

INCORPORATION OF DETAILED CHEMICAL MECHANISMS IN REACTIVE SIMULATIONS USING ELEMENT-FLUX ANALYSIS

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Summary

A dynamic mechanism reduction approach is proposed based on element flux analysis. The element flux analysis derives time-integrated and instantaneous pointers to quantify element transformations between species. This information is used to reduce the reaction mechanisms by excluding the steps that are not important in different time points. The reduction scheme is implemented *on-the-fly* in CFD code KIVA-3V to provide realistic engine simulations with detailed fuel chemistry. The results show that the on-the-fly reduction scheme is able to predict the combustion process accurately. Time-dependant information about species transformations is provided to capture the fuel oxidation kinetics underlying various combustion scenarios.

Keywords

Complex reacting flows, Reaction Path Analysis, Element Flux, On-the-fly reduction

Introduction

In recent studies detailed chemical kinetic mechanisms for realistic fuels have been developed to predict characteristics such as ignition delay, combustion efficiency, and pollutant formation. Detailed kinetic mechanisms can provide a more comprehensive description of fuel chemistry^{1, 2}. However, they usually consist of hundreds of species and thousands of reactions. The incorporation of these detailed mechanisms in computational fluid dynamics (CFD) calculations is computationally expensive, and often times prohibitive. Thus a number of approaches have been proposed to incorporate detailed kinetics in CFD while keep the computation task accessible to current computers. These approaches can be divided into two broad categories: (a) detailed flow calculation coupled with simplified kinetic models or reduced mechanisms^{3, 4}, and (b) detailed kinetic mechanisms coupled with simplified description of the flow field⁵.

In this work, a dynamic kinetic reduction method is proposed based on element flux analysis to allow the integration of comprehensive CFD models and detailed kinetic mechanisms. Element flux analysis provides an indicator to quantify species activity, which can be implemented in mechanism reduction to identify redundant species and reactions. The reduction scheme is implemented *on-the-fly* in CFD calculations to generate an accurate reduced mechanism for each computational cell at each time step based on local conditions. The on-the-fly scheme is demonstrated in CFD code KIVA-3V using

various engine models⁶. Excellent agreement on temperature, pressure and species composition history is observed between the on-the-fly scheme and the detailed simulation.

Mechanism Reduction based on Element Flux Analysis

The element flux analysis quantifies the element transformation between species in terms of sources and sinks in a reaction system. It provides an indicator to measure species activity, which can be further implemented in redundant species identification⁷. The element flux between all source-sink pairs in the system are sorted in a descending order and a user-selected cutoff is applied to the flux lists, with species above the cutoff retained in the reduced mechanism while species below the cutoff are excluded. The proposed reduction method can be either employed to develop a library of reduced mechanisms that address different reaction conditions⁸, or implemented dynamically during a reaction flow calculation to achieve on-the-fly reduction⁹. In order to incorporate different reaction networks, i.e., fuel oxidation, NOx formation, and soot formation in mechanism reduction, an efficient multi-element (C, H, O, N) flux analysis framework combined with a tree searching procedure are employed in the proposed reduction method¹⁰.

Integration in CFD

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The mechanism reduction scheme based on flux analysis provides an efficient method to couple detailed chemistry with CFD calculation. The on-the-fly reduction scheme performs element flux analysis for every computational cell and time step of the CFD calculation. A reduced mechanism is thus developed to describe the local chemistry. In this work, the on-the-fly reduction scheme is integrated in CFD code KIVA-3V for various engine simulations. A number of fuel mechanisms with increasing complexity have been incorporated in the simulation. Figure 1 shows the pressure and selected species concentration history of n-pentane combustion in HCCI engine. The on-the-fly scheme reproduces results of the detailed simulation with good accuracy while the CPU time is reduced by a factor of 20. In addition, the on-the-fly scheme provides full characterization of the combustion process. For example, one of the interesting phenomena in combustion process is the multiple ignition points in the engine chamber. By incorporating detailed chemistry in engine simulation, multiple ignition points in HCCI engines can be predicted and the dominant chemistry of different ignition sites can be captured by element flux analysis. Figure 2(a) shows a demonstration case which uses a 2-D numerical mesh to simulate HCCI combustion. Inhomogeneous initial temperature ranging from 700 K to 1000 K is assigned to the chamber, which is shown in Figure 2(b). Figure 3(a) shows in-cylinder temperature contour of n-heptane combustion in HCCI engine near ignition time. Two ignition sites, A and B, are identified which correspond to initial temperatures 1000 K and 800 K with the similar ignition delay (Figure 3(b)). Element flux analysis is performed to analyze the pathways of radical pool build up of the two ignition sites and revealed that dominant chemistry of two sites are different: site A follows beta scission pathways while site B undergoes oxygen addition to the original fuel radicals.

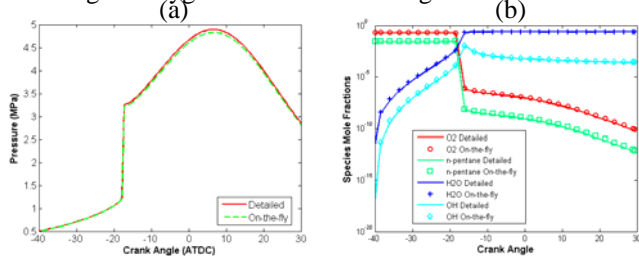


Figure 1. In-cylinder pressure (a) and species (b) profiles of n-pentane combustion in KIVA at 1000 K

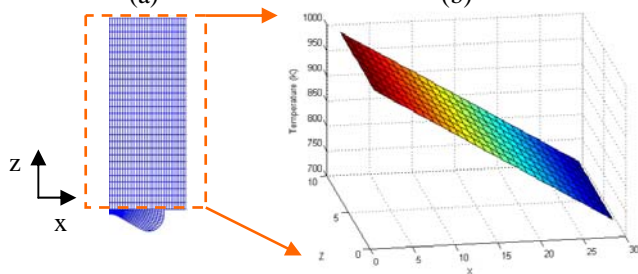


Figure 2. Case study of HCCI combustion in KIVA-3V. (a) 2-D numerical mesh, (b) initial temperature.

The flux analysis and the on-the-fly reduction scheme can be extended to other engine models and chemical mechanisms to provide species-dependant and time-dependant information of specific interest, which is usually not available in conventional experiments and simulations with simplified chemical kinetics.

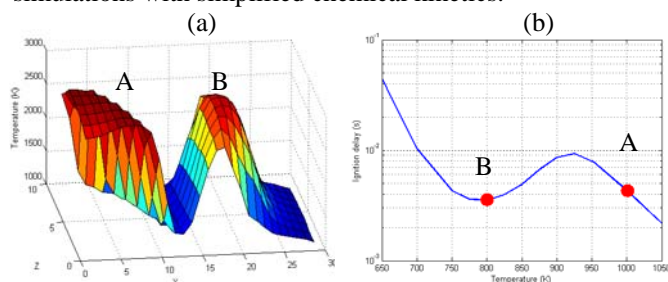


Figure 3. Multiple ignition sites in HCCI engine. (a) Temperature contour, (b) Ignition delay of n-heptane.

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