Temperature-Dependent Feature Sensitivity Analysis for Combustion Modeling

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Motivation

• Sensitivity analysis is one of the most widely used tools in kinetic modeling.
• Typically, it is performed by perturbing the A-factor of the individual reaction-rate or binary diffusion coefficients and monitoring the effect of these perturbations on the observations.
• However, the sensitivity coefficients obtained in this manner do not contain any information on possible temperature-dependent effects. Yet, in many combustion processes, temperature-dependent kinetic parameters are crucial because of local parameters and specific experimental conditions. The obtained information is determined to be of critical importance in understanding combustion processes and their sensitivity to changes in experimental conditions.

Temperature Dependent Sensitivity Analysis (TDSA)

• Sensitivity coefficients are calculated at every temperature in order to compute the sensitivity spectrums of the major source reactions at different origin (CO and HCO), the sensitivity windows for reaction (R2) in propylene flames will generally differ from those of CO flames.

Sensitivity Coefficients for (R2) and (R3)

As compared to the same reaction in CO flames and hydrogen flames, the reverse reaction (R3) is much more sensitive to temperature, while the reverse reaction (R1) is somewhat more sensitive to temperature, which is particularly true for CO flames and hydrogen flames. As with the forward reaction (R2), although the sensitivity is not dependent on pressure, conditions of higher temperature and lower pressure will result in larger sensitivity at the lower temperatures.

Summary and Conclusions

• A novel applied sensitivity analysis method using perturbed rate constants of reaction-dependent Dirac-delta-shaped profile similar to the range of temperatures and the corresponding sensitivity coefficients, which are determined by the temperature interval.
• Sensitivity results indicate that in the sensitivity spectrums, the temperature-dependent sensitivities are also visible and can be expected to change shapes at different temperatures.
• Sensitivity analysis in keeping with the change of temperature and kinetic development was also demonstrated.

Application: Choice of the Rate Coefficient

The rate curves closely follow the corresponding sensitivity coefficients for the C_5H_8 case. Clearly, in such cases, the sensitivity of the specific rate coefficients can be used to identify the most significant temperature dependence in the flame structure.


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Methanol Flame

Sensitivity Coefficients for Propylene Flame

As evidenced by the example of (R2) for CO/H_2 flame, the reaction rate, while closely following the corresponding sensitivity coefficients, can change sign at high pressures and fuel-rich conditions. As a result, the sensitivity coefficients estimated based on the reaction rate curve would be substantially underestimated.

Sensitivity Coefficients for H/He binary diffusion coefficient

The rate curves closely follow the corresponding sensitivity coefficients for the C_3H_8 case; clearly, in such cases, the sensitivity of the specific rate coefficients can be used to identify the most significant temperature dependence in the flame structure.

Sensitivity Coefficients for HCO/H_2 kinetic model

The rate curves closely follow the corresponding sensitivity coefficients for the C_3H_8 case; clearly, in such cases, the sensitivity of the specific rate coefficients can be used to identify the most significant temperature dependence in the flame structure.

Sensitivity Coefficients for CO/H_2 kinetic model

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Sensitivity Coefficients for H/He binary diffusion coefficient

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