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

João Rodrigo Andrade, jr_femec@yahoo.com.br
Aristeu Silveira-Neto, aristeus@mecanica.ufu.br
Francisco José de Souza, fjsouza@mecanica.ufu.br
João Marcelo Vedovoto, jmvedovoto@mecanica.ufu.br
Federal University of Uberlândia, Campus Santa Mônica, Laboratory of Fluid Mechanics, Avenue João Naves de Ávila, 2121, Uberlândia, MG.

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 was 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 andintegral 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

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.

Computer simulation is now truly on par with experiment and theory as a research tool to produce information that is not available by using any other technique. Computational Fluid Dynamics (CFD) is efficiently used to improve the design of aerodynamical systems, and today no real progress in design can be made without using CFD. With the same objects, many works have been devoted to combustion modeling, following a variety of approaches and distinct modeling strategies. This paper is intended to provide an integral model which is solved by a numerical method.

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. Outside the set, there is a force varying hyperbolically being applied directly in the piston. It's growing with the expansion of the internal volume of the system. 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 orde 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.

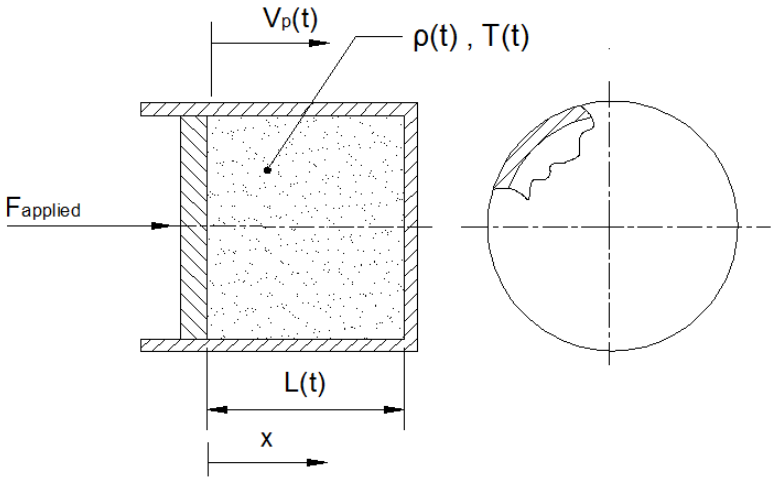

Figure 1. Sketch of the system studied.

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 ativation (kJ/mol)	-	-	-	8,36E+04

3. THEORY AND MATHEMATICAL MODELING

Applying seconds Newton's law to the piston. It basically states that the net external force on a system is equal to the rate of change of its linear momentum, in an inertial reference frame, results Eq. (1). In the horizontal coordinate we have Eq. (2).

$$\sum(\vec{F})_{external} = \frac{d(m\vec{v})}{dt}, \tag{1}$$

$$\sum(F)_{x\,piston} = F_{applied} - F_{gas} - C_{resist}V_p = m_p\frac{d(V_p)}{dt}, \tag{2}$$

$$F_{applied} = \frac{20}{0.3-L} + P_{atm}A\,. \tag{3}$$

The first term on right hand is the externally applied external force. The second term on the right-hand side is the force generated internally by the fluid and the third term is the force of mechanical resistance between the piston and the cylinder wall. 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 and an ideal gas or perfect gas is a theoretical gas composed of a set of randomly-moving, non-interacting point particle. 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.

The thermodynamic properties of an ideal gas can be described by the equation of state, given by Eq. (4):

$$P = \rho RT \, . \tag{4}$$

Applying the Eq. (4) at the gas of the system, Eq. (5) is obtained:

$$F_{gas} = \rho RTA \, . \tag{5}$$

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. The reaction considered in this paper is given by Eq. (6):

$$x \cdot CH_4 + 2x \cdot O_2 \rightarrow 2x \cdot H_2O + x \cdot CO_2 \, , \tag{6}$$

where x is the number of moles of methane.

When a fuel consisting of hydrocarbon is burned, the carbon and hydrogen are oxidized. In the combustion process several intermediates can be formed, but in this paper only the final products are considered. The minimum amount of air that supplies sufficient oxygen for complete combustion of carbon, hydrogen and other elements that can oxidize the fuel is called theoretical air. When it is possible to complete combustion of the reactants with the theoretical air, the resulting products do not contain oxygen. The mixture is considered to be stoichiometric in this paper. The reference thermodynamic state of the components admitted is defined at the temperature 298.15 K and pressure of 0.1 MPa.

In a chemical reaction, the difference between the enthalpy of the products and reagents gives us the heat transfer. In other words, it measures the total energy needed to break the bonds of the reactive elements and create connections needed to form the reaction product. This energy is based on the reference state. However, when it comes to states that are not the reference, the energy pattern is different and therefore it is necessary to correct formation enthalpy of each element. The enthalpy of formation of each constituent is given by Eq. (7):

$$\bar{h}_{T,P} = \left(\bar{h}_f^0\right)_{298\ k,0.1MPa} + \left(\Delta\bar{h}\right)_{298\ k,0.1MPa \rightarrow T,P} \, . \tag{7}$$

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. A chemical reaction takes place when a detectable number of molecules of one or more species have lost their identity and assumed a new form by change in the kind or number of atoms in the compound and/or by a change in structure or configuration of these atoms. The rate equation for reaction is an algebraic equation that is solely a function of the properties of the reacting materials, reaction conditions and the reaction mechanism. Each reaction has its own equation, in this paper the rate of reaction used is given by Eq. (8):

$$r_{CH_4} = k_{reaction} \cdot {C_{CH_4}}^2 . \tag{8}$$

Arrhenius assumed that only molecules that possess energy greater than E_a can react and that only these high energy molecules form products. Then factor Bolstzman is given by Eq. (9):

$$k_{reaction} = A_{reaction} \cdot e^{\left[\frac{-E_a}{(\bar{R} \cdot T)}\right]} . \tag{9}$$

The terms $A_{reaction}$ and E_a are constants dependent on the reaction, $\bar{R}$ is the universal gas constant and C_{CH_4} is the methane concentration

It is considered that there are no species entering or leaving the system and the volume of the system is varying. It is also assumed that the reaction mixture is perfect, so that there is no variation in the rate of reaction throughout the reactor volume. Molar balance is modeled by Eq. (10):

$$\frac{dC_{CH_4}}{dt} = -r_{CH_4} + \frac{C_{CH_4}}{\forall} \cdot \frac{d\forall}{dt}, \tag{10}$$

where $\forall$ is the volume of the system.

To convert a system analysis to a control volume analysis, it is necessary to transform the mathematics in order to apply it to a fixed region, instead of the individual masses. This transformation called Reynolds Transport Theorem (RTT) can be applied to all basic laws. In this paper, it is applied to energy and mass balances.

Considering a control volume deforming over time in an arbitrary manner, the rate of change of any magnitude B (energy, mass …) within the system is given by Eq. (11):

$$\frac{d}{dt}\left(B_{system}\right) = \frac{d}{dt}\left(\int_{C\forall} \beta\rho dv\right) + \int_{CS} \beta\rho\left(\vec{V}\cdot\vec{n}\right)dA, \tag{11}$$

where $\beta = dB/dm$.

It is possible to apply the RTT to mass conservation, it is considered $B = m$ and $\beta = 1$. Since by definition in a system of control no mass enters or leaves, the left-hand-side term on Eq. (11) is zero. Considering the system as perfectly sealed, there is not mass crossing the control surface, so the second term on the right hand of Eq. (11) is also zero. Equation (12) represents the RTT applied to the mass conservation:

$$\frac{d}{dt}(\rho\forall) = 0\ . \tag{12}$$

Simplifying Eq. (12) we obtain the rate of density change, given by Eq. (13).

$$\frac{d\rho}{dt} - \frac{A}{m_{gás}} \cdot V_p\rho^2 = 0\ . \tag{13}$$

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

To apply the RTT to the first law of thermodynamics, it is necessary to make some considerations first. The variable B in Eq. (11) becomes the energy E, and $\beta = dE/dm = e$ is the energy per unit mass. The Eq. (14), which represents the first law of thermodynamic, can be written as Eq. (15):

$$\frac{dQ}{dt} - \frac{dW}{dt} = \frac{dE}{dt}, \tag{14}$$

$$\frac{dE}{dt} = \frac{d}{dt}\left(\int_{\forall C} e\rho dv\right) + \int_{SC} \beta\rho\left(\vec{V}\cdot\vec{n}\right)dA. \tag{15}$$

The energy per unit of mass, e, is given by Eq. (16), neglecting the change of kinetic energy and considering only the internal energy, simplification.

$$e = \hat{u} = c_pT, \tag{16}$$

where c_p is the specific heat of the fluid.

The only work that the system performs is expanding due to piston movement. This term is given by Eq. (17):

$$\delta W_{pressure} = -P\delta\forall \rightarrow \frac{dW_{pressure}}{dt} = F_{applied}V_p\ . \tag{17}$$

In the system investigated two forms of rate of heat transfer are considered, first by conduction through the cylinder walls and second by generation with the combustion.

The mathematical model of the conduction through the walls of the system is given by Eq. (18), which is modeled as function of the thermal resistance:

$$\frac{dQ_{transf}}{dt} = \left[\frac{T_{ext}-T}{R_{eq}}\right], \tag{18}$$

where T_{ext} is the temperature outside the cylinder and R_{eq} is the thermal resistance between the internal and external sides.

Another term considered in the equation of energy is the combustion, given by Eq. (19):

$$\frac{dQ_{combustion}}{dt} = r_a \cdot \Delta H_R \cdot \forall \, . \tag{19}$$

By applying Eqs. (15), (16), (17), (18) and (19) in Eq. (14) it is possible to obtain the energy integral equation for the studied system, given by Eq. (20):

$$mc_v \frac{dT}{dt} = \frac{dQ_{convecção}}{dt} + \frac{dQ_{gerado}}{dt} + F_{ext} V_p \, , \tag{20}$$

where the specific heat present in Eq. (20) is the air specific heat.

The differential equations system that models the physical problem in this paper is given by Eqs. (21), (22), (23) and (24):

$$\frac{dV_p(t)}{dt} - \frac{F_{applied} - RA\rho(t)T(t) - C_{resist}V_p(t)}{m_p} = 0 \, , \tag{21}$$

$$\frac{dC_{CH_4}(t)}{dt} + A_{reaction} \cdot e^{\left[\frac{-E_a}{R \cdot T(t)}\right]} \cdot \left(C_{CH_4}(t)\right)^2 - \frac{A\rho(t)V_p(t)C_{CH_4}(t)}{m_{gas}} = 0 \, , \tag{22}$$

$$\frac{d\rho(t)}{dt} - \frac{A}{m_{gas}} \cdot V_p(t)\rho(t)^2 = 0 \, , \tag{23}$$

$$\frac{dT(t)}{dt} - \left(\frac{F_{applied}V_p(t)}{m_{gas}c_p}\right) - \frac{T_{ext} - T(t)}{R_{eq}} - \frac{(\Delta H_R(t))A_{reaction} \cdot e^{\left[\frac{-E_a}{R \cdot T(t)}\right]} \cdot \left(C_{CH_4}(t)\right)^2}{c_p m_{gas}} = 0 \, . \tag{24}$$

The initial conditions that characterize this system are given by Eqs. (25), (26), (27) and (28):

$$V_p(0) = 0 \; m/s \, , \tag{25}$$

$$T(t) = 1000 \; K \, , \tag{26}$$

$$C_{CH_4}(0) = \frac{p_{inicial}}{R_{CH_4} \cdot T \cdot M_{CH_4}} \, , \tag{27}$$

$$\rho(t) = \frac{p_{inicial}}{R_{ar} \cdot T} \, . \tag{28}$$

3.1. Numerical methods

To solve the differential equation system the fourth-order Runge-Kutta method is used. The verification of the code evaluates the implementation of the equations, boundary conditions and discretization schemes, aiming to ensure the absence of programming errors.

In this work the code verification is performed by comparing numerical solutions with a manufactured solution. The exact solution used in this article is obtained through the method of manufactured solutions as described in Roache (1998) and Roy (2005). This verification method involves the introduction of sources terms in governing equations, creating a mathematical problem for which an analytical solution is proposed. This analytic solution (manufactured) can be used for comparisons with the numerical solutions.

4. VERIFICATION OF THE COMPUTER CODE

To verify the computer code, each variable from the numerical and analytical results have been compared after its stabilization. Figure 2 shows the behavior of the error as a function of the inverse of time step used. The manufactured solutions are given by Eqs. (34), (35), (36) and (37).

$$f_\rho = -\frac{Ae^{-t}sin(t)\left(e^{-t}cos(t) + \frac{F_{applied}}{A \cdot T_{ext} \cdot R}\right)^2}{m_{gas}} \, , \tag{34}$$

$$f_V = -e^{-t}sin(t) + e^{-t}cos(t) - \frac{1}{m_p}\left(F_{applied} - R(e^{-t}sin(t) + T_{ext})A\left(e^{-t}cos(t) + \frac{F_{applied}}{A \cdot T_{ext} \cdot R}\right) - C_{resist}e^{-t}sin(t)\right) \, , \tag{35}$$

$$f_T = -e^{-t}sin(t) + e^{-t}cos(t) - \frac{F_{applied}e^{-t}sin(t)}{m_{gas}\cdot C_v} + \frac{e^{-t}sin(t)}{m_{gas}\cdot C_v \cdot R_{eq}} \ . \tag{36}$$

$$f_{C_{CH_4}} = -e^{-t}sin(t) + e^{-t}cos(t) + A_{reaction} \cdot e^{\left[\frac{-E_a}{R\cdot(e^{-t}sin(t)+T_{ext})}\right]} \cdot e^{-t}sin(t) - \frac{A\left(e^{-t}cos(t)+\frac{F_{applied}}{A\cdot T_{ext}\cdot R}\right)\left(e^{-t}sin(t)\right)^2}{m_{gas}} \ . \tag{37}$$

The results are consistent with the formal fourth-order of the method. These results provided confidence that programming errors are nonexistent and that the code was well established.

5. RESULTS AND ANALYSIS

Figure 3 shows the behavior of *model A*, in which is adiabatic, with no friction and without chemical reaction

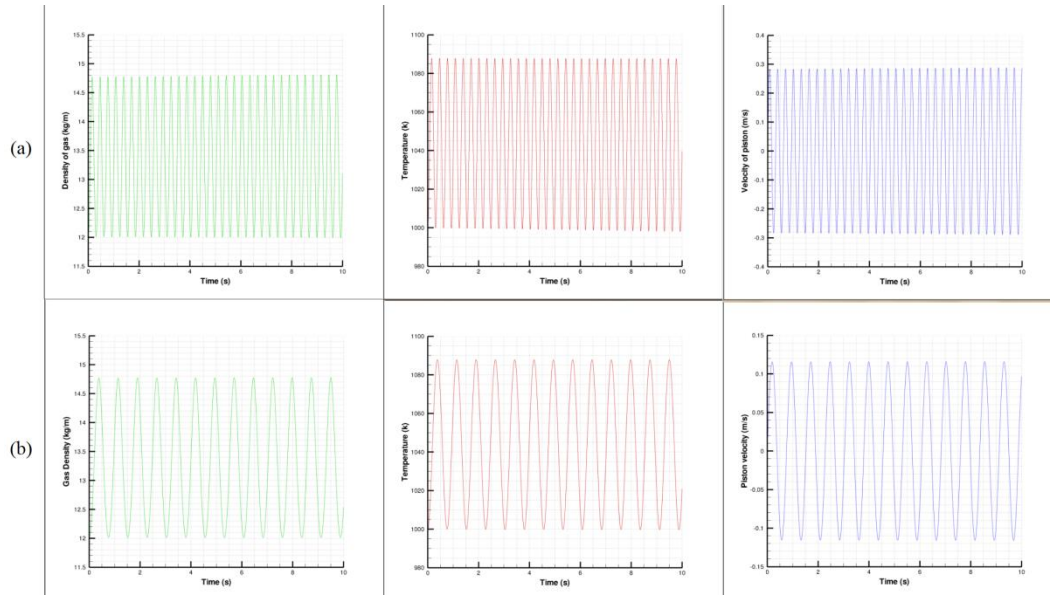

Figure 3. Behavior of velocity of the piston, temperature of the system and the density of the gas, in *model A*, versus the time, for two different mass of the piston; (a) $m_p = 5\ kg$; (b) $m_p = 30$.

The response presented by Fig. 3 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.

Figure 3 show that the frequency of oscillation is inversely proportional to the mass of the piston, the consequently of the mass increase is the increase of inertia of the piston. Figure 4 represents the *system B* response, which is similar to *system A*, but with a dissipative term. The analysis in Fig. 4 shows how the mechanical resistance influences the . It is possible to note that the variables tend to the same values but with different times to stabilize. Figure 5 presents the system response with heat transfer. A thermal resistance and a temperature difference between the internal and external environment were introduced. In Fig. 5 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. 6. 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.

6. 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.

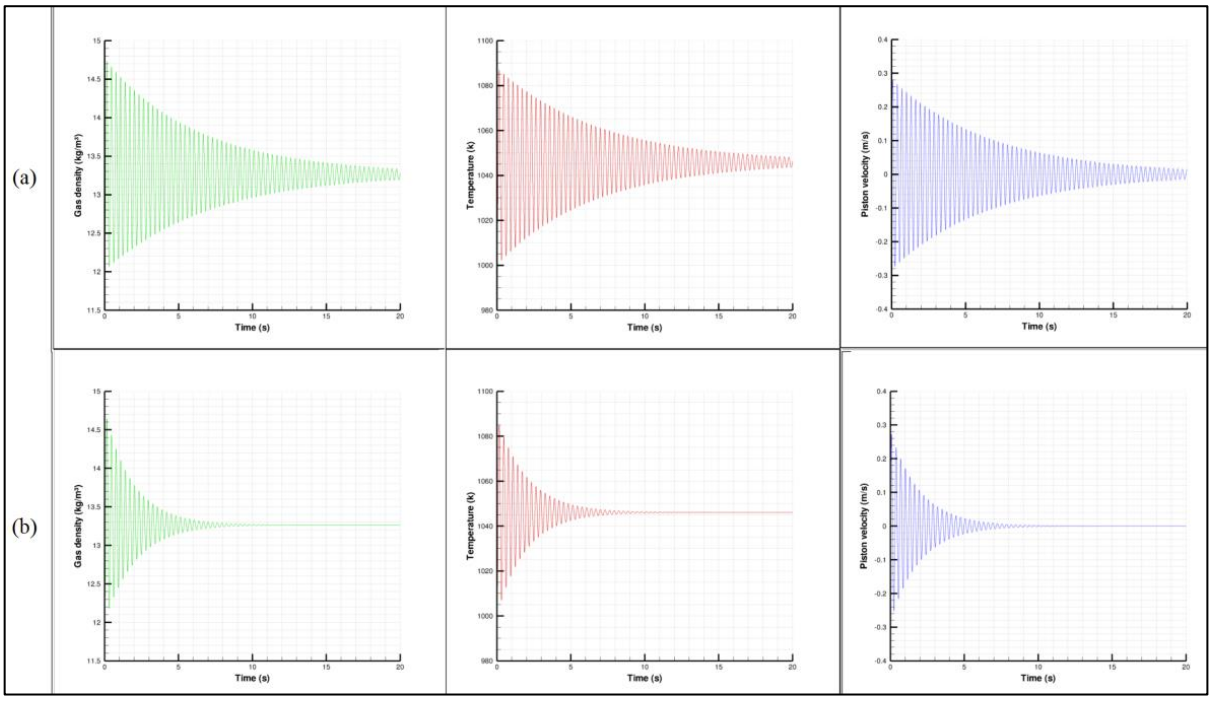

Figure 4. Behavior of the piston velocity, temperature of the system and the density of the gas, in *model B*, versus time for two different coefficients of resistance; (a) $C_{resist} = 0.5$; (b) $C_{resist} = 1.5$.

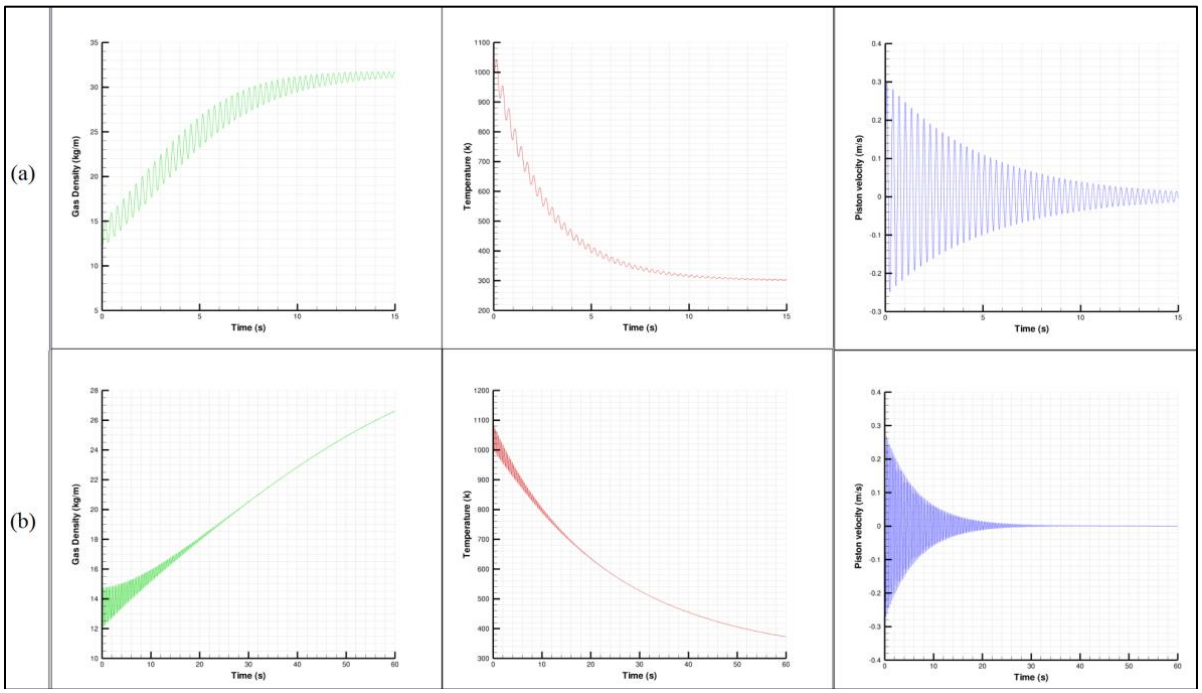

Figure 5. Behavior of the piston velocity, temperature of the system and the density of the gas, in *model C*, versus the time for two different thermal resistance; (a) $R_{eq} = 50\ K/W$; (b) $R_{eq} = 150\ K/W$.

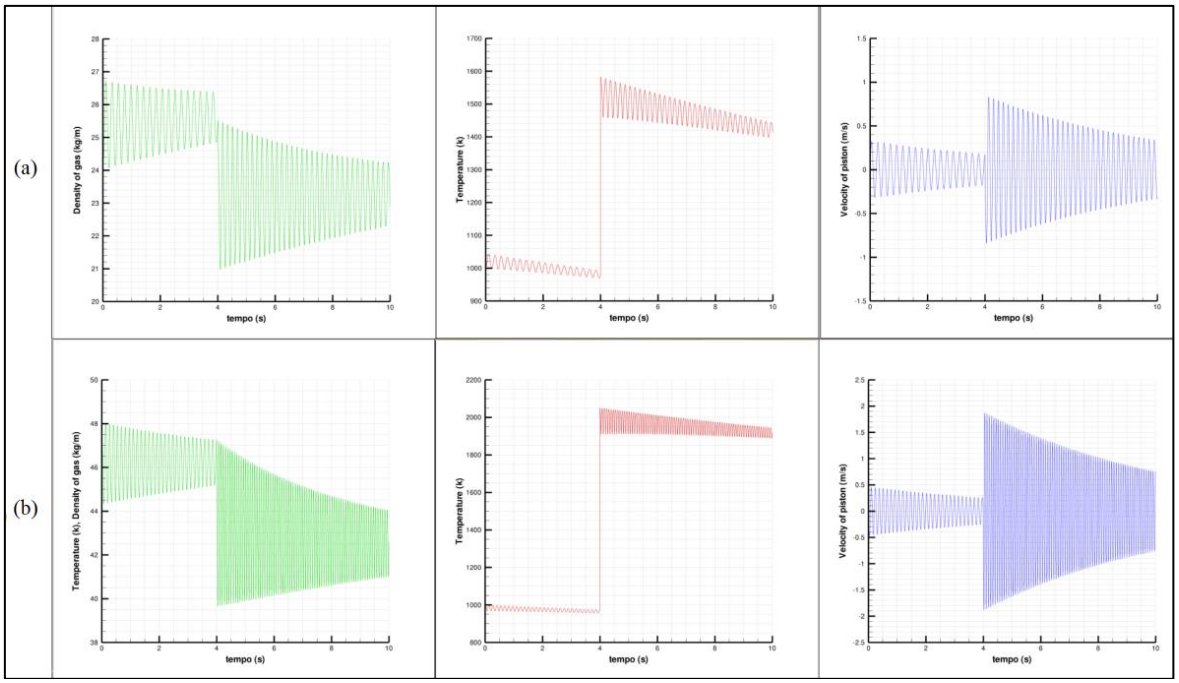

Figure 6. Behavior of the piston velocity, temperature of the system and the density of the gas, in *model D*, versus the time for two different initial internal pressure; (a) $P_{initial} = 6900\ kPa$; (b) $P_{initial} = 13800\ kPa$.

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8. RESPONSIBILITY NOTICE

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9. REFERENCES

Ferziger, J.H, Peric, M., 2002, "Computational Methods for Fluid Dynamics", Ed. Springer, New York.
Fogler, H.S, 1939, "Elementos de engenharia das reações químicas 4th ed.", Ed. LTC, Rio de Janeiro.
Çengel, Y.A, 2009, "Transferência de Calor e Massa", Ed. McGraw Hill, S. Paulo, Brazil.
Çengel, Y.A, Cimbala, J.M., 2006, "Mecânica dos Fluidos", Ed. McGraw Hill, S. Paulo, Brazil.
Franco, N.B., 2006, "Cálculo Numérico", Ed. Pearson Prentice Hall, S. Paulo, Brazil.
Anderson, J.D., 1995, "Computational fluid dynamics: the basic with applications", Ed. McGraw-Hill, New York.
Borgnakke, C., Sonntag, R.E., 2009, "Fundamentos da Termodinâmica", Ed. Edgard Blucher, S. Paulo, Brazil.
Çengel, Y.A, Cimbala, J.M., 2007, "Mecânica dos fluidos: Fundamentos e aplicações", Ed. McGraw-Hill, S. Paulo, Brazil.
Roy, C.J, "Review of Code and Solution Verification Procedures for Computational Simulation", Journal of Computational Physics, v.205(1), pp.131-156.
Roache, P.J, 1998, "Verification and Validation in Computational Science and Engineering", Hermona Publishers, New Mexico.
Mansur, S.S, Vieira, E.D.R., Silveira-Neto, A., 2010, "Turbulência", Rio de Janeiro : ABCM. :Il. – (Coleção Cadernos de Turbulência, v.7)..