \right) |M_X(u)|}{\|M_X(u)\|} du$$

(6)

where $\|M_X(u)\|$ denotes the Lebesque measure (e.g. length, for a real variable) of the set $M_X^{-1}(u)$.

It is crucial to note that the importance function does not map from one variable to another variable the way that a probability density function would map. That is, if one correctly propagates
the Dempster-Shafer uncertainty on $X$ to (for example) $Y = X^2$, the importance function of $X$ as defined by Equation 6 does not necessarily correspond or map in any way to the importance function of $Y$.

The importance function formula in Equation 6 only shifts the judgment call necessary in building a weight function. Instead of arbitrarily specifying the weight function, the analyst must now decide upon what transformations of the input variables the importance function formula will be applied to derive the weight function. Importance functions do not map through transformations, but weight functions in response surface methodologies do.

For example, in the dust uncertainty quantification problem, $\nu$ is interval-uncertain. Therefore, $\ln(\nu)$ is also interval-uncertain. So, the importance functions for $\nu$ and $\ln(\nu)$ are both uniform. (They are simply uniform on different intervals.) However, to use the importance function of $\nu$ as the weight function and then derive samples on $\nu$ in accordance with that weight function will lead to a different response surface than would be obtained by using the importance function of $\ln(\nu)$ as the weight function, deriving samples on $\ln(\nu)$, and then mapping those samples back to $\nu$.

Since the Conrath parameter varies over multiple orders of magnitude, the response surface is written in terms of $\ln(\nu)$ with its marginal weight function being a uniform distribution on the interval $[\ln(0.003), \ln(0.17)]$. The importance function calculated by directly applying Equation 6 to the representation of total opacity given in the right half of Figure 3 is used as the marginal
weight function for total opacity. The joint weight function for $\tau_{tot}$ and $\ln(\nu)$ is simply taken as the product of the two marginal weight functions. In a probabilistic framework, such a treatment would reflect an assumption of stochastic independence between the two parameters. Here, the approach is merely meant to reflect that given a particular value of $\tau_{tot}$, all possible values of $\ln(\nu)$ are equally important (since their relative probabilities are unknown).

The sample inputs of total opacity and the Conrath parameter (see Figure 5) used in building the response surface are the 4th Order Gaussian Quadrature abscissas for the joint weight function just described. Gaussian Quadrature abscissas are chosen due to previous experience with weighted least squares polynomial approximations for simpler problems. Ultimately, a different type of response surface is utilized, but the abscissa-selection that was originally motivated by a least squares polynomial approach persists to the final response surface. These abscissas are listed in Table 1.

B. Non-intrusive polynomial chaos

The original intent in this project was to use a non-intrusive polynomial chaos (NIPC) expansion to model the density response to perturbations in the dust parameters. An NIPC expansion is a truncated orthogonal polynomial series, the coefficients of which are solved for using a quadrature or weighted least squares approach. The use of 4th Order Quadrature means that at most a 4th Order NIPC Expansion can be used. If $\Phi_i(\tau_{tot})$ represents the $i$th orthonormal polynomial on total opacity and $\Xi_j(\ln(\nu))$ represents the $j$th orthonormal polynomial on the natural logarithm of the Conrath parameter, then the 4th Order NIPC expansion of density at a given altitude, $R_4(z,\tau_{tot},\nu)$ is given by

$$R_4(z,\tau_{tot},\nu) = \sum_{i=0}^{4} \sum_{j=0}^{4-i} r_{i,j}(z) \Phi_i(\tau_{tot}) \Xi_j(\ln(\nu)).$$

Reorganizing this equation in terms of a new index, $k(i,j) = i + j - 4 + \sum_{m=0}^{i} (5 - m)$, gives

$$R_4(z,\{\tau_{tot},\nu\}) = \sum_{k=1}^{15} r_k(z) \Psi_k(\{\tau_{tot},\ln(\nu)\})$$

where $r_{k(i,j)}(z) = r_{i,j}(z)$ and $\Psi_{k(i,j)}(\{\tau_{tot},\ln(\nu)\}) = \Phi_i(\tau_{tot}) \Xi_j(\ln(\nu))$. The coefficients of this series, $r_k(z)$, at each altitude are calculated to minimize the error in the response surface values in the least squares sense. That is, the coefficients are calculated to minimize the error norm, $J(z)$, defined as

$$J(z) = \sum_{m=1}^{25} w_m(R_4(z,\{\tau_{tot},\nu\}_m) - \rho(z,\{\tau_{tot},\nu\}_m))^2$$

where $\rho(z,\{\tau_{tot},\nu\}_m)$ is the PRAMS output value of density and $w_m$ is the quadrature weight attached to the $m$th abscissas. At a given altitude, the values for $r_k(z)$ that minimize $J(z)$ are

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<th>$\tau_{tot}$</th>
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<th>$\tau_{tot}$</th>
<th>$\nu \times 10^3$</th>
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<td>6.696</td>
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<td>6.696</td>
</tr>
</tbody>
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solved by the matrix equation

$$\vec{r}(z) = (A^TWA)^{-1}A^T W \vec{\rho}(z)$$

where $A$ is the $25 \times 15$ collocation matrix whose entries, $a_{m,k}$, are given by

$$a_{m,k} = \Psi_k \left( \{\tau_{tot}, \ln(\nu)\}_m \right),$$

and $W$ is the diagonal weight matrix whose non-zero entries are the quadrature weights, $w_m$. It is worth noting that since Gaussian Quadrature abscissas and weights are used, the weighted least squares approach is identical to the quadrature approach; that is, $A^TWA$ is the identity matrix given Gaussian Quadrature abscissas and weights.

The NIPC expansion for density at an altitude of 41 km over Holden crater generated using Equation 7 is plotted in Figure 7. The performance of the response surfaces at this altitude is typical for the performance at all altitudes. Since the least squares approach is overdetermined, it is almost a foregone conclusion that the reconstituted response surface points will have some error. As it turns out, this error is significant. At a total opacity value of roughly 0.26, the error in the reconstituted samples is roughly on the same scale as the deviation of the response from reference density. As total opacity rises, the errors grow precipitously - especially for extreme values of the Conrath parameter. For values of total opacity with a cumulative belief value of 90% or less (see Figure 3), the error in the density response surface doesn’t seem to exceed 3%. Moreover, the NIPC expansion is relatively well behaved, only exhibiting suspicious extrema in high total opacity regions, which carry very little weight. So, the NIPC expansion is a mixed bag. A 3% error in the response surface is nothing to scoff at, as the deviations from the reference density are of that same magnitude. At the very least, since the response surface is reasonably-behaved, the reconstituted

Figure 7. NIPC response surface for density at 41 km. Reference density of $1.73 \times 10^{-4} \text{ kg m}^{-3}$. Sample inputs and sample response deviation from reference density given in black. Error in response surface reconstruction of sample points given in red for NIPC. Illustrated values are normalized with respect to reference density.
sample points give a reference for assessing error in the response surface. There is much to be said for a response surface with, at least, semi-estimable error; even if that error is higher than desired.

C. Lagrange polynomial

Lagrange polynomials constitute an interesting counter-point to the NIPC expansion. By design, a Lagrange polynomial will match the abscissa-outputs exactly. However, Lagrange polynomials are notorious for generating suspicious extrema - especially as the number of points being interpolated increases. Lagrange polynomials offer a simple direct method for matching abscissas but must be handled with care.

A Lagrange polynomial, \( L_n(x) \), in one dimension approximating \( y \) as a function of \( x \) is calculated using the following formula:

\[
L_n(x) = \sum_{i=0}^{n} y(x_i) \lambda_i(x)
\]

where \( n + 1 \) is the number of input points, \( n \) is the order of the approximating polynomial, and \( \lambda_i(x) \) is calculated using

\[
\lambda_i(x) = \prod_{j=0, j \neq i}^{n} \frac{x - x_j}{x_i - x_j}
\]

Since the twenty-five response surface abscissas form a full tensor product set (that is, they form the complete set of combinations of the five abscissas in each dimension), a multi-dimensional Lagrange polynomial surface can be computed. If \( k \) indexes the total opacity abscissas and \( m \) indexes
Figure 9. PCHIP response surface at 41 km. Reference density of $1.73 \times 10^{-4} \text{kg/m}^3$. Sample inputs and sample response deviation from reference density given in black.

the Conrath parameter abscissas, the two-dimensional Lagrange polynomial is computed using

$$L(z, \{\tau_{tot}, \nu\}) = \sum_{k=0}^{5} \sum_{m=0}^{5} \rho(z, \{\tau_{tot_k}, \nu_m\}) \lambda_k(\tau_{tot}) \lambda_m(\nu).$$

The Lagrange polynomial response surface for density at 41 km is illustrated in Figure 8. This response surface generates suspicious extrema at the edges of the domain and in the vicinity of $\tau_{tot} = 0.6, \nu = 0.006$. It is the extreme dive at the left hand edge of the domain ($\tau_{tot} \to 0$) that is most concerning. All of the other suspicious extrema happen in regions of the domain that will not greatly influence the uncertainty structure. However, the left edge of the domain is a high probability area. The difficulty with the Lagrange polynomial is that one cannot automatically claim that suspicious extrema are wrong. Without propagating additional samples through PRAMS to check the response surface, it is impossible to tell how good a fit the Lagrange polynomial is.

D. Piecewise cubic Hermite interpolating polynomial

In contrast with the Lagrange polynomial, the piecewise cubic Hermite interpolating polynomial (PCHIP) is as mundane as any response surface could be. In one dimension, a PCHIP interpolates between two points using the unique cubic polynomial that matches the values and slopes of the two abscissas. If the lower of these two points is labeled $a$ and the upper is labeled $b$, then the interpolating polynomial approximating $y(x)$ for a point $x \in [a, b]$

$$H(x) = h_a(x|a, b) y(a) + h_b(x|a, b) y(b) + \dot{h}_a(x|a, b) \left[ \frac{dy}{dx} \right]_{x=a} - \dot{h}_b(x|a, b) \left[ \frac{dy}{dx} \right]_{x=b}$$
where
\[ h_a(x|a, b) = \left[ 1 + 2 \left( \frac{x - a}{b - a} \right) \right] \left( \frac{b - x}{b - a} \right)^2 \]
and
\[ h_b(x|a, b) = \left[ 1 + 2 \left( \frac{b - x}{b - a} \right) \right] \left( \frac{x - a}{b - a} \right)^2 \]

\[ \hat{h}_a(x|a, b) = (x - a) \left( \frac{b - x}{b - a} \right)^2 \]
\[ \hat{h}_b(x|a, b) = (x - x) \left( \frac{x - a}{b - a} \right)^2 \]

For a function of two variables, \( x_1 \) and \( x_2 \), the two-variable PCHIP response surface may be written as
\[ H(x_1, x_2) = h_a(x_1|a_1, b_1) h_a(x_2|a_2, b_2) y(a_1, a_2) + h_b(x_1|a_1, b_1) h_a(x_2|a_2, b_2) y(b_1, a_2) + h_a(x_1|a_1, b_1) h_b(x_2|a_2, b_2) y(a_1, b_2) + h_b(x_1|a_1, b_1) h_b(x_2|a_2, b_2) y(b_1, b_2) \]
\[ + \hat{h}_a(x_1|a_1, b_1) \left( h_a(x_2|a_2, b_2) \left[ \frac{\partial y}{\partial x_1} \right]_{x_1 = a_1, x_2 = a_2} + h_b(x_2|a_2, b_2) \left[ \frac{\partial y}{\partial x_1} \right]_{x_1 = a_1, x_2 = b_2} \right) \]
\[ + \hat{h}_b(x_1|a_1, b_1) \left( h_a(x_2|a_2, b_2) \left[ \frac{\partial y}{\partial x_1} \right]_{x_1 = b_1, x_2 = a_2} + h_b(x_2|a_2, b_2) \left[ \frac{\partial y}{\partial x_1} \right]_{x_1 = b_1, x_2 = b_2} \right) \]
\[ - \hat{h}_a(x_1|a_1, b_1) \left( h_a(x_2|a_2, b_2) \left[ \frac{\partial y}{\partial x_2} \right]_{x_1 = a_1, x_2 = a_2} + h_b(x_2|a_2, b_2) \left[ \frac{\partial y}{\partial x_2} \right]_{x_1 = a_1, x_2 = b_2} \right) \]
\[ + \hat{h}_b(x_1|a_1, b_1) \left( h_a(x_2|a_2, b_2) \left[ \frac{\partial y}{\partial x_2} \right]_{x_1 = b_1, x_2 = a_2} + h_b(x_2|a_2, b_2) \left[ \frac{\partial y}{\partial x_2} \right]_{x_1 = b_1, x_2 = b_2} \right) \]

for any point inside the rectangle whose vertices are \( \{a_1, a_2\}, \{b_1, a_2\}, \{a_1, b_2\}, \) and \( \{b_1, b_2\} \). The functions \( h_a(x|a, b), h_b(x|a, b) \), \( \hat{h}_a(x|a, b) \), and \( \hat{h}_b(x|a, b) \) retain the same definitions given for a one-dimensional PCHIP response surface. Substituting in \( \tau_{tot} \) for \( x_1 \), \( \nu \) for \( x_2 \), and density at a specific altitude for \( y \), transforms Equation 9 into the formula for the PCHIP response surface at that altitude.

There are two issues that must be resolved before applying this formula. First, PRAMS does not provide the partial derivatives of density with respect to total opacity or the Conrath parameter. Therefore, the derivatives must be estimated at each of the sample points. Secondly, although the interior of the grid outlined by the sample points illustrated in Figure 5 can clearly be subdivided into rectangles to which Equation 9 may be applied, this grid does not encompass the entire domain. The enclosure problem is managed by simply applying Equation 9 using the vertices of the nearest rectangle for points that are not enclosed by the samples drawn. For example, the point \( \{\tau_{tot} = 0.01, \nu = 0.05\} \) is interpolated using \( a_{\tau_{tot}} = 0.026542, b_{\tau_{tot}} = 0.124145, a_\nu = 0.022583, \) and \( b_\nu = 0.066964 \) even though \( \{\tau_{tot} = 0.01, \nu = 0.05\} \) does not fall within the rectangle formed by these vertices.

The derivatives in each dimension at each sample point are estimated by taking the derivative of a 2nd Order Lagrange polynomial based on the point itself and its two closest neighbors along that dimension. So, the resulting PCHIP response surface is not a true PCHIP, since it is based on an estimate of the slopes, rather than the true slopes. The result is a response surface that is continuous and differentiable at all points and behaves with a high degree regularity. Whereas the NIPC response surface suffers significant errors at the sample locations and the Lagrange polynomial undergoes suspicious oscillations, the PCHIP response surface shows extrema only where the sample values seem to indicate extrema. It is just a more intuitive response surface. Therefore, the PCHIP response surface is used in this work to propagate uncertainty from the dust parameters to atmospheric density.
E. Propagation of uncertainty across response surface

With an efficient response surface in hand, propagating uncertainty from the dust parameters to density is a relatively simple matter. The first step is to heavily sample the response surface. To this end, all one million combinations of a thousand points in total opacity and Conrath parameter each were processed through the response surface. This collection of points is labeled the stratified sample. Then, one thousand Monte-Carlo focal elements were drawn from the joint Dempster-Shafer structure on the dust parameters described at the end of Section III. For each input Monte-Carlo focal element, the resulting output focal element on density (at each altitude) is the closed interval bounded by the minimum and maximum output values resulting from the input points from the stratified sample that fall within the input focal element. These output focal elements, stacked upon each other (each with a height of 1/1000) are illustrated in Figure 10. These stacked focal elements form an approximation to the mapping-formalism representation of density uncertainty due to the dust parameter uncertainty.

V. Results

A. Dempster-Shafer structures on density

The Dempster-Shafer representations of density uncertainty at four different altitudes are given in Figure 10. These maps are used below to calculate canonical nested belief intervals. If one wished to compute the belief and plausibility value of the density at a particular altitude falling within some set, $A$, one need only apply Equations 3-4. Supposing that the original Dempster-Shafer representation of uncertainty in total opacity and the Conrath parameter are conservative, then the resulting belief and plausibility values on density will conservatively represent the uncertainty in density due to uncertainty in the dust (given the initial and boundary conditions of the Holden Crater simulation, level of grid refinement, etc etc).

Although perhaps of interest in their own right, these altitude-specific Dempster-Shafer representations of uncertainty are of little direct use to entry, descent, and landing (EDL) calculations. It is not the uncertainty in density at each altitude that matters for an EDL mission, but rather uncertainty in the entire density profile. The Dempster-Shafer representation of a density profile, while theoretically possible, would involve focal elements consisting of a continuum of density profiles (just as an interval focal element on a scalar variable is a continuum of points). The practical
Figure 11. Canonical nested belief intervals on density using various input representations of the dust parameters

representation of a continuum of density profiles is a mathematically arduous task. Nevertheless, the Dempster-Shafer approach to uncertainty and the response surface linking dust parameters to density profile would be of enormous value to EDL uncertainty quantification. If one wanted to propagate dust parameter uncertainty to uncertainty in a mission-critical quantity (such as landing location), one could supply sample density profiles to an EDL dynamics predictions code using the dust-to-density response surface. One could then build a response surface linking the dust parameters (and other perturbed inputs) to landing location and propagate uncertainty from the dust parameters to landing location the same way it has been propagated to density in this report. So, although the density uncertainties plotted in Figure 10 may not constitute a part of future EDL uncertainty quantification, they do result from the same process by which EDL uncertainty quantification would be conducted.

B. Contrast with Bayesian analysis

The Mars atmosphere uncertainty problem explored in this report illustrates the practical difference between the probability-bounds approach and Bayesian uncertainty analysis. Given only the information in Section III, it is impossible to build a joint frequentist probability distribution function for total opacity and the Conrath parameter without applying some baseless assumptions. The purpose of the analysis so far has been to demonstrate that the probability-bounds approach allows the analyst to avoid making the kind of spurious statistical assumptions necessary for a purely
probabilistic analysis.

Figure 11 demonstrates just how much false confidence is engendered by making standard probabilistic assumptions. Panel A of this figure illustrates the nested central belief intervals in density at each altitude using the Dempster-Shafer representation of uncertainty in the dust parameters. The remaining five panels are the results of different probabilistic analyses based on different possible assumptions about the probability distribution of the Conrath parameter and its relationship with total opacity. For Panels B-F, total opacity is assumed to have a gamma distribution, described by the following probability density function:

\[ f(\tau_{\text{tot}}) = \frac{1}{\Gamma(\alpha)\beta^\alpha} \tau_{\text{tot}}^{(\alpha-1)}e^{-\tau_{\text{tot}}/\beta} \]

where \( \Gamma(\alpha) = \int_0^\infty t^{\alpha-1}e^{-t}dt, \alpha = 1.877 \text{ and } \beta = 0.07719. \) The CDF of this distribution threads nicely through the middle of the map-function for total opacity illustrated in the right-hand panel of Figure 3.

The nested central belief intervals illustrated in Panel B are based on the assumption that the Conrath parameter is uniformly distributed on \([0.003, 0.17]\) and is stochastically independent of total opacity. To treat an interval-uncertain quantity as being uniformly distributed is common practice in probabilistic uncertainty analysis today. Assuming stochastic independence between two variables when their relationship is unknown is also a common practice. Panel B of Figure 11, therefore, gives the representation of uncertainty in density one could expect from a standard Bayesian analysis.

There is in the Mars atmosphere literature\(^{18,19}\) some indication that the Conrath parameter and total opacity should be inversely related. The reasoning is that as the Conrath parameter gets smaller, dust penetrates higher into the atmosphere. It is thought that a higher total opacity (and hence total dust content) will be linked to a higher relative distribution of dust. Panel C shows the resulting nested central belief intervals on density garnered by assuming that the Conrath parameter is uniformly distributed on \([0.003, 0.17]\) and that total opacity and the Conrath parameter have a relationship of opposite dependence. Opposite dependence is characterized by the following relationship:\(^{13}\)

\[ F_\nu(\nu) = 1 - F_{\tau_{\text{tot}}}(\tau_{\text{tot}}) \]

where \( F_{\tau_{\text{tot}}} \) and \( F_\nu \) are the cumulative distribution functions used to model total opacity and the Conrath parameter respectively. Opposite dependence is not necessarily the best way to represent a relationship that is vaguely known to be inverse, but it may be the simplest. For the representation of dust uncertainty, it is certainly no worse than assuming independence.

As was explored in Section IV, given interval uncertainty in a quantity, it may make more sense to represent a monotonic function of that quantity, rather than the quantity itself, with a uniform probability distribution. Panels D and E of Figure 11 are based on treating the natural logarithm of the Conrath parameter as being uniformly distributed on the interval \([\ln(0.003), \ln(0.17)]\). Modeling a uniform distribution on the logarithm of an interval uncertain quantity rather than the quantity itself is not unheard of when representing a quantity that varies over more than one order of magnitude. For representing uncertainty on the Mars dust parameters, this approach does generate wider nested central belief intervals than assuming that the Conrath parameter itself is uniformly distributed. However, even with this alternative assumption, the Bayesian approach still generates substantially tighter (i.e. less conservative) nested central belief intervals than the probability-bounds approach.

Panel F of Figure 11 illustrates the results of a best-guess estimation of the variability in the dust parameters. Rather than trying to stick a uniform distribution on the Conrath parameter or some simple monotone function thereof, the Conrath parameter is modeled as the following function of total opacity:

\[ \ln(\nu) = \ln(0.17) - \frac{\tau_{\text{tot}}}{0.834}(\ln(0.17) - \ln(0.003)) \]
Figure 12. Density focal elements using NIPC (red) and PCHIP (black) response surfaces.

Figure 13. Density focal elements using Lagrange polynomial (red) and PCHIP (black) response surfaces.

This function keeps the Conrath parameter bounded within the interval $[0.003, 0.17]$ and reflects knowledge of a vague inverse relationship between the Conrath parameter and total opacity.

The most notable value of these probabilistic analyses is that they represent the kind of reduction in uncertainty that is possible as knowledge about total opacity and the Conrath parameter is improved. There is a baseline level of variability in these two parameters. Of the different analyses presented here, it is the Author’s opinion that Panel F of Figure 11 gives the best-attempted representation of the uncertainty due to this variability alone. However, the probabilistic analyses are all guesses. A guess is not a representation of uncertainty. Only the Dempster-Shafer representation, resulting in the density nested central belief intervals in Panel A of Figure 11, accurately reflects the information for the dust parameters given in Section III.

C. Comparison of alternative response surfaces

As it turns out, the differences between the three response surfaces explored in the Section IV are fairly unimportant for the Mars dust uncertainty problem. As Figures 12 and 13 illustrate, the resulting mapping representations of density at a given altitude are largely similar. So, although
the PCHIP response surface is trusted most out of the three response surfaces explored, the fact is, any of these three response surfaces could be used to propagate uncertainty with a fair degree of assurance that the results will not be excessively erroneous.

As a whole, neither the NIPC expansion nor the Lagrange polynomial can be said to match the PCHIP response surface better than the other. The flat regions of the mapping representation of density at a given altitude, which result from the existence of a local minimum or maximum in the response surface, seem to match between the NIPC response surface and the PCHIP response surface better than either matches the Lagrange polynomial response surface. On the other hand, the nested central belief intervals using the Lagrange polynomial response surface match those obtained using the PCHIP response surface better than either matches the nested central belief intervals developed using the NIPC response surface, as illustrated in Figure 14. Nevertheless, it bears reiteration that the results obtained using the three response surfaces do not differ much in any event.

VI. Conclusions

Uncertainty in dust parameters alone leads to a roughly ±10% uncertainty in Mars atmospheric density at the 95% belief level. Dust-engendered uncertainty in density may be apportioned as being half due to variability in the dust loading and half due to ignorance about the shape and scale of the dust distribution. That is, the probabilistic analyses presented in this paper indicate that it would be reasonable to expect the nested central belief intervals on density to be reduced in width by roughly a factor of two were ignorance about the dust parameters eliminated. This is a rough estimate, however, as the various Bayesian probability distributions that were explored in Section B resulted in different estimates of the variability in the density profiles.

This paper has demonstrated that probability bounds analysis using Dempster-Shafer mathematics is practically feasible. The probability bounds approach requires more computational effort than the Bayesian approach, but it also requires fewer assumptions. The Mars atmosphere uncertainty analysis has demonstrated that the two approaches lead to significantly different results, with significantly different meanings. The different Bayesian analyses all result in approximately half as much uncertainty as that obtained via the probability bounds approach using Dempster-Shafer mathematics. The two approaches cannot be considered equivalent.

The question for an engineer quantifying Mars atmosphere uncertainty for a Mars lander project is which approach will lead to better design decisions. The Bayesian approach will almost certainly lead to thinner design margins than the probability bounds approach can justify. That, on its own, is
an attractive feature as it would justify a more cost-effective design. However, the Bayesian approach results in probabilities that express personal betting preference, a subjective quantity whose value does not directly relate to any concrete predictions about the state of the Mars atmosphere. In contrast, the probability bounds analysis supports the concrete claim that deviations of the density from the norm will fall within the stated 95% bounds (i.e. roughly \( \pm 10\% \); Panel A of Figure 11 gives a more detailed breakdown) in at least 95% of the situations similar (i.e. similar latitude and time of year) to the situation that the Mars Science Laboratory would encounter during a landing mission at Holden Crater. The validity of this prediction depends on the accuracy of the atmospheric model and the relevance of the data used for the dust parameters, both of which may be subject to question; but, at least, it is a claim that can be verified or refuted with future measurement. Bayesian analysis supports no such empirical claim; or, to put it more precisely, a subjectivist Baycsian statistician would state that it does not matter if the 95% bounds do or do not capture the atmospheric density 95% of the time.\(^4\)\(^5\) Under the subjectivist standard, it only matters that the probability values precisely represent the analysts’ collective personal willingness to commit to a proposition.\(^2\)\(^3\)\(^4\)\(^5\)\(^8\) The reader can judge which standard is more appropriate for design analysis on a Mars lander project. There is still an alternative case to be made for the best-guess Bayesian analysis (i.e. Panel F of Figure 11) as a good-faith estimate of the real underlying atmospheric variability; and this might be an appropriate representation of uncertainty, if the purpose of uncertainty quantification is an estimate of variability for variability’s sake. However, if the purpose of uncertainty quantification is to support the selection of rational and empirically justified design margins, then there is a strong case to be made for the more conservative probability bounds approach.

References


