



Chemistry acceleration with tabulated dynamic adaptive chemistry in a realistic engine with a primary reference fuel



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HIGHLIGHTS

- Efficient chemistry calculation via combined ISAT–DAC.
- Chemistry acceleration effected by temperature inhomogeneity.
- Performance of ISAT–DAC with different error tolerance values.
- Low temperature chemistry is very important.

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ABSTRACT

Detailed kinetic reaction mechanisms are necessary for accurate prediction of combustion characteristics such as ignition and emissions in realistic engines. However, the calculation of chemically reacting flows with detailed chemistry is computational expensive due to the large number of species and reactions involved. In this study, a combined approach of dynamic adaptive chemistry (DAC) and *in situ* adaptive tabulation (ISAT) for efficient chemistry calculations has been implemented into a three-dimensional flow solver to simulate a homogenous charged compression ignition (HCCI) engine with a primary reference fuel (PRF). In the combined method, ISAT speeds up the chemistry calculation by reducing the number of integrations of ordinary differential equations (ODEs) governing chemical kinetics through tabulating and re-using the ODE solutions. At the meantime, DAC accelerates the necessary ODE integrations via the use of locally valid reduced mechanisms, which are obtained using the direct relation graph (DRG) method. The study shows that ISAT–DAC can achieve a speedup factor of about three with accurate prediction of composition and heat release even for the pressure-varying transient engine simulation with significant composition inhomogeneity resulting from wall heat loss. A detailed analysis reveals that the combined method effectively reduces the computational cost through taking advantage of the respective acceleration characteristics of DAC and ISAT at different combustion stages. In the low temperature combustion stage between about 650 K and 1000 K, even though the reduction in the mechanism size and consequently the ODE integration of the chemical kinetics by DAC is not significant, the combined method can still reach a speed-up factor of more than 100 due to the fact that the tabulated entries can effectively be reused. For the high temperature region, even though the tabulated entries cannot be reused due to the rapid change of the pressure and large composition inhomogeneity resulting from the active combustion and heat loss, DAC can effectively reduce the size of the needed ODE integrations by freezing a significant number of unimportant species and reactions. The study further quantifies the effect of composition inhomogeneity on the computation efficiency in detailed chemistry calculations in realistic engine simulations. For the case considered, the temperature inhomogeneity due to the wall heat loss obviously increases at around top dead center (TDC), reaching a level of 350 K difference in temperature within the combustion chamber. Consequently, the overall computational efficiency in chemistry calculation by the combined method has been reduced by 40% compared to the case without heat loss.

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1. Introduction

Practical engine fuels, such as gasoline and diesel, consist of multi-component with variant classes of chemical structures [1]. It is widely accepted that the oxidation processes of n-heptane and iso-octane can represent the ignition and combustion characteristics of diesel and gasoline fuels well. The multi-component surrogate fuels of diesel and gasoline, such as primary reference fuel (PRF) [2–6], n-heptane/toluene/ethanol blends [7], and toluene reference fuel (TRF) [8], are applied in numerical simulation researches. PRF is widely used as a surrogate fuel of practical fuels, which is a mixture of n-heptane and iso-octane [2] with the octane number ranging from 0 to 100. It provides detailed chemical information with detailed chemistry kinetic mechanisms to predict the ignition, flame propagation, and emission processes in internal combustion engine (ICE) accurately.

The major computational challenge of the IC engine simulations with detailed chemistry is the time-intensive nature of chemical integration, which may account for more than 90% of the overall simulation time [9]. Over the last decades, significant progresses have been made to accelerate the chemistry calculations in engine combustion simulations [9–19], such as *in situ* adaptive tabulation (ISAT) [16]; cell agglomeration methods such as multi-zone models [11], and dynamic adaptive chemistry (DAC) [20,21]. The DAC approach accelerates the time-integration of ODEs through the use of locally (spatially and temporally) valid skeletal mechanisms, which are obtained by invoking the directed relation graph method [22,23] or its variants [24–26] for each CFD cell to perform on-the-fly mechanism reduction at the local thermochemical condition. DAC has been successfully demonstrated for chemistry acceleration in internal combustion engine (ICE) simulations [9]. In contrast, ISAT algorithm presented by Pope [27] offers the unique feature of storing and retrieving the chemical integration results. By tabulating solutions of ordinary differential equations (ODEs) system governing chemical kinetics and reusing them, ISAT can substantially reduce the number of direct chemical kinetic integrations and significantly speedup the chemistry calculations. The computational efficiency of the ISAT algorithm is higher when the tabulated information can be re-used more frequently. For instance, speedup factors of 100–1000 can be achieved using ISAT for statistically stationary reactive flows [27].

More recently, the combined use of ISAT and DAC (ISAT–DAC) was employed by Contino et al. [28] and Ren et al. [13] for highly efficient ICE simulations with detailed chemistry. For example, with ISAT–DAC, a speed-up factor of hundreds to thousands for chemistry calculations has been achieved in a simple 2D HCCI simulation [28]. However, ISAT–DAC with extreme high speed up factor is only achieved so far for simple configurations and close-to-homogeneity conditions. Its performance is still unclear for challenging simulations with complex configurations and significant composition inhomogeneity. In recent study [29], Gianluca et al. carried out a heavy-duty diesel engine simulation with the ISAT–DAC similar to that proposed by Contino et al. [28]. It was found that an overall speed-up factor of only 1.2 was achieved compared to direct integration (DI) due to the significant composition inhomogeneity in the simulation, although a detailed analysis of the influence of the temperature and compositions inhomogeneity on the chemistry calculation acceleration is not provided.

The object of this work is to investigate the performance of the ISAT–DAC method for practical engine simulations with significant temperature inhomogeneity, which is the case even for HCCI engine due to wall heat loss. To do so, the ISAT–DAC method has been implemented into a three-dimensional flow solver to simulate a homogenous charged compression ignition (HCCI) engine with a primary reference fuel (PRF). A detailed analysis has been

performed to investigate the acceleration characteristics of DAC and ISAT at different combustion stages. The study further quantifies the effect of composition inhomogeneity on the computation efficiency. As an outline of the paper, the acceleration methods DAC, ISAT, ISAT–DAC and the computational model are reviewed in Section 2. In Section 3, the performance of the ISAT–DAC in HCCI engine simulations is analyzed. Conclusions are in Section 4.

2. Model description

For a gas-phase reacting mixture consisting of n_s chemical species participating in n_k elementary reactions, its thermo-chemical state is described by the pressure P , temperature T , mixture sensible enthalpy h_s and the n_s -sized vector \mathbf{Y} of species mass fractions. In reaction sub-steps of the simulations with an operator splitting scheme [30,31], the compositions $\Phi \equiv \{Y, h_s, Ps\}$ of each cell is governed by a set of nonlinear stiff ordinary differential equations:

$$\frac{d\Phi}{dt} = \mathbf{S}(\Phi), \quad (1)$$

where \mathbf{S} is the rate of change due to chemical reactions. Note that this source term has contributions from all the n_k reactions in the mechanism.

2.1. Combined method implemented into CFD

The DAC approach accelerates the time-integration of Eq. (1) through the use of locally (spatially and temporally) valid reduced mechanisms, which is obtained using the direct relation graph (DRG) method [22]. The DRG method eliminates the species that do not significantly affect the reaction rates of the major species based on a threshold, ε_{DAC} , for the truncation of weak species couplings. Details on the DAC method can be found in Refs. [13,20]. Note that the starting species need to be provided at each combustion step. In the present study, 6 species including three maximum mass fractions and three fixed species like CO, NO and HO₂ are selected as starting species for each given local composition based on the past studies [9,14].

For the ISAT, from the initial condition Φ^0 at time t_0 , Eq. (1) is integrated for a time Δt to obtain $\Phi(t_0 + \Delta t)$. For fixed Δt , the reaction is mapping $R(\Phi^0) = \Phi(t_0 + \Delta t)$. In practice, the typical combustion system involves dozens of chemical species and the stiffness of Eq. (1) is very strong, direct integration (DI) is a computational intensive process and requires significant computational resources. However, ISAT uses the ODE solver DDASAC to integrate Eq. (1) and stores the relevant information in a binary tree, with each termination node representing a record consisting of the tabulation points, the reaction mapping f , and the mapping gradient matrix A . Thus, for a given query composition x^q close to a tabulated point x , from the tabulated quantities at x , a linear approximation to $f^{l,n}$ can be obtained with a small error tolerance ε_{ISAT} as

$$f^{l,n} = f^n + A^n(x^q - x^n), \quad (2)$$

The detailed explanation can be found in Ref. [13].

In this work, the combined use of ISAT and DAC, denoted as ISAT–DAC is implemented into the multi-dimensional CFD code KIVA3V [32] and the reaction sub-step of a CFD simulation is shown in Fig. 1. The composition, $\phi \equiv \{Y, h_s, P\}$ involving the entire reaction species in a detailed chemical kinetic mechanism is solved in CFD solver. For the reaction sub-step in CFD the species mass fractions are used to describe species variations and enthalpy is used to evaluate the energy or temperature variation. Besides, the local pressure is a known parameter. For the reaction sub-step with ISAT–DAC, the composition $\phi(\Delta t)$ is determined based

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