Sensitivity Analysis - Overview

In the current context, the goal of sensitivity analysis is to determine which parameters most strongly affect a given quantity of interest (QoI). Only parameters to which a given QoI is sensitive will be informed by calibrations based on data for that QoI.

Scenario:
- 1-D, steady shock.
- Upstream speed $= 8000$ m/s.
- Upstream number density $= 3.22 \times 10^{21} \, \text{m}^{-3}$.
- Upstream composition by volume: 79% $N_2$, 21% $O_2$.
- Upstream temperature $= 300 \, K$.

Parameters:
Our current sensitivity analysis focused on the rate constants for reactions which take place in five-species air.

Sensitivity Analysis - Results

QoI: We are not yet at a point where the DSMC simulation results can be compared with experimental shock tube results from EAST, and so we must choose a surrogate QoI. For this work, we have chosen the density of NO as our QoI. We have found in past work that this QoI is sensitive to several of our parameters. We are not concerned with just one specific point downstream of the shock, instead we are interested in how changes in the rate constants affect the non-equilibrium chemistry in the post-shock region. For this reason, we need to treat our QoI as a vector, where each component of that vector represents $\rho_{NO}$ at a specific $x$-location. The sensitivity analysis methods we will use, however, are intended for a scalar QoI. To overcome this problem, we treat the vector QoI as a set of scalar QoIs. We apply the full sensitivity analysis procedure to each scalar QoI and then combine the results of those individual analyses.

Conclusions

- Global, Monte Carlo based sensitivity analysis can provide a great deal of insight into how various parameters affect a given QoI.
- Sensitivities based on $\rho^2$ are similar to those based on the mutual information, but there are notable differences for some parameters.
- We find that our surrogate QoI, $\rho_{NO}$, is most strongly affected by the rates for $NO$ dissociation reactions, the $NO$ exchange reactions, and the dissociation of $N_2$, by $N$. These results are not unexpected, and fit with our prior understanding of the chemistry which takes place behind an 8 km/s shock.

Future Work

- Synthetic data calibrations for a 1-D shock with the current code.
- Upgrade the code to allow modeling of ionization and electronic excitation.
- Couple the code with a radiation solver.
- Sensitivity analysis for a 1-D shock with the additional physics included.
- Synthetic data calibrations with the upgraded code.
- Calibrations with experimental data from EAST or similar facility.