An approach to the efficient modelling of lean, premixed HCCI-operation

A. Schubert*[1], O. Maiwald†[1], K. König[1], R. Schießl[1], U. Maas[1]
[1]Institut für Technische Thermodynamik, Universität Karlsruhe (TH), Germany

Abstract
A model for the efficient simulation of lean, premixed self–ignition under HCCI conditions is introduced. In the model the in–cylinder gas is described by an ensemble of independent, homogeneous chemical reactors, which develop according to detailed chemistry. Essential information used in the model to describe the HCCI behaviour is the spatial fluctuation of temperature in the cylinder gases. Laser–Induced Fluorescence (LIF) of formaldehyde is used to approximately determine temperature fluctuations in an optically accessible HCCI–engine. These fluctuations are used to initialize the reactor ensemble, which predicts the onset of ignition and the measured pressure trace of the same engine very well. Detailed simulations evidenced that the consideration of temperature fluctuations with a reactor ensemble is sufficient to predict pressure traces with good accuracy for HCCI with lean, homogeneous mixtures.

Introduction

Homogeneous charge compression ignition (HCCI) offers the potential for increased fuel economy [1] and lower NO_x emissions than those from a comparable spark ignition (SI) engine operated at the same load. But the HCCI–engine is more difficult to control with respect to the onset of ignition. To develop strategies for a better control, reliable simulation tools are helpful.

Modelling can help to acquire profound understanding of the self–ignition in engines and the underlying physical and chemical processes. A simulation that considers detailed chemical reactions and physical processes (diffusion, heat conduction, momentum and all aspects of flow) would be optimal. Currently, however these fully detailed simulations are computationally prohibitive.

The purpose of the present work is to introduce and apply a simplified efficient model for the simulation of lean, premixed self–ignition under HCCI conditions. In the model, the in–cylinder combustion process is described by an ensemble of independent, homogeneous chemical reactors, which react according to detailed chemistry and according to the boundary conditions imposed by the engine. The use of this model is justified by 1D–simulation used to identify the importance of physical and chemical processes for lean, premixed HCCI conditions before self–ignition. The results of the simulations indicate that, for the mentioned conditions the influence of transport processes is negligible, so that independent reactors are appropriate for modelling.

The essential feature of our modelling approach is that the individual reactors are initialized with slightly varying temperatures. This is motivated by optical observations in engines [2] and rapid compression machines [3]. These give evidence that the temperature in the combustion chamber is not homogeneous, but that spatial temperature fluctuations exist in the cylinder gas prior to ignition. Detailed numerical simulations show that the variation of the temperature fluctuations is of paramount influence to the subsequent behaviour: for small fluctuations and lean mixtures, the temporal change of in–cylinder gases is dominated by chemical reactions, physical processes like diffusion or gasdynamical effects being negligible. Therefore, under thes conditions the central information used in the model is the temperature fluctuation.

It is shown that the consideration of temperature fluctuations with an ensemble of homogeneous, independent chemical reactors, is sufficient to predict the observed cylinder pressure traces (under sufficiently lean conditions and with premixed fuel/air mixture) with good accuracy.

Detailed numerical investigations

The state of the in–cylinder load can be described by the temperature T, pressure p and chemical composition, e.g. defined by the concentrations c_i of the i–th species, for all times t and all locations z. For a more efficient notation, we write the quantities as state vector:

$$\psi(z,t) = (T(z,t), p(z,t), c_i(z,t))$$

A solution of the conservation equations with detailed chemical and physical consideration is

*Corresponding author: schubert@itt.mach.uni-karlsruhe.de
†Current address: IAV GmbH, Ingenieurgesellschaft Auto und Verkehr, Vorentwicklung Dieselmotor, Germany

difficult and computationaly prohibitive. Therefore, it is useful and necessary to refrain from a detailed treatment, and to apply simplifications. The question is, which degree of detail is needed for a realistic model.

1D-simulation is used to address this question, because it can handle detailed chemistry and detailed transport processes. In order to mimic the broad range of scenarios that appear during operation of a HCCI–engine, we performed a set of representative detailed numerical simulations. These simulations are not intended to directly simulate a real engine, but are used to infer essential characteristics of the physical and chemical processes in the cylinder. Especially, the relative importance of chemical source terms and physical processes (transport and gasdynamical effects) on the temperature change are taken from these model calculations. Similar studies were performed, e.g. in [4, 5]. In each calculation, the temporal evolution of spatial profiles of the state variables is computed by solving the system of partial differential equations established by the conservation equation for total mass, species mass, energy and momentum and using the ideal gas law [6, 7].

For the simulation, the conditions near top dead center (TDC), just before self–ignition are used as initial conditions. The initial pressure is adopted directly from the experimental pressure traces. In the simulation, 34 gridpoints were used. To estimate the influence of the heat conduction, different sinusoidal initial temperature profiles are specified. Initial conditions like the conditions investigated in the engine were used (see below). The average temperature is varied between 1025 K and 2025 K, the fluctuation amplitudes were varied between 25 K and 50 K and the fluctuation wavelenghts are varied between 11.13 mm and 22.25 mm. Likewise, the influence of diffusion is estimated with varying initial temperature and concentrations. For the evaluation of the chemical source term, a detailed iso–octane mechanism [8] is used (84 chemical species and 824 elementary reactions).

The simplest way to simulate the compression and the self–ignition of a mixture is by a homogeneous chemical reactor. This can by described by the following differential–algebraic equation system:

$$
\begin{aligned}
\frac{\mathrm{d}V}{\mathrm{d}t} &= \left(\frac{\mathrm{d}V}{\mathrm{d}t}\right)_{\text{ext.}} \\
\frac{\mathrm{d}U}{\mathrm{d}t} &= -p\frac{\mathrm{d}V}{\mathrm{d}t} + \frac{\mathrm{d}Q}{\mathrm{d}t}
\end{aligned}
$$

$$
\begin{aligned}
p &= RT\sum_{i=1}^{n_s} c_i \qquad (1) \\
U &= \sum_{i=1}^{n_s} w_i U_i\,(t) \\
\frac{\mathrm{d}c_i}{\mathrm{d}t} &= \dot{\omega}_{\text{chem.}} - \frac{c_i}{V}\frac{\mathrm{d}V}{\mathrm{d}t} + \frac{\mathrm{d}c_{i,\text{loss}}}{\mathrm{d}t}
\end{aligned}
$$

V is the volume, $\left(\frac{\mathrm{d}V}{\mathrm{d}t}\right)_{\text{ext.}}$ is the temporal change of the volume that is imposed to the system by the moving piston. $\mathrm{d}Q/\mathrm{d}t$, $\mathrm{d}c_i/\mathrm{d}t$ describe the heat- and mass loss of the system (e.g. by wall heat losses, blow–by) and U, U_i are the specific internal energy of the mixture and of the i–th species. w_i is the mass fraction, c_i the concentration of the i–th species and $\dot{\omega}_{\text{chem.}}$ is the chemical source term (on a molar scale). R is the universal gas constant, $R = 8.314\mathrm{J/(molK)}$.

The initial conditions are set according to the experimental results, with a homogeneous chemical composition, pressure and temperature field.

Experimental Determination of Temperature-Fluctuations

Laser-based investigations in an optically acessible experimental 2–stroke–engine were performed, providing information about mixture homogeneity and spatial temperature fluctuations in the in–cylinder load. The engine has been described in previous publications [9, 10], therefore only a short account is given here. The combustion chamber has optical access by a quartz glass ring at the cylinder top, which is closed by a quartz glass block. Laser radiation can be coupled through the ring and the resulting fluoresence can be observed through the quartz block. This enables a complete and distortion–free observation of the combustion chamber.

The mixture homogeneity was investigated with planar laser–induced fluoresence (PLIF) [11] of acetone used as a fuel tracer. For the excitation the output of a pulsed XeCl–excimer Laser (Lambda Physik LPX 200, wavelength 308 nm) was formed into a thin light sheet using cylindrical lenses. Additionally the fluoresence of formaldehyde, that is formed during the ignition phase as an intermediate species, was observed and used for visualization of the temperature fluctuations, according to the method described in [2]. The $2_0^1 4_0^1$ vibrational band of the $\mathrm{A^1A_2 - X^1A_1}$ electronic transition of $\mathrm{CH_2O}$ was excited with a pulsed dye laser (Lambda Physik FL3002, wavelength 339.3 nm [12]) pumped by a XeCl–excimer laser (Lambda Physik LPX 200). Pressure was measured using two Kistler transducer (Kistler 6001 and Kistler 4045-A20). The measured pressure traces are used to judge on the accuracy and the

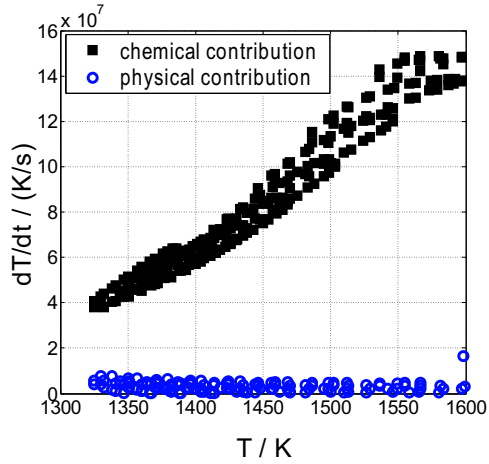

Figure 1: Contributions of chemical reactions and physical processes to the temporal change of temperature, as a function of temperature in different volume elements in a 1D-model

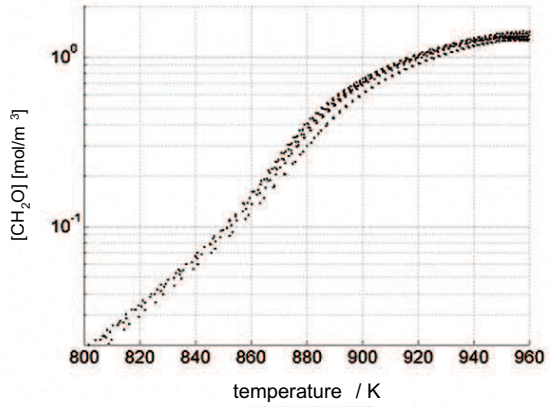

Figure 2: Correlation between $[CH_2O]$ and T, determined for the engine at 1000 rpm; various experimental cylinder pressure traces are applied as temporal constraint to the system.

predictive power of various computational models. Previous publications [2, 9, 13] show that for the conditions of the compressed endgas, the gas temperature and the formaldehyde concentration $[CH_2O]$ are strongly correlated (Figure 2). A characteristic feature of these correlations is an approximation of the form $\log [CH_2O] = A + BT$ with constants A and B, which is valid in temperature ranges, like they occur in the combustion chamber immediately before self–ignition. A and B can be determined by simulations of defined engine conditions. In the interesting temperature and pressure range, the formaldehyde fluoresence–intensity signal I in a single–shot measurement is, in good approximation, proportional to the formaldehyde number density. The temperature fluctuation ΔT can then be determined from the LIF–signal I and the constant B by $\Delta T = \Delta \log I/B$ [2].

Ensemble of homogeneous reactors

Since the single reactor model a–priori has the shortcoming of assuming a complete homogeneous mixture, an improvement can be expected by using a multi–reactor model. In this model, the temporal evolutions of many individual reactors with varying initial temperatures reflecting the essential characteristics of the temperature fluctuations observed in the experiment are used.

These empirical temperature fluctuations are projected onto an ensemble of homogeneous reactors as initial condition. Each member of the ensemble evolves according to the equations 1. At this degree of model complexity, no interaction between reactors occurs, transport processes like heat conduction and transport of mass by diffusion are not contained in the model.

Results and Discussion

The 1D-simulation show that for conditions like small temperature fluctuations and lean mixtures, which are typical for HCCI–combustion, the influence of the physical processes, like diffusion or heat conduction, is much smaller than the influence of chemical reactions $\left(\left|\left(\frac{\partial T}{\partial t}\right)_{\text{chem.}}\right| \gg \left|\left(\frac{\partial T}{\partial t}\right)_{\text{phys.}}\right|\right)$ (see Figure 1) [14].

Since in the considered case of a lean, premixed in–cylinder gas the influence of physical processes is negligible it is possible to simulate the compression and the self–ignition of the mixture by a homogeneous chemical reactor. The homogeneous reactor predicted the experimental pressure traces during the compression, up to TDC, quite well. The simulated point of the initiation of combustion matches well with the experimental initiation of combustion. But the computed pressure gradient is much too large compared to the experiment (see Figure 4) [15].

To understand the cause for the too large pressure gradient of the simulation, the results of the laser-based investigations in an optically acessible experimental 2–stroke–engine were considered. As outlined above, from the combined information of the acetone- and formaldehyde LIF–experiment, and using the results of numerical simulations, temperature fluctuations in the in–cylinder gases can be estimated. Figure 3 shows a typical LIF–result and the corresponding derived temperature fluctuation curve.

Since spatial temperature fluctuations are present in the cylinder gases, it is clear that the single reactor model a–priori has the shortcoming of assuming a completely uniform tempera-

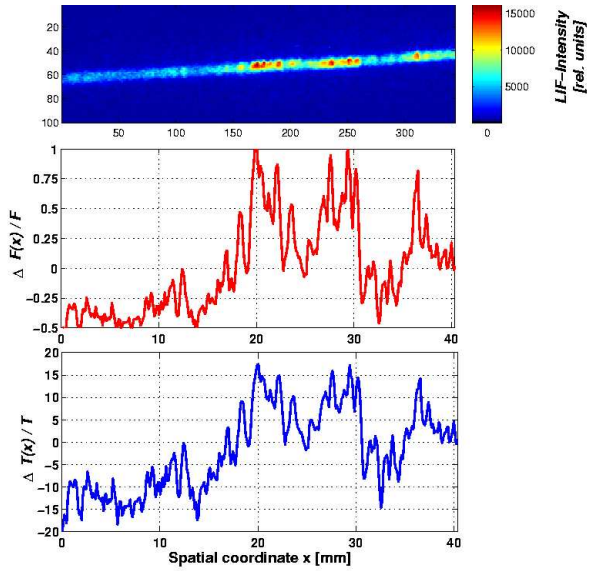

Figure 3: top: CH_2O LIF-Image. middle: the corresponding normalised fluctuations. bottom: the derived temperature fluctuation profile.

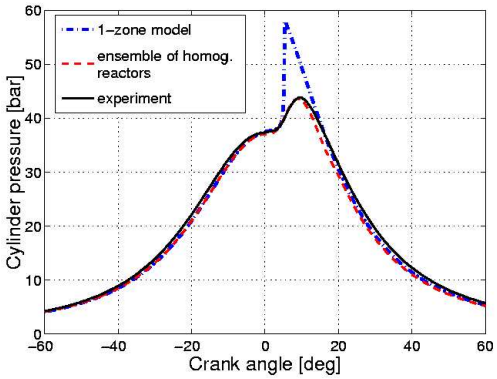

Figure 4: Calculated cylinder pressure traces of a HCCI–engine, using a single homogeneous reactor (blue curve), and an ensemble of homogeneous reactors (red curve), which was initialised according to measured temperature fluctuations. For comparison, an experimental pressure trace is shown.

ture. Figure 4 shows the behaviour of the reactor–ensemble in form of the calculated pressure trace. In those calculations, an ensemble with several reactors was considered. The ensemble members displayed slightly varying temperatures taken from a random gaussian distribution, with a standard deviation for the initial temperature of $\Delta T = 5$K, leading to a deviation of $\Delta T = 11$K near TDC. This corresponds to the temperature fluctuations deduced from the LIF–formaldehyde measurements. As a consequence of the progressing chemical reactions, each member of the ensemble sequentially starts to ignite, and to increase its pressure. The overall pressure trace is obtained from the individual pressure traces by averaging. Since the ignition events do not occur simultaneously, the ensemble–averaged pressure trace displays a smooth temporal increase. Those pressure traces indeed match very well to the experimentally observed pressure traces (see Figure 4).

Conclusion

A numerical model for the description of self–ignition in HCCI–engines is introduced and applied. This model exploits the fact, that in the specified range of conditions (typical HCCI operation range with respect to equivalence ratio), the chemical processes dominate over physical processes by orders of magnitudes in the late compression phase. For these operation ranges, physical processes can be neglected in the numerical treatment. An essential feature of the model is the consideration of temperature fluctuations, which are incorporated into the model by homogeneous reactor ensemble.

To obtain information about temperature fluctuations in a test engine, laser–induced fluorescence of in–cylinder mixture is used to determine formaldehyde (CH_2O) concentration fluctuations. This measurement, combined with correlations between gas temperature and intermediate species concentrations yields spatially resolved profiles of temperature fluctuations.

As demonstrated in Figure 5, the fuel/air load can be modelled as an ensemble of independent homogenous chemical reactors with good accuracy. The simulated pressure trace matches well with the experimental pressure trace, if an ensemble of homogeneous reactors, reflecting the experimentally determined temperature fluctuations, is used. An important feature of the model is also that it is efficient and computationally not expensive, making it attractive for use in practical applications. The transformation of the fuel/air mixture to exhaust gas and heat is under these conditions not a flamelike combustion, which is controlled strongly by transport processes, and also not a knocking combustion mode, which is generated or accompanied by pressure waves. Instead, it is a successive, independent self–ignition of different regions in the combustion chamber, which is controlled by the local ignition delay time according to the local temperature: a process that is mainly kinetically controlled.

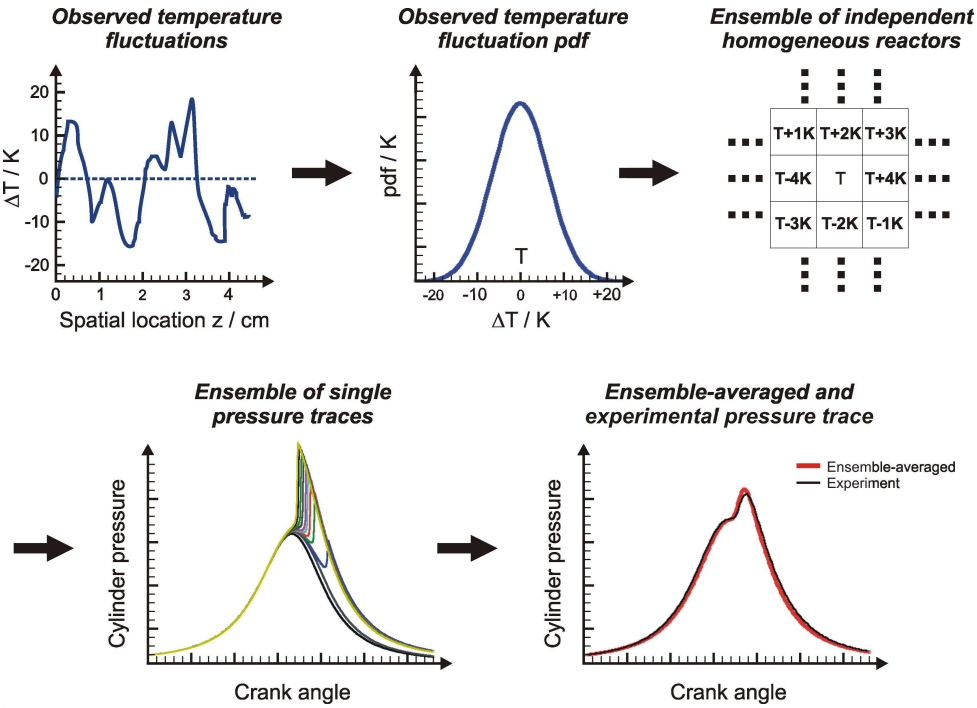

Figure 5: Schematic of the computation of the ensemble–averaged pressure trace.

References

[1] F. Zhao. *Homogeneous Charge Compression Ignition (HCCI): Key Research and Development Issues*. SAE Press, 2003.

[2] R. Schießl and U. Maas. *Combustion and Flame*, 133:19–27, 2003.

[3] J.F. Griffiths, J.P. MacNamara, C.G.W. Sheppard, D.A. Turton and B.J. Whitaker. *Fuel*, 81:2219–2225, 2002.

[4] H.-J. Weber, A. Mack and P. Roth. *Combustion and Flame*, 97:281–295, 1994.

[5] G. Goyal, U. Maas and J. Warnatz. *Combust. Sci. and Tech.*, 105:4–6, 1993.

[6] U. Maas and J. Warnatz. *Combustion and Flame*, 74:53–69, 1988.

[7] U. Maas and J. Warnatz. *Twenty-Second Symposium (International) on Combustion / The Combustion Institute*, pages 1695–1704, 1988.

[8] V. Golovitchev. *http://www.tfd.chalmers.se/~valeri/MECH.html*, 2004.

[9] O. Maiwald, R. Schießl and U. Maas. In *Beitrag in Berichte zur Energie- und Verfahrenstechnik: Motorische Verbrennung, VI. Tagung*, pages 209–217, München, 2003.

[10] O. Maiwald. PhD thesis, Universität Karlsruhe, 2005.

[11] A.C. Eckbreth. *Laser Diagnostics for Combustion Temperature and Species*. Gordan and Breach Publishers, 1996. 2^{rd}edition.

[12] R. Schießl, P. Pixner, A. Dreizler and U. Maas. *Combust. Sci. and Tech.*, 149:339–360, 1999.

[13] R. Schießl, O. Maiwald, K. König and U. Maas. In *6. Internationales Symposium für Verbrennungsdiagnostik*, pages 95–104, Baden-Baden, 2004.

[14] P. Maigaard, F. Mauss and M. Kraft. In *2000 Spring Technical Conference, ASME*, volume ICE-34-2, Paper No. 2000-ICE-275, 2000.

[15] J.-Y. Chen, R.W. Dibble, J. Kolbu and R. Homma. *Combust. Sci. and Tech.*, 175:373–392, 2003.