Mechanism reduction strategies for gasoline surrogate fuels

Kyle Niemeyer[1,2] and Chih-Jen Sung[2]

[1]Case Western Reserve University, Cleveland, OH, USA; [2]University of Connecticut, Storrs, CT, USA

Detailed mechanisms need reduction

Modeling complex transportation fuels such as gasoline is difficult due to the near-continuous spectrum of hydrocarbon components. One solution is to use a "surrogate," which represents the real fuel with a mixture of specific hydrocarbon components.

While this approach can successfully match the physical and chemical properties of fuels, it unfortunately results in very large detailed mechanisms, as seen in Figure 1.

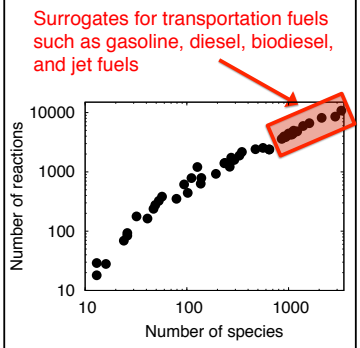

Figure 1. Sizes of detailed mechanisms for hydrocarbon fuels.

Reduction techniques may be performed in order to reduce the size and complexity of detailed mechanisms. Figure 2 shows our multi-stage approach, based on the work of Lu and Law [1]; our strategy centered on the directed relation graph with error propagation and sensitivity analysis (DRGEPSA) skeletal reduction method [2].

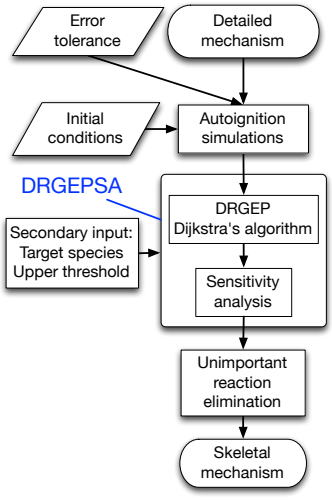

Figure 2. DRGEPSA-based mechanism reduction strategy.

Reduction of gasoline surrogate

In this work we focused on the recently developed surrogate for gasoline of Mehl et al. [3,4], which emulates experimental engine data, flame speeds, shock tube ignition delays, and more recently rapid compression machine autoignition [5] using research-grade gasoline. It consists of 1389 species and 5936 reversible reactions—far too large to be used in practical engine simulations. Further, it consists of four components: n-heptane, iso-octane, toluene, and 2-hexene.

Here, we targeted HCCI operating conditions for a reduction of the gasoline mechanism, using autoignition initial conditions covering 700–1200 K, 10–60 atm, and $0.2 \leq \phi \leq 1.0$. We specified an error limit of 10% with respect to ignition delay.

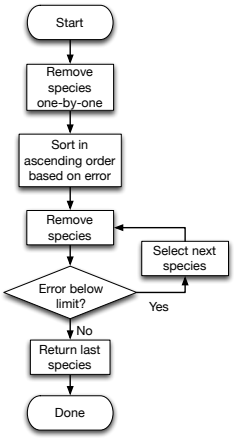

Figure 3. Original (naïve) sensitivity analysis algorithm.

Greedy sensitivity analysis

In order to reduce the gasoline surrogate mechanism further, we introduced a new sensitivity analysis algorithm for DRGEPSA: the greedy SA approach. Figures 3 and 4 show the original and greedy versions of SA, respectively. By reevaluating the induced error of each species after a removal, the algorithm is able to use the most up-to-date information about species, rather than relying on the original induced error information.

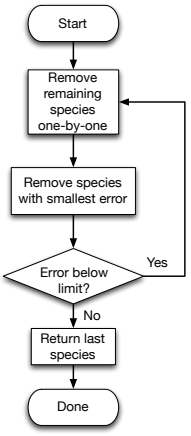

Figure 4. New greedy sensitivity analysis algorithm.

Resulting skeletal mechanisms

The combined DRGEPSA and unimportant reaction elimination methods, when used with each of the SA algorithms, resulted in skeletal mechanisms with:

- Original (naive) SA: **344 species & 1297 reactions**
- Greedy SA: **233 species & 910 reactions**

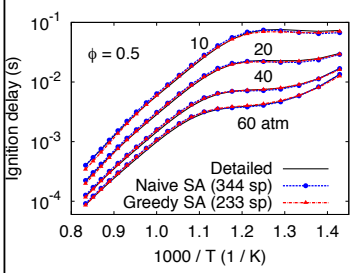

Figure 5. Ignition delay validation of gasoline skeletal mechanisms, for ϕ = 0.5. Comparisons for ϕ = 0.2 and ϕ = 1.0 show similar good agreement.

Validation

We performed validation studies of both skeletal mechanisms, using homogeneous autoignition, as demonstrated in Figure 5, and single-zone HCCI simulations, as shown in Figure 6. In all cases considered, both skeletal mechanisms performed nearly indistinguishably and with good agreement compared to the detailed mechanism.

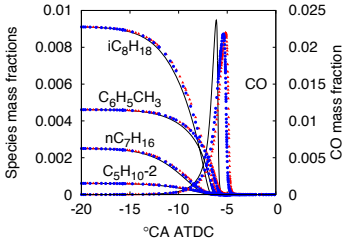

Figure 6. Species profiles for HCCI simulations using both skeletal mechanisms, for initial conditions of 447 K, 1 atm, and ϕ = 0.5; compression ratio = 14 and engine speed = 900 rpm.

Conclusions

Detailed mechanisms for surrogate fuels can be used to closely emulate the physical and chemical properties of complex transportation fuels such as gasoline, but are typically too large to be used unchanged. In this work, we

- applied a multi-stage reduction approach to a detailed mechanism for gasoline surrogates, using DRGEPSA followed by further unimportant reaction elimination,
- demonstrated a new greedy sensitivity analysis algorithm that reduced significantly more species (~100) using the same error limit,
- generated skeletal mechanisms with 344 and 233 species using the original (naïve) and greedy algorithms, respectively, and
- showed that both mechanisms performed well compared against the detailed mechanism in autoignition and HCCI simulations.

Similar strategies can be used to reduce detailed mechanisms for other multicomponent surrogate fuels, such as for diesel, biodiesel, and jet fuels. Our future plans include further study of the new greedy sensitivity analysis, the inclusion of additional reduction stages including isomer lumping and CSP-based QSS reduction.

Literature cited

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Further information

Kyle Niemeyer
kyle.niemeyer@case.edu
www.kyleniemeyer.com

Chih-Jen Sung
cjsung@engr.uconn.edu
http://combdiaglab.engr.uconn.edu/

CASE WESTERN RESERVE UNIVERSITY EST. 1826

University of Connecticut