



Full Length Article

Two-stage Lagrangian modeling of ignition processes in ignition quality tester and constant volume combustion chambers

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HIGHLIGHTS

- TSL model was used to simulate ignition delay time in the IQT and in the CVCC.
- TSL model is good in simulating IQT of long ignition delay time fuels and CVCC experiments.
- TSL approach demonstrates the suitability of using detailed models to provide insights into spray combustion.

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ABSTRACT

The ignition characteristics of isooctane and *n*-heptane in an ignition quality tester (IQT) were simulated using a two-stage Lagrangian (TSL) model, which is a zero-dimensional (0-D) reactor network method. The TSL model was also used to simulate the ignition delay of *n*-dodecane and *n*-heptane in a constant volume combustion chamber (CVCC), which is archived in the engine combustion network (ECN) library (<http://www.ca.sandia.gov/ecn>). A detailed chemical kinetic model for gasoline surrogates from the Lawrence Livermore National Laboratory (LLNL) was utilized for the simulation of *n*-heptane and isooctane. Additional simulations were performed using an optimized gasoline surrogate mechanism from RWTH Aachen University. Validations of the simulated data were also performed with experimental results from an IQT at KAUST. For simulation of *n*-dodecane in the CVCC, two *n*-dodecane kinetic models from the literature were utilized. The primary aim of this study is to test the ability of TSL to replicate ignition timings in the IQT and the CVCC. The agreement between the model and the experiment is acceptable except for isooctane in the IQT and *n*-heptane and *n*-dodecane in the CVCC. The ability of the simulations to replicate observable trends in ignition delay times with regard to changes in ambient temperature and pressure allows the model to provide insights into the reactions contributing towards ignition. Thus, the TSL model was further employed to investigate the physical and chemical processes responsible for controlling the overall ignition under various conditions. The effects of exothermicity, ambient pressure, and ambient oxygen concentration on first stage ignition were also studied. Increasing ambient pressure and oxygen concentration was found to shorten the overall ignition delay time, but does not affect the timing of the first stage ignition. Additionally, the temperature at the end of the first stage ignition was found to increase at higher ambient pressure and oxygen concentration.

Sensitivity analysis was performed using the TSL model to elucidate the reactions that control the overall ignition process. The present TSL modeling approach demonstrates the suitability of using detailed chemical kinetic models to provide insights into spray combustion processes.

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1. Introduction

An enhanced understanding of physical and chemical processes occurring during autoignition is paramount to the development of advanced combustion engine technologies and future fuels. Such engines include homogeneous charge compression ignition (HCCI) engines and low-temperature combustion (LTC) engines. Combustion processes in these engines are shown to be dominated by the

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Nomenclature

IQT	ignition quality tester	W_k	molecular weight of species k
TSL	two-stage Lagrangian	ρ	density
CVCC	constant volume combustion chamber	ρ_o	jet source density
ECN	engine combustion network	\dot{m}	mass flow rate in the jet
LLNL	Lawrence Livermore National Laboratory	\dot{m}_o	initial jet mass flow rate
KAUST	King Abdullah University of Science and Technology	c_p	specific heat (at constant pressure)
CFD	computational fluid dynamic	q_R	radiation loss
τ_f	first stage ignition delay time	f	fuel mixture fraction
τ_s	second stage ignition delay time	$a_{j,k}$	number of atoms of element j in species k
τ_t	total ignition delay time	M_j	atomic mass of element j
T_{ef}	temperature at the end of first stage ignition delay time	ε	number to avoid the singularity where f_h passes stoichiometric
A	jet cross-sectional area	B	expression that controls the homogeneous stream entering the flame-sheet reactor
Y_k	mass fraction of species k		
K	number of species		
h_k	enthalpy of species k		
$\dot{\omega}_k$	species molar production rate		

kinetics of intermediate and low-temperature ignition [1]. Autoignition is related to the increase in the rate of chain branching reactions that can drive a combustion system to completion in a short period. More knowledge on this phenomenon is useful for enhancing the performance of the engine, reducing NO_x and CO₂ emissions, and improving fuel economy. Such knowledge can be achieved by the development and application of simulation tools with accurate chemical kinetic models.

The development of reliable chemical kinetic models for autoignition relies on well-defined experiments for validation. These include experiments in homogeneous systems such shock tubes [2–4], rapid compression machines [5–10], and the jet stirred reactors [11]. These systems are however mostly limited to gas phase studies. Heterogeneous combustion facilities such as ignition quality tester (IQT) offer an alternative where ignition properties of liquid sprays could be explored. An IQT is a constant volume combustion chamber with a spray injection system. It is designed to measure the ignition delay time of various fuels including low volatility fuels [12]. The temperature, pressure, the mass of fuel injected and charge oxygen concentration in an IQT can be well controlled, which makes an IQT a useful system for producing experimental data for the validation of chemical kinetic models, provided that appropriate simulation tools are available. As reported in [12], a small fuel mass requirement in an IQT makes it an exemplary system to study ignition delay times of fuels that are not readily available in large quantity. Another experimental facility used in generating data for development of chemical kinetic models and computational fluid dynamic (CFD) simulations is a constant volume combustion chamber (CVCC) [13–17]. This is a high-pressure facility used for generating data for the Engine Combustion Network (ECN) [18–20], a library containing diesel spray experiments at various engine-relevant operating conditions.

In practical combustion systems, ignition delay time is the time difference between the start of injection (SOI) to the start of combustion (SOC). It consists of a physical ignition delay (atomization, vaporization and mixing of fuel and air) and a chemical ignition delay. The chemical ignition delay period of the overall ignition delay occur once the gaseous fuel/air mixture with a suitable temperature and mixture ratio is obtained, such that fast chemical reactions can be initiated [21,22]. The ignition delay in an IQT and a CVCC comprises of both physical and chemical ignition delay periods. Therefore, it is required for a modeling code to encompass both mixing as well as chemical kinetics for it to be used to predict accurately the ignition processes in these facilities. The two-stage

Lagrangian model (TSL) employed in this study describes mixing as a two-stage process that is seen in a frame moving downstream with the normal fluid motion. The model is capable of adopting detailed chemical kinetics while also simulating basic mixing processes that are important in turbulent gaseous-jet diffusion flames [18,19,22–26].

Only few studies were so far reported using the TSL model. These include the works of Pickett et al. [24], Broadwell and Lutz [25], and Han et al. [26]. Though these studies provided insight into how the TSL works, they however based their focus on soot and NO_x emission without particular emphasis on ignition. Using the TSL, Meijer et al. [19] studied the effects of mixing on ignition delay time of a diesel fuel surrogate in a constant volume combustion chamber. They found out that as a result of overmixing, the second stage ignition delay time of diesel fuel increases as the injection pressure increase from 1000 to 2000 bar, while the trend of first stage ignition shows the opposite. Cung et al. [27] studied the effect of temperature on ignition delay time of DME in a high-pressure facility using the TSL model. The present study would be among the few of its kind to use the TSL model to investigate, in detail, factors controlling ignition processes. In this study, the ignition delay times of isooctane and *n*-heptane in an IQT were investigated. Also, the model was used to simulate CVCC ignition delay data of *n*-dodecane and *n*-heptane available in the ECN library [20]. The study of isooctane and *n*-heptane ignition delay time is especially important because these are primary reference fuels (PRF) for octane ratings. *n*-Heptane and *n*-dodecane are used as diesel fuel surrogates [28–30].

The ignition properties of isooctane were previously investigated in shock tubes and RCMs in [9,30,31]. However, very little effort was made to study ignition properties of isooctane in IQTs. Similarly, the ignition characteristics of *n*-heptane fuel were extensively investigated in RCMs and shock tubes in [4,10,28,31]. *n*-Heptane ignition has been investigated experimentally and numerically in an IQT by Bogin et al. [32–34]. Key to the outcome of their study is the exhibition of negative temperature coefficient (NTC) behavior by alkanes, including C7 isomers. They also observed the two-stage behavior of alkanes in the NTC region. Dodecane ignition properties using CVCC facilities were also reported in [35–37]. Most of numerical studies on ignition in IQTs or CVCCs adopted reduced chemical kinetic models. Alternatively, the simpler TSL modeling tool can accommodate high-fidelity detailed kinetic models at a reduced computational cost in studying the ignition properties of these fuels in an IQT and CVCC. This

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