Applied Energy 156 (2015) 149–158

Contents lists available at ScienceDirect

Applied Energy

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

Combustion-response mapping procedure for internal-combustion engine emissions

T. Korakianitis [a,*], S. Imran [b,c], N. Chung [d], Hassan Ali [c], D.R. Emberson [c], R.J. Crookes [c]

[a] Parks College of Engineering, Aviation and Technology, Saint Louis University, St. Louis, MO 63103, USA
[b] Faculty of Mechanical Engineering, University of Engineering and Technology, Lahore, Pakistan
[c] School of Engineering and Materials Science, Queen Mary University of London, Mile End Road, E1 4NS, UK
[d] New Green Way Pte. Ltd., 51 Goldhill Plaza, #7-10/11, Singapore 308900, Singapore

HIGHLIGHTS

- Prediction of emissions by using CFD and detailed chemical kinetics reactions.
- Decoupling of CFD calculations during the combustion process.
- Pre-calculations of chemical kinetics for different thermodynamic conditions.
- Experimental validation of the technique for a CI and an SI engine.

ARTICLE INFO

Article history:
Received 20 November 2014
Received in revised form 12 May 2015
Accepted 17 June 2015

Keywords:
Combustion response mapping
Decoupling chemical kinetics
Combustion CFD

ABSTRACT

This paper describes a new method to predict emissions in internal combustion (IC) engines. The method couples a multi-dimensional engine modeling program with pre-integrated non-equilibrium chemical kinetics reaction results. Prior to engine simulation, detailed chemical kinetics reactions of air/fuel mixture at different temperatures, pressures, and compositions, are calculated using SENKIN, a subprogram in the CHEMKIN-II computer package. The reaction results are decoupled from their chemical eigenvalue (order of about 10^{-10} s), then integrated and saved in physical time scale (order of about 10^{-5} s) in a database file. In the database reaction results of different initial conditions (temperature, pressure, and species composition) are stored in different zones; the zones are indexed using their respective reaction conditions. Fluid dynamics and thermal dynamics of the movement of piston and valves, and spray droplets interaction are simulated by KIVA-3 V. Instead of calculating directly the non-equilibrium chemical reactions of the air/fuel mixture, reaction results are obtained from the database file via an interpolating subroutine, which returns temperature, heat release, and species concentrations after reaction to the main program. The approach avoids direct time consuming calculation of detailed chemical reactions as well as the errors introduced by coupling the physical and chemical processes. Emissions are predicted accurately since reaction of air/fuel mixture is calculated using the detailed chemical kinetics mechanism. The approach is applied to model a Caterpillar 3401 direct injection compression ignition (CI) diesel engine. In addition we carried out experimental tests on a Toledo 1500 SI gasoline engine, and those results are compared with the proposed computational approach. In all cases the predicted results agree well with the experimental data.

1. Introduction

The continued use of the internal combustion (IC) engine is highly dependent on new designs and new fuels: meeting ever stricter emissions regulation; and meeting customer demands for greater efficiencies reducing fueling costs. A greater understanding of the physics and chemistry taking place in the IC engine is key to meeting these demands. The field of engine research is very active with a number of strategies being employed in order to achieve this insight into engine operation. Research mainly consists of the development of an accurate and efficient method to simulate and model the internal combustion engine with a variety of configurations and fuels. This field can further be broken down into those conducting experimental work with real engines and those

* Corresponding author.
E-mail addresses: korakianitis@alum.mit.edu (T. Korakianitis), chung.nguyen@greenway.sg, chung9251@gmail.com (N. Chung).

http://dx.doi.org/10.1016/j.apenergy.2015.06.039
0306-2619/

Nomenclature

Latin

G	arbitrary variable
N_c	number of species in reaction
N_r	number of reaction
t	time

Greek

∇	difference operator

Superscripts

0	standard state, reference point
c	chemical
n	step index

Subscripts

1	species 1 (fuel)
b	backward
f	forward
m	species m

Abbreviations

AC	adaptive chemistry
CFD	computational fluid dynamics
CFR	fuel co-operative research
CI	compression ignition
CPU	central processing unit
DAC	dynamic adaptive chemistry
DME	dimethyl ether
HCCI	homogeneous charge compression ignition
IC	internal combustion
ILDM	intrinsic low dimensional manifold
ODE	ordinary differential equation
RME	rape methyl ester
SI	spark ignition
QSSA	quasi-steady-state assumptions

constructing accurate mathematical models to simulate the engine. Both of these fields feed into each other with the purpose to increase accuracy and efficiency at the design stage.

Alternative fueling of IC engines is predominated with experimental work in laboratory based engines with fuels such as RME and DME [1–3] used extensively along with natural gas, often in a compression ignition design. These works such as those by McTaggart Cowan [4] employ direct measurement of emissions and any performance analysis is firmly routed in the first law of thermodynamics frame work, with engine pressures and the heat release rate ubiquitous in the field. There is a need to model these alternative fuels on a mathematical basis without the need to resort to empirical data all the time and to address emissions along with performance.

The coupling of first law analysis to empirically collected data is used extensively to provide quick and easy to interpret data concerning an engines performance. The majority of these first law models, such as that developed by Payri et al. [5] are often described as zero-dimensional, with the combustion chamber treated as a single or number of zones. Within each zone the first law of thermodynamics is applied with respect to time (dt). Whilst this treatment allows for a computationally quick determination of heat releases, temperatures or pressures, emissions are often neglected from such a model or may be inferred as is demonstrated by Kegl [6]. Emissions predictions models have been previously employed based around these zero-dimensional models [7,8], here the combustion chamber is divided into 3 zones: unburned gas; burned gas; and burned gas zone adjacent to the combustion chamber walls. The burned gas and unburned gas zones are separated by the flame front. It is assumed that each zone, burned or unburned is completely and instantaneously mixed (uniform in temperature, pressure, and composition). The combustion is calculated based on the propagation speed of the flame front. The nitric oxide emissions are calculated using the extended Zeldovich kinetic scheme [9] with the steady-state assumptions made for N concentration and equilibrium values used for H, O, O_2, N_2, and OH concentrations. Because of the simplified assumptions made, this method is normally used only for parametric studies.

Multidimensional modeling of an IC engine really tries to address the complex fluid flows taking place in the engine throughout a cycle or over a number of cycles. Here the temporal and spatial variations of the flow field, temperature, composition, pressure and turbulence within the combustion chamber are dealt with [10]. These models may range from a less complex one dimensional model [11] to full three dimensional models examining the complex in-cylinder air motion characteristics of squish, swirl and turbulence [12]. This has become a major part of the engine design and development stage as both CI and SI engines have moved towards direct injection.

This paper deals with how complex multidimensional modeling is used to model an event involving combustion, as we do with IC engines. Researchers and designers have employed a number of techniques and with the rapid progress in computer technology, ever more detailed modeling techniques are available including: full CFD to model the flow field characteristics; and detailed chemical kinetics to detail the species formation during combustion.

There have been numerous methods to integrate the fluid dynamic to the combustion simulation. In the single zone approach [13,14], during the combustion process the combustion chamber is assumed to be a homogeneous volume (temperature, pressure, and composition are uniformly distributed over the considered volume). Modeling starts from the beginning of ignition to the end of combustion. The combustion of the air/fuel mixture is handled by detailed chemical kinetics, with a number of chemical kinetics modeling packages available, such as HCT [15] and SENKIN, a subprogram in CHEMKIN computer package [16] The state of fluid in the cylinder chamber at the beginning of combustion is specified using different methods. A CFD analysis of the cylinder describes the cylinder air/fuel mixture from the beginning of compression to the point of ignition. The results of this step are then used as input for the detailed chemical kinetics. An example of this two step scheme can be seen in the work of Ogink and Golovitchev [14]. Heat transfer between the mixture and the cylinder wall in the single-zone models is computed using the Woschni method [17]. Since combustion of the air/fuel mixture is calculated for the entire combustion chamber volume, this approach has several disadvantages: (1) fluid dynamics is not taken into account when calculating combustion and (2) the simplicity of the heat transfer model during the compression and expansion strokes does not describe the complexity of the thermal processes. The approach predicted well the trends (qualitative results) of emissions, but failed to predict emissions quantitatively.

A multi-zone approach [18] is really an extension of the single zone approach. Here the combustion chamber is divided into three typical zones: (1) constant volume zone representing crevices; (2) zone representing the thermal boundary layer; and (3) core zones.