An alternative approach of turbulent combustion modelling by BEM

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Abstract

An alternative approach of turbulent combustion modelling based on detailed chemical kinetics and simplified mixing is presented. The main conservation equations of mass energy and species mass have been solved numerically applying boundary-domain integral method. The model has been applied to the particular case of the premixed charge in a spark-ignited internal combustion engine. The model predictions are in good agreement with measurements.

1 Introduction

It is well accepted that the Navier-Stokes equations are an accurate description of turbulent reacting flows. These equations are easily posed and are easily cast into forms for numerical computations. The solution of the equations is computationally intensive and requires more time than most people can afford. Accordingly, simplifications to these equations are sought. Two limiting cases are identified. One case has a characteristic mixing time large compared to the chemical time, which is modelled with an assumption of chemical equilibrium. The other case has a mixing time small compared to the chemical time, which
is usually modelled, with an assumption of homogenous mixture. Between these limiting cases, neither mixing nor chemical reactions can be eliminated from consideration. The usual approach is to simplify the chemical kinetics, often by reducing many step mechanisms to one or two global steps, and retaining details of fluid mixing and dynamics. In so doing details of combustion processes such as prediction of oxides of nitrogen and carbon monoxide are not in the model. However, much of the impetus in combustion research is management of carbon monoxide and oxides of nitrogen while maintaining high fuel efficiency. Accordingly, a model introduced here, retains detailed chemical kinetics and simplifies the fluid dynamics regarding especially its velocity field. The model represents improved model developed by J.Y. Chen [1] where detailed chemical kinetics and simplified mixing applying well-mixed reactor technique (WMR) have been considered. Presented model is applied to the particular case of the premixed charge in a spark-ignited internal combustion engine for the investigation of NO formation. The model divides the continuous flow and reaction field inside the combustion chamber into a series of concentric deformable shells than can be arbitrarily convoluted by convection and turbulence, each of which is modelled by partially-mixed reactor (PMR). Thermochemical data and the detailed chemical kinetics for each PMR are computed by the CHEMKIN package of numerical codes. The model predictions are in good agreement with measurements and giving also better results in comparison with model based on WMR only [2].

2 Governing equations

2.1 Single partial-mixed reactor (PMR)

For a single PMR as shown in Figure 1, the basic differential equations can be derived from conservation of mass, species, and energy, respectively

\[ \frac{dm}{dt} = \sum_{i=1}^{N_t} \dot{m}_i - \dot{m}_e, \tag{1} \]

\[ \frac{\partial \xi_s}{\partial t} + \frac{\partial}{\partial x_k} \left( \nu_m \xi_s \right) - D_{sm} \frac{\partial^2 \xi_s}{\partial x_k^2} = \frac{1}{m} \sum_{i=1}^{N_t} \dot{m}_i (\xi_{is} - \xi_s) + \frac{\dot{W}_s}{\rho}, \tag{2} \]

\[ \frac{\partial T}{\partial t} + \frac{\partial}{\partial x_k} \left( \nu_m T \right) - a_T \frac{\partial^2 T}{\partial x_k^2} = \frac{1}{c_p m} \sum_{i=1}^{N_t} \dot{m}_i \left[ \sum_{s=1}^{N_s} (h_{is} - h_s) \xi_{is} \right] - \sum_{s=1}^{N_s} \frac{\dot{Q}_{loss}}{\rho c_p} - \frac{\dot{Q}_{loss}}{c_p m} \frac{\partial p}{\partial t}, \tag{3} \]
where: \( m \) - mass inside of reactor, \( \dot{m}_i \) - mass flow rate into reactor at inlet \( i \), \( \dot{m}_e \) - total mass flow rate out of the reactor, \( N_i \) - number of inlets, \( D_{sm} \) - species diffusion coefficient, \( a_T \) - thermal diffusivity, \( \xi_s \) - mass fraction of species \( s \), \( \dot{\xi}_i \) - species \( s \) production rate at inlet \( i \), \( N_s \) - number of chemical species, \( \dot{\omega}_s \) - species \( s \) production rate (calculated using CHEMKIN), \( M_s \) - molecular mass of species \( s \), \( \rho \) - mass density in the reactor, \( T \) - temperature, \( \bar{c}_p \) - mean specific heat at constant pressure in the reactor, \( p \) - pressure, \( t \) - time, \( v_m \) - modified gas speed given by eqn (6).

**Figure 1.** A partially-mixed reactor (PMR) showing multiple inlets and a single outlet.

\( Q_{\text{loss}} \) in eqn (3) represents the heat transfer to the combustion chamber walls and it is given by a modified form of the Woschni [3]

\[
\dot{Q}_{\text{loss}} = \alpha_w A(T - T_w), \tag{4}
\]

where: \( T \) - gas temperature, \( T_w \) - wall temperature, \( A \) - instantaneous gas-wall interface area, \( \alpha_w \) - instantaneous convective heat transfer coefficient.

The Woschni [3] correlation is a dimensional correlation and gives the instantaneous heat transfer coefficient as:

\[
\alpha_w = 3.26 \left( \frac{p v_m}{b^{0.2} T^{0.55}} \right)^{0.8}, \tag{5}
\]

where: \( p \) - pressure [kPa], \( T \) - gas temperature [K], \( b \) - cylinder bore [m] and \( v_m \) is a modified gas speed given by:

\[
v_w = 2.28 s_m + 3.24 \times 10^{-3} \frac{V_s T_i}{p_1 V_1} (p - p_0) \tag{6}
\]

for the combustion and expansion phase of the cycle, where: \( s_m \) - mean piston speed [m/s], \( V_s \) - cylinder volume [m\(^3\)], \( T_i, p_i, V_i \) - temperature [K], pressure [kPa] and volume [m\(^3\)] at the beginning of the combustion, \( p_0 \) - pressure that would exist if combustion did not occur, or, the pressure that would exist in a motored engine under the same conditions.

Consideration of eqn (4) in eqn (3) leads to the simplification of the boundary conditions in later use.
2.2 Matching the turbulent reacting flow

Turbulent reacting flow can be matched applying the multiple PMR’s technique. In this case, as shown in Figure 2, the outlets of one reactor become the inlets of the adjacent reactors. If the first reactor were ignited, hot gas would flow into the second reactor, which would soon reach the ignition temperature and ignite. This ignition process repeats itself as the hot gas in the second reactor goes into the third reactor and so forth. By adjusting the mass flow rates between reactors one can vary the mass burn rate to match an engine. Since the fluid properties are the same at all exits, the flow at all exits may be lumped together into a single exit flow, even though there may be more than one exit.

![Figure 2. A series of PMR's.](image1)

Applying the series of various number of PMR’s of different size the combustion chamber of spark-ignited engine can be modelled as shows a conceptual picture of a 12 reactor system in Figure 3.

![Figure 3. Conceptual picture of typical locations of the reactors.](image2)

In this case of multiple PMR’s the actual formula for \( \dot{Q}_{\text{loss}} \) has been changed due to the following equation

\[
\dot{Q}_{\text{loss}} = \alpha_w K_r (T_r - T_w) A_{\text{total}} \frac{m_r}{m_{\text{total}}}
\]  

written now for each of the PMR, where: \( K_r \) – heat transfer factor for reactor \( r \), \( T_r \) – temperature of reactor \( r \), \( A_{\text{total}} \) – total surface area of combustion chamber,
calculated from engine geometry, \( \dot{m}_r \) - massflow through reactor, \( m_{\text{total}} \) – total mass of system.

The total area, \( A_{\text{total}} \) is calculated from engine geometry. The implicit assumption made in eqn (7) is that the heat transfer from each reactor scales directly with the fraction of mass in that reactor, and with the total surface area (of all reactors).

The \( \frac{\partial p}{\partial t} \) term is modelled by assuming that all reactors have the same pressure and noting that:

\[
p = \frac{R_m}{V} \sum_{r=1}^{N_r} \frac{m_r T_r}{M_r},
\]

where: \( R_m \) – universal gas constant, \( V \) – total volume of all reactors, \( M_r \) – mean molecular weight of the gas in reactor.

Differentiating eqn (8) with respect to time and considering that combustion occurs at the constant volume gives an expression for \( \frac{\partial p}{\partial t} \) which can be rearranged to give:

\[
\frac{V}{R_m} \frac{\partial p}{\partial t} = \sum_{r=1}^{N_r} m_r T_r \sum_{s=1}^{N_s} \frac{1}{M_s} \frac{\partial \xi_{rs}}{\partial t} + \sum_{r=1}^{N_r} m_r \frac{\partial T_r}{\partial t} \sum_{s=1}^{N_s} \frac{\xi_{rs}}{M_s} + \sum_{r=1}^{N_r} T_r \frac{\partial m_r}{\partial t} \sum_{s=1}^{N_s} \frac{\xi_{rs}}{M_s}.
\]

For of the \( N_r \) reactors there is an energy eqn (3) for \( \frac{\partial T_r}{\partial t} \) which contains \( \frac{\partial p}{\partial t} \). The eqn (9) which is the formula for \( \frac{\partial p}{\partial t} \) also contains \( \frac{\partial T_r}{\partial t} \) of each of the reactors. This forms a set of \( N_r \) of eqn (3) in \( N_r \) unknowns that must be solved simultaneously to give the \( \frac{\partial T_r}{\partial t} \) terms. All differential eqn’s of (1) through (3) can be solved applying the boundary-domain integral method.

3 Solution method

3.1 Boundary-domain integral equations

Differential eqn’s from (2) through (3) can be written in a general non-steady diffusive-convective transport equation for an arbitrary scalar quantity \( u \) [4]:

\[
\frac{\partial u}{\partial t} + \frac{\partial}{\partial x_j} (\nu_m u) - a \frac{\partial^2 u}{\partial x_j^2} + S_u = 0,
\]

where \( a \) is a diffusivity (\( a_T \) or \( D_{sm} \)), \( \nu_m \) velocity and \( S_u \) a source term including now the right hand side terms of eqn’s (2) through (3). This equation represents
with known boundary and initial conditions a parabolic initial-boundary value problem.

Introducing a finite difference expression to approximate the time derivative

\[
\frac{\partial u}{\partial t} = \frac{u_F - u_{F-1}}{\Delta t}
\]  

(11)

and decomposing the velocity into constant and variable part

\[
u_m = \overline{v}_m + \tilde{v}_m
\]  

(12)

the eqn (10) can be rewritten in the next form

\[-a \frac{\partial^2 u}{\partial x_j^2} + \overline{v}_m \frac{\partial u}{\partial x_j} + \frac{\partial}{\partial x_j} (\overline{v}_m u) + \frac{u - u_{F-1}}{\Delta t} + S_u = 0.
\]  

(13)

Introducing the pseudo-body force term

\[
b = S_u - \frac{\partial}{\partial x_j} (\overline{v}_m u) + \frac{u_{F-1}}{\Delta t},
\]  

(14)

eqn (13) may be rewritten in the following form

\[-a \frac{\partial^2 u}{\partial x_j^2} - \overline{v}_m \frac{\partial u}{\partial x_j} - \frac{u}{\Delta t} + b = 0.
\]  

(15)

The above differential formulation can now be transformed into an equivalent integral statement using a weighted residual technique or Green’s theorems [5] for scalar functions, resulting in the following integral formulation

\[c(\xi)u(\xi) + \int_\Gamma a u \frac{\partial u}{\partial n}^* d\Gamma = \int_\Gamma \left( a \frac{\partial u}{\partial n} - \overline{v}_n u \right) u^* d\Gamma + \int_\Omega b u^* d\Omega
\]  

(16)

or applying the equation (14) and combining some terms, the final form of integral representation of diffusive-convective equation may be derived

\[c(\xi)u(\xi) + \int_\Gamma u \frac{\partial u}{\partial n}^* d\Gamma = \frac{1}{a} \int_\Gamma \left( a \frac{\partial u}{\partial n} - \nu_n u \right) u^* d\Gamma + \frac{1}{a} \int_\Omega \overline{v}_m u \tilde{v} u^* d\Omega \]

\[+ \int_\Omega \left( \beta u_{F-1} + \frac{S_u}{a} \right) u^* d\Omega,
\]  

(17)

where the following equality \(\nu_n = \nu_m \overline{n} = \overline{v}_m + \tilde{v}_m\) is considered.

The fundamental solution \(u^*\) involved in integral statement (17) contains the influences of convection and diffusion [6]
\[ u^* = \frac{1}{2\pi a} K_0(\mu r) \exp\left(\frac{\bar{v}_j r_j}{2a}\right), \]  
\[ \mu = \sqrt{\left(\frac{\bar{v}}{2a}\right)^2 + \beta}. \]

where \( \beta = 1/\alpha \Delta t \).

### 3.2 Discretized boundary-domain integral equation

Boundary-domain integral equation (17) is solved numerically in a discrete form. A discrete form of integral formulation (17) can be written in the form as follows [7]:

\[ [H][u] = \frac{1}{a} [G]\left\{ a \frac{\partial u}{\partial n} - \nu_n u \right\} + \frac{1}{a} [D_x]\{\bar{v}_m u\} + [B]\left\{ \beta u_{F-1} + \frac{S_n}{a} \right\} \]  

Matrices \([G]\) and \([H]\) consist of boundary integrals of fundamental solution \( u^* \) and its normal derivations, respectively. Domain integrals of fundamental solution \( u^* \) and its coordinate derivations are involved, respectively, in matrices \([B]\) and \([D_x]\). Each formulation can be written for whole domain or for each subdomain if applied [8].

### 3.3 Numerical model

Each of PMR’s has been discretized by mesh of 10 x 10 equally spaced geometric nodes as shown in Figure 4. Each quadrilateral internal cell represents one subdomain bounded by four boundary elements. Discretized domain representing \( i \)-th PMR is bounded on top and bottom by impassable and adiabatic walls.

![Figure 4. Discretization of PMR’s](image-url)
Inlet boundary conditions are constant \((u_0)\) representing the velocity, temperature and species mass fractions out-coming from the previous PMR. First reactor involves fuel only while the other reactors involve the corresponding amount of air regarding given air/fuel ratio. Mass flow rate through each reactor is the same and one part of it could be returned to match the turbulent mixing conditions between each reactor what strongly depends on the engine operating conditions.

4 Results and discussion

The combustion process with 0.5 equivalence ratio in a spark-ignited engine has been calculated applying fully developed natural gas chemical mechanism [9]. The stroke was reported but the connecting rod length was not and reasonable value was assumed. The volume vs. time curve for the cylinder is a weak function of the ratio of connecting rod length to stroke. This approximation is not believed to cause any appreciable error. The engine speed, spark timing, and compression ratio were reported, thus the approximate volume as a function of time for the entire combustion and expansion phase is known. It was assumed that no reaction happened prior to the spark. The input variables that were considered to be unknown were primarily the mixing rates between reactors.

![Temperature vs. time profiles for reactors 3, 7, and 11 (14 PMR's)](image)

Figure 5. Temperature vs. time profiles for reactors 3, 7, and 11 (14 PMR’s)
The central assumption of this method is that if the mixing rates are adjusted so the rate of burning of the mass is roughly equal to that in the real engine, the formation of all the product gases should also follow that of the engine. It has to be noted that this drawback is typical for WMR model and now has been improved taking into account the convection and diffusion in the PMR model. However, the initial temperature was also adjusted, but never far from that predicted by analysis of the compression phase. All calculations have been performed applying 14 reactors’ model.

Figure 5. shows the comparison of the temperature profiles vs. time trace for several of the reactors for different calculation models. Note that each reactor undergoes sudden combustion, with the lower numbered reactors igniting first.

Figure 6. shows the amount of NOx and CO in the combustion chamber as a function of time calculated by WMR and PMR model. The freezing of the NOx reactions after the expansion has begun is apparent. The steps in the latter portion of the CO trace are caused by the ignition of the large middle reactors. Ignition tends to oxidise most of the CO in the reactor suddenly. A significant improvement especially in the CO calculation applying modified PMR seems to be the consequence of the more proper flow description considering the convective and diffusive terms in transport equations.

![Graph](image1)

![Graph](image2)

Figure 6. NOx and CO mass fractions in the cylinder

5 Conclusions

An improved PMR modelling process has been developed in comparison with WMR model which, in general, is useful for systems which have competing reaction and turbulent mixing effects. The model presented emphasises detailed chemistry considering partially also the fluid dynamics. On that way a major drawback of the WMR model representing the heuristically prescription of the mixing rates has been mostly avoided. Specifically, the model was used to
model the combustion of an internal combustion spark ignition engine. By matching the mass burned curves of the actual engine one obtains reasonable pressure and temperature curves and obtains acceptable prediction of combustion products. However, there are a lot of evidences that suggest this model can be used to predict knock also.

References


