

Hexadecane mechanisms: Comparison of hand-generated and automatically generated with pathways

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1. A detailed hexadecane mechanism with 2176 species and 7269 (reversible) reactions was developed
2. The hexadecane mechanism was created with the automatic generation system: REACTION.
3. A systematic comparison showed that a automatic generation and by hand generation can be similar.
4. Ignition delay times and the sensitivity of different reaction classes was calculated.

Abstract

In this paper, the automatically generated mechanism for hexadecane with both high and low temperature chemistry included is compared to a systematically generated mechanism by hand. In contrast to other systems for automatic generation, the REACTION system uses pathways to organize the application of reaction classes. A pathway is a sequence of reaction classes where only those species produced by the previous step of the pathway are used in the current step of the pathway. This "controlled" generation process not only mimics what is done by hand, but also helps to limit the size of the generated mechanisms. Both systematic reaction by reaction comparisons and numerical simulation (zero-dimensional constant volume) comparisons were done and the mechanisms were found to have minor differences. Both mechanisms used the same set of reaction classes to model the high and low temperature combustion chemistry of all n-alkanes up to hexadecane. In addition, a sensitivity analysis of all the reaction classes was performed. The generated mechanism has 2176 species and 7269 (reversible) reactions.