An automated target species selection method for dynamic adaptive chemistry simulations

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ABSTRACT

The relative importance index (RII) method for determining appropriate target species for dynamic adaptive chemistry (DAC) simulations using the directed relation graph with error propagation (DRGEP) method is developed. The adequacy and effectiveness of this RII method is validated for two fuels: n-heptane and isopentanol, representatives of a ground transportation fuel component and bio-alcohol, respectively.

The conventional method of DRGEP target species selection involves picking an unchanging (static) set of target species based on the combustion processes of interest; however, these static target species may not remain important throughout the entire combustion simulation, adversely affecting the accuracy of the method. In particular, this behavior may significantly reduce the accuracy of the DRGEP-based DAC approach in complex multidimensional simulations where the encountered combustion conditions cannot be known a priori with high certainty. Moreover, testing multiple sets of static target species to ensure the accuracy of the method is generally computationally prohibitive. Instead, the RII method determines appropriate DRGEP target species solely from the local thermo-chemical state of the simulation, ensuring that accuracy will be maintained. Further, the RII method reduces the expertise required of users to select DRGEP target species sets appropriate to the combustion phenomena under consideration.

Constant volume autoignition simulations run over a wide range of initial conditions using detailed reaction mechanisms for n-heptane and isopentanol show that the RII method is able to maintain accuracy even when traditional static target species sets fail, and are even more accurate than expert-selected target species sets. Additionally, the accuracy and efficiency of the RII method are compared to those of static target species sets in single-cell engine simulations under homogeneous charge compression ignition conditions. For simulations using more stringent DRGEP thresholds, the RII method performs similarly to that of the static target species sets. With a larger DRGEP threshold, the RII method is significantly more accurate than the static target species sets without imposing significant computational overhead.

Furthermore, the applicability of the RII method to a DRG-based DAC scheme is discussed.

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1. Introduction

The use of detailed reaction mechanisms is essential for high-fidelity predictions of important combustion phenomena such as pollutant emissions [1] and local flame extinction [2]—a cause of lean blowout [3]—as well as in the design of next-generation combustion devices such as homogeneous charge compression ignition (HCCI) engines [4]. However, the large size and high chemical stiffness of transportation-relevant fuel mechanisms prohibit their use in realistic simulations. For multidimensional reacting flow simulations, the chemistry time integration can take up to 75–99% of the total simulation time [5–8]. In order to utilize large chemical reaction mechanisms for transportation-relevant fuels in realistic simulations, accurate mechanism reduction and chemical stiffness removal strategies must be employed.

Detailed reaction mechanisms are constructed to be valid over a wide range of thermo-chemical states, and therefore tend to contain many species and reactions that are not important in all combustion regimes. A skeletal mechanism is created by removing species and reactions considered unimportant for the thermo-chemical state space under consideration. A comprehensive

skeletal mechanism is constructed for a broad thermo-chemical state space, while a local skeletal mechanism is created for a specific, limited range of thermo-chemical states.

Several systematic techniques to generate skeletal mechanisms by removal of unimportant species and reactions from a detailed mechanism have been developed; the directed relation graph (DRG) method [9–11] and the directed relation graph with error propagation (DRGEP) [12] are two skeletal reduction methods popularly used due to their efficiency and reliability. Other commonly used skeletal reduction methods include sensitivity analysis [13–15], principal component analysis [16], level of importance analysis [17–19], and methods based on computational singular perturbation [20–22] modified for skeletal reduction [23,24]. To generate even more compact skeletal mechanisms, the DRG and DRGEP methods are often combined with sensitivity analysis, as in the DRG-aided sensitivity analysis [11] and DRGEP-aided sensitivity analysis [25,26] methods.

In order to further optimize comprehensive skeletal mechanisms, dimension reduction methods are often employed. For example, chemical timescale analysis is utilized to exploit the tendency of reaction mechanisms to be attracted to lower dimensional manifolds, constraining the dimensionality of the reaction mechanism and thus simplifying integration. Methods such as the quasi-steady state [27] and partial equilibrium approximations [28,29] assume a species or reaction quickly reaches a steady state after initial transience, and thus can be solved for algebraically. More systematic dimension reduction methods include the computational singular perturbation [20–22] and the intrinsic low-dimensional manifold [30] methods, which analyze the Jacobian matrix to decouple the fast and slow chemical reaction modes to reduce chemical stiffness.

Finally, to accelerate chemical integration, tabulation methods that store and reuse previous solution information to cheaply construct approximate solutions of chemical integrations are often used. Common examples include in situ adaptive tabulation [31] (ISAT), piecewise reusable implementation of solution mapping [32], and artificial neural networks [33].

Most skeletal reduction approaches create a single, comprehensive skeletal mechanism for use over a prescribed range of conditions expected to be encountered. However, this approach is inherently at a disadvantage in multidimensional simulations because the same level of detail must be applied to the entire domain. Inside the flame zone, a highly detailed skeletal mechanism will likely be necessary to maintain accuracy, but in computational cells where combustion is mostly completed or weakly reacting a much smaller skeletal mechanism may be sufficient.

Recently, Liang et al. [34,35] proposed a dynamic adaptive chemistry (DAC) scheme to exploit this observation, where the DRGEP skeletal reduction method was applied to a thermo-chemical state under consideration to generate a smaller, locally accurate skeletal mechanism. The local skeletal mechanism was then integrated for a single simulation time-step and discarded; this process was repeated at the next time step. The reduced expense resulting from integrating the smaller, locally accurate mechanism outweighed the overhead of the reduction method, leading to time savings overall. For this reason, reduction methods that scale linearly with the problem size (e.g., DRG, DRGEP, element flux analysis [36]) are typically used in DAC schemes.

Liang et al. [34] utilized this method to achieve a 30-fold speedup with high accuracy for single cell HCCI simulations of n-heptane. Later, they demonstrated the applicability of the method for n-heptane/isooctane/toluene blends in HCCI and homogeneous autoignition simulations [35]. By pairing an element flux analysis method with the DAC scheme, He et al. [36] achieved a 25-fold speedup in a simulation of n-pentane in a pairwise mixed stirred reactor; however, the overhead of the flux-based reduction method

consumed nearly 20% of the total simulation time. Yang et al. [37] paired the DAC scheme with the DRG method in turbulent methane flame simulations. They found that the DRG-based DAC method accurately reproduced the combustion process of a partially stirred reactor with significant levels of non-equilibrium chemistry. Furthermore, for simulations with longer flow time scales (e.g., 10^{-4} s or longer) it was more efficient to generate a larger skeletal mechanism to be used for the whole flow time step, rather than performing multiple reduction/integrations steps within a single flow time step due to the overhead of the mechanism reduction [37].

Tosatto et al. [38] formulated a DRG-based DAC scheme that additionally considered transport fluxes, achieving speedup factors of 5 and 10 for a steady JP-8 flame and a time-dependent ethylene flame, respectively. Gou et al. [39] paired a simplified version of the path flux analysis method [40] with the DAC scheme to develop a method of error control for DAC simulations. Data tabulated from simple zero-dimensional simulations were combined with a reaction progress variable—the mass fraction of oxygen—to automatically select appropriate reduction thresholds during the simulation. This method reached speedup factors of 5–100 with high accuracy. However, the use of pre-tabulated data and choice of reaction progress variable may lack generality in turbulent reacting systems where the combustion conditions are unknown a priori and mixing plays a much stronger role. Therefore, more investigation is needed in this direction.

Contino et al. [41,42] proposed the tabulation of dynamic adaptive chemistry (TDAC) method that combines the strengths of tabulation methods (e.g., ISAT) and the DAC scheme. In the base ISAT method, when integrating the reaction mechanism at a thermo-chemical state, a database is first queried to determine if a similar state (and corresponding state after integration) are stored. If an appropriate state is found, an approximation to the integration of the queried state is cheaply constructed from the stored data. Otherwise, the reaction mechanism is directly integrated at the queried state and, following integration, the database is updated with the original and integrated states. In the TDAC method, the direct integration of the reaction mechanism is accelerated using a DAC scheme resulting in further computational savings. A speedup factor of ~500 was reported for premixed combustion cases, and ~9 for non-premixed cases with high fidelity predictions of species concentrations and pressure traces. Ren et al. [43,44] applied a similar scheme to computationally intensive partially stirred reactor simulations, showing up to ~1000 speedup factor for premixed cases and a 30% improvement in computational efficiency over the base ISAT method for a non-premixed case.

Apart from the reduction thresholds explored by Gou et al. [39], the other major factor controlling the performance and accuracy of DRG/DRGEP-based DAC methods is the selection of target species (i.e., search-initiating species). These species are selected for their expected importance to the combustion processes under consideration, and control the reduction of the detailed mechanism. The skeletal mechanisms generated by DRG/DRGEP-based methods include only species whose removal would introduce large error into the production or consumption of these target species. Traditionally, these species are selected before the simulation and treated as target species throughout; however, as discussed by Shi et al. [8], this methodology may overestimate the importance of these target species in certain combustion regimes. For example, while the fuel molecule is almost always used as a target species, in high-temperature, post-ignition combustion almost all the large hydrocarbons have broken down into small molecules and the fuel molecule no longer plays an important role. To address this problem, Shi et al. [8] proposed an extended DAC scheme (EDAC) that switches between a small number of target species