Predictive Flame Propagation Model for Stochastic Reactor Model Based Engine Simulations

Simon Bjerkborn[1], Cathleen Perlman[1], Karin Fröjd[1], and Fabian Mauss[2]

[1]Lund Combustion Engineering — LOGE AB, Lund, Sweden
[2]Brandenburg University of Technology — BTU, Cottbus, Germany

1 Introduction

A stochastic reactor model (SRM) based spark-ignition engine simulation code allowing for detailed chemistry based knock prediction [1] has been extended with a predictive flame propagation model. The previously used Wiebe function approach, has been replaced by a turbulent flame propagation model where the underlying laminar flame speeds rely on detailed chemistry calculations. This new model development allows for studying the effects of fuel chemistry on the flame propagation event, in addition to determining the knock limit.

The turbulent flame propagation model derived by Kolla et al. [2] was combined with a laminar flame speed library for iso-octane to obtain a predictive flame propagation model. The flame development was simulated for arbitrary cylinder shapes using a flexible Monte Carlo geometry model, echoing and improving on a study published by Poulos & Heywood in 1983 [3].

The turbulent flame propagation model is based on a formula derived by Kolla et al. from Kolmogorov-Petrovskii-Piskunov (KPP) analysis [2]. It was simplified to better suit the application, while retaining the features allowing for general application. Parameters which could be assumed constant for a large spectrum of situations were replaced by three parameters. For cases with low ratio between the turbulent velocity fluctuation and the laminar flame speed, where the molecular diffusivity cannot be neglected as in KPP analysis [4], a simple turbulence model was used with suitable parameters.

Validation was made qualitatively, against the predictions of Poulos & Heywood [3], and against experimental data.

2 Model Description

2.1 The Stochastic Reactor Model

As a basis for this work the zero dimensional two-zone stochastic reactor model, available in the DARS [5] software package, was used. This model assumes stochastical homogeneity in the burned and the unburned zones. No spatial resolution is calculated, but instead a mass-discretized probability

Correspondence to: maussf@tu-cottbus.de

density function is used to describe state variables. Mass transport between the zones is given by the flame propagation. Until now, a simple Wiebe function has been used. In this work a predictive model for turbulent flame propagation was developed, and proven to be usable as a complement or a replacement for the non-predictive Wiebe model.

2.2 The Turbulent Flame Propagation Model

Foundations for the used turbulent flame propagation model can be found in reference [2], where an inclusive turbulence model was derived from a scalar dissipation rate model. The resulting equation was:

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

This model has been thoroughly validated for a wide range of experimental data, well covering the parameter regions relevant for SI engine combustion [2]. Furthermore the model offers good applicability compared to more simplistic turbulence models, while still being easy to use due to the manageable number of user parameters. The model works within a wide operation range, since it is based on first principles.

Assuming invariance in some model parameters, the following approximation can be done:

$$\frac{S_T}{S_L} \approx \left(\left(b - a\cdot\left(1 + \left(\frac{u'}{S_L}\right)^{1.5}\left(\frac{\delta_L}{l_L}\right)^{0.5}\right)^{-0.4}\right)\frac{T_{ad} - T_u}{T_u}\cdot\frac{l_L}{\delta_L}\cdot\frac{u'}{S_L} + \frac{d}{\left(\frac{u'}{S_L}\right)^{0.75} + \left(\frac{\delta_L}{l_L}\right)^{-0.25}}\cdot\left(\frac{u'}{S_L}\right)^{2.75}\right)^{1/2} \quad (2)$$

The values of parameters *a* and *d* can be derived from the analytical expression of Kolla et al., but can also be tweaked to give optimal results for a particular application. The parameter *b* is dependent on the fuel and the equivalence ratio. All other parameters can either be approximated or are calculated in the existing SRM model. The turbulence velocity is calculated using the given turbulence length scale and a turbulent mixing time, which can be described either as a constant or using any time-dependent profile.

The laminar flame speed is retrieved from a laminar flame speed library for iso-octane, calculated for a wide parameter range given in Table 1. For fast access to the values an advanced correlation function was developed. A mean relative error of 9 % was achieved for the full parameter range. The table values vs the correlation function is illustrated in Figure 1 below.

Equivalence ratio	0.2 - 4.0
Temperature	300 K - autoignition
Pressure	1 - 130 bar
EGR	0 - 50%

Table 1 – Parameter ranges for the laminar flame speed library

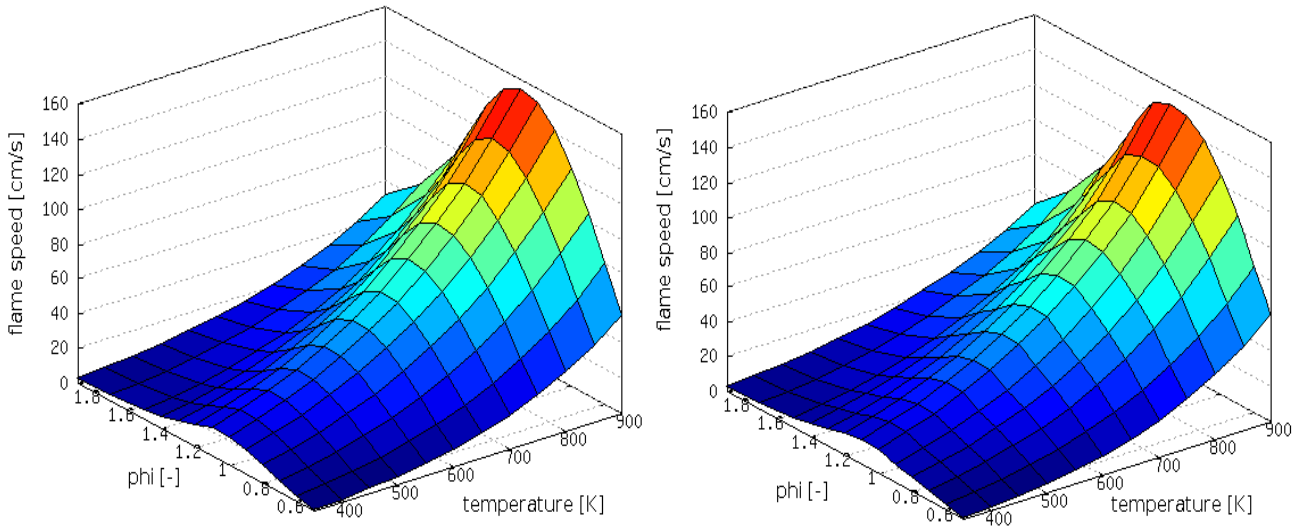

Figure 1 – Comparison of library data (left) and correlation function (right) for laminar flame speed at 10 bar and 10% EGR.

2.3 Geometry

The SRM is a zero-dimensional model, without spatial resolution. Still, geometrical data is needed to calculate the flame evolution. This is taken into account by a Monte Carlo geometry model, assuming a spherical flame propagation and a user defined cylinder geometry. The geometry input is a set of two dimensional coordinates describing the cylinder profile and the spark plug location. Rotational symmetry is assumed in the current implementation of the model.

The use of a Monte Carlo model for calculating the flame volume allows for calculations of specific fractions of the flame volume, such as the volume of the flame within a distance from the cylinder walls. This in turn can be used for developing advanced flame quenching models.

3 Results & discussion

Poulos & Heywood [3] report a study using a similar Monte Carlo model for the geometry, where a number of cylinder/piston geometries are investigated together with various spark plug positions. The flame propagation model is however substantially different from the one used in this study, and not using detailed kinetic calculations for the laminar flame speed. It is limited to one engine case, and therefore many of the effects seen in the study cannot be assumed to be general. The SRM code was used to recreate a similar, though not identical, case as used in [3], and the results compared to [3] are presented in fig. 2.

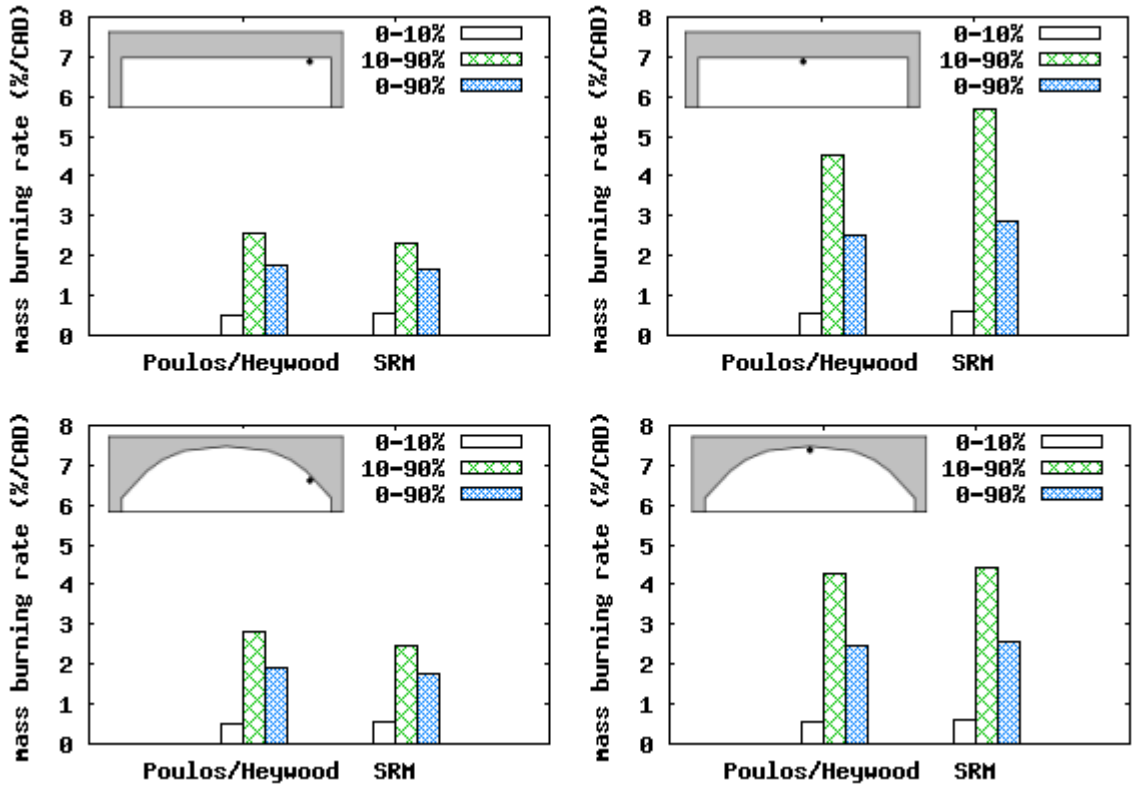

Fig. 2 – Comparison between the burning speed (percent of the total mass burned per crank angle degree) in the SRM model and for results derived by Poulos & Heywood. Schematic drawings of the four studied cylinder profiles inserted, black dot marks spark plug position.

The general trends are similar, but the discrepancies highlights the non-generalizability of some of the phenomena observed in [3]. It was observed that cylinder head geometry, compression ratio and equivalence ratio has a significant influence on the combustion process.

The model was also tested against a 4 cylinder passenger car engine. The behaviour of three of the four cylinders could be well predicted by adjusting the initial temperature at 130 CAD BTC by ±15 K. The dissonant behaviour for the fourth cylinder could be explained by leaking piston rings or deviations in the relative air/fuel ratio (λ). Experimental pressure traces and model predictions for three of the four cylinders are presented in fig. 3. The deviation in pressure after 20 CAD can be explained by the use of an approximated geometry and spark plug location. At 20 CAD the flame radius was found to be in the region of 4 cm, similar to the cylinder radius. At this stage the flame makes contact with the cylinder walls, and the exact cylinder geometry and spark plug position is highly relevant for the flame propagation.

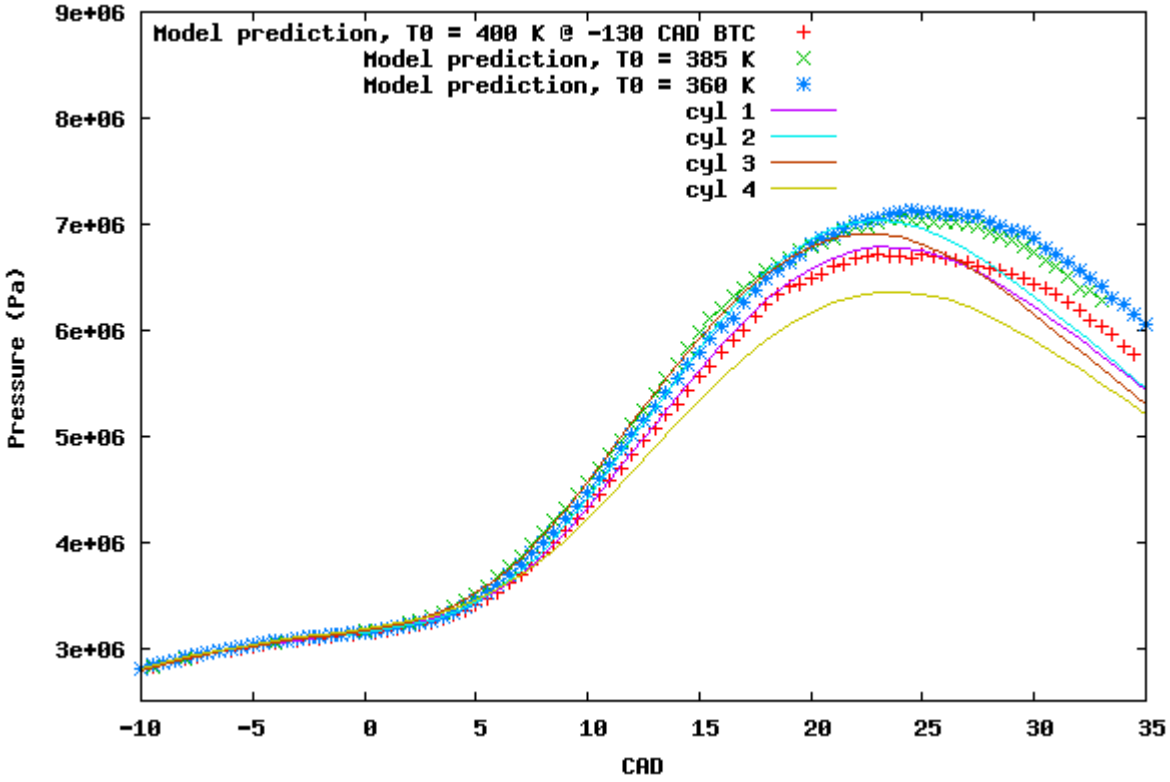

Fig. 3 – Measured and predicted pressure for a four cylinder engine. Experimental pressure traces are cycle-averaged.

It should be noted that no equation parameters in the turbulent flame propagation model needed to be changed. The parameters that depend on operating conditions and engine geometry, i.e. u', l_L and δ_L were adjusted.

4 Conclusion

The zero-dimensional SRM code was extended with a predictive turbulent flame propagation model, and a Monte Carlo model for describing the geometry of a spherical flame propagating in an arbitrary cylinder geometry.

The Monte Carlo model shows general agreement with previous simulations performed by Poulos and Heywood, but makes use of a more advanced reactor model. Technological advances since the study in ref. [3] means that the code can easily be used to quickly simulate individual engines, rather than just a few general cases.

Good agreement with experimental data from a multicylinder SI engine is achieved. The deviation between individual cylinders can be caught by adjusting the initial temperature within experimental uncertainty.

The flame propagation model produces results with comparable or better accuracy than a fitted Wiebe curve, but with further predictive capabilities. It was shown that it is possible to apply the model to varying operating conditions by adjusting parameters depending on geometry and operating conditions.

Nomenclature

S_T	Turbulent flame propagation speed
S_L	Laminar flame speed
u'	Turbulence velocity
l_L	Integral length scale
δ_L	Laminar flame thickness
$C_\mu, C_m, C_3, C_4, K_c^*, \tau$	Equation parameters in eq. 1, see ref. [2]
a,b,d	Equation parameters in eq. 2
T_u	Unburnt temperature
T_a	Adiabatic temperature

References

[1] Gogan, A., Sundén B., Lehtiniemi, H. and Mauss, F. (2004) "Stochastic model for the investigation of the influence of turbulent mixing on engine knock", SAE paper 2004-01-2999.

[2] Kolla, H., Rogerson, J.W., Chakraborty, N., Swaminathan, N. (2009) "Scalar dissipation rate modeling and its validation", Combustion Science and Technology, 181:3, p 518-535

[3] Poulos, S. G., Heywood, J. B. (1983) "The effect of chamber geometry on spark-ignition engine combustion", SAE paper 830334, SAE Trans. vol. 92

[4] Libby, P.A. (1989) "Characteristics of laminar lifted flames in a partially premixed jet", Combustion Science and Technology, 68:1-3, p 15-33

[5] http://www.diganars.com