

MODELING AND SIMULATION OF A COMPRESSION CYLINDER-PISTON SYSTEM WITH COMBUSTION REACTION

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Abstract. In flammable gases, due to the energy stored in its molecular bonds, the construction of systems to transform the chemical energy into mechanical energy was possible. These systems were named motor. With the combustion reaction, a high rate of energy is supplied to the system in the form of heat. Expanding it suddenly and due to the action of an external force against this expansion, the movement becomes oscillatory. Within this context, the present paper contributes to the computational simulation and study of sensitivity of the velocity of the piston, the temperature and the density of the gas in the combustion process, in an integral formulation, given equations for mass, energy, momentum and molar concentration balance. The Arrhenius' equation, numerical methods for solving differentials equations system and integral formulation using Reynolds Transport Theorem (RTT) are also used. The study is done gradually in order to understand in detail all the variables from ideal conditions. The gas is assumed to be ideal, the cylinder is perfectly sealed and the flow is assumed to be instantaneously homogeneous. The system works as a set containing gas, which is compressed by an external force. Initially, there is no friction and the system is considered adiabatic. So it was possible to understand the variation of the parameters in a model that does not lose energy. Conversely, it is conservative. The final system has friction between the piston and the cylinder wall, change of heat through the wall of the system and combustion reaction, then comparison and analysis were done. The first model response is an oscillatory system with perpetual motion, because there is no dissipation and energy is always constant. The last model response is also oscillatory, but the system tends to be static, due to the non conservation of energy. Heat transfer through the cylinder walls was observed and the temperature oscillates, tending to the prescribed temperature. As a response the density decreases, showing that the volume of the system increases, characterizing the behavior of the pressure and temperature of an ideal gas. When the chemical reaction of combustion is added, there is a very sudden increase of the temperature and volume of the system, because the rate of energy was very high.

Keywords: combustion, cylinder-piston, compression, 0-dimensional model engine model, heat

1. INTRODUCTION

Turns (2000) says the number of combustion systems used in transformation and transportation industries is rapidly growing. This induces pollution and environmental problems, becoming into critical factors in our society. The accurate control of combustion reaction therefore appears as a real challenge.

2. PROPOSED PROBLEM

The model studied, sketched in Fig. (1), is a cylinder-piston system, which is initially filled with an ideal mixture of atmospheric air and methane. To simplify the problem, the following assumptions are initially used: ideal gas, tight sealing, adiabatic, no friction and instantaneous homogeneity of gas. This model is called *model A*. Next mechanical resistance between piston and cylinder wall was added, this model is called *model B*. In order to have the system close to reality, In *model C* the change of heat through the walls of system was introduced. With all the parameters previously studied, the combustion reaction was added to the system, the last model is named *model D*.

The objective of this paper is to study the sensitivity of temperature and the specific mass of the gas inside the container and the velocity of the piston. The problem was solved by applying the integral formulation of the first law of thermodynamic to an integral volume aided by RTT, balance of momentum applied to the piston, mass conservation to the gas and molar balance of the mixture components. The time integration was accomplished by the fourth-order Runge-Kutta.

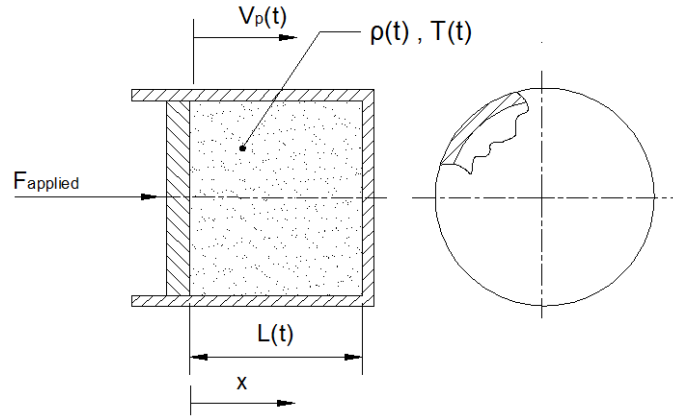


Figure 1. Sketch of the system studied.

The parameters used in the simulations are given by Tab. 1.

Table 1. Parameters used in simulations.

	Model A	Model B	Model C	Model D
Internal radius (m)	1,00E-01	1,00E-01	1,00E-01	1,00E-01
Initial position (m)	1,50E-01	1,50E-01	1,50E-01	2,24E-01 2,50E-01
Initial velocity (m/s)	0,00E+00	0,00E+00	0,00E+00	0,00E+00
Initial temperature (K)	1,00E+03	1,00E+03	1,00E+03	1,00E+03
Mass of the piston (kg)	5,00E+00 3,00E+01	5,00E+00	5,00E+00	5,00E+00
Coefficient of friction	-	1,50E+00 5,00E+00	1,50E+00	1,50E+00
Thermal resistance (K/W)	-	-	5,00E+01 1,50E+02	1,50E+02
External temperature (K)	-	-	3,00E+02	3,00E+02
Initial Internal pressure (kPa)	3,45E+03	3,45E+03	3,45E+03	6,90E+03 1,38E+04
Constant pre-exponential (1/s)	-	-	-	1,08E+09
Energy of activation (kJ/mol)	-	-	-	8,36E+04

3. THEORY AND MATHEMATICAL MODELING

Applying seconds Newton's law to the piston.

$$F_{applied} = \frac{20}{0.3-L} + P_{atm}A . \quad (1)$$

At the right-hand, the letter m means the mass and V the velocity, subscript p means that refers to the piston.

In this paper it is considered the gas as ideal. The ideal gas concept is useful because it obeys the ideal gas law, a simplified equation of state, and is amenable to analysis under statistical mechanics.

Applying the equation of state at the gas of the system (Borgnakke, 2009), Eq. (2) is obtained:

$$F_{gas} = \rho RTA . \quad (2)$$

In the right-hand-side, R is the ratio of the universal gas constant and the molar mass of a certain element, A is the area of the piston in contact with the gas and ρ is the density of the gas. T is the gas temperature, which is constant in space.

The combustion process involves the oxidation of the fuel components that are oxidizable and can therefore be represented by a chemical equation. In the combustion process, mass conservation should be taken into account.



where x is the number of moles of methane.

In a chemical reaction, the difference between the enthalpy of the products and reagents gives us the heat transfer.

$$\bar{h}_{T,P} = (\bar{h}_f^0)_{298\text{ K}, 0.1\text{ MPa}} + (\Delta\bar{h})_{298\text{ K}, 0.1\text{ MPa} \rightarrow T,P} \quad (4)$$

The first term on right-hand-side is the enthalpy of formation in the reference state and the second represents the difference between the enthalpy in any state.

The rate of reaction is how fast a number of moles of one chemical species are being consumed to form another chemical species (Fogler, 1939). Each reaction has its own equation, in this paper the rate of reaction used is given by Eq. (5):

$$\frac{dC_{CH_4}}{dt} = -r_{CH_4} + \frac{C_{CH_4}}{V} \cdot \frac{dV}{dt}, \quad (5)$$

where V is the volume of the system.

Applying the equation of mass conservation, considering the system as perfectly sealed, there is not mass crossing the control surface.

$$\frac{d\rho}{dt} - \frac{A}{m_{gas}} \cdot V_p \rho^2 = 0. \quad (6)$$

The term m_{gas} means the mass of the gas inside the cylinder.

The first law of thermodynamics, neglecting the change of kinetic energy and considering only the internal energy with the only work that the system performs is expanding due to piston movement and with two forms of rate of heat transfer are considered, first by conduction through the cylinder walls and second by generation with the combustion.

$$mC_v \frac{dT}{dt} = \frac{dQ_{convecção}}{dt} + \frac{dQ_{gerado}}{dt} + F_{ext} V_p, \quad (7)$$

where c_p is the specific heat of the fluid, T_{ext} is the temperature outside the cylinder and R_{eq} is the thermal resistance between the internal and external sides.

4. RESULTS AND ANALYSIS

The behavior of *model A*, in which is adiabatic, with no friction and without chemical reaction indicates that the oscillation of the system is perpetual, because there is no dissipation of energy. The variations of the parameters are direct consequences of the initials conditions.

The *system B* response, which is similar to *system A*, but with a dissipative term, the responses tend to constant values but with different times to stabilize.

In *system C*, which thermal resistance and a temperature difference between the internal and external environment were introduced, it is noticed that the temperature of the system tends to approximate to the outside temperature. It is also possible observe that the system expands, as the density of the gas increases. This behavior occurs because the external temperature is initially lower than the internal temperature, then energy leaves the system as heat.

The response of *Model D* is given by Fig. (2). This model represents the system with combustion. The reaction starts at the fourth second. *Model D* response shows is the behavior of the energy of the combustion is in the system studied in this paper. The temperature increases almost instantaneously at the exact moment the combustion starts. Another interesting fact is the increase of the frequency of oscillation. By comparing simulations (a) and (b) in Fig. (6), it can inferred that, for a higher initial pressure, the temperature after the combustion is higher, which is due to the gas concentration and consequently a greater energy released. The velocity of the piston in the simulation of Fig. (6-b) is also greater, since with the temperature increase. There is an expansion in the system and then the stroke is larger.

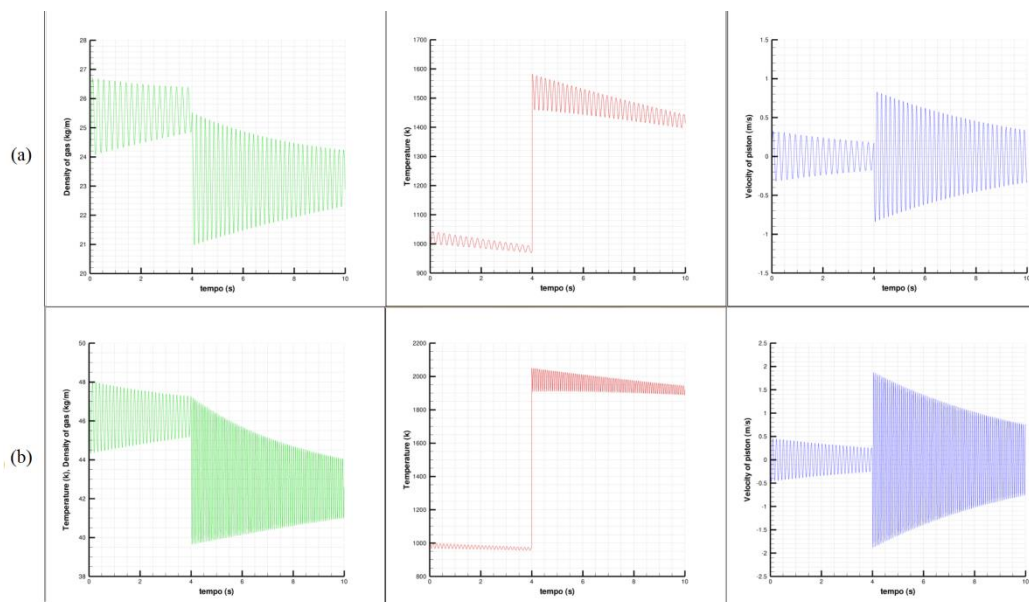


Figure 2. Behavior of the piston velocity, temperature of the system and the density of the gas, in *model D*, versus the time for two different initial internal pressure; (a) $P_{initial} = 6900 \text{ kPa}$; (b) $P_{initial} = 13800 \text{ kPa}$.

5. CONCLUSION

The conclusion is that the studied system has an oscillatory behavior and when the combustion reaction occurs, the system receives a high-energy, increasing its temperature and its rate of oscillation. The combustion reaction releases high energy almost instantaneously, which significantly influences the system. A high control of such a system is necessary when applying it to practical purposes, since, as shown in the paper, variations on parameters cause different responses.

It is possible to state that the control of the system, to obtain satisfactory results, in accordance to the practical characteristics involves many parameters. In this work, it was possible to understand the influence of some of them.

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