

Large Eddy Simulation of an n-Heptane Spray Flame with Dynamic Adaptive Chemistry under Different Oxygen Concentrations

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ABSTRACT

Detailed chemical kinetics is essential for accurate prediction of combustion performance as well as emissions in practical combustion engines. However, implementation of that is challenging. In this work, dynamic adaptive chemistry (DAC) is integrated into large eddy simulations (LES) of an n-heptane spray flame in a constant volume chamber (CVC) with realistic application conditions. DAC accelerates the time integration of the governing ordinary differential equations (ODEs) for chemical kinetics through the use of locally (spatially and temporally) valid skeletal mechanisms. Instantaneous flame structures and global combustion characteristics such as ignition delay time, flame lift-off length (LOL) and emissions are investigated to assess the effect of DAC on LES-DAC results. The study reveals that in LES-DAC simulations, the auto-ignition time and LOL obtain a well agreement with experiment data under different oxygen concentrations. The produced time of NO_x induced by the high temperature and a certain equivalent ratio is close to the inflection point (increasing timing) of CO₂ variation.

CITATION: Zhou, L., Lu, Z., Ren, Z., Lu, T. et al., "Large Eddy Simulation of an n-Heptane Spray Flame with Dynamic Adaptive Chemistry under Different Oxygen Concentrations," *SAE Int. J. Engines* 8(2):2015, doi:10.4271/2015-01-0400.

INTRODUCTION

Understanding and controlling spray combustion process is an essential part of the research in diesel engine, which can significantly improve efficiency and drastically reduce emissions. High-fidelity simulation of spray combustion has become an indispensable and effective method to comprehend the complex physical process, such as temperature, composition distribution and pollutant formation. Thus, multi-dimensional computational fluid dynamic (CFD) coupled with detailed chemistry is strictly required in order to capture spray flame features accurately.

Detailed chemistry have been applied to auto-ignition process in diesel engine conditions. However, the large number of species, which participate in hundreds to thousands of reactions, brings about huge computational cost. It makes the detailed chemistry inaccessible for multi-dimensional simulations, especially for LES or even direct numerical simulation (DNS) Therefore, an increasing number of studies have been proposed to reduce the computational cost imposed by the use of detailed chemistry[1, 2, 3, 4, 5, 6]. Currently, there are main three approaches to radically decrease the computational time. They are the development of skeletal mechanisms from large detailed mechanisms by the elimination of inconsequential species and reactions; dimension-reduction techniques; and tabulation strategies.

In dimension reduction, composition in reactive flows are assumed to lie on a low-dimensional manifold in the full composition space; and the chemistry is described in terms of the reduced composition variables. Many dimension reduction methods have been proposed, such as the quasi-steady state assumption (QSSA)[7], rate-controlled constrained equilibrium (RCCE)[8], intrinsic low-dimensional manifolds(ILDM)[9]. As for the tabulation strategies, the most popular method is storage/ retrieval strategy-in situ adaptive tabulation (ISAT algorithm) presented by Pope [10]. ISAT originally was developed in the context of particle based probability density function (PDF) methods for chemically reacting turbulent flows. Then this method is used to numerical simulation of internal combustion engine[11,12]. Instead of solving the chemistry ordinary differential equations (ODEs) directly for every point in space, the ISAT method only solve the ODES for some significant ad special number of points, and use the values in these points to interpolate the solution for the other similar points under similar thermodynamic conditions. Recently, two similar methods based on flamelet calculations named FPI(Flame Prolongation of ILDM)[13,14] and FGM(Flame-Generated Manifold)[15] were proposed. Basically, the two methods are based on the tabulation of a set of unstrained premixed laminar flames.

In this work, the dynamic adaptive chemistry method is used. The DAC methodology involving on-the-fly chemical mechanism reduction has been demonstrated to be able to accelerate the chemistry calculations. The DAC is achieved through directed relation graph (DRG) [3] with effective error propagation (DRGEP) method, which is invoked for each computational cell to obtain a locally, instantaneously valid smaller mechanism for local thermochemical condition. After that, only a small subset of species and reactions in the full mechanism is kept to capture the domain reaction pathway for each cell. Consequently, the stiff nonlinear ODEs system governing chemical kinetics during the reaction fractional step is reduced in size due to eliminating unimportant species and related reactions. The DAC method was first proposed by Liang et al. [2] to obviously reduce CPU times for a homogeneously charged compressed ignition (HCCI) combustion process with CHEMKIN. After that, many researchers have used and improved this method. Shi et al. [16] applied the DAC method for a DI engine. In their study, DAC can significantly improve the computational efficiency compared to the full chemistry solver for multi-dimensional engine simulations. Yang et al. [17] investigated the use of DRG based DAC in partially stirred reactor (PaSR), involving methane/air at both premixed and non-premixed conditions with different chemistry mechanisms. For the PaSR simulations, DAC achieves a speedup factor of three to six for different chemistry mechanisms with good accuracy in both temperature and species concentrations. Viggiano and Magi [18] extended DAC to multidimensional simulations of ethanol HCCI/Partially charged compressed ignition (PCCI) engines. Through analyzing and comparing different values of tolerance and the choice of different species as search-initiating set, about 50% computational time is saved in the multidimensional simulation with a 57 species mechanism. However, the current studies of DAC mainly concentrate on simple cases and single phase flow, few studies have considered the transient performance using DAC on liquid spray combustion process.

Low temperature combustion (LTC) is a combustion concept in diesel engine that can simultaneously reduce NO_x and PM emissions using exhaust gas recirculation (EGR) technique. Many researches are very interested in this combustion pattern. Sandia National Laboratories has made a lot of fundamental experiments investigating the liquid spray and combustion process under different oxygen concentrations (similar EGR) in a constant volume combustion chamber [19,20]. The engine combustion network (ECN) [21] provides high-fidelity measurements data such as spray shape, liquid and vapor penetration length, mixture-fraction, ignition delay, flame lift-off length and soot emissions, which is a well-defined test case for spray and combustion models. The aim of this paper is validating present models against ECN data and investigating transition characteristics of n-heptane spray combustion process with LES and DAC with different oxygen concentrations.

As an outline of the paper, DAC approach and other computational models will be reviewed in section 2. Next in section 3 we demonstrate the DAC approach was used to spray combustion process with LES methodology. Conclusions are presented in Section 4.

THE COMPUTATIONAL MODEL

Flow Solver

The spray combustion process was calculated in this study by using the multi-dimensional two-phase flow KIVA3VLES solver coupled with CHEMKIN II developed by our groups based on original KIVA3V [22], which has found widespread applications for the IC engine simulations. The numerical scheme is based on the Arbitrary Lagrangian-Eulerian (ALE) method with finite volume method. For continuum phase, KIVA3VLES has been extended to a LES solver using $k - \epsilon$ sub-grid turbulent kinetic energy or other algebraic sub-grid models (Smagorinsky model, Dynamic Smagorinsky model and WALE model). Details about these models can be found in [23]. Originally, KIVA only offers first or second order Quasi-Second Order Upwind (QSOU) convective scheme. In this work, the Monotone Upstream-centered Schemes for Conservation Laws (MUSCL) differencing scheme proposed by Van Leer [24] was employed to calculate the convective term for LES, which has third order accuracy. The main idea is a piecewise linear reconstruction of the solution to achieve higher accuracy while preserving stability. For combustion process, a parallelization algorithm with uniform random distribution has been used to accelerate the chemical fractional step.

For the discrete phase, the Discrete Droplet Model (DDM) was applied in which the droplet particles are considered and tracked by solving their droplet velocity, mass and temperature equations using Lagrangian method in a time step. The interaction between gas phase and droplet is also considered. The two phase coupling involves two aspects, “gas-to-liquid” and “liquid-to-gas”. In “gas-to-liquid”, the change of the droplet velocity in computational domain is calculated by the drag force $F_{i,d}$ on droplet, which is calculated by the relative velocity between droplet and gas. In “liquid-to-gas” aspect, the effect of liquid motion on gas phase is treated as the Lagrangian source terms in the Eulerian momentum equation. It was noted that for LES the subgrid dispersion velocity model and spray source term model [25,26] are also involved.

The breakup of liquid fuel jet is a very complex physical phenomenon associated with aerodynamic liquid-gas interaction, physical and thermal properties of the fuel, and the ambient environment. In the present study, the Kelvin-Helmholtz and Rayleigh-Taylor (KH-RT) model [27] which have been widely used in the recent literatures were implemented in the KIVA code to predict the primary and subsequent secondary breakup.

Dynamic Adaptive Chemistry

Dynamic chemistry adaption (DAC) can be achieved through the DRG-based methods, which are employed to eliminate as many unimportant species and related reactions as possible to accelerate chemical step and simultaneously maintain the prediction accuracy results compared to the detailed mechanism. In this study, we consider a reacting gas-phase mixture consisting of n_s chemical species, composed of n_e elements. The local thermochemical state of the mixture is completely characterized by the local pressure P , the local mixture sensible enthalpy h_s , and the vector Y of local species mass fractions.



The DRG method is based on the observation that many species are only weakly coupled during combustion process, such that the species that do not significantly affect the reaction rates of the major species can be eliminated from the mechanism. The first step in DRG is to quantify species couplings by the pair-wise errors, $r_{A,B}$, induced to a species A by the elimination of another species B for a given reaction states that consists of temperature and species concentrations

$$r_{A,B} \equiv \frac{\max_i |v_{A,i} \omega_i \delta_{B,i}|}{\max_i |v_{A,i} \omega_i|} \quad (1)$$

with $\delta_{B,i}=1$ if the i th reaction involves B, otherwise, $\delta_{B,i}=0$. In above equation, ω_i is the net reaction rate of the i th reaction and $v_{A,i}$ is the stoichiometric coefficient of species A in the i th reaction. Thus, a pre-specified reduction threshold or error threshold ε_{DAC} is used to determine the important of species B to A. Simply, if $r_{A,B} > \varepsilon_{DAC}$ it indicates species B is important for the reaction rate of species A.

Numerical Setup

At the start of the simplification procedure, the DRG method requires one or more species (e.g., major species, important radicals and/or other interesting species) as the search-initiating Starting from these species of interest, the Depth-First Search (DFS) algorithm can be employed to identify all the species that are strongly coupled to the starting species. These species together with the starting species are retained in the local skeletal mechanism. Note that the eliminated species may still act as third-bodies.

In previous works, the starting species are manually specified, e.g. to include the fuel components together with CO, H and NO. In this study, with a given local composition, the M starting species are selected as follows with M being a user-specified small integer, e.g.6 used in this study. By default, species H, CO and NO were fixed as search-initiating species. The remaining starting species are selected from the non-inert species in the mechanism base on their abundance in mass until M variables are reached. This automatic procedure avoids the ambiguity in the fixed species strategies when the concentrations of one (more) specified search-initiating species approach zero and can dynamically select the species of importance based on the progress of the combustion process.

For spray modeling, the collision and coalescence model used in this study is that of O'Rourke[28]. The atomization model is the KH-RT model with the velocity interpolation model[29]. No-slip wall boundary conditions were applied to all solid walls. For calculating the combustion process, an n-heptane reduced mechanism involving 94

species and 400 reactions including Lu's 88 species and 387 reactions[30] and 13-steps NOx mechanism was used in this work. The fully three-dimensional (3D) simulations were conducted in a cylindrical domain with 30mm in diameter and 100 mm, as base grid, based on the studies of Bharadwaj et al.[25], Hori et al[31], and Zhou et al[23]. The overall computational grids are about 800,000 with the time step from $1 \cdot 10^{-8}$ s to $1 \cdot 10^{-6}$ s. Table 1 is the main experimental conditions by Lyle et al.[32]. These measurement data come from then standard database for n-heptane fuel sprays in ECN, and is often used to validate different spray and combustion models. For the numerical calculation the supercomputer workstation with Linux system in Tsinghua High-Performance Computing Center was employed.

THE COMPUTATIONAL MODEL

In this work, the experiments with n-heptane from the public database(ECN) of Sandia National Laboratories have been selected as a reference for the current model. The engine combustion network (ECN) [21] provides high-fidelity measurements data which is a well-defined test case for spray and combustion models. Experiments were conducted in a constant-volume combustion vessel under simulated, quiescent diesel engine conditions. The experimental conditions are chosen because of their similarity to conditions expected near top- dead-center(TDC) in an engine[33]. In this paper, the experiment imagines of combustion cases are presented by the high-temperature chemiluminescence using a high-speed CMOS camera. Fig.1 presents predicted and measured liquid spray and fuel vapor penetration at different times after start of injection (ASOI) in non-reacting case. Liquid penetration initially increases with time and then stabilizes at a quasi-steady value after about 0.1 ms. Although the LES results slightly over-predicted the vapor penetration, simulations are able to capture the overall penetration characteristics.

Fig.2 qualitatively shows the effect of the oxygen concentration on ignition delay time and flame lift-off length (LOL) with different error threshold values of ε_{DAC} compared with measured data with initial ambient temperature of 1000 K. The lift-off length is defined at the location where the temperature reaches half of the total temperature in the entire combustion process in the domain. Note that the definition of flame LOL using this half temperature method in the work is same as that of using OH radical distribution method[34]. The overall trends of ignition delay time and LOL are consistent with experiment data. It can be seen that with increase in the oxygen concentration, the ignition delay time and consequently the flame LOL decrease, as the flame position moves upstream as expected. As expected, the accuracy of LES-DAC simulation increases with decrease of the DAC threshold.

Table 1. Experimental conditions

Fuel	Hole diameter (mm)	Injection duration (ms)	Injection pressure (MPa)	Fuel mass (mg)	fuel temperature (K)	ambient gas oxygen	Ambient density (kg/m ³)	Ambient temperature (K)
C7H16	0.1	6.8	150	17.8	373	10%-21%(reacting)	14.8.	1000