Sensitivity and Uncertainty Analysis of a Polyurethane Foam Decomposition Model

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Abstract

Sensitivity/uncertainty analyses are not commonly performed on complex, finite-element engineering models because the analyses are time consuming, CPU intensive, nontrivial exercises that can lead to deceptive results. To illustrate these ideas, an analytical sensitivity/uncertainty analysis is used to determine the standard deviation and the primary factors affecting the burn velocity of polyurethane foam exposed to fire-like radiative boundary conditions. The complex, finite element model has 25 input parameters that include chemistry, polymer structure, and thermophysical properties. The response variable was selected as the steady-state burn velocity calculated as the derivative of the burn front location versus time. The standard deviation of the burn velocity was determined by taking numerical derivatives of the response variable with respect to each of the 25 input parameters. Since the response variable is also a derivative, the standard deviation is essentially determined from a second derivative that is extremely sensitive to numerical noise. To minimize the numerical noise, 50-micron elements and approximately 1-msec time steps were required to obtain stable uncertainty results. The primary effect variable was shown to be the emissivity of the foam.

Simplified Model

Figure 1.A shows a comparison between an X-ray and a 2-D finite element simulation of an 8.8-cm diameter right circular cylinder of polyurethane foam encapsulating a solid 3.8-cm diameter by 6.4-cm long right circular cylinder of 304 stainless steel. The X-ray and model show exceptional agreement when comparing the shape of the burn front after a 10-minute exposure to an incident flux of 25-W/cm². The 2-D serial simulation required 11 days and 16 hours

Figure 1. A) Original and B) simplified model

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* Burning is defined as material destruction by heat. Burning of polyurethane foam is an endothermic process that requires an external heat source to propagate a slow burning front.
of CPU time on a 400-Mhz SUN-Ultra-2 using 11,209 elements. Even with massively parallel computers, an uncertainty analysis for this CPU-intensive model is difficult. A simple representation of the complex model is needed for efficient sensitivity analysis. Figure 1.B shows a single row of elements with a radiation boundary condition. This simple 1-D model will be used in lieu of the complex 2-D model to do sensitivity/uncertainty analysis. Gartling et al. (1998), Chu et al. (1999), and Hobbs et al. (2000) give details about the finite element model, decomposition experiments, and decomposition model, respectively.

The response variable for the 1-D analysis was chosen as the steady-state "burn velocity" of the foam, calculated as the derivative of the burn front location versus the elapsed time for element death. Figure 2.A shows the front location calculated using 25-μm elements exposed to a 1,000° C radiative temperature. The burn front location is taken as the centroid of the element associated with the radiation boundary. Elements are removed when the condensed fraction drops below 1 percent.

**Numerical Issues**

Figure 2.B shows burn front velocities calculated using various element sizes. Table 1 gives the average time steps, decomposition front velocities, and CPU times for the solutions shown in Fig. 2. The larger time steps (large Δtave) are based on an auto time stepping scheme discussed by Gartling et al. (1998) with an integration convergence tolerance of 10^-4. The solutions obtained with smaller time steps (small Δtave) are based on the same convergence tolerance but are constrained to satisfy the following derivative smoothness criterion:

\[
\Delta t \leq 0.003 \Delta t/V,
\]

where Δt, Δx, and V represent the time step, element size, and burn velocity, respectively. In Fig. 2.B, the small time step solutions are smooth (solid lines, 0.5-mm and 1-mm) compared to the noisy solutions obtained with larger time steps. The small time step

<table>
<thead>
<tr>
<th>Grid</th>
<th>Large Δtave (auto)</th>
<th>Small Δtave (Eq. 1)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25 μm</td>
<td>Δtave = 0.066 sec</td>
<td>Δtave = 0.00041 sec</td>
</tr>
<tr>
<td></td>
<td>Vave = 1.12 cm/min</td>
<td>Vave = 1.10 cm/min</td>
</tr>
<tr>
<td></td>
<td>CPU = 13 min</td>
<td>CPU = 5 hrs</td>
</tr>
<tr>
<td>50 μm</td>
<td>Δtave = 0.076 sec</td>
<td>Δtave = 0.00083 sec</td>
</tr>
<tr>
<td></td>
<td>Vave = 1.11 cm/min</td>
<td>Vave = 1.09 cm/min</td>
</tr>
<tr>
<td></td>
<td>CPU = 6 min</td>
<td>CPU = 1 hr</td>
</tr>
<tr>
<td>0.5 mm</td>
<td>Δtave = 0.14 sec</td>
<td>Δtave = 0.0095 sec</td>
</tr>
<tr>
<td></td>
<td>Vave = 0.94 cm/min</td>
<td>Vave = 0.91 cm/min</td>
</tr>
<tr>
<td></td>
<td>CPU = 70 sec</td>
<td>CPU = 110 sec</td>
</tr>
<tr>
<td>1.0 mm</td>
<td>Δtave = 0.202 sec</td>
<td>Δtave = 0.023 sec</td>
</tr>
<tr>
<td></td>
<td>Vave = 0.77 cm/min</td>
<td>Vave = 0.76 cm/min</td>
</tr>
<tr>
<td></td>
<td>CPU = 120 sec</td>
<td>CPU = 130 sec</td>
</tr>
</tbody>
</table>

Table 1: Time step and CPU requirement
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curves for 25- and 50-μm element solutions overlie each other, so the less costly 50-μm element using fixed time step results are effectively converged. The noisy velocities in Fig. 2.B resulted from taking excessively large time steps for the instantaneous derivative calculation. Rather than imposing the time step constraint in Eq. (1), the integration convergence tolerance could have been decreased with the same expense of increased CPU cost.

The numerical noise is related to the discrete removal of elements from the computational domain. Figure 3 shows the temperature gradient in element No. 20 for a 650°C radiation temperature using 0.6-mm elements. The first 20 elements are also shown in Fig. 3 centered about the time of “element death.” The noise is associated with the death of neighboring elements and is likely the source of the sensitivity to the computational time step.

The remainder of this paper will focus on determination of the standard deviation of the burn velocity and ranking the importance of the 25 model input parameters. Fully grid and time-step converged solutions using 50-μm elements and -1-msec time steps were used in the analysis.

**Mean Value Sensitivity/Uncertainty Analysis**

In the mean value (MV) method, the mean burn velocity, \( \mu_V \), and the standard deviation of the burn velocity, \( \sigma_V \), can be determined from a simple Taylor series expansion of the burn velocity, \( V(\vec{\xi}) \), about the mean of the individual random variables or input parameters, \( \vec{\xi} \), by neglecting higher order terms as follows:

\[
\mu_V = V(\vec{\xi}) \bigg|_{\vec{\xi} = \vec{\mu}} \\
\sigma_V^2 = \sum_{i=1}^{n} \left[ \sigma_i \left. \frac{\partial V(\vec{\xi})}{\partial \xi_i} \right|_{\vec{\xi} = \vec{\mu}} \right]^2.
\]

Equation (2) is a single-sample approximation of the mean burn velocity calculated with the finite element model with all input parameters equal to the mean values, \( \vec{\mu} \). In Eq. (3), \( \sigma_V \) is the standard deviation of the burn velocity (response variable) and \( \sigma_i \) is the standard deviation of the \( i^{th} \) input parameter (random variable). The derivatives in Eq. (3) were obtained using a central differencing technique using a finite difference step size of 0.001 times the mean input parameter. For each temperature, 51 function evalu-
tions (two for each random variable plus one evaluation at the mean input values) were required to obtain the derivatives for the 25 random variables.

The relative importance of each input variable to the uncertainty in the burn velocity can be determined from the sensitivity coefficients, \( \gamma_i \), defined as:

\[
\gamma_i = \frac{\sigma_r}{\sigma_y} \times \frac{\partial y}{\partial x_i},
\]

where

\[-1 \leq \gamma_i \leq 1 \quad (4)\]

and

\[\sum_{i=1}^{n} \gamma_i^2 = 1. \quad (5)\]

The input variables that contribute the most to the uncertainty in the burn velocity also have the largest absolute sensitivity values. The sign of the sensitivity coefficients indicate that an increase in the input parameter causes an increase in the response function. A negative sensitivity coefficient indicates that an increase in the input parameter causes a decrease in the response function. The square of the sensitivity coefficient multiplied by 100 gives an importance factor, \( 100 \times \gamma_i^2 \), that can be used to easily identify which input variables are important.

**Input parameters**

The means, \( \mu_i \), and standard deviations, \( \sigma_i \), of the following 25 input parameters are given in Table 2: the initial density and temperature of the foam (\( \rho_i \) and \( T_i \)), the temperature-dependent thermal conductivity and specific heat of the foam (\( k \) and \( C_p \)), the coordination number of the polymer lattice (\( s+1 \)), the initial lattice bridge population (\( L_i \)), the reaction enthalpy of the foam (\( h_r \)), the emissivity of the foam (\( \varepsilon \)), 16 activation energies (\( E_i \)), and the average standard deviation of all the activation energies (\( E_0 \)). The input parameters

<table>
<thead>
<tr>
<th>( \rho_i ) g/cc</th>
<th>( T_i )</th>
<th>( k )</th>
<th>( C_p )</th>
<th>( s+1 )</th>
<th>( h_r ) cal/cm³</th>
<th>( \varepsilon )</th>
<th>( E_1 )</th>
<th>( E_2 )</th>
<th>( E_3 )</th>
<th>( E_4 )</th>
<th>( E_5 )</th>
<th>( E_6 )</th>
</tr>
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<tr>
<td>0.353</td>
<td>300</td>
<td>1</td>
<td>1</td>
<td>2.8</td>
<td>0.78</td>
<td>15</td>
<td>0.8</td>
<td>48.8</td>
<td>50.5</td>
<td>49.7</td>
<td>50.2</td>
<td>49.4</td>
</tr>
<tr>
<td>0.0252</td>
<td>3</td>
<td>0.1</td>
<td>0.1</td>
<td>0.2</td>
<td>0.05</td>
<td>1.5</td>
<td>0.05</td>
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<td>0.3</td>
<td>0.3</td>
<td>0.3</td>
<td>0.3</td>
</tr>
<tr>
<td>( E_i )</td>
<td>( E_i )</td>
<td>( E_i )</td>
<td>( E_i )</td>
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<td>( E_i )</td>
<td>( E_i )</td>
<td>( E_i )</td>
<td>( E_i )</td>
</tr>
<tr>
<td>49.1</td>
<td>50.6</td>
<td>49.5</td>
<td>51.2</td>
<td>49.4</td>
<td>50.3</td>
<td>49.7</td>
<td>50.6</td>
<td>50.7</td>
<td>50.2</td>
<td>49.7</td>
<td>3.97</td>
<td></td>
</tr>
</tbody>
</table>

\| \( \mu_i \) \| \( \sigma_i \) \| 0.3 | 0.3 | 0.3 | 0.3 | 0.3 | 0.3 | 0.3 | 0.3 | 0.3 | 0.3 | 0.05 |

\( a \) The temperature-dependent thermal conductivity and heat capacity were multiplied by a factor.

\( b \) Activation energies in Kcal/mol

**Table 2: Means and standard deviations of input parameters**
are assumed to be independent random variables that are normally distributed. Some of the mean input parameters - e.g. activation energies - were determined by optimizing predicted mass loss to experimental Thermal Gravimetric Analysis (TGA) data. Other mean input parameters, such as thermal conductivity and specific heat, were measured at Purdue’s Thermophysical Properties Research Laboratory. The standard deviations for the input parameters were taken to be approximately 10 percent of the mean value for all parameters except the initial temperature which is thought to be known to within 3° C and the activation energies which are assumed to be within 300 Kcal/mol.

Sensitivity/Uncertainty Results

Figure 4 shows the mean with a 1.96-σ band and the standard deviation of burn velocity, the importance of the most significant input parameters, and various sensitivity coefficients as a function of the radiative boundary temperature. The most important input parameters are shown to be the emissivity of the foam followed by the foam heat capacity and density. The lattice coordination number and the activation energies associated with Reactions 5, 6, and 9 are also shown to be important factors in Fig. 4.B. An increase in emissivity will cause the burn velocity to increase, whereas an increase in density or heat capacity will cause the burn velocity to decrease.

![Figure 4. A) Velocity, B) importance factors, and C) sensitivity coefficients](image)

Experimental Design Techniques

The primary effects of various model parameters were also obtained using a simple two-level 28-run Plackett-Burman (PB) analysis. Parameter interactions could have been obtained using general factorial designs but were considered beyond the scope of the present study. Table 3 shows the top three primary effect factors calculated

<table>
<thead>
<tr>
<th>Rank</th>
<th>1.000° C</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>PB auto^*</td>
</tr>
<tr>
<td>1</td>
<td>C_σ</td>
</tr>
<tr>
<td>2</td>
<td>ρ_σ</td>
</tr>
<tr>
<td>3</td>
<td>ε</td>
</tr>
</tbody>
</table>
with 1) the PB analysis using the large, auto time step option (PB-auto); 2) the MV method using the large, auto time step option (MV-auto); and 3) the MV method using a small, stable time step of ~1-msec (MV-1-msec). The MV-1-msec results give the best estimate of the true ranking of the importance factors. Note that the PB analysis gives the correct top three primary effect variables, even with the coarser auto time step option.

Summary and Conclusions

The sensitivity and uncertainty associated with burning of rigid polyurethane foam has been examined using a mean value analysis for radiation boundary temperatures ranging from 600° C to 1,000° C. Numerical noise caused the sensitivity/uncertainty analyses on this complex engineering model to be frustrating and time consuming. For example, the sensitivity/uncertainty analysis was repeated numerous times when the elements and/or time steps were found to be too large to obtain adequate sensitivity coefficients resulting in thousands of additional functional evaluations. A lot of frustration could have been avoided if a thorough study of the problem numerics had been initiated before beginning the sensitivity/uncertainty analysis. Also, the sensitivity analysis was repeated multiple times as the uncertainties in input parameters were refined.

The numerical noise associated with the sensitivity coefficients was related to the discrete removal of elements from the computational domain. When an element was removed, the radiation boundary condition was reapplied to the newly exposed element. This discrete change in the surface temperature of the exposed element caused large fluctuations in the temperature gradient within elements that were within close proximity of the advancing decomposition front. Using small time steps reduced the numerical instability considerably. In the current work, fully converged solutions required 50-μm elements with approximately 1-msec time steps.

Despite the difficulties in performing the sensitivity/uncertainty analysis on the complex finite element combustion model, stable burn velocities and sensitivity coefficients were obtained. The most important factors affecting the burn rate were shown to be the thermophysical properties of the foam (emissivity and thermal capacitance). These parameters were also shown to be important using a Plackett-Burman analysis using larger time steps.

References

