Simulation of the combustion of alternative fuels in spark ignition engines

Sebastian Verhelst

Abstract: The public and industrial transport impose a heavy burden on the environment. Because of this, there is increasing focus on alternative fuels such as natural gas, LPG and hydrogen. Their emission characteristics are considerably better than those of the fossil fuels gasoline and diesel.

In order to fully exploit the benefits of those cleaner fuels in internal combustion engines, those engines have to receive a proper set-up. Experiments on an engine test bench to determine this optimal set-up would demand substantial time and money.

A simulation programme for the combustion of alternative fuels in internal combustion engines is a very interesting solution. Such a programme combines sufficient accuracy with fast computation, allowing rapid evaluation of set-up designs or optimisations of the engine parameters. This paper clarifies the need for engines on alternative fuels and the need of simulation and discusses the elements of the simulation programme.

Keywords: SI engines, alternative fuels, simulation

I. INTRODUCTION

One of the most important topics of research in the Laboratory for Transporttechnology, part of the Department of Flow, Heat and Combustion Mechanics, is the use of alternative fuels in spark ignition (SI) engines. Such fuels, e.g. natural gas, LPG and hydrogen, are attractive alternatives to the traditional fossil fuels such as diesel and gasoline. The latter have serious disadvantages concerning exhaust emissions: the noxious components such as nitrogen oxides (NOx), unburned hydrocarbons (UHC) and particulate matter pose a threat to human health and the environment. Furthermore, the CO2 emissions are to large extent responsible for the global warming of the planet.

The major part of the research concerns hydrogen, the fuel that eliminates any harmful emissions (except NOx, which can be kept at very low levels), and of which there is an unlimited resource. This is an important advantage over fossil fuels, with their limited reserves.

In recent years, several engines have been converted to hydrogen. At the moment, the work has been focussed on two engines: a GM 7.4 litre V8 engine, and a one-cylinder CFR engine. The first is intended to deliver knowledge concerning practical aspects that arise from preparing the engine for propulsion purposes (e.g. for a city-bus) [1-2-3]. The second engine allows extensive research of the fundamental properties of the combustion of hydrogen.

Although much knowledge has been gathered from these engine tests, there is an important disadvantage and that is the cost, both in money and time. At the moment, hydrogen is still expensive (when compared to other fuels) and thus, the tests have to be restricted in time.

It is therefore very interesting to consider computer simulations. These can be done relatively cheap and can give results in a considerably shorter time.

II. SPARK IGNITION ENGINE CYCLE SIMULATION

The cycle of a four stroke SI engine consists of several parts: the intake of the fresh air-fuel mixture, the subsequent compression, the ignition resulting in the combustion of the mixture, the expansion (power stroke) and finally the exhaust of the burned mixture.

The gasdynamic part, i.e. intake and exhaust, can be modeled with algorithms obtained from computational fluid dynamics (CFD). In the thermodynamic part, the simulation of the compression and expansion strokes are fairly straightforward following the laws of thermodynamics and some assumptions which approximate the real processes accurately. The most difficult part is the combustion simulation. The combustion process is a set of complicated events comprising turbulent flow and chemical reactions, of which a large part remains fairly unknown at this moment. This uncertainty has led to a variety of simulation models.

To simulate the combustion processes in a SI engine, one can follow different paths. The simplest option is a “zero-dimensional” model, based on the first law of thermodynamics (conservation of energy). However, such a model requires several assumptions and can only give approximate results, due to its simplicity. On the other side of the spectrum of complexity, one has the multi-dimensional models. These consider the flow processes in the cylinder, the chemical kinetics and their interactions. The computation of these turbulent flows and their interaction with the combustion processes demand considerable computing power and CPU time, thus losing some of the advantages of computer simulation.

A compromise can be taken with a quasi-dimensional model. This is a model that takes some geometrical parameters into consideration and uses fenomenological models for the description of the turbulence and its interaction with the combustion process.

Thus, a reasonable accuracy can be combined with fast computation. In order to model the physical and chemical processes that occur, it is necessary to distinguish the important events and parameters from the less important ones. This provides a deeper understanding of these processes.
III. TWO-ZONE MODEL

The quasi-dimensional model that was chosen for the simulation of the combustion part in the thermodynamic cycle of a SI engine is a so-called “two-zone model". This model is based on the model originally proposed by Blizard and Keck [4], later adapted by numerous researchers as a better understanding of the occurring processes was gained.

The simulation programme uses the model in the form developed by Tabaczynski et al. [5]. This model considers two zones in the combustion chamber: a zone with burned gases and a zone with the unburned mixture, divided by a spherical flame front. The combustion process is assumed to occur in two phases: first, unburned mixture is entrained into the flame front. In a second phase, this unburned mixture is burned. The combustion speed is calculated out of two differential equations. These take into consideration the characteristics of the turbulence in the combustion chamber and the laminar flame speed of the fuel (dependant of the pressure, temperature, amount of combustion air and residual gas).

The combustion speed obtained with this model allows the evaluation of the equations determining the evolution of the pressure (assumed to be uniform throughout the cylinder) and the temperatures (uniform for each zone). These equations are derived from the first law of thermodynamics. A set of equations determines the composition of the cylinder gases by assuming chemical equilibrium at the given pressure and temperature.

IV. ADAPTION OF EXISTING CODE

A programme for the simulation of the gasdynamic and thermodynamic cycle of SI engines has been written by a former Ph. D. student [6]. The gasdynamic part has sufficient precision in the first instance: accurate predictions of the pressure waves in the inlet and exhaust manifold can be computed. In a later phase, this part can be extended in order to be able to compute the gas dynamics in the manifolds of multi-point injection (MPI) engines. However, the thermodynamic part asks for improvements.

The problem here is that the existing models for the simulation of the combustion process have been designed and validated for gasoline. SI engines working with alternative fuels have different characteristics and thus, the simulations with the existing models give less accurate results. For instance, a hydrogen fueled SI engine uses a large variation of the mixture-richness (that is, the ratio of air to fuel) to control the power delivery. On the contrary, a gasoline engine operates with a very narrow variation of the air to fuel ratio (the use of a catalyst demands a portion of air that is exactly equal to the amount needed to burn the delivered fuel completely, which is called 'stoichiometric combustion').

It can be expected that several elements of the simulation model will be different for the alternative fuels. It is known that the expression for the heat exchange of the cylinder gases with the cylinder walls has to be modified in case of lean mixtures (the amount of air exceeds the amount needed to burn the fuel completely). However, new, accurate, models have yet to be developed.

For hydrogen, there exists uncertainty about the proposed formulas for the laminar flame speed. None give accurate results when they are used in an engine simulation programme. A study of other formulas or maybe the proposal of a new formula is necessary.

As a final example: the details of the formation of nitrogen oxides (NOx) during the combustion in SI engines are still largely unknown. This implies difficulties in modeling the NOx formation and thus, only very few simulation programmes are capable of predicting NOx levels that approach the levels recorded during experiments. As NOx is the only noxious component of a hydrogen engine, it is clear that a precise prediction of the emission of NOx of a hydrogen engine can be very useful to come to an optimal setup of the engine.

V. USE OF THE RESULTS OF THE PH. D.

As can be clear from the above, the final goal of the Ph. D. is to enable the optimisation of SI engines operating on alternative fuels. It should be possible to optimise the setup of such engines by means of a simulation programme that can give results with minimum effort and within reasonable time. The programme should enable parameter studies, to determine the influence of the engine parameters such as the compression ratio, the ignition timing, the injection timing and duration, the sparkgap, …

The optimisation of these parameters can have different objectives: this could be maximum power and torque, minimum NOx emission or minimum fuel consumption. These objectives can be contradictory and it is possible that a compromise has to be searched for. The execution of experiments to determine this compromise would demand considerable time and would imply great costs. The simulation programme would decrease the time and significantly lessen the costs.

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REFERENCES


