

Numerical Study of the Influence of Hot Spot Formation and EGR on Knock Occurrence in SI-Engines

M. A. Liberman^{1*}, L.-E. Eriksson², M. F. Ivanov¹, D. Valiev¹

¹Department of Physics, Uppsala University, Box 530, S-751 21, Uppsala, Sweden

²Volvo Aero Corporation, Combustor Division, S-461 81, Trollhattan, Sweden

*Corresponding author, M. A. Liberman: Michael.Liberman@fysik.uu.se

Introduction

We present results of multidimensional numerical simulation of the autoignition onset in SI engine and compare the calculations with the experimental data. Combustion in SI engine and autoignition was studied by direct numerical simulation of 3D or 2D (if applicable) Navier-Stokes equations coupled with the chemical kinetic model, which takes into account both the low-temperature and high-temperature kinetics and yields correct induction times for hydrocarbon autoignition.

Much attention was paid to dynamics of the propagating flame, to the heat losses to the walls, and to the formation of non-uniformities in the end-gas, which can be identified with hot spots, and where subsequent autoignition of the unburned mixture starts. It was found that there is a considerable feedback between the autoignition onset, which is accompanied by the acceleration of the propagating flame and development of the autoignition in the end gas. The calculations show two feedback processes: flame is accelerated by the temperature increase due to development of the cool flames in the end gas, and development of the autoignition is enhanced by the flame acceleration (König, 1990). Knocking onset is the self-ignition of the end-gas, which occurs as a result of combined effects of the end-gas compression by the moving piston during the compression stroke and by the propagating flame together with expanding combustion products. Detailed analysis of the calculated temperature and pressure fields has shown that the development of the autoignition is tightly connected to the formation of hot spots that evolved from the non-uniformities caused by pressure waves emitted by the propagating flame. The developed model shows that the calculated dependence of the temperature and pressure on crank angle and predicted time of the autoignition onset for different engine operation conditions, in particular, for stoichiometric fuel mixture, and for different percentage of EGR are in a good agreement with the experimental data.

Numerical model and experimental data to be satisfied

Dynamics of the knock occurrence in SI engine was studied by means of direct numerical simulation of the complete system of hydrodynamic Navier-Stokes equations coupled with the reduced chemical model. The chemical kinetic model used in the present calculations is the kinetic model based on a modified Shell model (Halstead, et al. 1975; Halstead, Kirsch, Quinn, 1977). Since the Shell model is restricted basically to a low-temperature mechanism of autoignition, the present chemical model was extended to include the high-temperature and low-temperature schemes for the propagating flame and for the autoignition onset. A modified chemical model consists of reactions species for the fuel composition (C_8H_{18} , C_7H_{16} , O_2 , N_2) and the reaction products (CO , CO_2 , H_2O , NO_x). Due to small concentration of the intermediate radicals compared to major species and air their contribution to the thermodynamic characteristics is small and can be neglected.

Results of the numerical simulation were validated using the experimental data of the combustion and knock occurrence obtained from the experimental studies on a flat Volvo B230 cylinder head mounted on a single-cylinder Ricardo Hydra test-bed (Grandin et al, 2002). The experimental set-up has been described in detail in (Grandin et al, 2000). For convenience of measurements the head of a cylinder had the form of a horseshoe. The heat release in the end-gas prior to autoignition was investigated in the experiment using coherent anti-Stokes spectroscopy for instantaneous thermometry of the gas for mixtures of various equivalence ratios together with the average pressure measured as a function of the crank angle. The mixture of 75% iso-octane, 25% n-heptane and air was used as a charge. The charge was ignited by two spark plugs mounted opposite to the plane wall of the horseshoe with the angle of 120 degrees between the spark plugs.

Influence of the propagating flame on hot spot formation and autoignition onset

It was recognized that the propagating flame has a strong influence on the thermodynamic conditions at the end gas, where a body of the end gas is brought to a cool flame reaction under the influence of the high temperature and pressure established in the end gas by combined compression of piston motion and primary flame propagation. In particular, formation of the hot spots in the end gas is just because of the propagating flame; otherwise the end gas would be brought to a homogenous reaction by merely the piston compression. Formation of the hot spots and time of the autoignition onset are strongly influenced by the regular propagating flame, and hence depend on the flame structure and the flame velocity. One of the aims of the study was to reveal the mechanism of autoignition and to investigate the influence of heat losses to the walls and thermal boundary layer on the process.

It is obvious that the numerical grid must be fine enough to resolve structure of the flame front. In fact, the problem in question can be formulated in terms of computational requirements as following: When it is possible to use flamelet assumption, and how fine must be calculating mesh? How many points are required for obtaining reliable results of simulation? There are two principle factors that affect the choice of the grid: the characteristic combustion length scales, i.e. thickness of the flame front and turbulent scales from one side, and cost of the simulation. To find a compromise between all these factors sensitivity analysis of the calculated time of the onset of autoignition with respect to grid resolution, i.e. the total number of mesh points was performed. The calculated time of autoignition onset for grids with different number of cells per width of the propagating flame is shown in Fig.1 as a function of $L_f/\Delta x$, where L_f is width of the flame front, Δx is the cell size. It is seen that the autoignition time depends strongly on the cell size and tends to constant limit as cell size decreases.

Results of the numerical simulations

In essence, the dependence of the intensity of cool flame on temperature makes the autoignition process very sensitive to the local thermodynamic parameters in the end-gas, which results in formation at some mean temperature of unburned gas sites of unstable state at the end-gas, when even slight local increase of the temperature may lead to a rapid development of the autoignition. Fig. 2 shows the calculated temperature and pressure profiles at the end gas prior to the autoignition. Clearly seen are non-uniformities in temperature and

pressure formed by pressure waves generated by the propagating flame, which can be identified with hot spots.

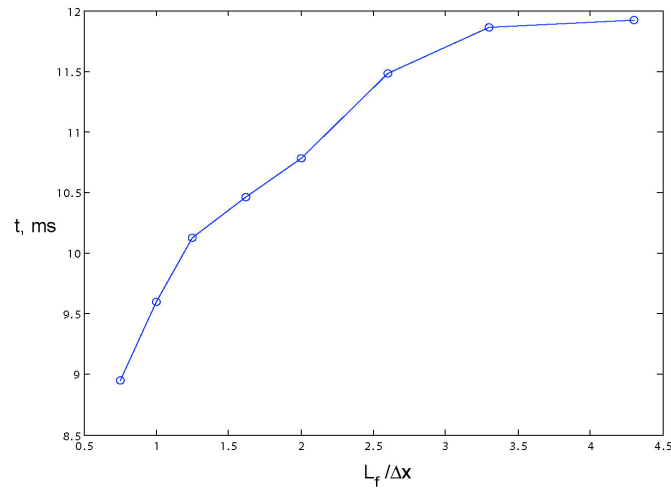


Figure 1. The calculated time of autoignition onset versus size of the grid cell

Results of the numerical simulations

In essence, the dependence of the intensity of cool flame on temperature makes the autoignition process very sensitive to the local thermodynamic parameters in the end-gas, which results in formation at some mean temperature of unburned gas sites of unstable state at the end-gas, when even slight local increase of the temperature may lead to a rapid development of the autoignition. Fig. 2(a,b) shows the calculated temperature and pressure profiles at the end gas prior to the autoignition. Clearly seen are non-uniformities in temperature and pressure formed by pressure waves generated by the propagating flame, which can be identified with hot spots.

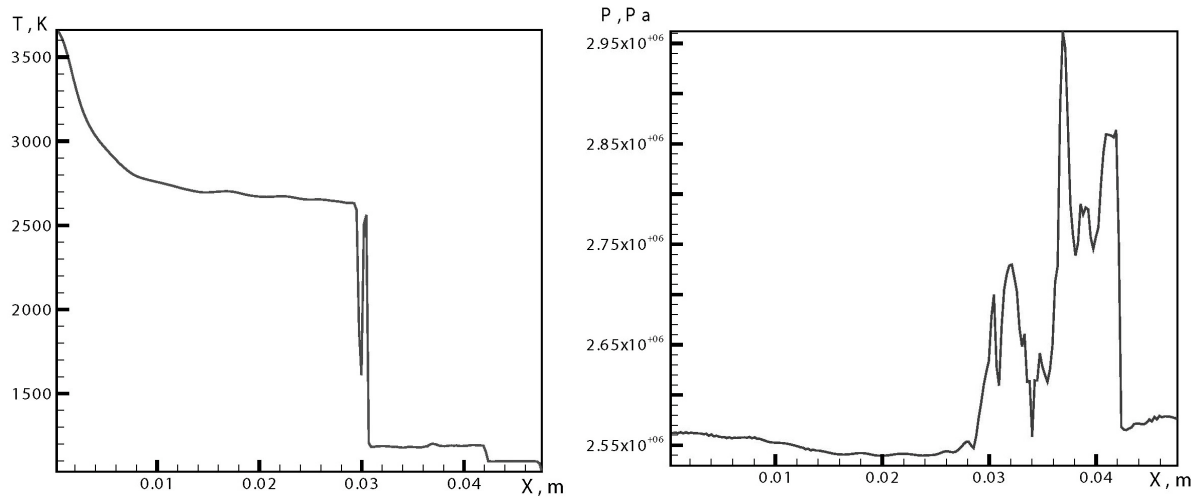


Figure 2. Temperature and pressure profiles at the end gas at the moment before autoignition.

The calculated temperature at the end gas and time of the autoignition are shown in Fig. 3 for stoichiometric mixture. The moments of the autoignition onset obtained in the numerical

simulations and observed in the experiment are designated by the star and diamond respectively. As it is seen, the calculated dependence of the temperature on CAD agrees well with the experimental data. The calculated crank angle at which the autoignition onset occurs is within $CAD = \pm 2$ compared to the experimentally measured value. Account of the heat losses to the walls and the gas-wall friction decrease slightly time when the autoignition starts: from 18.2CAD to 17.8 CAD, respectively.

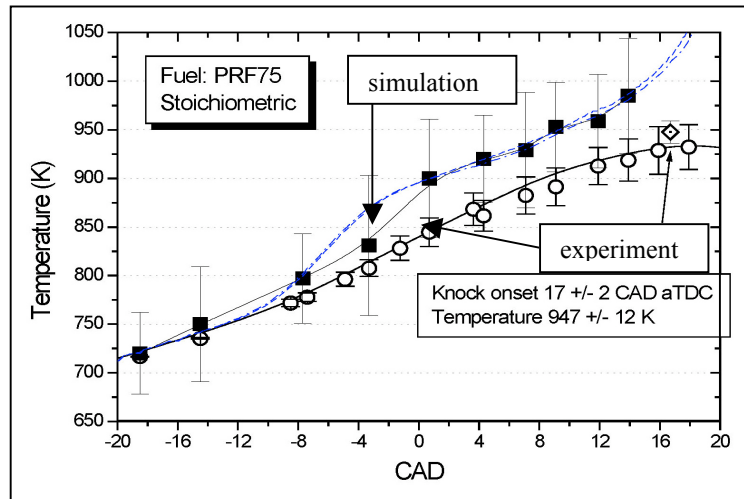


Figure 3. Dashed lines represent the calculated temperature variation versus the crank angle and the moment of the autoignition onset for the case of stoichiometric mixture. Compression ratio - 9.5, engine speed - 1200 rpm. The experimental data are from (Grandin et al 2002).

At the time when the propagating flame enters the top rectangular part of the horseshoe-like chamber the flame front becomes almost flat. This fact was observed in the experiment and was confirmed by 3D modeling. While the flow is essentially three-dimensional on the first stage of combustion, after the plug spark was ignited, and can be correctly modeled by means of 3D modeling, 2D modeling of the combustion process is suitable for describing the process with satisfactory accuracy when the flame enters the top rectangular part of the chamber. Taking into account high cost of the 3D modeling it was reasonable to combine 3D modeling at the beginning of the combustion with the 2D modeling at the later stage.

References

1. König G., Maly R. R., Bradley D., Lau A. K. C. and Sheppard C. G. W. (1990) SAE paper 902136.
2. Halstead M. P., Kirsch L. J., Prothero A., and Quinn C. P. (1975) Proc. Roy. Soc. London A 346, 515.
3. Halstead M. P., Kirsch L. J., and Quinn C. P. (1977) Combust. Flame, 30, 45.
4. Grandin B., Denbratt I., Bood J., Brackman C. and Bengtsson P. E. (2002) SAE paper 010239. Grandin B., Denbratt I., Bood J., Brackman C., Bengtsson P. E. (2000) SAE paper 2000-01-2831.
5. Liberman M. A., Eriksson L. E., Ivanov M. F., Valiev D. M., (2004) Numerical Modeling of Propagating Flame and Knock Occurrence in SI-engines, Comb. Sci. Tech. 177, 32.