

Combustion and Autoignition Modelling in a Turbocharged SI Engine

Ahmed F. Khan and Alexey Burluka
The University of Leeds

Jens Neumeister, Dave OudeNijeweme, Paul Freeland, and John Mitcalf
Mahle Powertrain Ltd

ABSTRACT

A holistic modelling approach has been employed to predict combustion, cyclic variability and knock propensity of a turbocharged downsized SI engine fuelled with gasoline. A quasi-dimensional, thermodynamic combustion modelling approach has been coupled with chemical kinetics modelling of autoignition using reduced mechanisms for realistic gasoline surrogates. The quasi-dimensional approach allows a fast and appreciably accurate prediction of the effects of operating conditions on the burn-rate and makes it possible to evaluate engine performance. It has also provided an insight into the nature of the turbulent flame as the boost pressure and speed is varied. In order to assess the sensitivity of the end-gas chemical kinetics to cyclic variability, the in-cylinder turbulence and charge composition were perturbed according to a Gaussian distribution. Coupling cyclic variability with autoignition modelling allowed prediction of the autoignition propensity for the entire spectrum of cyclic variations in cylinder pressure.

The models have been validated against engine test data from a technology demonstrator downsized, turbocharged engine. The knock-limited spark advance was predicted for a RON 95 and RON 102 gasoline within 2° of crank angle. This work demonstrates the viability of chemical kinetics for gasoline surrogates coupled with 0-dimensional thermodynamic modelling approach as a fast and reliable development tool for high performance engines.

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INTRODUCTION

The most significant factors in the development of new engine technologies are the emissions legislation, improvement in fuel efficiency as well as viability of renewable and synthetic fuels for engine use. For SI engines, the first two issues have been targeted in the past decade or so through the use of technologies such as gasoline direct injection, variable valve timing, turbocharging and after-treatment systems. One approach which has seen vast application is 'engine downsizing' that is a reduction in the engine displacement, invariably accompanied by turbocharging. The end result is an improvement in part-load performance owing to reduced frictional and pumping losses and increased volumetric efficiency. The peak load performance is maintained through pressure charging. Substantial improvements in fuel efficiency have been reported, e.g. 25-30% improvement in fuel consumption for a 50% downsized engine [1], 20% for a 60% downsized engine [2] and 17% for a 40% downsized engine [3].

One of the key challenges in SI engine development remains to be of the engine knock and for turbocharged engines, the higher in-cylinder pressures may result in an even greater likelihood of autoignition of the unburned air-fuel mixture or the so-called 'end gas', possibly resulting in knock. The effects of high pressures on the nature of the

reactions in the end gas leading up to the autoignition are not properly understood [4]. This is because of the lack of information on reaction rates and ignition delay times at high pressures for gasoline-like complex fuel blends.

The ability to predict autoignition during SI engine development is indispensable in order to meet the emissions and performance challenges. This can be achieved by modelling the autoignition reactions through reduced chemical kinetics for gasoline surrogates. The chemical reactions leading to auto-ignition are driven by the end gas pressure-temperature (p - T) history which is determined by motion of the piston and the rate of propagation of the main flame. The easiest method allowing calculation of the (p - T) history is a quasi-dimensional thermodynamic model predicting the combustion rate and thermodynamic states of the burned and unburned gases [5, 6]. This work aims to develop such modelling tools and their application to a downsized turbocharged SI engine.

Current work makes use of set of subroutines from the Leeds University Spark Ignition Engine (LUSIE) code coupled with GT-Power from Gamma Technologies Inc. [<https://www.gtisoft.com/gt-suite/gt-suite-overview/>]. Such coupling referred to as GT-LU was made earlier [7, 8] and the current work extends the previous work by applying GT-LU to high intake pressures and engine speeds.

conditions challenging for any model, be it quasi-dimensional or CFD. Compared to the earlier studies, this work makes greater use of GT-Power and highlights the challenges arising in attempts of making the quasi-dimensional combustion modelling predictive. The most novel element of the present work is a systematic account of interaction between the autoignition pre-flame reactions and cycle-to-cycle variations of the combustion rate accounted through a simple model [7]. These modelling approaches are described in the following sections.

MODELS OF VARIOUS COMBUSTION SUB-PROCESSES

Figure 1 shows the flowchart of the thermodynamic simulations accepted in this work. It may be seen that the overall strategy of the simulation is that adopted in GT-suite, in particular, the combustion is described in the frame of the so-called "three-zone" model [6]. This model assumes that the in-cylinder charge consists of the burnt and fresh gas zones separated by an entrainment zone of a finite thickness representing the turbulent flame brush. In this "three zone" model, the rate of mixture entrainment and the rate of its 'after-burning' are calculated separately. For the main flame propagation, GT-LU subroutines provide the GT-power with the values of the rate of entrainment of the fresh gas, U_{te} , into the entrainment zone, or the flame brush:

$$\frac{dm_e}{dt} = \rho_u A_{fe} U_{te} \quad (1)$$

where, A_{fe} is active surface area of the entrainment front, m_e is the mixture mass behind the entrainment front, and ρ_u is the fresh gas density.

The entrainment velocity was calculated using the Turbulent Flame Speed Closure, or Zimont- Lipatnikov model, which is an extension [9] of the earlier model of Zimont [10] of a fully developed turbulent premixed flame. Original Zimont model [10] assumes that within a fully developed premixed turbulent flame brush there exists an equilibrium between large-scale turbulence which increases the flux of the fresh gas into the flame brush, small-scale turbulence which effectively widens the flame front, and the flame wrinkling caused by the large and inertial scale turbulence. Under these assumptions, the consumption flame speed relative to the fresh gas is derived as:

$$U_t^0 = C_Z u' Da^{1/4} \quad (2)$$

where u' is the root-mean-square (rms) velocity, and $Da = \tau_p / \tau_{ch}$ is the Damköhler number, a ratio of the τ_p , the integral time scale, to the chemical time-scale τ_{ch} . Eq. (2) has been put to extensive tests and proved to perform well when the constant $C_Z = 0.5$ [9, 11, 12]. Nonetheless, in SI engines, as in many other applications, the propagating turbulent flames may not attain the equilibrium state represented by Eq. (2) [9, 12]. In SI engines, three rather distinct stages of flame propagation may be discerned [12]: initial fast flow acceleration, propagation at an approximately constant speed and, finally deceleration caused by proximity to the chamber walls. The flame brush thickness grows at the first two stages [9].

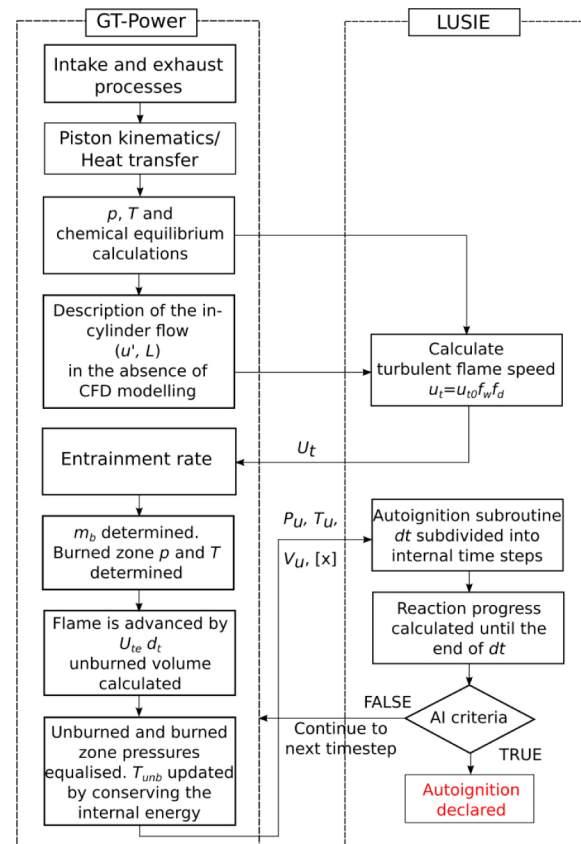


Figure 1. Flowchart showing flow of data and sequence of operations carried out in GT-LU.

Initial period of flame development is modelled in Zimont-Lipatnikov model by analogy with Taylor diffusion of a cloud in turbulent atmosphere:

$$U_t(t) = U_t^0 \left(1 + \frac{\tau_t}{t} \cdot \left[\exp\left(\frac{-t}{\tau_t}\right) - 1 \right] \right)^{1/2} \quad (3)$$

where, t is the time elapsed since ignition. Original Zimont model, Eq. 2, and the subsequent analysis [9] neglected the effects of the thermal expansion; this means that no distinction was made between the consumption and propagation velocity of the turbulent flame. According to Taylor diffusion picture, the flame brush thickness, δ_p , grows as:

$$\delta_t = L \left\{ \frac{2t}{\tau_t} \left[1 - \frac{\tau_t}{t} \cdot \left(1 - \exp\left(\frac{-t}{\tau_t}\right) \right) \right] \right\}^{1/2} \quad (4)$$

When the flame brush thickness is not constant, relationship between consumption and propagation speeds is very complex, so here a rather simple approach was undertaken. The entrainment rate U_{te} which corresponds to the propagation rather than consumption speed, U_p , the relationship for constant flame width:

$$U_{te} = \frac{\rho_u}{\rho_b} \cdot U_t \quad (5)$$

was used and the model constant C_Z was slightly reduced from recommended value of 0.5 to 0.35 to account for growing flame thickness. The latter value was found previously [13] from comparison of simulations with measurements in an optical ported engine and no adjustments were made in the current work, modelling very different type of engines.

The final period of flame deceleration caused by the flame brush truncation by the chamber walls is responsible for the burning of the largest mass proportion of the charge [5, 11, 12] but it had so far attracted little attention. The reduction of the turbulent consumption velocity of propagating spherical flame may be derived under certain assumptions compatible with Eqs. (2, 3, 4) as the following multiplier for U_t :

$$f_w = \operatorname{erf}\left(\frac{R_w - R_{fl}}{\delta_t(t)}\right) \quad (6)$$

where "erf" is the error function, R_w is the bore radius, R_{fl} is the current flame radius. Thus the final expression for the entrainment velocity which GT-LU passes on to GT-Power is:

$$U_{te} = U_L + U_t \cdot f_w \quad (7)$$

GT-power takes the entrainment velocity calculated by GT-LU, Eq. (7), and then uses Eq. (1) to calculate an increase in the amount of the entrained mass. The increment of the burnt mass is calculated by GT-Power using standard model [6] and it proved impossible to modify this procedure to make it entirely coherent with the assumptions about the flame structure embedded in Eqs. (2, 3, 4, 5, 6, 7, 8). As will be shown later, the results are sensitive to the rate of the conversion of the entrained mass to the fully burnt state.

Modelling of Cyclic Variability

Variability of the combustion from one cycle to another was represented on the premise that its main causes are the random variations of the turbulent rms velocity intensity u' of the charge and the equivalence ratio, ϕ . The variation of u' comes from the fact that the time for combustion does not usually exceed a few integral time scales hence the flame does not experience perfect averages. The variation of ϕ is brought in by factors such as a fluctuation in amount of injected fuel in direct injection engines or action of large scale turbulence in intake runners for multipoint injection. A cyclic variation of the global equivalence ratio will effectively change the spread of localised charge composition leading to slightly different burning rates. This variations of both u' and ϕ are sampled from Gaussian distributions with the nominal averages and standard deviation of 12.5% and 5%, respectively [7]. These fluctuations were used to perturb u' and ϕ in the beginning of each new cycle. The particular values of the standard deviations for these perturbations

was previously derived from analysis of measurements in an optical ported engine [13] and no attempt was made here to adjust those in order to achieve better agreement.

Chemical Kinetics of Autoignition

A literature review of the reduced and semi-detailed kinetics mechanisms revealed that several mechanisms of the size of about 100 species and 400 - 600 reactions describing pathways for oxidation of key gasoline surrogate components such as iso-octane, n-heptane, toluene, ethanol and different olefins and naphthenes, typically, iso-butene and cyclo-hexane. An earlier comparison of 8 mechanisms ranging from simpler skeletal models to fully detailed mechanisms [14] showed that such reduced mechanisms offer appreciable accuracy of prediction of autoignition delay time for different blends in a wide range of pressures, temperatures (p - T) and equivalence ratios at feasible computational times. From these comparisons, three most versatile reduced mechanisms have been retained for this work for autoignition simulations. Those three mechanisms are Andrae model [15] which comprises 144 species and 673 reactions, Golovitchev model [16] comprising 121 species and 681 reactions and the Reitz model [17], also known as the MultiChem model, which comprises 113 species and 487 reactions. Thermochemical data and the data of the reaction rate constants for these mechanisms were available in the so-called Chemkin format and they were read through an in-house Fortran code. The code assembles the stiff ordinary differential equations for the rate of change of concentrations. The kinetic equations are then integrated using a numerical library, MEBDFI, which is an implementation of a (M)odified (E)xtended (B)ackward (D)ifferentiation (F)ormulae for fully (I)mplicit equations developed by J. Cash [18].

ENGINE AND OPERATING CONDITIONS

The engine studied in this work, referred here as the Di3 engine, is a 3 cylinder, 1.2 liter, turbocharged GDI engine, developed at Mahle Powertrain Ltd and previously introduced in [19].

The engine operating conditions chosen for simulation studies are shown in Fig. 2 along with the peak bmep curve. The main fuel used in engine tests was an E5 gasoline of RON 95 and MON 85 with some limited amount of tests done with higher RON number gasoline; formulation of surrogate blends for both gasolines is described in later sections. Autoignition studies were made for the three load-speed points shown as I, III and IV in Fig. 2; all lie under the peak bmep curve as comprehensive experimental data were only available for these points in the knocking regime. Typically, low speed and high load points are of interest as there is a higher propensity of knock at these conditions. However, for the objectives of this work the low load points were sufficient. Operating points, II, IV and V represent a change in either the engine speed or the load (boost pressure). This allowed a modelling study of the effects of variation in speed and load on the flame structure by plotting a Borghi regime diagram, see Fig. 7.

Before any predictive modelling of the auto-ignition chemistry could be done, the GT-Power model was thoroughly validated against experimental measurements. Heat release analysis of the measured cylinder pressures provided the fuel mass burning rates which were used in an initial set of simulations to correctly model the in-cylinder pressure. This allowed various other flow-related, thermodynamic and engine performance quantities to be validated against measurements. The predicted pressures and flow rates in the intake and exhaust runners were used as boundary conditions for the CFD modelling to predict the in-cylinder turbulence which would in turn be fed as input to the calculations of the flame speed in the GT-LU model. The correlated GT-Power model was able to correctly predict the gas exchange process thereby achieving the correct volumetric efficiency, fuel flow rate and heat transfer which made it certain that with the use of predictive GT-LU combustion model, any deviation of cylinder pressure was caused by the combustion model and not due to the initial and boundary conditions in various other submodels of GT-Power.

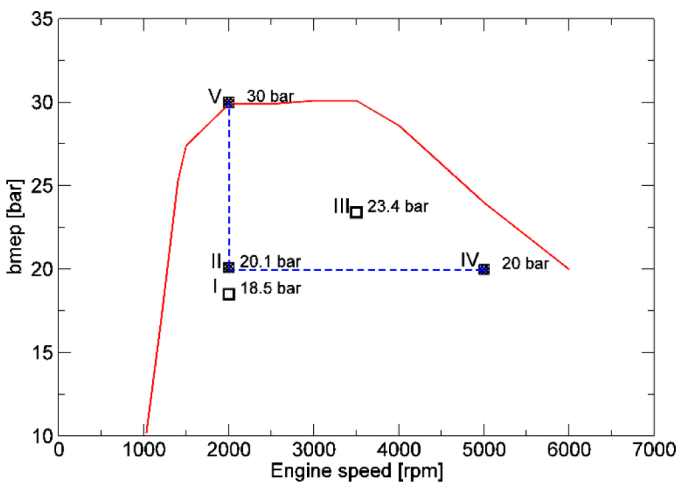


Figure 2. Peak bmep curve of the Di3 engine with five operating points studied in this work.

MODELLING RESULTS AND DISCUSSION

CFD Modelling

In the thermodynamic modelling the rate of combustion is determined by a few turbulence parameters (u' and τ_p) averaged over the entire chamber volume. Even though GT-Power software enables use of a homogeneous "k- ϵ " model, here use of CFD was preferred as detailed chamber geometry could be considered and the details of the modelling methodologies are well known.

The 3-D CFD modelling of cold flow was done from the intake valve opening until the crank angle at which combustion was expected to finish. A correlated GT-Power model was used to generate the boundary conditions for the CFD modelling. A RNG "k- ϵ " turbulence model was employed in Star-CD solver with the meshing and the problem preparation done in ES-ICE by CD-Adapco. The mass averaged rms turbulent velocity u' and the integral length scale L for the five operating points shown in Fig. 2 were determined and are presented in Fig. 3.

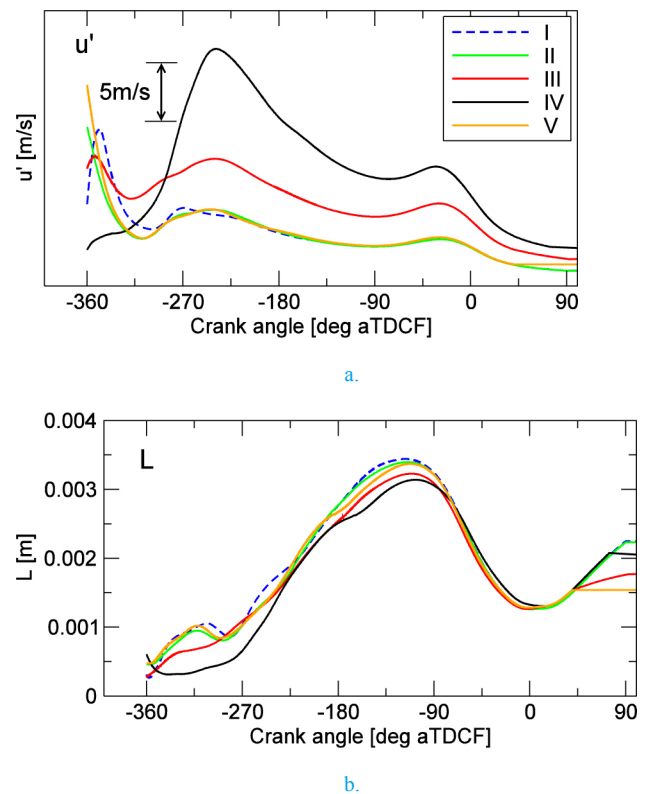


Figure 3. CFD modelling results showing u' and L for the five operating conditions studied.

Increase in engine speed expectedly increases the rms turbulent velocity u' as it relates to the intake jet velocity which scales up with the piston speed. The initial bulk flow in the cylinder is set up by the interaction of the intake jet with the chamber walls. Different valve timings for different conditions result in an interaction of the intake jet with the piston at different positions resulting in variations in the bulk flow pattern. This difference in flow pattern induces then a visible difference of the integral length scale during the intake and early parts of the compression stroke, see Fig. 3. As the piston nears TDC towards the end of compression, the larger bulk flow patterns break down into smaller eddies and the memory of initial differences is lost. This can be seen as a convergence of integral length scale curves to nearly the same value around TDC for all five conditions. It can also be inferred from Fig. 3a that an increase in engine load and a corresponding increase in intake pressure, does not affect the turbulent rms velocity, see 2000 rpm cases.

The turbulence intensity (u') predicted by both the k-epsilon model in GT-Power and the CFD modelling produced very similar results at various engine speed and loads. The difference was that the k-epsilon model in GT-Power produced much larger integral length scales at higher engine speeds, almost greater than twice the CFD modelling predictions. As no measurements were available of the integral length scale it was impossible to say conclusively which modelling approach was the correct one. The integral length scale is not expected to change greatly as the engine speed is changed, CFD modelling