

A Monte Carlo Based Turbulent Flame Propagation Model for Predictive SI In-Cylinder Engine Simulations Employing Detailed Chemistry for Accurate Knock Prediction

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ABSTRACT

This paper reports on a turbulent flame propagation model combined with a zero-dimensional two-zone stochastic reactor model (SRM) for efficient predictive SI in-cylinder combustion calculations. The SRM is a probability density function based model utilizing detailed chemistry, which allows for accurate knock prediction. The new model makes it possible to - in addition - study the effects of fuel chemistry on flame propagation, yielding a predictive tool for efficient SI in-cylinder calculations with all benefits of detailed kinetics.

The turbulent flame propagation model is based on a recent analytically derived formula by Kolla et al. It was simplified to better suit SI engine modelling, while retaining the features allowing for general application. Parameters which could be assumed constant for a large spectrum of situations were replaced with a small number of user parameters, for which assumed default values were found to provide a good fit to a range of cases. Only one parameter, the turbulence intensity, needed tuning to obtain excellent agreement for various cases. The laminar flame speed is obtained from a laminar flame speed library generated using detailed chemistry.

The flame development was calculated from the turbulent flame speed under the assumption of a spherical flame. A Monte Carlo geometry calculation was applied to cater for arbitrary cylinder geometries and spark plug positions, modelling the geometrical properties of the flame with high precision. In later stages of the project, a polygon based description of the flame surface was used, to achieve faster computational times than those of the Monte Carlo model.

CITATION: Bjerkborn, S., Frojd, K., Perlman, C. and Mauss, F., "A Monte Carlo Based Turbulent Flame Propagation Model for Predictive SI In-Cylinder Engine Simulations Employing Detailed Chemistry for Accurate Knock Prediction," *SAE Int. J. Engines* 5(4):2012, doi:10.4271/2012-01-1680.

INTRODUCTION

Many phenomena significant for the internal combustion engine can be well modelled using only the statistical distribution of properties in the combustion chamber gas. Zero-dimensional models such as the stochastic reactor model (SRM), available in the DARS-ESM software packageⁱ, have proven to be time-efficient ways of predicting for example engine knock and emission characteristicsⁱⁱ. Some phenomena, however, are still highly dependent on spatial effects, requiring either calculation-heavy three dimensional models or approximations requiring tweaking.ⁱⁱⁱ One of these phenomena is of course the flame growth.

In an SI engine, the propagation of the turbulent flame front, and the heat release characteristics that it gives rise to, is of utmost importance to the behaviour of the engine. In zero-dimensional models, the Wiebe function is often used to characterize the combustion rate. This is a mathematical description of the burned mass fraction (MFB) as a function of time, which requires a re-fit every time a parameter affecting the flame propagation is changed.

This paper deals with the tracking of a three-dimensional flame front in a user-defined combustion chamber, and the integration of this model in the zero-dimensional SRM code. Two alternative approaches for the flame volume calculations are proposed. SRM models have previously successfully been

used to study engine behaviour, with different approaches to the flame growth modelling^{iv}.

METHODS

The SRM Model

In the two-zone SI-SRM model, the mass of the cylinder gas is divided into two separate zones, burned and unburned, and the mass of each zone is divided into a number of particles. The particles, however, carry no spatial information and are merely a discretization of the mass. The distribution of state variables is described using probability density functions. In each time step, a new probability density function is calculated by numerically solving its transport equation. Individual processes in the cylinder (see Fig. 1) are solved for each time step in an operator splitting loop. Including detailed chemistry enables the model to predict knock onset and emissions.

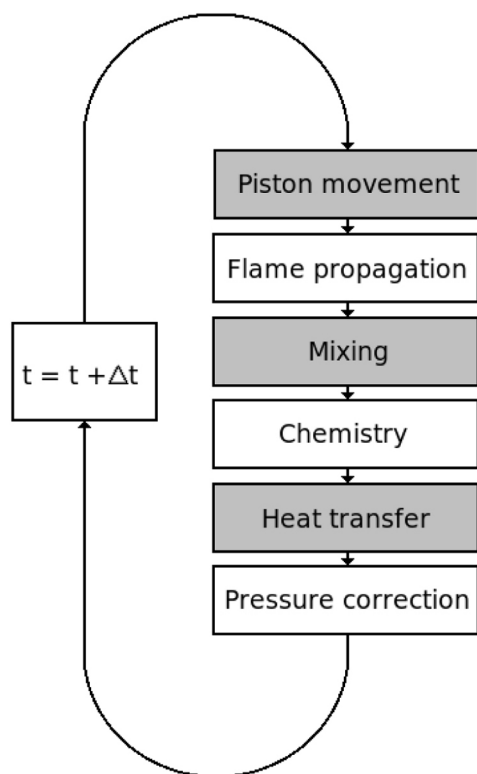


Figure 1. The operator splitting loop for the SI-SRM

Chemistry

The distribution of mass fractions for a particular species between the particles is initialized according to a probability density function. This evolution of this distribution is modelled by stochastic mixing between the particles. Chemical reactions, with corresponding heat release, are calculated based on reaction coefficients defined in the chemistry mechanism. During the development of the flame propagation model, the 200 species NICE 4.02 PRF

mechanism for n-heptane and iso-octane was used. The same model was used by the model to determine if and when autoignition conditions occur in the unburned zone.

The Wiebe Function

The previously used method for describing flame propagation was to let the burned mass ratio follow a defined Wiebe function, on the general form of Eq. 1.

$$x_b = 1 - e^{-a\left(\frac{\theta - \theta_0}{\Delta\theta}\right)^{m+1}} \quad (1)$$

The mass of the gas in the burnt zone (normalized to the total cylinder mass) is denoted by x_b , while a and m are user parameters determining the exact shape of the function. θ_0 is the time of ignition in crank angle degrees, and $\Delta\theta$ denotes the total duration of combustion. Most or all of these parameters need to be tweaked for every individual case. The limitations it imposes on the model's range of applications are obvious.

Fig. 2 shows a typical example of a Wiebe generated burned mass fraction.

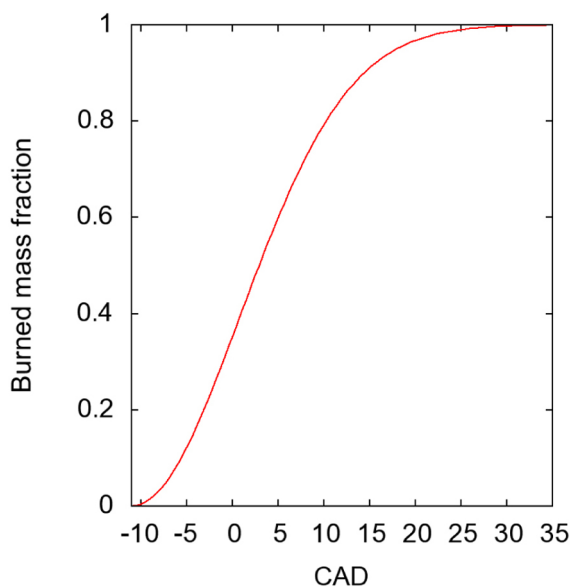


Figure 2. The mass fraction burned (MFB) curve generated by a Wiebe function with typical parameters.

Turbulent Flame Propagation Model

In the developed flame propagation model, the flame brush is assumed to expand approximately spherically, centred at the defined spark plug location and limited by the cylinder walls and the piston. The turbulent flame speed is calculated using a correlation between laminar and turbulent flame speed, using a laminar flame speed library calculated in DARS using detailed chemistry.

The assumption of a spherically propagating flame might not be valid for all engines (turbulence, swirl and tumble effects might distort the flame shape, in engines might make

use of stratified combustion to prevent flame-wall contact), but is likely the best approach which can be achieved without calculating the actual flow field. Although the flame volume is calculated in three dimensions, the turbulence is still calculated without spatial resolution, which in turns allows for significantly faster calculations.

Enthalpy losses to the cylinder walls are described using Woschni's heat transfer equation. For simplicity it was assumed that the heat transfer did not affect the spherical flame shape, while the total heat loss to the walls manifested itself via the temperature dependency in the laminar flame speed library.

Turbulent Flame Speed

As a tool for validating a scalar dissipation rate model, Kolla et al.^V derived and validated an expression for the turbulent flame propagation speed, according to Eq. 2.

$$\frac{S_T}{S_L} = \sqrt{\left(\frac{18C_\mu}{(2C_m-1)\beta'}\right) \left([2K_C^* - \tau C_4] \frac{l_L}{\delta_L} \frac{u'}{S_L} + C_3 \frac{2}{3} \left(\frac{u'}{S_L}\right)^2\right)} \quad (2)$$

S_T and S_L is the turbulent and laminar flame propagation speed, respectively. The values of C_μ , C_m and β' are given in the articles of Kolla et al. as $C_m \approx 0.7$, $C_\mu = 0.09$ and $\beta' = 6.7$. K_C^* is dependent of the flamelet structure, and is found to be roughly 0.85τ for methane/air-flames, with a slight dependency (in the region of $\pm 10\%$) on the equivalence ratio. It is thought to be in a similar order of magnitude for other fuels. The parameter τ is the heat release parameter, defined according to $\tau = \frac{T_{ad}-T_u}{T_u}$. C_4 and C_3 are equation parameters, l_L is the integral length scale of the system, δ_L is the laminar flame thickness and u' is the turbulence intensity.

The turbulence model has been showing good correlation^{VI} to a large number of experimental cases, for different turbulent combustion regions, engine speeds and loads. It is however overly complex for the application, and therefore the following simplification was made. Expanding Eq. 2 using definitions from^{II} gives

$$\frac{S_T}{S_L} = \left(\frac{\frac{18C_\mu}{(2C_m-1)\beta'} \left(\tau \cdot 1.1 \left(1 + \left(\frac{u'}{S_L} \right)^{1.5} \left(\frac{\delta_L}{l_L} \right)^{0.5} \right)^{-0.4} \right)}{\left(\frac{u'}{S_L} \frac{l_L}{\delta_L} \right) + \frac{18C_\mu}{(2C_m-1)\beta'} \frac{2}{3} \frac{1.5 \cdot \left(\frac{u'}{S_L} \right)^{1.5} \left(\frac{\delta_L}{l_L} \right)^{0.5}}{1 + \left(\frac{u'}{S_L} \right)^{1.5} \left(\frac{\delta_L}{l_L} \right)^{0.5}} \left(\frac{u'}{S_L} \right)^2} \right)^{0.5} \quad (3)$$

which via the introduction of the variables a , b and d , and an approximation of the relationship between K_C^* and τ , yields

$$\frac{S_T}{S_L} = \left(\left(b - a \cdot \left(1 + \left(\frac{u'}{S_L} \right)^{1.5} \left(\frac{\delta_L}{l_L} \right)^{0.5} \right)^{-0.4} \right) \frac{T_{ad}-T_u}{T_u} \frac{l_L}{\delta_L} \frac{u'}{S_L} + \left(d \cdot \left(\left(\frac{u'}{S_L} \right)^2 + \left(\frac{\delta_L}{l_L} \right)^{-0.25} \left(\frac{u'}{S_L} \right)^{-2.25} \right) \right)^{-1} \right)^{0.5} \quad (4)$$

$$a = \frac{1.1}{d} \quad (5)$$

$$b \approx \frac{1.6}{d} \quad (6)$$

$$d \approx 1.654 \quad (7)$$

In Eq. 4, all parameters which are not calculated in the SRM code have been replaced with three user-tuneable parameters (the expected values of which can be approximated from the formula by Kolla et al., and can be found in Eq. 5,6,7). The relationship between parameters b and d depends on the relationship between K_C^* and τ for the fuel and equivalence ratio in question. The laminar flame thickness, integral length scale and turbulence intensity can all be defined by the user.

It should be pointed out that neither Eq. 3 nor 4 are valid for near-laminar systems, where the turbulence intensity approaches zero. Although it falls beyond what would be a realistic scenario in a typical passenger car engine, the model included a more simplistic approach to the turbulent flame propagation speed for this region. This model, unlike Eq. 4, tends towards $S_T/S_L = 1$ when u' goes towards 0.

Flame Geometry Calculations

Monte Carlo Methods

In order to offer the most precise volume calculations of the flame sphere which would be possible without the need to calculate a flow field, a Monte Carlo algorithm was developed. Randomizing coordinates within the cylinder space and sorting them based on whether or not they are within the flame radius echoes on a study by Poulos & Heywood in 1983^{VIII}, allowing the model to capture the effects of combustion chamber geometry, piston position and spark plug position on the flame propagation with very good precision. A large set of coordinates ($i = 1 \dots n_{MC}$) were randomized within a known volume V_{REF} . For each randomized coordinate i , a value was calculated from the product of four step functions: A , B , C and D , defined respectively as 1 inside the flame radius (propagating with the speed S_T from the spark position), below an arbitrarily defined cylinder roof, within the cylinder walls and above the piston surface, and 0 outside these regions. For a sufficiently large amount of Monte Carlo points, the volume can be well approximated according to Eq. 8.

$$V_{flame} = V_{ref} \frac{\sum n_{MC}(A_i B_i C_i D_i)}{n_{MC}} \quad (8)$$

For this project, all simulations were performed using a time step of 0.5 CAD at engine speed intervals of 1200-2500 rpm. During the phase with the most rapid combustion, the volume of a typical flame (going from 0 to 90% burnt mass in 25-30 CAD) is thought to increase with 25 %/CAD. In order to capture the flame growth between two consecutive time steps, it is therefore important that the stochastic fluctuations in the Monte Carlo volume is kept smaller than 0.125% (one percent of the expected maximum volume growth during one time step). To achieve this, the reference volume within which the Monte Carlo points are randomized must enclose the flame as closely as possible. The algorithm in use was tested for calculating the volume of a hemisphere, with a well-defined volume. The discretized probability density function of the deviation from the analytically calculated volume is presented in Fig. 3 and 4 below. The Monte Carlo algorithm was set to calculate the volume of a hemisphere with a fix radius using 10,000,000 and 20,000,000 randomly distributed particles. This calculation was repeated 4000 times, and the likelihood for a particular deviation from the analytically calculated volume was plotted.

It was found that for a value of 10,000,000 Monte Carlo points, the desired precision was reached in 98.2% of the calculations, and for a value of 20,000,000 Monte Carlo points it was reached in 99.9% of the calculations. For increased robustness, the algorithm assumes a lowest possible growth per time step, and applies this in the unlikely event that the Monte Carlo simulation should return a negative growth for a particular time step.

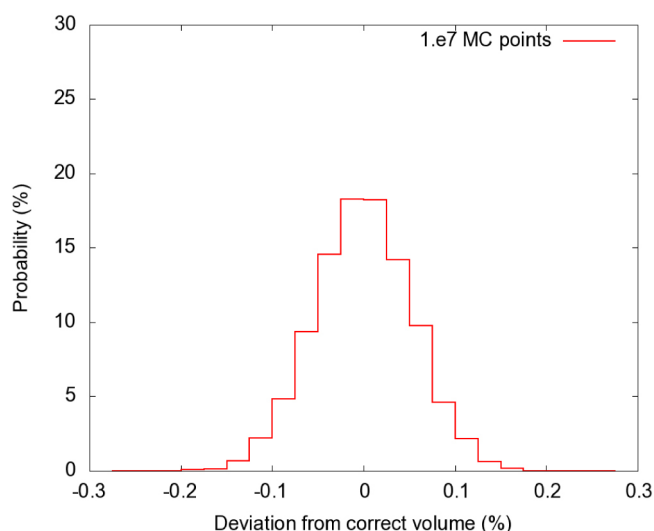


Figure 3. Discretized probability density function for the volume deviations in the Monte Carlo algorithm, using 10^7 Monte Carlo points.

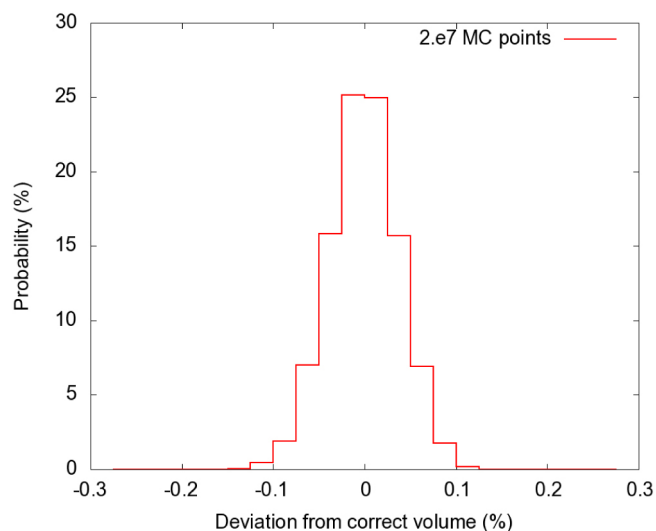


Figure 4. Discretized probability density function for the volume deviations in the Monte Carlo algorithm, using $2 \cdot 10^7$ Monte Carlo points.

The Monte Carlo model was written to calculate flame volumes for user-defined three dimensional cylinder and piston profiles. This enables the flame propagation model to capture three-dimensional spatial effects, despite being integrated in a zero-dimensional combustion model. When running on a single CPU, on a typical consumer PC, the total flame volume calculations for one cycle simulated in steps of 0.5 CAD took approximately 30 minutes for $2 \cdot 10^7$ Monte Carlo points.

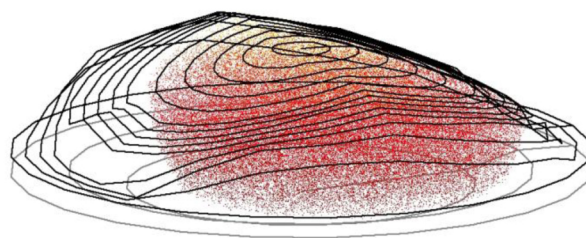


Figure 5. Visualization of Monte Carlo coordinates for a flame radius of 30 mm in a given cylinder geometry.

POLYGON BASED GEOMETRY

To decrease CPU time, the algorithm was adapted to calculate the flame volume using a polygon model. The flame sphere was approximated as a set of tetrahedrons, each with an analytically solvable volume. This approach was also chosen to simplify future inclusion of local variations in for example temperature. The flame surface is represented as a set of nodes, each of which can propagate outwards from the flame centre with a flame speed defined by local conditions. In his work statistical homogeneity was assumed, and the flame propagation speed was hence thought to be equal for all nodes.