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Global Sensitivity Analysis for Chemical Kinetics of Hydrocarbon Combustion

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Introduction

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- Numerical predictions of combustion need to account for uncertainties in model parameters for reliability purposes
- Global sensitivity analysis (GSA) informs reduction of stochastic dimensionality for uncertainty quantification analysis
- Objective: Perform GSA in reaction kinetic models for combustion of complex hydrocarbons

Local vs. Global SA

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Local Sensitivity Analysis

- emphasizes the local impact (at a point) of the parameters on the model
  - Differential analysis falls under this category
- not useful in this case because the model is nonlinear over a range of parameters

Global Sensitivity Analysis

- emphasizes the contribution of each parameter to the overall uncertainty in the output
  - Sampling approach
  - Monte Carlo analysis, method of Sobol', and Fourier amplitude sensitivity test (FAST) are some examples

Background

- Temperature dependence of rate coefficients
  - A + B + … $\xrightarrow{k}$ C + D + …

    where k = rate coefficient of the reaction
  - Arrhenius model: $k = AT^n \exp(-\frac{E}{RT})$
  - Assume all uncertainty in k is due to uncertainty in A
    (in this instance only; in general there is uncertainty in A, n, and E)
- Dimensionality ~ number of reactions
  - Konnov hydrogen mechanism – 30 reactions, 33 dimensions
  - Tomlin n-butane mechanism – 1111 reactions, 1127 dimensions
- Investigating 0-D Ignition
  - Quantity of interest: ignition-delay time for 0-D ignition
  - Factors: initial conditions (temperature, pressure, mole fractions); number of samples; uncertainty factors (for each rate coefficient)

Method

- Use TChem (open source tool to analyze reaction kinetic models) and CVODE (tool to numerically integrate initial value problems) to simulate ignition, obtain *A* coefficients and ignition-delay times
- Calculate total effect indices, derived from method of Sobol':
  - total order sensitivity indices, or total effect indices, measure an input variable's contribution to the variance of the output
  - here, the total effect index, S_j^T, for the j[th] factor:

$$S_j^T = \frac{E_{x_{\sim i}}(V(y \mid x_{\sim j}))}{V(y)}$$

    - $x = (x_1,\ldots,x_n)$
    - $y = f(x)$

  - estimate using Monte Carlo sampling:

$$S_i^T = \frac{1}{2V}\left(\frac{1}{N}\sum_{j=1}^{N}\left(f(x^j) - f(x_{-i}^j \cup x_i''^j)\right)^2\right)$$

Konnov Mechanism

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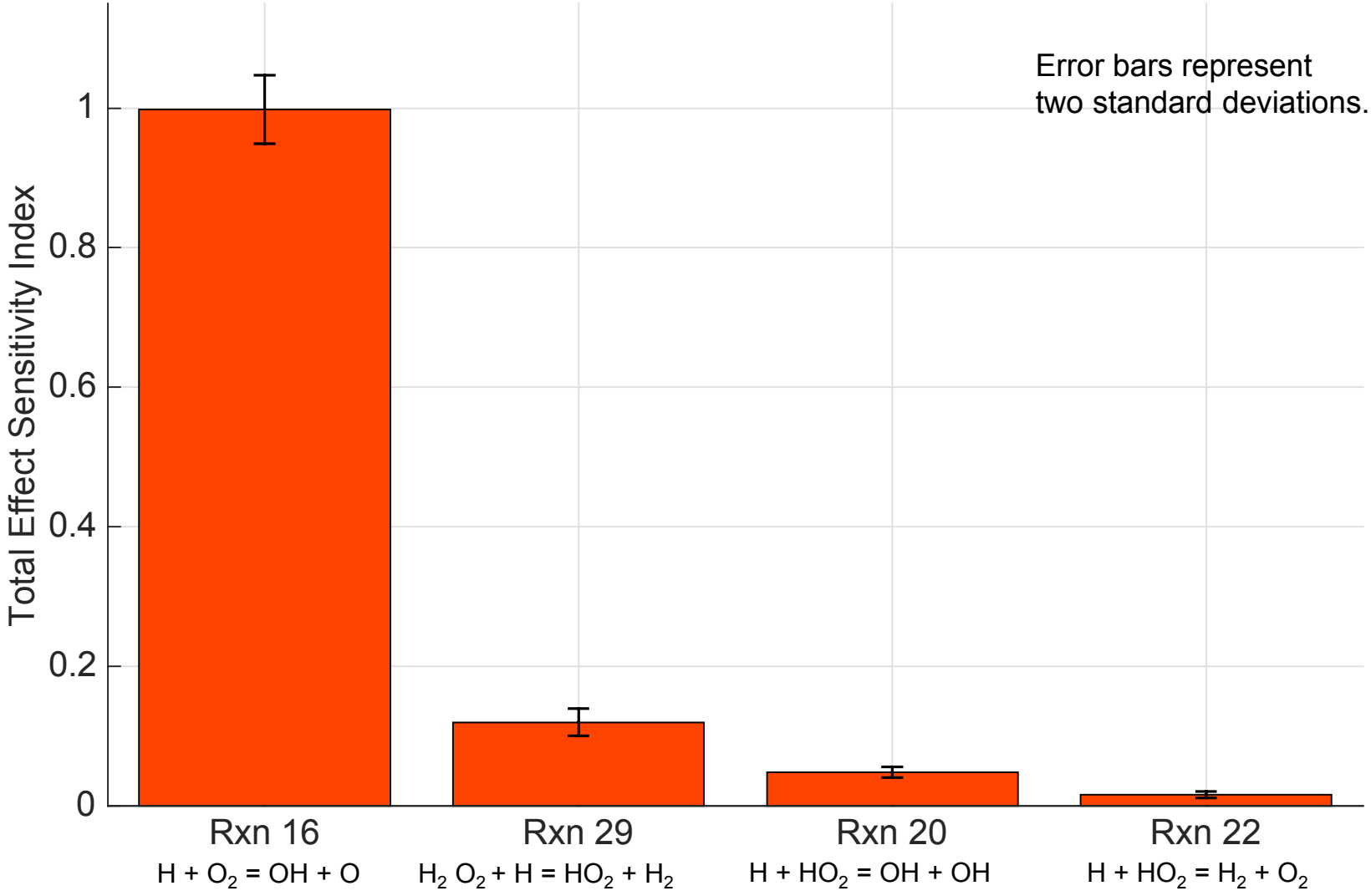
- Hydrogen, H_2
- 33 dimensions
- 10,000 samples
- Initial conditions: T = 1000K, P = 1 atm, stoich. mixture
- Computational expense:
  - execution time goes up with number of species, number of reactions, and numerical stiffness of the mechanism
  - 0.020 sec to run one ignition
- Results
  - include indices over 0.01
  - Chain branching – Rxn 16: $H + O_2 = OH + O$
  - Chain termination – Rxn 29: $H_2O_2 + H = HO_2 + H_2$

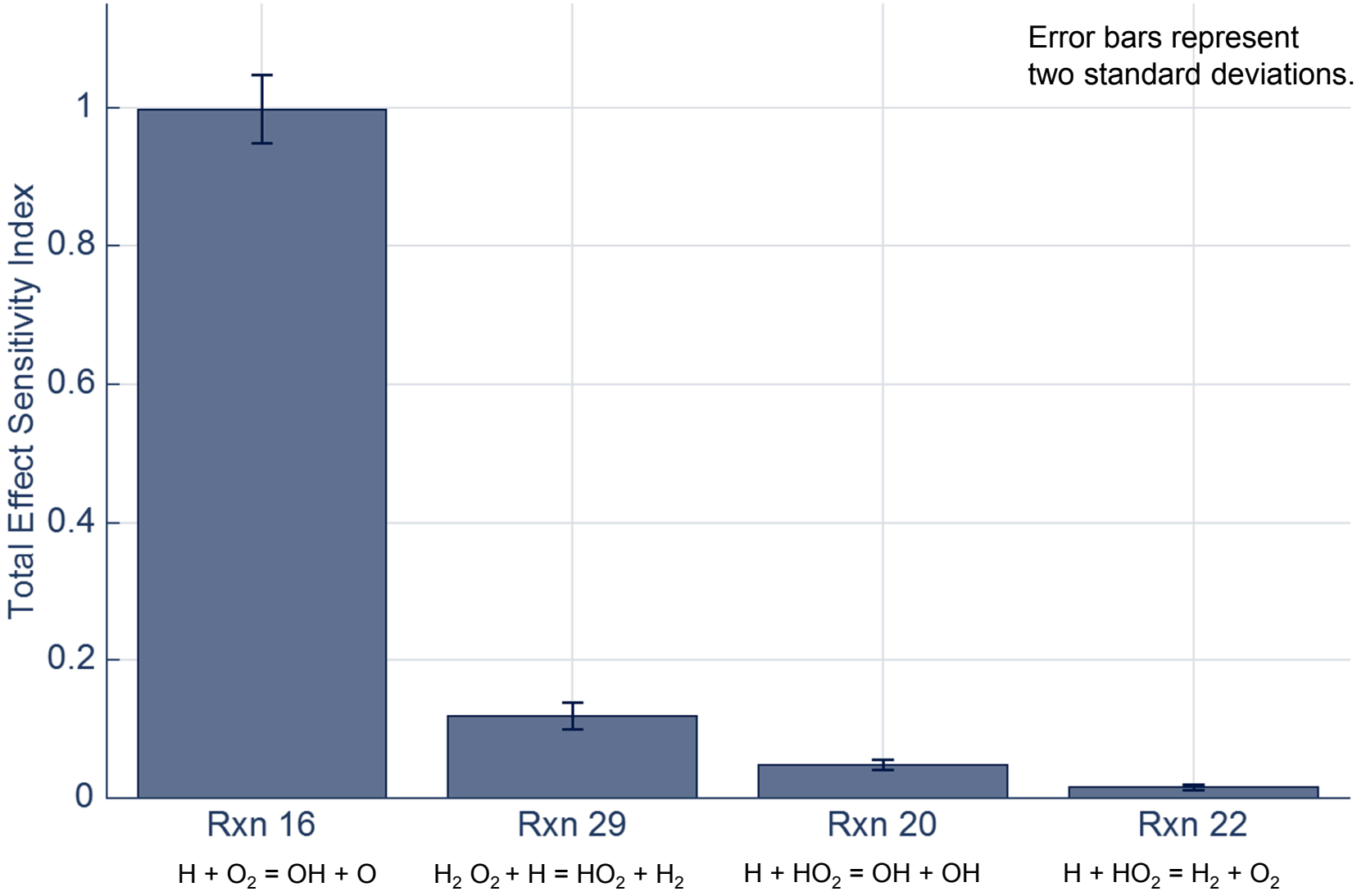
Total Effect Indices for the Konnov Hydrogen Mechanism



Tomlin Mechanism

- n-butane, C_4H_{10}
- 1127 dimensions
- 500 samples
- Initial conditions: T = 1000K, P = 1 atm, stoich. mixture
- Computational expense:
  - execution time goes up with number of species (177 vs. 12), number of reactions (1111 vs. 30), and numerical stiffness of the mechanism
  - 9.70 sec to run one ignition

Total Effect Indices for the Konnov Hydrogen Mechanism



Conclusion

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- For the Konnov mechanism, ~4 important reactions
- For the Tomlin n-butane mechanism, ~5-10 important reactions
  - if Tomlin results show 5 – 10 indices above 1%, then this indicates that as dimensionality increases from 33 to 1127 (which is 34x), the number of important indices does not multiply by 34x (number of important indices is independent of dimensionality)
- Execution time
  - much longer than proportional to run n-butane than hydrogen
  - hydrogen: 0.020 sec vs. n-butane: 9.70 sec to run 1 ignition

Future Work

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- Observe the scatter of the sensitivity indices for the n-butane mechanism to determine if dimensionality influences the level of accuracy associated with a certain number of samples
- Perform more extensive GSA on a subset of the parameters deemed important from the initial analysis
- Examine effect of initial conditions on sensitivity indices
- Examine different quantities of interest
  - species' concentration profiles
  - flame speed (flame calculations)

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