Combustion and Flame 171 (2016) 185–197

Contents lists available at ScienceDirect

Combustion and Flame

journal homepage: www.elsevier.com/locate/combustflame

Application of a multi-zone model for the prediction of species concentrations in rapid compression machine experiments

David Wilson*, Casey Allen

Department of Mechanical Engineering, Marquette University, Milwaukee, WI 53233, USA

ARTICLE INFO

Article history:
Received 5 February 2016
Revised 20 May 2016
Accepted 21 May 2016

Keywords:
Autoignition
Ignition delay time
Rapid compression machine
Primary reference fuels

ABSTRACT

A multi-zone model for simulating rapid compression machine (RCM) experiments is integrated with a chemistry solver for robust, computationally-efficient speciation predictions. The model builds upon previous work (Goldsborough et al., 2012) by simulating chemical kinetics in each temperature-varying main combustion chamber zone. The accuracies of the model predictions are evaluated by a comparison to results from computational fluid dynamics (CFD) simulations. The present model is shown to yield significant improvement over a homogeneous modeling approach in predicting chemical species mole fractions, as well as accurate predictions of temperature and pressure. Species mole fractions predicted by the present model are on average within ~15% of CFD predictions, while the difference in predicted mole fractions between a homogeneous model and CFD are ~90% on average. The improvement in species predictions is due to the fact that the present model simulates chemical reaction throughout the entire main reaction chamber in an RCM, while the homogeneous model utilizes a reactor model that simulates conditions inside the core of the reaction chamber only. The enhanced model will enable direct comparison to cylinder-averaged experimental speciation data that is obtained by expanding a reactive mixture to quench the reaction.

1. Introduction

Depleting fossil fuel and oil reserves as well as geopolitical and environmental concerns associated with the use of petroleum based fuels have motivated the advancement of internal combustion engine technology and biomass based fuels. The predictive accuracy of chemical kinetic models are integral to the development of alternative fuels since they play a key role in engine simulations [1,2]. Common tools that are used to validate kinetic mechanisms include flow reactors [3,4], shock tubes [5,6], laminar flames [7,8], and rapid compression machines (RCMs) [9,10]. RCMs generate a well-defined reaction environment by rapidly compressing a reactive gas mixture and then maintaining a constant volume during post-compression. Typically, RCM experiments are conducted in order to acquire ignition delay data. The obtained ignition delay data is then compared to ignition delay data predicted by RCM simulations coupled with a chemical kinetic mechanism, in order to validate the mechanism. While ignition delay measurements can be an important benchmark for confirming a mechanism's ability to predict the rate of global reactions, they do not by themselves provide insight into reaction pathways. Comparison between simulation and experimentation based on species concentrations and paths of chemical reactions is more telling of the predictive accuracy of a chemical kinetic mechanism [11,12]. Speciation data is a reflection of exactly what mechanisms are trying to predict: reaction rates and species evolution. There are existing studies that have done "quenching" experiments, where the contents inside an RCM are rapidly cooled in order to terminate further chemical reaction [13–15]. The mixture is then removed and analyzed to determine its chemical composition. While these kinds of experiments are a necessary piece for validating kinetic mechanisms based on species concentrations, they require an efficient model capable of accounting for heat loss and temperature inhomogeneity within the main chamber, and predicting species data throughout the entire RCM reaction chamber.

Both of these requirements can be achieved with the use of computational fluid dynamics (CFD). Although rigorous and highly accurate, CFD simulations can be very computationally expensive, especially when detailed chemical kinetic models with many species and chemical reactions are used [16,17]. Chemical reaction and species evolution must be simulated for every cell in a CFD simulation, making this method intractable. Other modeling techniques to account for heat loss have been implemented, including an effective volume approach which models the influence of heat loss by including a volume expansion term in the adiabatic energy equation [15,18,19]. This approach forms the basis of a

* Corresponding author.
E-mail address: david.wilson@mu.edu (D. Wilson).

http://dx.doi.org/10.1016/j.combustflame.2016.05.018
0010-2180/

Nomenclature

A	area
B	bore length
c_v	constant volume specific heat
h	enthalpy
h_{conv}	convection coefficient
k	thermal conductivity
l	axial length
m	mass
n	number of zones
Nu	Nusselt number
P	pressure
Pr	Prandtl number
Q	heat transfer
q	heat flux
Re	Reynolds number
sp	chemical species
$\boldsymbol{T}$	temperature
t	time
t_o	outermost zone thickness
u	specific internal energy
v	velocity
V	volume
x	distance
X	mole fraction
Y	mass fraction

Greek letters

α	zone growth factor
γ	ratio of specific heats
ρ	density
τ	shear stress
ζ	characteristic length

Subscripts

crev	piston crevice volume
ex	exit
gap	tapered gap between piston crown and cylinder wall
in	inlet
pist	piston
r	zone resizing
RC	reaction chamber
surf	surface
wall	wall

zero-dimensional model known as the "homogeneous reactor model" (HRM). The HRM approach has been largely satisfactory for making ignition delay time predictions, but it requires non-reactive pressure data for each test condition being modeled. These tests are time consuming, making a model based approach attractive. Furthermore, it is known that the HRM cannot be used to make speciation predictions for quenching experiments, which are sensitive to the temperature and concentration distributions that evolve during the experiment [20,21].

Goldsborough et al. [22,23] eliminated the need for non-reactive experiments with the creation of a computationally efficient, physics-based multi-zone model (MZM) which can be integrated with kinetic mechanisms for predicting temperature and pressure evolution in an RCM experiment. This model utilizes the adiabatic core hypothesis as described above. However, instead of deriving the volume profile from a non-reacting experiment, the extent of the isentropic expansion of the adiabatic core is calculated from the pressure profile derived from a separate physics-based zonal model. The pressure profile is then used to calculate an effective volume profile for the HRM, which simulates chemical reaction in the core region of the main reaction chamber of an RCM. This model is comprised of the main reaction chamber, piston crevice, tapered gap (which connects the main reaction chamber and crevice), and the ringpack, which accounts for blowby. The main reaction chamber is divided into multiple concentric, cylindrical zones. Each zone has a unique temperature yet identical chemical composition. Throughout compression and the ignition delay period, the energy evolution of each zone is calculated according to conduction (which is induced by the temperature gradient between zones), enthalpy loss to the crevice (induced from the pressure differential between the main reaction chamber and crevice), and boundary work from compression. Mass flow from the main reaction chamber to the crevice is calculated by employing a quasi-steady formulation of the mass, momentum and energy transfer of the tapered gap. An iterative method is used to converge on the correct inlet and exit velocities, and the exit temperature at each time step. The goal of this paper is to present an extension of this model that simulates chemistry in each of the main reaction chamber zones, so that the model can be used as a validation tool based on species concentrations from quenching experiments.

The physics-based multi-zone model was shown to be effective for predicting temperature and pressure evolution for non-reacting simulations through comparison to CFD simulations. Ignition delay predictions similar to those from CFD simulations were also seen for a few cases [22]. However, one limitation of this modeling approach is that chemical reaction is simulated in the adiabatic core reactor model only, and the MZM assumes uniform composition and an absence of chemical evolution. Therefore, this model cannot be used as a rigorous validation tool for chemical kinetic mechanisms based on intermediate species concentrations from quenching experiments. The species concentrations calculated from the adiabatic core reactor model itself will not accurately reflect the average concentration within the RCM. Also, failing to account for chemical reaction in the outer regions not only produces a lower predicted energy in the main reaction chamber, but also results in inaccurate calculation of thermodynamic and transport properties, both of which are a function of chemical composition. This study proposes an extension of the MZM developed by Goldsborough et al. [22] that simulates chemical kinetics in the entire main reaction chamber, allowing for a more rigorous validation of chemical kinetic mechanisms that is based on speciation data from quenching experiments, as opposed to ignition delay alone. A description of the proposed model is presented in the next section. This is followed by a Results and Discussion section with a presentation of the new model's predictions compared with CFD results for various cases. A summary of the work and suggestions for future explorations, such as validating the present model with quenching experiments, is then provided.

2. Methods

2.1. Multi-zone model description

An extension of the multi-zone model developed by Goldsborough et al. [22] is presented below. Throughout the paper, the model by Goldsborough et al. is referred to as the original model, while the model presented in this study is called the modified model. A significant distinction that makes the modified model different from the original model is the absence of an integrated homogeneous reactor model (HRM). The original model utilizes an HRM, separate from the MZM, which represents the "adiabatic core" or the hot central region in the main reaction chamber. The purpose of the HRM is to simulate the effects of chemical reaction