COMBUSTION MODELING OF A COMPRESSION IGNITION ENGINE

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Abstract. *Since the nineteenth century the internal combustion engines had its development linked to thermodynamic models that have described its works. The research progress has increased the computational tools utilization which reduces costs and work time against the purely experimental methods. That last one has required, during the last decades, high investments and large return time. Despite that the comprehension and control of a thermal engine operation are extremely complex due the large diversity of phenomena inherent to many scientific fields such as chemistry, fluid mechanics, heat and mass transfer and mechanical vibrations. Under the gaze of that context, this paper describes the development of a mathematics-computational model which was accomplished on the ambiance Simulink®, of Matlab®. The model is able to represent and evaluate the combustion in a compression ignition engine (Diesel). The modeling is zero-dimensional, established and based on the first law of thermodynamics, considering the cylinder's borders as the control volume boundaries, having the crank angle as the only independent variable. The thermodynamic variables such as pressure and temperature are considered as uniform in whole cylinder volume, at each crank shaft position. The modeling on Simulink® consists in the elaboration of a subsystems library in which each subsystem represents an engine component, a theoretical model or a calculator block. The logical and operational linkage between the subsystems builds up the proposed modeling. Two ignition compression engines were evaluated employing the modeling: one to assess a performance engine behavior and another to validate the mathematics-computational model capability in representing the reality. Test bench data acquired were exploited in order to validate the mathematics-computational model capability in represent the reality.*

Keywords: *Numerical Simulation, Diesel, Ignition Compression Engine, Combustion, Simulink.*

1. INTRODUCTION

The internal combustion engines have always fascinated the world due to them applications and importance in several high-technology fields, mainly into energy systems, energy production and transformation and transport fields. Despite that the comprehension and control of a thermal engine operation are extremely complex due the large diversity of phenomena inherent to many scientific fields such as chemistry, fluid mechanics, heat and mass transfer and mechanical vibrations. Barros (2003) mentions that since the nineteenth century this kind of engines has had its development linked to thermodynamic models, which have described and simulated them operation. A simulation model allows studying engine behavior, to develop a better comprehension on its process and phenomena, to identify important operational parameters, to reduce experimental research costs, time and resources with prototypes and predicting the influence of chemically different fuels, as long as obeying the engine model under study. Nowadays the research progress has improved the computational tools utilization, which reduces costs and work time against the purely experimental methods.

Actually simulation models don't describe the combustion faithfully and because of that the comprehension about the theory and hypotheses is very relevant in order to adjust the model under study in relation to its accuracy and quickness. The hypotheses serve to simplify the simulation, whereas the disaccording among the reality and simulation will be as little as models are more accurate and as such less quick (Becerra, 1996). The models can be classified in two main modeling groups: the dimensional (or multidimensional) and the thermodynamic (or zero-dimensional) models. The grandeurs vary only as function of time in the zero-dimensional models and as such like the same manner in the quasi-dimensional models (Souza, 2009).

Thereby this paper describes the development of a mathematics-computational model that was accomplished on Simulink®, of Matlab®, employing mathematical models such as thermodynamic cycles analysis on internal combustion engines. The modeling is able to represent and evaluate the combustion related to a compression ignition engine (Diesel). Test bench data acquired were exploited in order to validate the mathematics-computational model capability in represent the reality.

2. COMPRESSION IGNITION ENGINES

The thermal engine involves several kinds of engine: steam engine, combustion engine, turbine, there are many other examples. The engines are classified in relation to combustion model as internal combustion engines (or endothermic) or external combustion engines (or exothermic). About the first one the combustion takes place in the working fluid. About the second one the combustion takes place out of the working fluid. Also, the endothermic engines are classified in relation to them operation as reciprocating, rotary or jet engines. They are classified in relation to the combustion mode as spark-ignition (SI) engines (Otto engines) or compression-ignition (CI) engines (Diesel engines). About them operative cycle they are classified as 2-stroke or 4-stroke engines (Magot-Cuvru, 1981). The CI models have a greater number of physical and chemical phenomena than the SI engines. Actually, in homogeneous SI engines, the average velocity with which the flame travels across the combustion chamber controls the heat-release rate.

Nevertheless, in CI engines, the essential features of the combustion process are fuel injection, carburant pulverization, fuel spray penetration, spray evaporation, physical mechanisms which start up the combustion and another factor of influence that is the own combustion, which occurs at several points of the combustion chamber simultaneously (Higelin and Jaine, 2009; Moreira, 2000).

The discussion on CI engines combustion involves similarly many concepts such as mass and energy conservation, ideal gas concept, penetration of liquid fuel sprays under condition typical of those found in CI engines, flame length and heat transfer rate in order to find the main engine performance parameters, consummation and pollutants production. Therefore about compression engine modeling it's very important to enumerate the main phenomena in order to have an adequate analysis. In according to Higelin and Jaine (2009), these fundamental phenomena can be summarized as follows:

- Carburant injection rate and fuel jet penetration/pulverization rates, model describing the carburant/fuel injections within the combustion chamber;
- Fuel spray droplets vaporization – model concerning its transformation from liquefied condition to vapor;
- Air drag with relation to the fuel-air mixture. This model is divided in two parts: the first one describes the air movement as function of carburant injection, the second one describes the interaction between the air and the carburant vapor which set up the fuel-air mixture;
- The turbulence is characterized by the combustion chamber internal aerodynamics, while the combustion occurs;
- The self-inflammation delay describes the duration since injection discharge up to combustion initiation;
- The combustion of pre-mixed fuel-air mixture (pre-mixed flame or rapid-burning) and diffusive combustion (diffusion flame or flame development) are combined allowing to compute the fuel's mass fraction burned and hence the heat-release rate.

3. INTERNAL COMBUSTION MODELING AND SIMULATION

There is a larger number of works about Otto than on Diesel engines. The most of works into both fields employs zero-dimensional models. A vast number of simulations employ software such as KIVA-II[1], KIVA-III, CFD, and Simulink; hence they are compared in relation to experimental tests as such in order to achieve a validation. At this present work it was developed a zero-dimensional computational algorithm using C++ language with approaches based on engine modeling state-of-the-art.

3.1 Numerical fundaments

The working fluid within the combustion cylinder comprises the fuel-air mixture and combustion products. The physical and chemical analysis about it is accomplished through equations considering that the cylinder's borders as the control-volume boundaries and also that it is working as a direct injection CI engine. Thus, the model evaluates that the delimited cylinder only modifies its volume when the crank angle value varies. The range of those values takes from the closing admission valve up to opening exhaust valve, valuing the compression, combustion and expansion processes, which comprise the main phenomena related to engine useful work (Heywood, 1988). The working fluids inside the control-volume can be considered as the air that enters into the combustion cylinder (during admission and compression) and as the Diesel oil that enters from the injection nozzle and produces mixture with the air (during combustion, expansion and exhaust). In according to some hypotheses the working fluids inside the cylinder behaves as an ideal gas (Hauck, 2010).

3.1.1 Energy balance – Combustion and Expansion

An energy balance based to the 1st Thermodynamic Law is employed on the control-volume, which contains the working fluid. The energy balance evaluates the internal energy variation (dU) of the mixture within the control-volume, the fuel heat-release, the heat transfer to combustion chamber walls and the work-transfer delivered by the cylinder gases on the pistons. Then, disregarding kinetic and potential energy variations the energy balance can also provide other relevant equations and in according to Heywood (1988), the equation is given by

$$\dot{Q}_f - \dot{Q}_w + \dot{m}_a \cdot h_a + \dot{m}_f \cdot h_f = \frac{dU}{dt} + \dot{W} - \dot{m}_e \cdot h_e \tag{1}$$

In the Eq. (1), $\dot{Q}_f$ (kW) is the fuel heat-release rate; $\dot{Q}_w$ (kW) is the heat transfer rate to the combustion chamber walls; $\dot{m}_a$ and $\dot{m}_e$ (kg/s) are the mass flow rates across the admission and exhaust valve, respectively; $\dot{m}_f$ (kg/s) is the fuel mass flow rate being injected into engine; h_f (kJ/kg) is the fuel specific enthalpy; h_a and h_e (kJ/kg) are the specific

[1] *Kiva is a software family concerning combustion computational modeling (KIVA-3V distributed as KIVA-II, KIVA-4 in grad not-structured version and KivA-4mpi which is a parallel version in relation to KIVA-4). Kiva is a transient, multiphasic, tridimensional and multicomponent code for analysis developed by Los Alamos National Laboratory.*

enthalpy of the mass flowing across admission and exhaust valve, respectively; *dU/dt* (kW) is the internal energy variation rate of the mixture within the control-volume and $\dot{W}$ (kW) is the work-transfer rate delivered by the cylinder gases on pistons.

3.1.2 Heat transfer to cylinder walls and fuel heat-release

The heat transfer to the cylinder walls is given by the Annand's correlation. This correlation is empiric and includes the convection and radiation terms. In according to Hauck (2010) and Prasath *et al* (2010), the equation to calculate the heat transfer rate to the cylinder walls is given by

$$\dot{Q}_w = \sum A_w \cdot \left[c_1 \cdot \frac{k}{D} \cdot \mathrm{Re}^{c_2} \cdot \left(T - T_w\right) + c_3 \cdot \left(T^4 - T_w^4\right) \right] \tag{2}$$

In the Eq. (2), *Re* is the Reynolds' number; *D* (m) is the cylinder diameter; T and T_w (K) are the average temperatures in the cylinder and at the cylinder walls, respectively; c_1, c_2 and c_3 are Annand's constants that are necessary in order to the empiric adjustment; k (kW/m.K) is the thermal conductivity and A_w (m²) is the heat transfer area that represents the control-volume boundaries (the top of the piston, the lateral walls of the cylinder and the engine head stock).

The fuel heat-release rate is a function of the mass fraction burned and it is expressed by

$$\dot{Q}_f = m_c \cdot LHV \cdot \frac{d\chi}{d\theta} \tag{3}$$

In the Eq. (3), m_c (kg) is the whole mass of fuel injected during one engine's cycle; *LHV* (kJ/kg) is the lower heating value of the fuel; $d\chi/d\theta$ is the mass fraction burned rate in relation to the crank angle variation. Indeed, the CI engines combustion has two steps (double phase combustion): pre-mixture combustion (pre-mixed flame) and diffusive combustion (diffusion flame). Then, Watson et al. (1980) and Miyamoto et al. (1985) proposed to modify the simple Wiebe's function, taking it as soon as the double Wiebe's function, which expresses the mass fraction burned and is given by

$$\chi = 1 - \chi_p \cdot \exp\left[-a_b \cdot \left(\frac{\theta - \theta_{ig}}{\Delta\theta_p} \right)^{m_p+1} \right] - \chi_{di} \cdot \exp\left[-a_b \cdot \left(\frac{\theta - \theta_{ig}}{\Delta\theta_{di}} \right)^{m_{di}+1} \right] \tag{4}$$

In the Eq. (4), χ_p and χ_{di} are the mass fraction burned at the pre-mixed flame and diffusion flame combustion phases, respectively, hence $\chi_p + \chi_{di} = 1$; a_b is the combustion efficiency parameter; θ_{ig} (degrees) is the angle of the ignition initiation; $\Delta\theta_p$ and $\Delta\theta_{di}$ (degress) are the pre-mixed flame and diffusion flame combustion delays, respectively and m_p and m_{di} are the combustion chamber shape factors during the pre-mixed flame and diffusion flame combustions, respectively. The crank angle, indicated by θ (degrees), is the independent variable.

3.2 Methodology of elaboration of the combustion modeling on Simulink

Firstly, the modeling under question is zero-dimensional. Among the different categories of zero-dimensional models, the thermodynamic model used in this present work ponders the heat-transfer to the cylinder walls and considers the constant-specific-heat model as such. The computational ambiance Simulink allows simulating a physical-logical system in function of parameters and other multi-physical systems, which, at this case, are correlated to combustion phenomena. The modeling on Simulink consists in the elaboration of a subsystems library in which each subsystem represents an engine component (crankshaft, cylinder or admission and exhaust valves); a theoretical model (Annand's correlation or Wiebe's correlation) or a calculator block (integrator or logical operator).

3.2.1 Simulation parameters

During the simulations, the differential equation platform solver used was *ode-45 (Dormand-Price)*[2]. The *variable type* selected as simulation parameter was *variable step*. The *absolute* and *relative tolerances* were $1.0\text{x}10^{-6}$ and $1.0\text{x}10^{-3}$, respectively. The *number of consecutive min steps* was 10.

3.2.2 Algorithm structure

Next, the Fig. 1 illustrates the flowchart explaining the modeling's algorithm structure.

[2] *Ode-45: It is a Matlab's routine, which uses a variable step Runge-Kutta Method to solve differential equations numerically.*

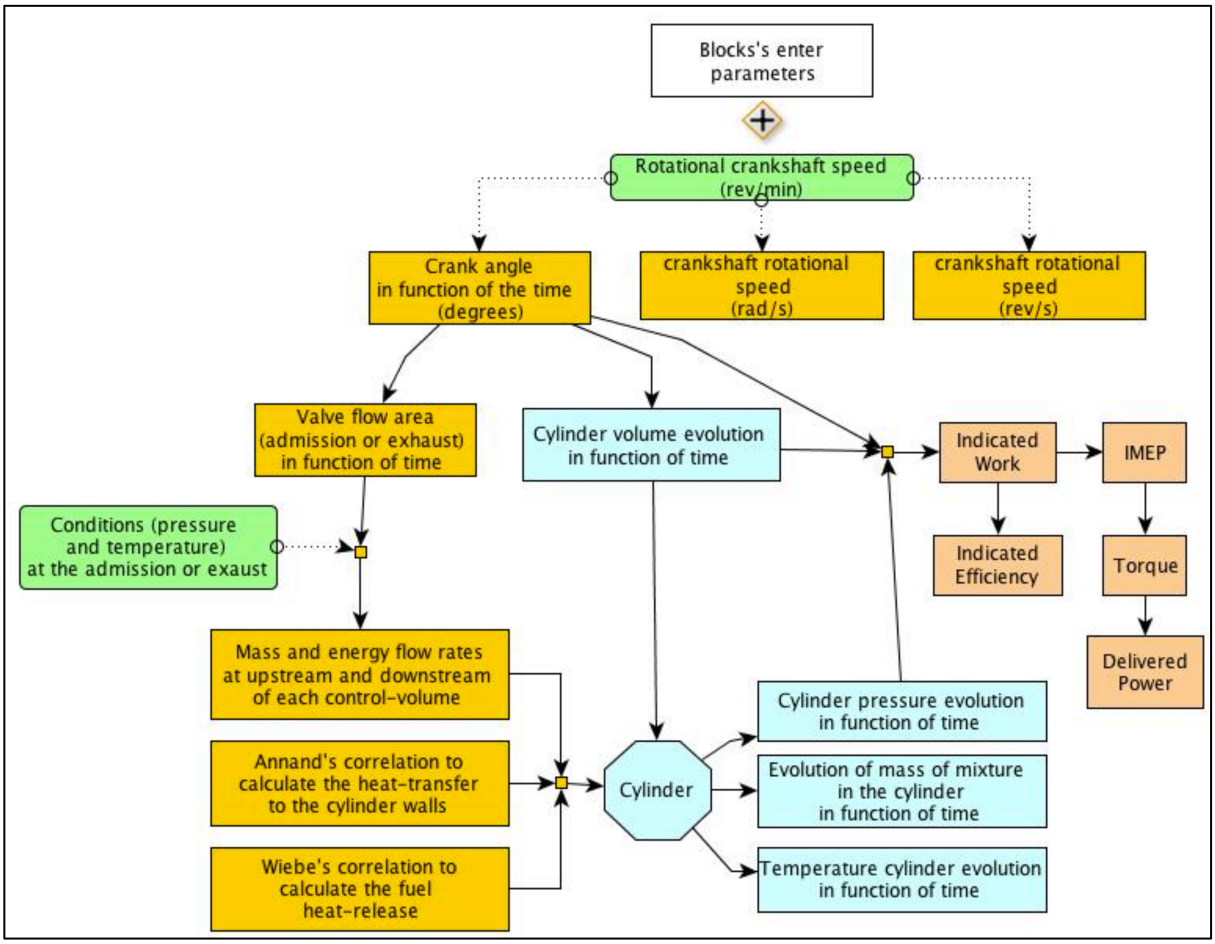

Figure 1. The modeling's algorithm structure.

4. RESULTS AND DISCUSSION

This section aims to explain the results regarding the simulations and experiments with the elaborated modeling.

At the first step of simulations the engine that has been chosen was the John Deere 4039TF, 4 cylinders. This step's main goal has consisted in assess the engine performance through the measurement concerning some global grandeurs such as performance curve, indicated engine torque, work, and efficiency, delivered power and IMEP (Indicated Mean Effective Pressure – obtained as a directly proportional grandeur with relation to the indicated work). Whether the simulation results are in according to the real engine behavior and to the theory it means that the modeling is representing well the combustion and the engine operation. Then, for the last step, another engine was simulated and some engine test bench data were also acquired in order to validate the mathematics-computational model capability in represent one real CI engine operation.

The both engine parameters are exposed in the Tab. 1 and 2.

Table 1. John Deere 4039TF's parameters.

Parameter	Value
Engine model	4 strokes – Diesel cycle – turbo
Cylinder number	4
Course (m)	110e-3
Cylinder diameter (m)	106.5e-3
Coupling rod length (m)	181e-3
Compression ratio	17.8:1
Maximum valve lift (m)	12.37e-3
Valve head diameter (m)	25e-3

Table 2. Second engine's parameter.

Parameter	Value
Engine model	4 strokes – Diesel cycle – turbo
Cylinder number	4
Course (m)	88.3e-3
Cylinder diameter (m)	75e-3
Coupling rod length (m)	136.8e-3
Compression ratio	16:1
Maximum valve lift (m)	9.25e-3
Valve head diameter (m)	42e-3

4.1 Simulations concerning the John Deere performance

The engine performance curve and its p-V diagram has been traced in a crankshaft rotational speed equal to 2800 rev/min, evaluating a duration equal to 2 seconds of operation, indicating the cylinder pressure evolution in function of the cylinder volume, which is delimited by the piston displacement. The curves in question are illustrated in the Fig. 2.

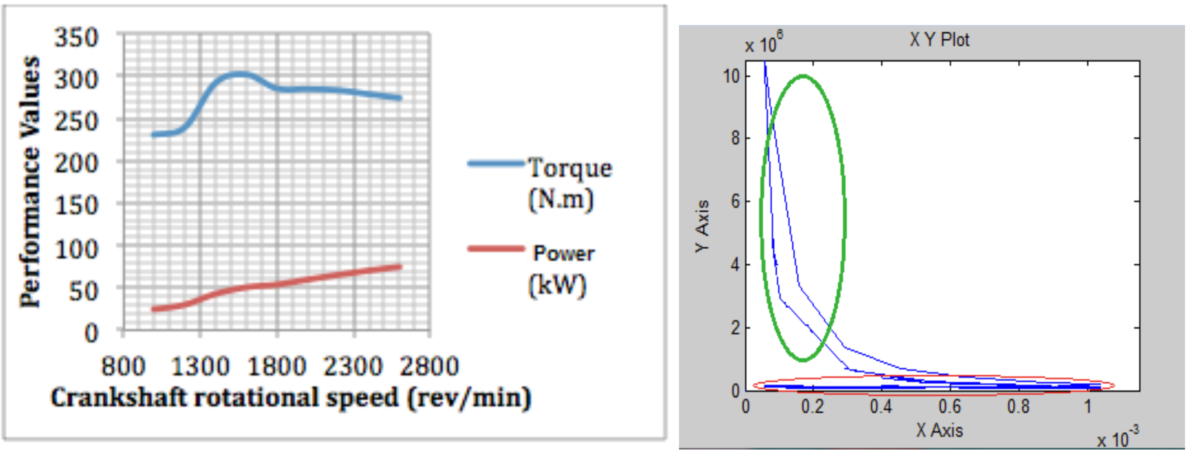

Figure 2. The performance curve (at left). The p-V diagram (at right) – Pressure (Pa) x Volume (m^3), for 2800 rev/min.

In the Fig. 2, about the p-V diagram, the green circle denotes the work (positive) delivered to the piston over the entire four-stroke cycle and is called brute work per cycle. The red circle denotes the energy (negative) lost due to friction i.e. the work transferred between the piston and the cylinder gases during the inlet and exhaust strokes and is called pumping work. Those results shall indicate if the simulation is in according to a normal CI engines behavior. The torque value is important, while the engine speed is low, and it increases in function of the engine speed until a certain value then it starts to decrease. That is the reason because is harder to have a relevant acceleration while the engine speed is high, even the power, which is proportional to the engine speed, continue developing. The power also will increase up to a maximum value, but this range is not exploited here.

4.2 Confrontation: simulation x reality

Test bench data acquired from a company into the automotive field has supplied experimental data concerning a compression ignition engine. Those data was exploited in order to validate the mathematics-computational model capability in represent the reality (confrontation between simulation and reality). The data comprises geometric and operational parameters that serve to be introduced as entry data in the simulation modeling in Simulink. The experimental results (engine rotational speed, IMEP and power delivered by the engine) obtained from the tests were also supplied. The experimental data, the simulation results and the relative error between the both cases are exposed in the Tab. 3.

Table 3. Experimental and simulated data used for the validation of the combustion modeling.

Engine speed (rev/min)	IMEP (E+05 Pa) (simulation)	IMEP (E+05 Pa) (experimental)	Power (kW) (simulation)	Power (kW) (experimental)	Relative error (IMEP) (%)	Relative error (Power) (%)
997	3,63	3,60	4,71	4,67	0,81	0,88
1497	4,89	4,80	9,52	9,34	1,93	1,92
1747	5,74	5,90	13,04	13,40	2,69	2,69
2247	6,43	6,40	18,78	18,70	0,43	0,50
2497	7,54	7,30	24,49	23,70	3,23	3,20
3748	7,88	7,90	38,44	38,49	0,13	0,25
3998	8,88	9,10	46,13	47,30	2,54	2,46

Consulting the Tab. 1, it is possible to note that the simulation results concerning IMEP and power delivered were significantly near than the experimental values. The relative errors were significantly low, being under 4% in all engine operation points (engine speeds). It is relevant to mention that the experimental results are sensible in relation to many factors such as fuel quality, engine efficiency sensibility in function of operation and air temperatures, metrology of measurement instruments and others influences. Nonetheless the simulation can assuage those influences as long as ranging the simulation time, ranging the engine speed nearly around the value in question, varying the relative and absolute tolerances (simulation parameters).

5. CONCLUSIONS

The thermodynamic numerical zero-dimensional modeling was developed successfully in the simulation ambiance Simulink. The work has consisted in an application of mathematical models, which represent several physical and chemical phenomena inherent to the combustion of compression ignition engines. The simulation has allowed the evaluation of various parameters concerning the engine efficiency. The model also allows evaluate any grandeur as long as they vary as a function of the crank angle. At the engine validation, all the engine regimes (rotational speed) have presented acceptable relative errors, indicating a plausible modeling validation.

The value of this work has an academic standpoint. The model can be intended by others to teach. It can also serve as pilot model for more advanced studies on consumption, pollutant formations, admission and gas treatment systems, electronic fuel-injection control systems, supercharging and turbocharging (many other new parameters), SCR (Selective Catalytic Reduction), DOC (Diesel Oxidation Catalyst) or CDPF (Catalytic Diesel Particulate Filter) and many other systems.

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