



## Full Length Article

# A generalized kinetic model with variable octane number for engine knock prediction



Zhi Wang\*, Fubai Li, Yingdi Wang

State Key Laboratory of Automotive Safety and Energy, Tsinghua University, Beijing 100084, China

## HIGHLIGHTS

- A reduced and generalized model for gasoline knocking prediction was developed.
- GRON can present gasoline fuels with various octane numbers.
- GRON was validated over a wide range of temperature, pressure and equivalence ratio.
- Pressure oscillations and important radicals during knocking was captured with CFD.
- GRON model significantly reduces computational time.

## ARTICLE INFO

## Article history:

Received 13 June 2016

Received in revised form 9 October 2016

Accepted 12 October 2016

Available online 17 October 2016

## Keywords:

Kinetic model

Engine knock

Octane number

CFD

## ABSTRACT

A generalized research octane number (GRON) model, including 22 species and 21 reactions, has been developed to simulate the hydrocarbon oxidation with the goal of predicting engine knock. The simplicity of the model enables to represent gasoline with different octane numbers by adjusting the global low-temperature reaction rate. The model was validated against shock tube experimental data obtained over a wide range of conditions, including equivalence ratios from 0.5 to 2.0, initial pressures from 13 to 55 bar, and initial temperatures from 700 to 1250 K. Both gasoline engine knock and normal combustion were investigated using Computational Fluid Dynamics (CFD) couple with the present GRON. The numerical results proved to be in good agreement with the experimental data. Both the cylinder pressure traces and the distribution of important radical species (CHO and OH) during knocking combustion can be predicted reasonably well. Compared to the CFD calculations using detailed mechanisms, the generalized kinetic model enables a reduction of the computational time by more than 90%.

© 2016 Elsevier Ltd. All rights reserved.

## 1. Introduction

Fuel consumption regulation are driving the technical development of internal combustion engines worldwide. The required CO<sub>2</sub> reductions between 2014 and 2020 are 17%, 24%, 30%, and 28% for Japan, Europe, USA, and China, respectively [1]. In the recent decades, China initiated a “863” project aiming at achieving less than 200 g/kW h fuel consumption for gasoline engines. Japan started a project named Research Association of Automotive Internal Combustion Engines (AICE), aiming at improving gasoline engine thermal efficiency to an unprecedented level of 50% by 2020. In Europe, the highly downsized gasoline engines with ultra-boost have been investigated intensively [2]. Improving compression ratio and boost ratio are the two major approaches for gasoline

spark ignition engines to meet the stringent fuel consumption regulations. However, the obstacle for further increasing compression ratio and boost ratio is engine knock. Accurate predictions of knocking combustion in spark ignition engines are critical for developing future high efficiency IC engines.

Based on a literature review, five categories of models employed for engine knock prediction were identified and are listed in Table 1 by increasing order of complexity. Table 1 also indicates the advantages, drawbacks and applicability of the different models. For gasoline engine knock prediction, the first model proposed was the Livengood-Wu correlation [3], which is based on ignition delay time calculation using a global reaction model in a zero-dimensional (0D) reactor. The quasi-dimensional model described the combustion chamber as a two-zone reactor composed of a burned zone and an unburned zone [4]. Noda et al. [5] accurately observed the engine knock onset using a quasi-dimensional two-zone model with a detailed primary

\* Corresponding author at: Automobile Research Institute, Tsinghua University, Beijing 100084, China.

E-mail address: [wangzhi@tsinghua.edu.cn](mailto:wangzhi@tsinghua.edu.cn) (Z. Wang).

**Table 1**  
Comparisons of engine knock models.

Knock model	Reaction number of mechanism	Advantages	Disadvantages	Applications	Calculation time (min)
0D single-zone [3]	Global reaction to 8-step reaction	Simple, ignition delay prediction with low computational cost	HC and CO incapable Pressure oscillation can't be simulated	Fast prediction of knock onset	<1
Quasi-dimensional two-zone with detailed chemistry [4,5]	10 <sup>2</sup> –10 <sup>3</sup>	End gas auto-ignition process can be described accurately before knock onset	Combustion chamber geometry is neglected	HC, CO and NO <sub>x</sub> emissions as well as heat release rate prediction	<10
1D CFD with detailed chemistry [5–8]	10 <sup>2</sup> –10 <sup>3</sup>	Aero-thermo-chemistry interaction with high calculation efficiency	Turbulence-combustion interaction is neglected	Combustion mode identification	<10 <sup>2</sup>
Multi-D CFD with simplified chemistry [10–13]	8–10 <sup>2</sup>	Fuel spray, flow and turbulence, mixture formation considered	Simplified pre-reaction and post-oxidation process	Optimization of SI combustion system	10 <sup>2</sup> –10 <sup>3</sup>
Multi-D CFD with detailed chemistry [14–17]	10 <sup>2</sup> –10 <sup>3</sup>	Detailed fluid dynamics, chemical kinetics and emission formation considered	High computational cost	HC, CO, NO <sub>x</sub> , Soot, heat release and pressure oscillation prediction	10 <sup>3</sup> –10 <sup>5</sup>

reference fuel (PRF) mechanism. Bradley et al. [6,7], Dai et al. [8], Wang et al. [9] employed one-dimensional (1D) computational fluid dynamics (CFD) with detailed syngas, *n*-heptane and iso-octane mechanisms in order to capture the auto-ignition and pressure wave in HCCI and super-knock conditions. However, 0D or 1D models could only capture the ignition delay time or heat release induced pressure rise. Since knock is a spatial-temporal combustion process, multi-dimensional model have been widely applied to analyze engine knock [10–17]. Using three-dimensional CFD with detailed chemistry, turbulent flame propagation, auto-ignition induced pressure oscillation as well as emissions could be predicted [13–16].

As seen from Table 1, the tendency in researches on knock modeling is from 0D to 3D models, with simple reaction models being substituted by detailed chemical kinetics. The challenges are the greatly increased calculation time and the uncertainty associated with the complex composition of the real gasoline fuel. In recent years, a series of gasoline surrogate mechanisms have been developed, such as iso-octane and *n*-heptane [18,19]; iso-octane, *n*-heptane and toluene [20,21]; iso-octane, *n*-heptane, toluene and 2-pentene [22]; iso-octane, *n*-heptane, toluene, 1-pentene, methyl cyclohexane [23]; iso-octane, *n*-heptane *n*-hexadecane and iso-cetane [24]; iso-octane, *n*-heptane, ethanol, toluene, and diisobutylene (DIB) [25,26]. Although these mechanisms enable an increasingly accurate description of the gasoline main components, they are still far away representing the gasoline characteristics in detail because real gasoline fuel is composed of hundreds of hydrocarbon species with different chemical and physical properties. In addition, the computational time is extremely long when coupling multi-dimensional CFD with these surrogate mechanisms which include hundreds or even thousands of reactions. Even with a parallel computing approach, single working cycle simulation of internal combustion engine necessitates more than 100 h [27]. This limits the practical application of multi-dimensional CFD in internal combustion engine simulation, especially for engine knock prediction.

For engineering application of engine knock prediction, the most important factors of gasoline surrogate model are carbon/hydrogen ratio, ignition delay time, heat release rate, concentration of important radicals, and the main pollutant emissions. To capture knocking combustion in gasoline engines, the model needs to focus on the following four aspects: (1) Ignition delay. The uncertainties of ignition delay time should be less than 0.1 ms (about 1 °CA at 1666 rpm) to capture engine knock under stoichiometric conditions; (2) Concentration of crucial radicals,

such as CHO and OH distribution; (3) Size of mechanism. Appropriate amount of reactions and species are needed for reasonable computational time, usually less than 8 h for engineering application; (4) Capability of representing gasolines with different octane numbers, for example, RON can be varied from 0 to 100. The objective of the study was to develop a practical and generalized gasoline oxidation model that enables computationally inexpensive multi-dimensional SI engines CFD simulations under conditions of both normal and knocking combustion of gasolines with various RONs.

## 2. Model construction

Gasoline fuels are typically composed of three main hydrocarbon families, alkanes, alkenes and aromatics. As for alkanes, significant differences in terms of reactivity exist between *n*-alkanes and branched alkanes. Generally, the oxidation of hydrocarbons can be divided into three temperature ranges: low temperature range (less than 850 K), intermediate temperature range (about 850–1050 K), and high temperature range (above 1050 K). Despite the difference of reactivity between the hydrocarbon families, the dominant chemical pathways are essentially similar in the low-temperature range are similar, as shown in Fig. 1 [28].

Under IC engine-like conditions, hydrocarbon fuel oxidize very slowly during the early stage of the process (often below 600 K). During the process of compression, temperature increases promptly, stepping into the low temperature reaction range (600–850 K). In this stage, reaction is initiated by the abstraction of H from a hydrocarbon fuel by O<sub>2</sub> to form an R<sup>•</sup> radical and HO<sub>2</sub> (R1). Following H abstraction, the R<sup>•</sup> radical undergoes successive O<sub>2</sub> addition and isomerization to form a QOOH radical (R2). The QOOH radical undergoes a second O<sub>2</sub> addition (R3) followed by OH elimination (R4) which leads to the formation of ketohydroperoxide species. OH radical further reacts with the fuel molecule to form R<sup>•</sup> radical and H<sub>2</sub>O (R5). The chemical sequence R2–R5 is exothermic and induces low temperature heat release. The initiation reaction (R1) controls the total reaction process whereas (R2) controls the low temperature heat release rate.



Download English Version:

<https://daneshyari.com/en/article/6475857>

Download Persian Version:

<https://daneshyari.com/article/6475857>

[Daneshyari.com](https://daneshyari.com)