# International Journal of Thermodynamics

Volume No. 28 Issue No. 1 January - April 2025



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# International Journal of Thermodynamics

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The purpose and scope of the International Journal of Thermodynamics (IJoT) is

- to provide a forum for the publication of original theoretical and applied work in the field of thermodynamics as it relates to systems, states, processes, and both non-equilibrium and equilibrium phenomena at all temporal and spatial scales.
- to provide a multidisciplinary and international platform for the dissemination to academia and industry of both scientific and engineering contributions, which touch upon a broad class of disciplines that are foundationally linked to thermodynamics and the methods and analyses derived there from.
- to assess how both the first and particularly the second laws of thermodynamics touch upon these disciplines.
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#### Effects of Nozzle Diameter and Holes Number on the Performance and Emissions of a Gasoline Direct Injection Engine

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#### ABSTRACT

The goal of the current study is to estimate how a gasoline direct injection (GDI) engine's performance and emissions are affected by the fuel injector nozzle diameter and hole number of its injectors. A thermodynamic mathematical modelling has been created utilizing a software program written in the MATLAB language to simulate the two-zone combustion process of a four-stroke direct injection engine running on gasoline at (Rotation Engine Speed 3000 revolution per minute (rpm), 40 MPa injection pressure, compression ratio 9.5, and spark timing 145°). The first law of thermodynamics, equation of energy, mass conserving, equation of state, and mass fraction burnedwere all used in the creation of the software program. The study was carried out at five different nozzle diameters (0.250, 0.350, 0.450, 0.550, and 0.650 mm) and nozzle hole numbers (4,6,8,10,12). The results show that the GDI engine's performance and emissions are significantly influenced by variations in nozzle hole diameter and number. It was shown that engine power, heat transfer, cylinder pressure, and temperature increased with increasing nozzle hole diameter and number of nozzle holes and the maximum value was seen with nozzle hole diameter 0.650 mm and (12) holes. The lowest value for the nozzle hole diameter and number of holes was found to be 0.250 mm and 4 nozzle holes, which resulted in the lowest emissions of carbon monoxide CO and nitrogen monoxide NO. The study was also conducted for different operating conditions (Rotation Engine speed of 1000, 2000, 3000, 4000, 5000 rpm, 35 Mpainjection pressure, compression ratio of 11.5, and spark timing of 140°) and the same nozzle diameters and nozzle holes number mentioned previously to estimate the maximum values for temperature, pressure, power, heat transfer and emissions. The results of the second part of the study showed that the highest of maximum values of temperature, pressure, and emissions were at of 1000 rpm, a nozzle diameter of 0.650 mm, and (12) holes. The highest values for maximum power at 4000 rpm, a nozzle diameter of 0.650 mm and (12) holes, while the highest maximum values for heat transfer are at 5000 rpm, a diameter of 0.65mm and (12) holes.

*Keywords: Gasoline direct injection engine (GDI); nozzle diameter; hole number; mathematical model; performance; emissions* 

#### INTRODUCTION

(GDI) engine technology has sparked considerable interest in recent years due to its several advantages over traditional fuel injection (PFI) engines, including reduced fuel consumption, improved efficiency, and lower hazardous emissions to comply with environmental requirements[1], [2]. Although GDI engines provide rapid reaction and flexible control, several aspects impact engine performance and

engine emissions, including ignition and injection timings, injection pressure, injection duration, diameter of nozzles, and aperture numbers, among others .Studying combustion engines experimentally is a very challenging issue because of the sophisticated experimental facilities that are required to perform the experiments. Therefore, researchers tend to perform theoretical or analytical analyses such as simulation and numerical analysis before conducting any experimental activity.

Cost and time may be saved by using a simulation approach that enables GDI engine designers to adjust and examine a variety of factors with no need to actually create any real part or even an entire engine. Numerous mathematical models, including combustion phasing modeling, thermophysical property models, injector models, and flow models into and out of a cylinder engine, have been developed to aid in understanding, correlating, and investigating the process of engine cycles [3].

The impact of engine settings on a DI engine's performance and emission characteristics has been examined in several studies related to diesel and gasoline. Kumbhar et al. [4] used computation fluid dynamics CFD codes with a combustion model to test four different nozzle throat diameters and their influence upon the engine performance, emissions, as well as spraying features. They discovered that improvements in spray cone angle, fuel atomization, and effective air-fuel mixture resulted to a 0.230 mm nozzle throat diameter, which led to the highest in-cylinder temperatures and pressures. Hydrocarbon (HC), Carbon monoxide (CO), and soot emission got decreased as nozzle hole diameter dropped; nevertheless, Nitric oxide (NO)emissions were reported to rise because of improved atomizing as well as a general increase within cylinder gas temperatures of nozzle holes by smaller sizes. As a result, nozzle throats having smaller diameters have a tendency to lower emission at the cost of increased NOx emission. Lee et al. [5] investigated the development of fuel spray-air mixing, combustion, and emitting as the number of injector throats changed. The researchers found that there is a optimal number of holes for better efficiency and emission of the diesel engine. Furthermore, the findings demonstrate that evaporating, atomizing, and combustion are significantly impacted by the amount of holes present. On the other hand, when the number of injector holes exceeds a certain limit, the combustion and emissions deteriorate as a result of an absence of air entraining necessary to create a stoichiometric mixture. By using a flux dynamometer, a four-stroke single cylinder diesel engine, a water-cooled direct injection dieselengine operated by computer, a typical injection timescale of 23° before top dead center(BTDC), and a variety of throat diameters, Kumar et al. [6] studied the performance, combustion, and emitting of the engine for the different nozzles hole dimension (3 holes ×  $\emptyset = 0.20 \text{ mm}$ ), (3 holes  $\times \emptyset = 0.28 \text{ mm}$ ) and (3 holes  $\times \emptyset = 0.20 \text{ mm}$ ) as shown in figure 1. The results of this study showed that among all different nozzle throats, the 3 holes  $\times \emptyset = 0.20$  mm (adapted) improved the time. The findings were outstanding in terms of performance, combustion, and emitting.

The only disadvantage was that NOx numbers rise when the aperture nozzle hole size is reduced.



Figure 1. Schematic drawing of 3-holes of different nozzle diameters(a)  $\emptyset = 0.20 \text{ mm}$ , (b)  $\emptyset = 0.28 \text{ mm}$ , (c)  $\emptyset = 0.31 \text{ mm}$ .

Jiang C and Parker M., et al. [7] studied the influence of injection nozzle design upon the (GDI) engine fuel spray features. Inside a pressure- and temperature-controlled constant volume chamber as well as outside, testing on two custom three-hole injectors were carried out. The measuring was made at intervals of 15 mm, 25 mm, and 40 mm from the injection tip, radially outwards from the injection axis to the external edge of the jet. The researchers found that the spray penetration length before collapsing is determined by the injection pressure rise within extending such length. To understand the performance during flash boiling circumstances, average velocity and droplet diameter information were also studied. Additionally, the results showed that droplet size decreases whereas droplet velocity greatly rises during flash boiling circumstances. Researchers discovered that various hole geometries had distinct effects on sprays when exposed to a flash boiling setting. Some hole configurations provide more protection from spray collapsing. The researchers discovered that the spray produced by the middle of the three-hole sizes studied dispersed more easily than the spray produced by either smaller and greater hole diameters. Moreover, the convergent hole was more likely to show spray collapsing during flash boiling circumstances. Ahmed and Mekonen [8] conducted a simulation study by using ANSYS the influence of different injector nozzle hole numbers (INHNs) and fuel injection pressures (IPs) of the performance, and emissions characteristics of engine. The study performed for different fuel IPs 190, 200, 210, and 220 bar with a change of INHN of 1 (default), 3, and 4), each 0.84, 0.33, and 0.25 mm in orifice diameter, respectively as showing in figure 2. The results show the increasing of INHNs and fuel IPs have an essential improvement of atomization and mixing rates, as well as combustion and engine efficiency as well as minimize of CO and HC emissions with a small raise in Nox.



Figure 2. A diagram of fluid in nozzles: (a) single hole, (b) 3-holes, (c) 4-holes.

Reddy and Mallikarjuna [9] studied the impact of fuel injection settings on the performance, combustion, and emitting features of GDI engines by using CFD. For a variety of fuel injection pressures, spark timing, holes number, and multiple stage injection strategies, turbulence, combustion, and fuel spraying break-up analyses were carried out. The findings demonstrate that, relative to 110-bar fuel injection pressure, soot emission decreased for various fuel injection pressures by roughly 77.8 and 88.5% for 150 and 200-bar fuel injection pressures, respectively. When spark timing was advanced, the soot emission rose by an amount that was about 3.3 and 4.5 orders of magnitude more, correspondingly, at the spark time of 15° and 20° BTDC than at the spark time of 7.5° BTDC. Additionally, relative to a 6hole injection, the soot emission is lower when 8 or 10 fuel injection holes were employed. The soot emission dropped by around 72.8 and 76.1%, correspondingly, in comparison to single-stage fuel injection, when two different multiple stage fuel injection techniques were taken into account. Eventually, it was determined that a GDI engine's preparing of the mixture and soot emission are significantly influenced by the fuel injection pressure, amount of injection holes, spark time, and multiple stage fuel injection technique. Employing (CFD) research and information from literatures, Jadhav and Mallikarjuna [10] investigated the impact of fuel injectionhole diameter and fuel injection time upon the mix formation in a four-stroke, wall-guided GDI type of engines. GDI engine at a compression ratio of 11.5. CFD simulating is run at an engine velocity of 2000 revs per minute. Three crank angle measures, three fuel injection times, as well as three fuel injection hole sizes of 0.1, 0.14, and 0.18 mm were used. The findings demonstrate that larger nozzle-hole diameters produced extremely rich mixing zones close to the spark plug. Furthermore, a greater suggested mean effective pressure was seen with a smaller nozzle-hole diameter and delayed fuel injection time.

According to the preceding discussion, numerous researchers have concentrated on various elements of engine parameters of GDI engines utilizing various approaches and techniques. The injector setting effect upon the performance as well as emitting characteristics of a GDI engine, on the other hand, has not been well examined. As a result, the present work aims at using MATLAB to investigate such effect. This work will be useful in enhancing the GDI engine settings for optimal performance.

#### 2. Theoretical Model

This model examines a direct injection engine. The model depends on a two-zone thermodynamic study of the combustion process, which separates the combustionchamber into burned and unburned areas. The ideal gas law is assumed for the in-cylinder gases, and the first law of thermodynamics, state equation, and mass and volume conservation are used. For the temperature, pressure, mass, and volume of the burned and unburned gases, a set of equations may be constructed. The Wiebe function has the following definition. [11]:

$$X_{b(\theta)} = 1 - \exp\left[-a \left[\frac{\theta_{(j)} - \theta_{(\theta)}}{\theta_{(b)}}\right]^{k+1}\right]$$
(1)

here  $\Theta(i)$  represents the immediate crank angle,  $\Theta(o)$  represents the spark angle at the beginning of combustion, and  $\Theta(b)$  represents the combustion duration. The values of a and k represent adjustable constants (5 and 2 are typical values). The burn profile is engine-specific, and the constants a and k can be changed on a specific engine or application since the burn profile is engine-specific. The following equation is created by differentiating the ideal gas equation of state:

$$\frac{dp}{d\theta} = \left(-\frac{P}{V}\right) \left(\frac{dV}{d\theta}\right) + \left(\frac{P}{T}\right) \left(\frac{dT}{d\theta}\right)$$
(2)

In which the instantaneous quantities P, V, T, are modeled in relation to the crank angle of the engine. The first law of thermodynamics, which has the following formal formulation, may be implemented using the same procedure:

$$\Delta U = Q - W \tag{3}$$

Here Q represents the overall heat input into the system, W represents the work output from the system, and U represents the change in internal energy inside the system. Equation 4 may be produced by diffusing "Eq. (3)" [11]:

$$\frac{dU}{d\theta} = \left(\frac{dQ}{d\theta}\right) - \left(\frac{dW}{d\theta}\right) = mC_v \left(\frac{dT}{d\theta}\right) \tag{4}$$

Here Cv denotes the specific heat of the gas in the combustion chamber. The change in temperature as a function of crank angle is given by "Eq. (5)", which we get at by dividing the specific heat by the universal gas constant, utilizing  $\Pi$  (the combustion efficiency), and L.H.V. (the lower heating values of the provided fuel):

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$$\frac{dT}{d\theta} = T(\gamma - I) \left[ \left( \frac{I}{PV} \right) \left( \frac{dQ}{d\theta} \right) - \left( \frac{I}{V} \right) \left( \frac{dV}{d\theta} \right) \right]$$
(5)

The changing in pressure as a product of the crank angle may be determined using the heat input from the fuel. The definition of the fuel's heat input is [12]:

$$Q_{in} = \eta_{\rm c} \, . \, {\rm LHV}\left(\frac{l}{{\rm AF}_{\rm ac}}\right) \left(\frac{P}{RT}\right) {\rm V}_{\rm d}$$
 (6)

In which the actual air-fuel rate is  $Q_{in}$  in. The final definition of the pressure change would be:

$$\frac{dP}{d\theta} = \left(\frac{-\gamma P}{V}\right) \left(\frac{dV}{d\theta}\right) + \left(\frac{\gamma - I}{V}\right) Q_{in} \frac{dX_b}{d\theta} + (\gamma - I) \left(\frac{I}{V}\right) \left(\frac{dQ_w}{d\theta}\right)$$
(7)

"Eq. (7)" serves as the foundation for a numeric model that mimics engine performance.

#### 2.1 Modeling Engine Friction

The Several studies, notably Heywood [11] and Blair [13], have used general linear equations to forecast Friction mean effective pressure FMEP loses like a function of rpm. Although this approach only offers rough estimates of friction loses, it serves as a starting point for a numerical simulation. The following is Blair's equation for the linear FMEP loss:

$$FMEP = a + b(L)(RPM)$$
(8)

In which L represents the engine's stroke [m], rpm represents the engine speed [rev/min], while a and b represent constants that depend on the type of engine. According to the engine displacement, Blair has aspired to several variations of the FMEP loss equations for a sparkignition engine with simple internal bearings( $(V_d > 500 \text{ cm}^3)$  and  $(V_d < 500 \text{ cm}^3)$  respectively :

$$FMEP = 100000 + 350(L)(RPM)$$
 (8a)

 $FMEP = 100000 + 100(500 - V_d) + 350(L)(RPM)$  (8b)

The indicated, relative FMEP losses are given in [Pa] units.

#### 2.2 Burned and Unburned Areas

Assumptions must be made regarding the burned and unburned areas because this model ignores heat transmission between the burned and unburned zones and doesn't explore the geometric location of the flame front. The definitions of the unburned and burned zones are given in Rakopoulos and Michos' article [14]:

$$A_{u}(i) = A(i) \left( 1 - (X_{b}(i))^{\frac{1}{2}} \right)$$
(9)

$$A_{b}(i) = A(i) \left( \frac{X_{b}(i)}{(X_{b}(i))^{\frac{1}{2}}} \right)$$
(10)

The mass fraction burned like a function of crank angle gets denoted by Xb. The area of the cylinder that is now in touch with combustion chamber gases is known as A(i).

Although this technique ignores heat transmission between zones and presupposes a surface area of the cylinder head, it could be demonstrated to have physical consistency because the fractional heat transfer between the burned gas and the cylinder wall has always been greater in the burned region [18].

# 2.3 Burned, Unburned Mass, Volume, Temperature Calculations

The equation of state can be applied to the unburned and burned gas regions at any instant:

$$PV_b = m_b R_b T_b \tag{11a}$$

$$PV_u = m_u R_u T_u \tag{11b}$$

For the assumption of no mass loss from the combustion chamber, the total mass in the system at any stage can be expressed as:

$$m = m_b + m_u \tag{12}$$

The total volume at any stage

$$V = V_b + V_u \tag{13}$$

These are the main equations used; at any instant during combustion, there are seven unknown parameters to be solved ( $T_b$ ,  $T_u$ ,  $m_b$ ,  $m_u$ ,  $V_b$ ,  $V_u$ , P). In order to solve these parameters, an extra equation that specifies the burning rate is required. In the simple form of the model, the burning rate can be expressed by the exponential form of Wiebe function "Eq. (1)",

# 2.4 Heat Transfer Estimation

The main modes of heat transfer from each zone are convection and radiation, this heat is determined using relationships based on the work of Annand [15]. Nusselt and Reynolds number correlations for forced convection are:

$$Nu_i = 0.94 \ Re^{0.7}$$
 (14)

The coefficient of radiation heat transferring is calculated as:

$$hr = 4.25 * 10^{-9} * (\frac{T^4 - T_w^4}{T - T_w})$$
 (15)

Convective losses into the wall are calculated as a function of the crank angle as follows:

$$DQ_{I} = (hg(i) + hr(i))A_{b}(i)(T_{b}(i) - T_{w}) * \frac{60}{360 * RPM} + (hg(i) + hr(i))A_{u}(i)(T_{u}(i) - T_{w}) * \frac{60}{360 * RPM}$$
(16)

Calculates change in heat transfer (total) as A function of crank angle

$$DQ_2 = \eta^* m_f * \text{L.H.V} * Dx_i - DQ_1$$
(17)

### 2.5 Injector Calculations

Fuel velocity in model accounts as follows [16]:

$$U_{fuel} = \frac{C_{d}}{C_{a}} \sqrt{\frac{2^{*}(P_{inj}-P)^{*1000}}{\rho_{fuel}}} \left(\frac{m}{s}\right)$$
(18)

The following is accounted for by mass flow ratio in kilograms per millisecond:

$$\dot{m}_f = C_a A_{inj} \rho_f U_f (kg/s)$$
(19)

The following is how mass flow rate per crank angle unit is calculated:

$$\dot{m}_{CA} = \frac{holes * \dot{m}_f}{0.006 * N_s * MW_f} \left(\frac{\mathrm{kmol}}{\mathrm{deg}}\right) \tag{20}$$

Crank angle unit injection duration is calculated as follows:

$$dur_{CA} = \frac{m_f}{\dot{m}_{CA}} \text{ (deg)}$$

The following relationship is accounted for by the pressure injection for each time step:

$$P_{inj} = P_{injmin} + \left(\frac{P_{injmax} - P_{injmin}}{dur_{CA}}\right) * \theta$$
(22)

Where,  $Pinj_{max}$  is maximum injection pressure,  $Pinj_{min}$  is minimum injection pressure, and  $\theta$  is crank angle.

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#### 2.6 Power, Torque, and Efficiency Calculations

The power is represented by the braking power Wb, and the engine torque  $\tau$ , represents the amount of work completed per unit revolution (radians) of the crank [12].

$$\dot{W}_b = 2\pi \tau N \tag{23}$$

The network transmitted from the gas to the piston throughout a cycle is the stated work  $W_i$ , that represents the integration of the pressure over the cylinder volume.

$$W_i = \int P dV \tag{24}$$

while the designated power  $W_i$ , for any engine using  $\eta_c$  cylinders, is

$$\dot{W}_i = \eta_c W_i N/2 \tag{25}$$

Mechanical efficiency  $\eta_m$  is determined by the braking power to indicate power rate:

$$\eta_m = \frac{\dot{W}_b}{W_i} \tag{26}$$

### 2.7 The Combustion Reaction (Equilibrium Equations) [17]

$$CaH_{b}O_{c}N_{d} + \frac{a_{s}}{\phi}(O_{2} + 3.76N_{2}) \rightarrow n_{1}CO_{2} + n_{2}H_{2}O + n_{3}N_{2} + n_{4}O_{2} + n_{5}CO + n_{6}H_{2} + n_{7}H + n_{8}O + n_{9}OH + n_{10}NO$$
(27)

Where  $a_s$  and  $\phi$  are stoichiometric air--fuel ratio and equivalence ratio. The following four formulas are produced via atom balance:

C: 
$$a = (y_1 + y_5)N$$
  
H:  $b = (2y_2 + 2y_6 + y_7 + y_9)N$   
O:  $c + \frac{2a_s}{\phi} = (2y_1 + y_2 + 2y_4 + y_5 + y_8 + y_9 + y_{10})N$   
N:  $d + 7.52a_s/\phi = (2y_3 + y_{10})N$  (28)

where N stands for moles' total number. By definition, the mole fractions sum to 1:

$$\sum_{i=1}^{10} y_i = 1$$
 (29)

These equations define the following three constants:

$$d_1 = \frac{b}{a}$$
,  $d_2 = \frac{c}{a} + 2\frac{a_s}{\phi a}$ ,  $d_3 = \frac{d}{a} + \frac{7.52a_s}{\phi a}$  (30)

After some rearranging and replacement into the atom balancing equations, we have:

$$2y_{1}+2y_{6}+y_{7}+y_{9}+d_{1}y_{1}-d_{1}y_{5}=0$$

$$2y_{2}+y_{2}+2y_{4}+y_{5}+y_{8}+y_{9}+y_{10}-d_{2}y_{1}-d_{2}y_{5}=0$$

$$2y_{3}+y_{10}-d_{3}y_{1}-d_{3}y_{5}=0$$

$$\sum y_{i}=1$$
(31)

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Six gas-phase equilibrium processes are now shown. Such reactions result in the creation of OH and NO as well as the dissociating of hydrogen, oxygen, water, and carbon dioxide:

$$\frac{1}{2}H_{2} \rightleftharpoons H \quad K_{1} = \frac{y_{7}P^{\frac{1}{2}}}{y_{6}^{\frac{1}{2}}}$$

$$\frac{1}{2}O_{2} \rightleftharpoons O \qquad K_{2} = \frac{y_{8}P^{\frac{1}{2}}}{y_{4}^{\frac{1}{2}}}$$

$$\frac{1}{2}H_{2} + \frac{1}{2}O_{2} \rightleftharpoons OH \qquad K_{3} = \frac{y_{9}}{y_{4}^{\frac{1}{2}}y_{6}^{\frac{1}{2}}}$$

$$\frac{1}{2}O_{2} + \frac{1}{2}N_{2} \rightleftharpoons NO \qquad K_{4} = \frac{y_{10}}{y_{4}^{\frac{1}{2}}y_{5}^{\frac{1}{2}}}$$

$$H_{2} + \frac{1}{2}O_{2} \rightleftharpoons H_{2}O \qquad K_{5} = \frac{y_{2}}{y_{4}^{\frac{1}{2}}y_{6}P^{\frac{1}{2}}}$$

$$CO + \frac{1}{2}O_{2} \rightleftharpoons CO2 \qquad K_{6} = \frac{y_{1}}{y_{4}^{\frac{1}{2}}y_{5}P^{\frac{1}{2}}}$$

$$\log_{10} K_i(T) = A_i \ln \left(\frac{T}{1000}\right) + \frac{B_i}{T} + C_i + D_i T + E_i T^2$$
(33)

(32)

Where T is the temperature kelvin, in and  $(A_i, B_i, C_i, D_i, E_i)$  are the curve-fitting equilibrium constants. The unburned and burned mixed zones are regarded as independent open systems according to thermal characteristics. The atom balance equations are changed to correspond to six separate equilibrium the reacting equations, resulting in four equations with four unknowns  $(y_3, y_4, y_5, y_6)$ . Such four equations have numerical solutions.

# 2.8 Variable Specific Heats Ratio Model

For combustion processes including iso-octane and other fuels, Krieger and Borman created this polynomial approach in 1966 [19]. The Krieger and Borman technique simulates changes in internal energy by using "correction factors" for ideal gas constants that correlate to temperature variations (based on a given reference temperature). Using this

approach and the related polynomials, it is possible to derive the exact heats rate as a temperature function.

### 3. MATLAB Model

Figure 3 illustrates the flow chart of the model's mathematical formulation. Sub-models are created by the primary model to carry out certain tasks. The mathematical model's structure is as follows,

The piston's isentropic compressing and expanding in the cylinder are simulated by the isentropic sub-model. This model calculates the thermodynamic properties of cylinder in each step, which is theta equal 1 of crank angle degree, in piston movement according to the isentropic relation and by employing the engine geometry relations.

### 3.1 Injection sub-model

It replicates the processes of fuel injection and association, such as combustion, heat release, and heat transfer. This model, which is regarded as the most significant model, includes a number of sub-models for the injector, fuel characteristics, heat releasing and transmission, and ignition delay.

# 3.2 Equilibrium Sub-Model

In this model, the mole fraction of the combustion products and their specifications are calculated. The general algorithm of this model is shown in figure 4. The equilibrium model comprises several sub-models, such as minimum step *fmin* sub-model, guess sub-model, newton sub-model, and line search sub-model.





Figure.4 Algorithm of Equilibrium Model.

### 4. Results and Discussion 4.1Validation of the Matlab Model

Figure 5 shows the comparison of in-cylinder pressures obtained from the present Matlab Model and CFD simulation results of [Reddy A. et al., 9] for holes number 8 and compression ratio 9.3. From Figure 3, It can be observed that, there is a reasonably good agreement among the results. Therefore, the models used in this Matlab Model are working well and therefore they can be used with confidence for further study.



Figure 5. Comparison of in-cylinder pressures.

### 4.2 Variation of Orifice Diameter

The mathematical model for a GDI engine at (3000 rpm and 40 MPa injection pressure and compression ratio 9.5 spark timing 145°) is shown in Figure 6 the influence of nozzle hole diameter on the variation of cylinder pressure with crank angle. Increasing the hole diameter led to increase the cylinder pressure, as it can be observed. The maximum value of in-cylinder pressure is at the nozzle hole with a diameter of 0.650 mm due to due to the increase in injection area, which led to an increasing within fuel mass flow rate and quantity of heat release.



Figure 6. Cylinder pressure for different hole diameters.

The impact of nozzle hole diameter on the changing burned and unburned gas temperatures with crank angle is shown in figure 7. Although the impact of hole width on unburned gas temperature is minimal, it has a significant influence on burned temperature. By increased the diameter of the nozzle as it can be noticed, the burned gas temperature also increased. The 0.650 mm diameter nozzle hole produced a greater in-cylinder gas temperature due to the increased injection area, increased fuel mass flow rate, and increased heat release.



Figure 7. burned and unburned gas temperature for different hole diameters.

Figures 8 and 9 depict the impact of hole diameter on engine power and heat transfer as a function of crank angle. By increment the diameter of the nozzle as it can be observed, the engine power and heat transfer also increase because of the increased gas pressure brought on by an increase in the injection area, which leads to increase the fuel mass flow rate and heat release.





Figure 9. Heat transfer for different hole diameters.

Figure 10 shows CO emissions, as a function of crank angle at various fuel injector nozzle-hole sizes. These emissions of CO rise as the diameter of the nozzle hole increases. This is due to the fact that local rich zones begin to form as the injection area and fuel mass flow rate increase.





Figures 12 and 13 demonstrate the greatest power per cycle and optimal nozzle diameter vs. engine compression ratio as the number of holes is varied. It was shown that the greatest engine power per cycle was attained when the nozzle diameter (0.630 mm) and compression ratio (11) with (6) holes number were used.



Figure 12. Maximum power for nozzle diameter variation for different compression ratio & holes number.



Figure 13. Nozzle diameter variation give maximum power for different compression ratio & holes number.

# 4.3 Variation of Orifice Diameter with Rotation Engine Speed.

Data in the table 1 show the influence of the variation of nozzle hole diameter on the maximum values for temperature, pressure, power, heat transfer and emissions. The mathematical model for a GDI engine at (Rotation Engine speed of 1000, 2000, 3000, 4000, 5000 rpm ,35 MPa injection pressure, compression ratio of 11.5, and spark timing of 140°). The highest of maximum values of temperature, pressure, and emissions were at a 1000 rpm and diameter of 0.650 mm. The highest values for maximum power at 4000 rpm and nozzle diameter of 0.650 mm, while the highest maximum values for heat transfer are at 5000 rpm and diameter of 0.65mm.

#### 4.4 Variation of the Number of Nozzle Holes

Figure 14 shows the effect of injector holes' number on the variation in-cylinder pressure with crank angle as determined by the mathematical model for the GDI engine at (3000 rpm, 40 MPa injection pressure, compression ratio 9.5, and spark timing 145°) by using the MATLAB software. Because of the regular distribution of equivalence ratios throughout the spark plug area, it is observed that when the fuel injector holes' number rises, the in-cylinder pressure also rises. This is due to the creation of excellent fuel droplets with an increasing within the fuel injector holes number.

Figure 15 depicts the influence of hole number on burned and unburned gas temperatures as a function of crank angle. The influence of hole number on unburned temperature is minimal, whereas the hole number influence upon burned gas temperature is significant. By increased the injector holes number as it can be noticed, the burned gas temperature also increased. and highest gas temperature among the others at (12) nozzle holes number.



Figure 14. Cylinder pressure for different holes number.



Figure15. Burned and unburned gas temperature for different holes number.

Table 1. Variation of Maximum Values of Operating Engine Parameters with Nozzle Diameter.

Tempera	Speed (rpm)					
D(mm)	1000	2000	3000	4000	5000	
0.25	1767	1789	1536	1356	1124	
0.35	1916	1921	1754	1527	1343	
0.45	2467	2671	2224	1734	1542	
0.55	2976	2987	2685	2223	1936	
0.65	3187	3165	3013	2775	2430	

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(IZ)

Pressure (kPa)						
Speed (rpm)						
D(mm)	1000	2000	3000	4000	5000	
0.25	5284	4471	3852	3541	3354	
0.35	7331	6300	5088	4474	4103	
0.45	8974	7724	6729	5715	5102	
0.55	9750	8654	7773	6563	6028	
0.65	10674	9476	8537	7663	6940	
Power (k	(W)					
		Sp	eed (rpm)			
D(mm)	1000	2000	3000	4000	5000	
0.25	2.261	1.807	1.183	0.5134	0.3456	
0.35	4.918	5.051	4.639	4.095	3.492	
0.45	7.667	9.19	9.118	8.767	8.296	
0.55	11.48	13.34	14.56	14.48	14.19	
0.65	11.35	20.92	21.38	24.84	21.16	
Heat tran	sfer (kW)					
	Speed (rpm)					
D(mm)	1000	2000	3000	4000	5000	
0.25	8.643	8.991	9.352	9.793	10.04	
0.35	17	17.35	17.42	17.8	18.39	
0.45	27.79	28.8	29.05	30.16	30.97	
0.55	37.54	42.85	43.53	44.79	45.93	
0.65	52.36	59.07	60.72	61.17	63.56	

Mole fraction of CO (Xi)							
Speed (rpm)							
D(mm)	1000	2000	3000	4000	5000		
0.25	6.1 e-04	2.3 e-07	1.47e-06	1.8 e-6	7.53e-07		
0.35	0.02874	6.24 e-04	3.47e-05	6.33 e-06	8.53e-06		
0.45	0.07289	0.01387	0.00132	1.83 e-07	3.63e-05		
0.55	0.08544	0.053	0.01437	0.002918	0.00068		
0.65	0.1582	0.07495	0.05509	0.03227	0.00592		
Mole fra	Mole fraction of NO(Xi)						
		Spee	ed (rpm)				
D(mm)	1000	2000	3000	4000	5000		
0.25	0.00021	3.61 e-06	7.74e-06	4.79e-07	4.49e-07		
0.35	0.00989	0.000222	1.37e-05	3.88e-06	3.88e-06		
0.45	0.02439	0.004718	0.00046	6.79E-05	1.44e-05		
0.55	0.03021	0.01895	0.00489	0.001002	0.00024		
0.65	0.03976	0.0258	0.02021	0.01134	0.00201		

Figures 16 and 17 demonstrate impact of nozzle hole number on engine power and heat transfer as a function of crank angle. we can notice as the number of holes rise, so does engine power and heat transfer. This is due to increase in-cylinder pressures, as well as better atomization and a faster heat transfer rate.



Figure.16. Engine power for different holes numbers.

The CO emissions are shown in Figure 18 at different fuel injector nozzle-hole numeral as a function of the crank angle. We can see that as the of nozzle-holes increase, so do the amount of CO emissions. This is because increased injection area and subsequent rise in fuel mass flow rate that result in local rich zones and dissociation of combustion products at high temperatures.





Figure 18. Effect of holes number on emissions of CO.

Figure 19 explain NO emissions as a function of crank at various fuel injector nozzle-hole numeral. We can observe that NO emissions increase with increase in nozzle holes number. This is because the generation of NO is known to be significantly influenced by the thermal NO mechanism, which is extremely dependent on the temperature and the environment inside the cylinder. Higher numbers of nozzle holes result rich mixture zone and then higher in-cylinder temperature.



Figures (20) and (21) show the maximum power per cycle and the ideal number of nozzle holes in relation to engine compression ratio and nozzle diameter change. Figure 18 shows that the highest power per cycle generated at nozzle diameter (0.450 mm), the number of holes is (14) and the compression ratio is (12).



Figure 20. Maximum power for holes number variation for different compression ratio & nozzle diameter.



Figure 21. Holes number variation give maximum power for different compression ratio & Nozzle diameter.

4.5 Variation of the Number of Nozzle Holes with Rotation Engine Speed.

Data in the table 2 show the influence of the variation of nozzle diameter number on the maximum values for temperature, pressure, power, heat transfer and emissions. for the mathematical model for a GDI engine at (Rotation Engine speed of 1000, 2000, 3000, 4000, 5000 rpm ,35 MPa injection pressure, compression ratio of 11.5, and spark timing of 140°). The highest of maximum values of temperature, pressure, and emissions were at a rotation engine speed of 1000, and (12) holes. The highest values for maximum power at 4000 rpm and (12) holes, while the highest maximum values for heat transfer are at 5000 rpm and (12) holes.

### 5. Conclusion

A 4-stroke cycle of a gasoline direct injection engine was mathematically modeled. The mathematical model may be used to analyze the emissions of pollutants from a gasoline direct injection engine as well as its performance. Modeling the combustion with various nozzle hole diameters and numbers was done using the MATLAB algorithm. The following are the key findings from the current investigation.

- Cylinder pressure and temperature were observed to rise as nozzle hole diameter increased, as did maximum peak pressure and burned temperature when nozzle hole diameter was 0.650mm.
- Engine power and heat transfer increased as nozzle hole diameter increased, with a maximum value when nozzle hole diameter was 0.650mm.
- The lowest value of nozzle hole diameter, 0.250mm, was found to have the lowest CO and NO emissions.

Temperatur	e(K)				
		Spe	eed (rpm)		
holes	1000	2000	3000	4000	5000
4	2203	2040	1825	1559	1367
6	2653	2506	2361	1970	1728
8	3087	2984	2883	2372	2057
10	3156	3080	2929	2759	2381
12	3347	3230	3189	3019	2693
Pressure (kl	Pa)				
		Spe	eed (rpm)		
holes	1000	2000	3000	4000	5000
4	7954	7643	5997	5161	4656
6	8198	7892	7704	6453	5695
8	8973	8763	8460	7742	6734
10	9983	9958	9763	9014	7770
12	11019	10943	9987	9597	8805
Power (kW	/)				
		S	Speed (rpm)		
Speed rpm/holes	1000	2000	3000	4000	5000
4	7.736	6.364	6.132	5.691	5.16
6	9.133	7.364	11.73	12.5	13.12
8	11.57	14.95	16.53	16.23	17
10	11.3	26.92	20.3	20.93	16
12	10.7	21.58	24.63	45.01	25.62

Table 2. Variation of Maximum Values Operating Engine Parameters s with Nozzle Holes Number.

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Heat transf	er (kW)				
		Speed	d (rpm)		
Speed rpm/holes	1000	2000	3000	4000	5000
4	22.97	23.69	24.86	25.91	27.92
6	33.82	35.59	36.95	38.13	38.22
8	44.99	47.35	49.99	50.31	51.49
10	51.42	58.12	59.54	61.47	63.73
12	58.53	70.01	72	74.72	75.95
Mole fracti	on of CO (2	Ki)			
		Speed	d (rpm)		
Speed rpm/holes	1000	2000	3000	4000	5000
4	0.06334	0.004746	0.000341	4.32e-05	8.53e-06
6	0.07814	0.03322	0.005082	0.000828	0.000175
8	0.08852	0.06363	0.02332	0.005306	0.001334
10	0.09082	0.07345	0.09452	0.01744	0.005479
12	0.1049	0.07875	0.06435	0.03249	0.01471
Mole fractio	on of NO (X	(i)			
		Speed	l (rpm)		
Speed rpm/holes	1000	2000	3000	4000	5000
4	0.02345	0.001616	0.000124	1.69e-05	8.74e-06
6	0.02549	0.01172	0.001729	0.000292	6.5e-05
8	0.02768	0.02338	0.008061	0.001807	0.000465
10	0.03028	0.02504	0.009561	0.005969	0.001865
12	0.3568	0.0258	0.01872	0.01114	0.005018
- When using a nozzle diameter of 0.630 mm and a compression ratio of 11, with nozzle holes ranging from 6 to 12, the maximum power per cycle for the engine was obtained.
- The cylinder pressure and temperature were observed to rise as the number of nozzle holes increased, with 12 nozzle holes producing the highest peak pressure and burned temperature.
- By increasing the number of nozzle holes, up to a maximum of 12, engine power and heat transfer increased.
- With lowest nozzle holes number (four nozzle holes) it was found that CO and NO emissions were the lowest.
- Maximum power per cycle (0.450 mm) and the ideal number of nozzle holes in relation to engine compression ratio with respect to nozzle diameter variation were found to be (14) for nozzle holes and (12) for compression ratio, respectively.
- The highest of maximum values of temperature, pressure, and emissions were at a speed of 1000, and nozzle diameter of 0.650 mm, and (12) holes. The highest values for maximum power at 4000 rpm and nozzle diameter of 0.650 mm and (12) holes, while the highest maximum values for heat transfer are at 5000 rpm, a diameter of 0.65mm and (12) holes.

From the conclusions above, injector parameters (nozzle diameter & holes number) it plays an important role in engine performance and emissions. Knowing the optimal injector parameters and its effect with other parameters on engine performance is necessary. Accordingly, fuel injector must be designed for best engine operation and emissions as low as possible. Therefore, in the future, it is necessary to know the effect of the rest of the parameters, such as fuel injection pressure, engine load, and engine geometry etc., with injector parameters on the performance and emissions of the GDI engine.

# Acknowledgements:

The authors are grateful for the assistance they received from the staff at the Mechanical Department of the University of Technology-Iraq.

Nomenclature					
$a_s$	airfuel ratio	Unit less			
$A_{inj}$	Orifice Area	m <sup>2</sup>			
$A_u$	unburned area	m <sup>2</sup>			
$A_b$	Burnt area	m <sup>2</sup>			
Cv	specific heat	kJ/kg.k			
$C_d$	Discharge Coefficient	Unit less			
Ca	Area Contraction Coefficient	Unit less			
(CR)	compression ratio	Unit less			
$DQ_1$	Convective losses	kW			
$DQ_2$	change in heat transfer	KW			
$dur_{CA}$	Injection Duration	degree			
FMEP	Friction mean effective	Pa			
	pressure				
hr	radiation heat coefficient	W/m <sup>2</sup> .K			
Н	Heat transfer coefficient	W/m <sup>2</sup> .K			
L	engine's stroke	m			

LH V	lower heating values of the provided fuel	kJ/kg	
m ṁ <sub>f</sub>	mass Fuel flow rate	Kg kmol/s	
$\dot{m}_{CA}$	Fuel flow rate		kmol/deg
$MW_f$	Molecular weight		kmol/kg
Ns	Rotation Engine Velocity		rpm
Nu <sub>i</sub>	Nusselt number		Unit less
Р	Pressure		kPs
$P_{inj}$	Injection Pressure		kPa
Pinjmax	Maximum Injection Pressu	re	kPa
Pinjmin	Minimum Injection Pressur	kPa	
Q	overall energy input into th	e	kJ
	system		
$U_{fuel}$	Fuel velocity		m/s
$\Delta U$	changing within internal	kJ	
	energy		
R	Gas constant	kJ/	kg.k
Re	Reynolds number	Un	it less
Т	Temperature	K	
Tw	Wall temperature	K	
V	Volume	m <sup>3</sup>	
$V_d$	Displaced Volume of Engine	m <sup>3</sup>	
W	work output from the system	kJ	
$\dot{W_b}$	Brake power	kW	7
Wi	Work	kJ	
Ŵ,	indicate power	kW	7
Xb	mass fraction	Un	it less

Greek Sy	ymbols	
η	combusting efficiency	Unit less
$\eta_m$	Mechanic efficiency	Unit less
τ	torque	N.m
γ	Gas index	Unit less
θ	crank angle.	degree
0 (i)	immediate crank angle	degree
θ(o)	spark angle at the beginning	degree
	of combustion	
<del>O</del> (b)	the burn length	degree
$\phi$	equivalence ratio	
$\rho_{fuel}$	Fuel Density	kg/m <sup>3</sup>
Subscrip	ots	
В	burn	
U	unburned	

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# **Computational Fluid Dynamics Analysis of a Solar Dryer with** Various Phase Change Materials

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# ABSTRACT

A phase change material (PCM) is an organic (or inorganic) chemical that may store and release thermal energy in latent form as it changes physical states. This investigation aims to see how phase transition materials influence the thermal efficiency of the solar dryer. For the performance analysis, three PCMs were used: paraffin wax, lauric acid, and palmitic acid. As drying material, 5 mm thick potato slices were employed. According to the computational results, the total input thermal energy for the dryer for paraffin wax, lauric acid, and palmitic acid was about 17.36 MJ, 18.46 MJ, and 17.76 MJ, respectively, for 2 kg drying mass. When paraffin wax, lauric acid, and palmitic acid were utilized, the overall efficiency of the dryer increased by about 87%, 40.2%, and 12.4%, respectively, compared to the conventional dryer. By comparing the results of simulations and predictions, it is concluded that paraffin wax is the best-performing PCM for solar dryers as the energy storage material.

*Keywords:* Computational fluid dynamics; heat transfer; lauric acid; palmitic acid; paraffin wax; phase change materials.

### Introduction

Since ages, food and agricultural harvests have been dried under the sun. On the other side, this procedure is troubled with issues, such as items hampered by weather conditions, including rain, wind, humidity, birds and dust. Besides this, the method is labor-intensive, time-consuming, and necessitates extensive product dispersion to dry. The alternative ways of drying those products using heat from electricity or burning biomass are expensive and not environmentally friendly. In this situation, solar drying can be applied. Small food processing businesses may employ solar dryer technology to create nutritious, premium food products. As per National Horticulture Database (3rd Advance Estimates) published by National Horticulture Board, during 2021-22, India produced 107.24 million metric tons of fruits and 204.84 million metric tons of vegetables [1-3].

Significant moisture levels may be found in various fruits and vegetables. The food sector uses hightech drying apparatus, including ice cream, drum, and steam dryers, which control the market for food goods. Such dryers have a high market value. Thus, only substantial businesses can afford them. Most small-scale grocery businesses that work with the farmer cannot pay for the pricing owing to the hefty start-up expenses. As a result, such companies and farmers have started to favor low-cost and simple drying solutions. For thousands of years, farming and other foodstuffs have been dried in sunlight & air outside. In several developing nations, solar dryers are one of the most effective and efficient methods to use energy from the sun for drying and space heating. Solar dryers in emerging markets are widelyused for drying tobacco, tea, jaggery, coffee, grammes, grapes and spices [4-6].

Herbal and spice products are commonly dried in several South East Asian nations. However, because of weather circumstances, the application of sunlight for drying is restricted owing to loss due to the body's reaction on unpredictable wet days. It has been found that prolonged contact of agricultural goods with the sunlight on hot days might cause hardening. Hardening occurs without the use of crop goods. It traps humidity within the exterior layer, causing crops to be spoiled. For these reasons, solar drying emerges as a novel method for its preservation [7-9].

## 2. Literature Review

Lower thermal efficiency is the primary reason behind the unpopularity of solar drying in society. Hence, some arrangement is necessary to improve the solar dryer's thermal performance. Therefore, a literature review was conducted to understand methods for improving the thermal efficiency of solar dryers.

Hii et al., [1] showed that solar drying (placing the crops beneath direct sunlight) was feasible; however, the product obtained was of inferior quality due to contamination because of dirt, bugs, winged animals, dogs, and even precipitation. Furthermore, direct exposure to bright beams caused a depletion of vitamins and nutrients, dietary supplements, and have taken a long time to dry out.

Umogbai et al., [2] investigated the difference between solar drying and sunlight-based drying. They discovered that sunlight-based dryers produce greater temperatures, lesser relative humidity, less product wetness, and lesser



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degradation throughout the drying process. Rajeshwari and Ramalingam [10] showed that when sunoriented dryers were used instead of outdoor drying, drying time was reduced by roughly 20%, while the dried products were of a more excellent standard.

Some of the publications on tunnel dryers, halfway and half dryers and even, vertical dryers, multiplepass dryers, and dynamically detached dryers are all investigated in various sizes and designs. They came up with common conclusions that their systems were energy efficient and will effective for drying applications [11-18].

The effectiveness of an indirectly conduction-driven solar chilly dryer paired with a thermal storage material was constructed by Megha S. Sontakke and Sanjay P. Salve [19]. The chilies were dried in the bottom and upper containers, ranging from a starting humidity level of 72.8% to ending humidity levels of 9.2% and 9.7% (wet premise), respectively.

Toshniwal et al., [20] demonstrated the design and construction of a direct natural convection sun drier for drying tapioca in remote places. The study showed that an entire batch of 100 kg of cassava had been dried in 20 hours (2-day drying cycle), which requires a solar panel with a minimum size of 7.56 m2. Seemingly, 79% and 10% moist basis were the first and ultimate moisture content rates. Given a peak everyday total radiation level from the sun on the ground's surface of 13 MJ/m2/day, the typical surroundings are 320C air temperature and 74% relative humidity [21-22].

The primary goal of the current research is to maximize the efficiency of the solar dryer during offsunshine hoursUsing ANSYS flow simulation software, every aspect of assessment was completed.

The novelty of this research is that PCM tubes were kept horizontally at the bottom of the absorber copper plate instead of vertically at the top of the absorber copper plate, which was generally found in the literature.

# 3. Methodology

The various steps used to conduct the analysis were as follows:

a) Design of solar dryer equipped with PCM.

b) Finalize the dimensions.

c) Drawing in Catia V5 software.

d) CFD simulations

e) Analyzing the results.

SolidWorks flow simulation V-2020 was used to analyses the solar dryer. The computations were necessary to design the model to investigate the interaction of liquids and gases with the surfaces determined by boundary conditions. Software enhanced the precision and speed of complicated modelling situations, including turbulent flows, as the result of continuing studies.

## 3.1 Design Model

SolidWorks structures from the analysis system have been selected; then, the properties of the materials have been added from engineering data or material library. The material chosen for analysis was copper plate mounted on mild steel as the base part, clear glass, which produced a greenhouse effect and paraffin wax, lauric acid and palmitic acid for energy storage. The 3-dimensional sketch was designed in geometry and open design modeler. Figure 1 shows the 3D structure of a solar dryer.

A CAD model based on the phase change characteristics of several materials was developed to conduct a CFD analysis of the solar dryer. The solar dryer has two parts, mainly duct and drying cabinet. The air channel consists of glass, copper absorber plate and copper tubes filled with PCM. On the other hand, the drying cabinet where materials to be dried located, consists of shelves and exhaust fan used to intake the air from the atmosphere through the duct channel and the drying cabinet.

The function of air heaters is to heat the air. Therefore, the hot air from the atmosphere enters the duct bottom area, which releases heat to the PCM tubes and furthers the air exhaust through the drying cabinet. Hence, in this way, PCM materials store heat from the hot air and release it during offsunshine hours for drying. Palmitic acid, lauric acid, and paraffin wax were the investigated materials. They were placed in copper tubes on the underside of the absorber copper plate.

Properties of several materials used in the construction of solar dryer are depicted in Table 1.

The absorber tubes have been modelled for the material's types and boundary conditions. According to the fluid condition (hydraulic diameter and fluid velocity), turbulence conditions are applied for investigation. The mesh size in this analysis is kept at standard state. The properties of PCMs used are listed in Table 2.

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Tuble 1. I	ropernes of	sona materiais	used in a solar aryer.
Material	Density (K a/m <sup>3</sup> )	Specific heat	Thermal conductivity
	(Kg/m <sup>-</sup> )	(J/KgK)	(W/mK)
Copper	8954	383	386
Mild Steel	7680	445	45
Glass	2500	670	0.7443

Table 1. Properties of solid materials used in a solar dryer.

	Therese also include		PCM Material			
SN	properties	Units	Palmitic Acid	Lauric Acid	Paraffin Wax	
1	Density	kg/m <sup>3</sup>	860	880	900	
2	Specific heat	kJ/kg K	2.4	2.3	2.5	
3	Thermal conductivity	W/m K	0.2	0.18	0.23	
4	Latent heat of fusion	kJ/kg	200	230	220	
5	Melting	°C	63	44	60	

Table 2. Characteristics of the specified materials.

As seen in Table 2, lauric acid has a higher latent heat of fusion than palmitic acid and paraffin wax. In contrast, paraffin wax has a far higher density, specific heat, and thermal conductivity.

#### **3.2 Boundary Conditions**

The air input velocity is 1 m/sec at the atmospheric temperature of  $25^{\circ}$ C; the solar irradiation intensity is observed to be 733 W/m2. The following Table 3 lists all boundary conditions.

Boundary conditions					
Solar Irradiation	W/m <sup>2</sup>	733			
Inlet air conditions:					
Temperature	°C	25			
Humidity	%	50			
Velocity	m/s	1			
Ambient material temp	°C	25			
Outlet air conditions					
Temperature	°C	52			
Humidity	%	76			
Pressure	bar	1.01325			

Table 3. Boundary conditions of the Model.

### 3.3 Heat Transfer Rate

In a given system, heat transfer is the movement of heat across the system's boundaries due to a temperature difference between the system and its surroundings. As a result, it is an indicator of the particle's kinetic energy when there is a difference in temperature between a hot and cold body (or bodies). For a particular system, the rate of heat transfer relies on the mass (m) of the system, the specific heat capacity  $\mathbb{O}$ , and the temperature differential ( $\Delta T$ ) between the hot and cold bodies. As a result, the sensible heat transfer equation is as follows:

$$Q = mc\Delta T$$
 (1)

However, the heat transfer rate is governed by the wellknown three modes of heat transfer. They are described as below:

i) Heat transfer by conduction is the process of transmitting energy from one medium particle to another when the particles are in touch with each other.

$$Q = \frac{kA(T_{hot} - T_{cold})}{d}$$
(2)

This is called Fourier's law of heat conduction.ii) Heat transfer by convection is described as the movement of fluid molecules from higher to lower temperature zones.

$$Q = hA(T_{hot} - T_{cold})$$
(3)

The equation 3 is called Newton's law of cooling.

iii) Heat transfer by radiation refers to thermal radiation. The emission of electromagnetic waves produces thermal radiation. These waves carry away the energy from the producing body. Radiation is transmitted via a vacuum or a transparent material, whether solid or liquid. Thermal radiation is caused by the random movement of molecules in materials. The movement of charged electrons and protons causes the emission of electromagnetic radiation.

$$Q = \epsilon \sigma A (T_{Hot}^4 - T_{Cold}^4) \qquad (4)$$

This equation is called Stefen Boltzmann's law.

#### 4. Results & Discussions

This section illustrates the computational results obtained and its consequences on the performance of solar dryer.4.1 Temperature Distribution for Different PCMFigures 2 (2a, 2b, 2c) and 3 (3a, 3b, 3c) show the temperature distribution of lauric acid, palmitic acid and paraffin wax in the duct area. Nevertheless, Figure 4 (4a, 4b, 4c) shows that the temperature distribution of paraffin wax in the drying cabinet is satisfactorily greater than lauric acid and palmitic acid, respectively, because paraffin wax has higher thermal conductivity and specific heat than the othertwo.

### 4.2 Air Flow Velocity Contours Inside Chambers

Figures 5 (5a, 5b, 5c) and 6 (6a, 6b, 6c) show the airflow velocity contours inside the whole system and only inside the drying cabinet. It illustrated that although the air flow velocity is constant for all the three cases; the outlet temperature of air coming from duct fitted with paraffin wax has highest temperature as compared to other PCMs. The reason behind this is the superior thermo-physical properties of paraffin wax.

### 4.3 Temperature Distribution of Air

Figure 7 shows that the air temperature distribution in the entire system is better in paraffin wax compared to lauric acid and palmitic acid because it has high density and high thermal conductivity compared to the other two.

## 4.4 Temperature Distribution of Air at Chamber

Temperature analysis of air on the fluid at the drying chamber for lauric acid was an average of 530C, while in the case of palmitic acid, it was 51.20C and for paraffin wax, it was 56.30C as shown in figure 8.4.5 Model AnalysisOverall airflow and temperature distribution results clearly show the results in comparison between all three materials for PCM during the experiment in the solar dryer in CFD. Air temperature at the exhaust surface is shown in





*(b)* 



Figure 2. Temperature distribution of Copper Plate of Solar Dryer (Top View) in (a) Palmitic acid, (b) Lauric acid, © Paraffin.

Figure 9., where the Y axis denotes the change in temperature at 0o C. In contrast, the X axis indicates lauric acid, paraffin wax and palmitic acid. It has been concluded that paraffin wax has a much better temperature rise, as shown in Figure 9.

Heat transfer rate from paraffin wax has higher ascompared to lauric acid and palmitic acid, respectively, shown in Figure 10.









Figure 4. Temperature distribution in drying cabinet in (a) lauric acid (b) palmitic acid (c) paraffin wax. The heat transfer rate observed during analysis is represented by the Figure 10. It shows that the heat transfer rate of the paraffin wax is 252W, much more significant than lauric acid having 225W and palmitic acid having 210W, since paraffin wax has higher thermal conductivity, specific heat and density.

### 5. Conclusion

The present research investigates the best-performing PCM for solar dryers and air heaters. The three distinct PCMs, palmitic acid, lauric acid and paraffin wax, were analyzed using the latest simulation technology. From this investigation, the following conclusions are drawn:According to the computational analysis, the dryer needed about 17.36 MJ, 18.46 MJ, and 17.76 MJ of heat energy to dry 2 kg of potatoes using paraffin wax, lauric acid, and palmitic acid.





Figure 5. Air flow velocity contours (Top View) in (a) palmitic acid, (b) lauric acid, (c) paraffin wax.





Figure 6. Air flow velocity contours inside the chamber for(a) palmitic acid, (b) lauric acid (c) paraffin wax

When paraffin wax, lauric acid, and palmitic acid were used, the dryer was 87%, 40.2%, and 12.4% more efficient than a traditional dryer. Paraffin wax absorbs and transmits heat faster than lauric acid and palmitic acid.

Hence, paraffin wax emerged as the best-performing phase change material for solar dryers as the energy storage system.

These research findings are helpful for researchers and industry personnel in designing effective heat storage systems to reduce heat loss from solar dryers and solar air heaters. In future, multi-objective optimization and thermoeconomic analysis will be required to estimate the precise quantity of PCM for further investigations.



Figure 7. Temperature distribution of air at chambers for lauric acid, palmitic acid and paraffin wax respectively in (a) palmitic acid, (b) lauric acid, (c) paraffin wax.





Figure 8. Temperature distribution of air (top view) in (a) palmitic acid, (b) lauric acid (c) paraffin wax.



Figure 2. Air Temperature at the exhaust surface of the drying cabinet.



Figure 3.Heat transfer rate for PCMs.

# Nomenclature

- A Surface area (m<sup>2</sup>)
- C Specific heat capacity (J/kg K)
- d Thickness of copper plate (m)
- h Heat transfer coefficient (W/m<sup>2</sup> K)
- k Thermal conductivity (W/m K)
- m Mass (kg)
- Q Heat transfer rate (W/m<sup>2</sup>)
- T Temperature (<sup>0</sup>C)
- Tcold (fluid) temperature (<sup>0</sup>C)
- Thot Hot (surface) temperature (°C)
- σ Stefan Boltzmann constant (W/m<sup>2</sup> K<sup>4</sup>)
- ∈ Emissivity

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# Use the Thermodynamic State Equations to Analyze the Nonideality of Gas Mixtures

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# ABSTRACT

The assessment of gas behavior in chemical engineering systems necessitates a profound understanding of thermodynamic principles that govern the interactions among the components within a given system. To this end, the deviation from ideality in a single gas or gas mixture is associated with the disparity between the actual behavior of the gas or gas mixture and the behavior anticipated by the ideal gas model. This study is aimed at scrutinizing the deviation from ideal behavior in a gas mixture composed of CH4 and CO2. The analysis employs the cubic equations of state: Van Der Waals, Soave-Redlich-Kwong, and generalized Virial equations, truncated to the third term. These equations are widely recognized for their utility in characterizing substance behavior under specific thermodynamic conditions. The investigation involves an evaluation of the mixture's behavior by assessing variations in compressibility factor concerning pressure, volume, and pressure, using a thermodynamic calculator at 296.15 K and 15 bar. The findings of this study reveal the prevalence of attractive intermolecular forces at higher pressures and repulsive interactions at lower pressures. An analogous examination of the effect of altering the composition of Ch4was undertaken using the Soave-Redlich-Kwong equation, which incorporates parameters allowing for an evaluation of the impact of molecule size and intermolecular interactions within the mixture. Furthermore, experimental data were employed to validate the results obtained in this study. Consequently, it can be inferred that these equations provide insight into the influence of pressure on molecular interaction forces, encompassing repulsive and attractive forces, which in turn can define the new volume of a real system. Thus, based on the corroboration established herein, these equations demonstrate a high degree of consistency and applicability, thereby expanding the realm of thermodynamic inquiry.

*Keywords:* Equation of state; real gas; ideal gas; compressibility factor.

### 1. Introduction

The instruction of Chemical Engineering is founded on the examination of predicting the thermodynamic properties of both pure substances and mixtures of components within a given phase, which play a crucial role in separation systems capable of achieving phase equilibrium. The majority of the properties under discussion here pertain to the behavior of pure components, disregarding molecular interaction forces among various constituents within a given mixture.

Furthermore, separation operations, notably distillation, absorption, and liquid-liquid extraction, entail mixing phases in equilibrium, with process performance heavily contingent on an understanding of the

thermodynamic interactions between these phases. In such cases, employing equations of state for ideal gases (of the cubic, Virial-type, or generalized variety) is a common practice to enhance comprehension of the thermodynamic relationships at play. These equations establish a connection between the compressibility factor (Z) of either a pure substance or mixture and macroscopic, measurable parameters—Pressure, Volume, and Temperature, commonly referred to as PVT.

As posited by Muachia et al. [1], the thermodynamic relationships associated with PVT provide the means to assess the thermodynamic behavior of systems, as they offer mechanisms for experimental determination that yield knowledge of various physical relationships linked to perturbations of each one. The authors contend that pressurized systems, characterized by elevated pressure levels, lead to a reduction in system volume, thereby intensifying molecular interactions and augmenting the attractive and repulsive forces between the system's molecules.

Consequently, an examination of thermodynamic systems should initially be grounded in an understanding of the behavior of an ideal gas—a theoretical gas characterized by the absence of intermolecular forces, where collisions are non-existent or negligible. These phenomena are rooted in the principles of conservation of momentum and kinetic energy [2].

To comprehensively determine the state of a system composed of a mixture of pure components, it is imperative to possess knowledge of the intensive variables, with particular emphasis on pressure (P), volume (V), and temperature (T), as well as an understanding of the composition of the constituent components of the mixture slated for separation. The relationships between these intensive properties remain constant within the system as long as the composition remains unaltered. These relationships are predicated on the connections between volume, pressure, and work, as established by the principles of the first law of thermodynamics.

However, it is important to note that the behavior of most gas mixtures deviates from ideality, primarily due to the diverse interactions occurring among their constituent molecules. Moreover, variations in the shapes and sizes of the molecules within the mixture can also exert influence on the non-ideal behavior observed in gas-liquid mixtures. In such cases, Mamedov et al. [3] posit that the ideal behavior of gases can be represented by Clapeyron's equation (Equation 1), which is grounded in the fundamental principles of physics and frequently applied to address a wide array of practical challenges, particularly in the domain of chemical engineering. Equation 1 establishes a direct correlation between its principal parameters, thus characterizing thermodynamic ideality.

# PV = nRT

# (1)

When analyzing the ideal gas equation (Equation 1), Costa [4] asserts that it describes a gas composed of numerous molecules represented as rigid spheres with a diameter 'd.' These molecules exhibit random or disordered motion, governed by Newton's Laws. The author further contends that these particles possess a non-zero mass 'm' while their individual volumes are negligible relative to the container's volume.

In this context, intermolecular interactions involving attraction and repulsion are considered negligible, except during collisions with each other and with the container walls. Within this analytical framework, it is evident that the internal energy of the involved molecules is associated with translational kinetic energy, which propagates in a linear fashion. Finally, according to Costa [4], the collisions among these molecules are perfectly elastic, as kinetic energy is not converted into other forms of energy.

In alignment with this analysis, Mahan & Myers [11] propose that the macroscopic properties of an ideal gas entail the independent motion of molecules, particularly evident when measurements of pressure, molar volume, and temperature deviate from the behavior described by the Clapeyron equation, which represents non-ideal behavior. Deviations from ideality are observed in pure gases and mixtures of unreacted gases. At room temperature and low pressures, deviations from ideality are nearly nonexistent. However, as pressure increases, gas behavior deviates from that of ideal gases.

Under known temperature and pressure conditions, a real or non-ideal gas comprises material particles engaged in chaotic motion, subject to forces of attraction and repulsion, with significant mass and volume [6].

To assess the PVT (Pressure-Volume-Temperature) behavior of real gases, cubic equations of state and generalized correlations are employed. These mathematical models account for intermolecular interactions and describe actual behavior across various pressure ranges. Notable among these equations of state are Van der Waals, RedlichKwong, and Soave-Redlich-Kwong, alongside the Pitzer and Virial correlations [7].

The fundamental premise underlying deviations from ideality is attributed to intermolecular forces, both attractive and repulsive, which exert a predominant influence on the PVT behavior of a given fluid (Equation 2).

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$$P = P_R + P_A$$
(2)

In this scenario, repulsive forces contribute positively to pressure (PR > 0), while attractive forces yield a negative contribution to pressure (PA < 0). Consequently, the cubic Van der Waals (VDW) equation of state alters the ideal gas equation by incorporating the intermolecular forces present in a specific gas or gas mixture. Equation (3) characterizes this approach, taking into account intermolecular interactions, albeit with certain limitations. Nonetheless, Equation (3) proves valuable for depicting the behavior of real gases under conditions closely approximating those of ideal gases [8].

$$P = \frac{RT}{V-b} - \frac{a}{V^2}$$
(3)

Equation (2) can be applied to compute the thermodynamic parameters for gas mixing, which entails the utilization of the mixing parameters am and bm, as detailed in Equation (3).

$$P = \frac{RT}{V - b_m} - \frac{a_m}{V^2}$$
(4)

Where P represents the pressure of the gas in atm, V is the molar volume of the gas in cm3/mol, T is the temperature of the system in Kelvin (K), and R is the universal gas constant. Additionally, am and bm are the Van der Waals constants, which are defined according to Equations 5, 6, 7, 8, and 9.

$$a = \frac{27(RT_c)^2}{64P_c}$$
(5)

$$b = \frac{RT_c}{8P_c}$$
(6)

$$\mathbf{a}_{\mathrm{m}} = \sum \sum \mathbf{y}_{\mathrm{i}} \mathbf{y}_{\mathrm{j}} \mathbf{a}_{\mathrm{ij}} \tag{7}$$

$$\mathbf{a}_{ij} = \left(\mathbf{a}_i \mathbf{a}_j\right)^{0,5} \tag{8}$$

$$\mathbf{b}_{\mathrm{m}} = \sum \mathbf{y}_{\mathrm{i}} \mathbf{b}_{\mathrm{i}} \tag{9}$$

In the collision of gas molecules with any surface, the unopposed attractive forces of the molecules diminish the collision velocity. The additional term incorporated into the pressure equation serves to rectify the absence of counterbalancing attractive forces.

Conversely, the equation put forth in 1972 by SoaveRedlich-Kwong (SRK) represents one of the most extensively employed equations of state for elucidating the characteristics of both pure substances and gas mixtures (Equation 10). It is distinguished as an extension of the Van der Waals equation [6].

$$P = \frac{RT}{V-b} - \frac{a}{V^2 + Vb}$$
(10)

The utilization of Equation (10) is expanded to compute the thermodynamic properties of gas mixtures, encompassing the incorporation of mixing parameters am and bm, as delineated by Equation (11).

$$P = \frac{RT}{V - b_m} - \frac{a_m}{V^2 + V b_m}$$
(11)

In this context, P represents the gas pressure (in atm), V stands for the molar volume of the gas (in cm3/mol), T denotes the system's temperature (in K), while R signifies the universal gas constant. Additionally, a and b represent the substance-specific constants, and  $\alpha$  serves as a temperature dependent correction factor, in accordance with the descriptions provided in Equations (12), (13), (14), (15), and (16).

$$a_{\rm m} = \alpha a_{\rm c} \tag{12}$$

$$a_{c} = \frac{0.42748(RT_{c})^{2}}{P_{c}}$$
(13)

$$\alpha = [1 + m(1 - T_r)^{0.5}]^2$$
(14)

$$m = 0,048508 + 1,55171w - 0,15613w^2$$
(15)

$$b = 0,008664 \frac{RT_c}{P_c}$$
(16)

For Van Wylen et al. [9], assessing the departure from gas ideality involves the computation of the compressibility factor. This thermodynamic property quantifies the deviation of real gas behavior from ideal gas behavior. It is defined as the ratio between the molar volumes of real and ideal gases under identical temperature and pressure conditions. A compressibility factor of 1 (one) indicates ideal gas behavior, while values different from 1(one) suggest non-ideal behavior.

Given the aforementioned complexity, numerous equations of state have been developed to study gas behavior. Prominent among these are the cubic equations, including Van Der Waals, Redlich-Kwong, and Soave-RedlichKwong, among others [10].

Notably, Pitzer's correlation stands out among various approaches. It expresses the compressibility factor (Z) as a function of temperature (Tr), reduced pressure (Pr), and the acentric factor (w) for each component.

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The generalized Pitzer correlation serves as an empirical model that aids in comprehending molecular interaction forces, particularly in solutions where interactions occur between molecules of different sizes. Kenneth Pitzer introduced this correlation [10], which or ionic interactions in solution using linear combinations of parameters in a Virial-type expansion of the excess Gibbs free energy.

Consequently, the virial-type equation with emphasis on the third coefficient is employed to calculate the compressibility factor, as defined in Equation (17).

$$Z = 1 + (B^{0} + wB^{1})\frac{P_{r}}{T_{r}} + (C^{0} + wC^{1})\frac{P_{r}^{2}}{T_{r}^{2}}$$
(17)

$$P_{\rm r} = \frac{P}{P_{\rm c}} \tag{18}$$

$$T_{\rm r} = \frac{T}{T_{\rm c}} \tag{19}$$

On the contrary, the generalized equation incorporates the acentric factor (w), a parameter inherent to the molecular structure of the gas, which exhibits a significant correlation with the system's pressure and temperature. This factor is also interconnected with the dimensions of the constituent molecules within the examined mixture [14]. All functionsherein are interdependent with the reduced pressure and temperature, as elucidated in Equations (20), (21), (22), and (23) [11].

$$B^{o} = 0,083 - \frac{0,422}{T^{1,6}}$$
(20)

$$B^1 = 0,139 - \frac{0,172}{T^{4,2}}$$
(21)

$$C^{o} = 0,01407 + \frac{0,02432}{T_{r}} - \frac{0,00313}{T^{10,5}}$$
(22)

$$C^{1} = -0.02676 + \frac{0.05539}{T_{r}^{2.7}} - \frac{0.00242}{T^{10.5}}$$
(23)

Based on the provided theoretical framework, a thermodynamic assessment was conducted to analyze the behavior of the compressibility factor as a function of gas mixture pressure consisting of carbon dioxide (CO2) and methane (Ch4). This investigation explored the influence of varying proportions of these gas components. The obtained results were evaluated within the context of attractive and repulsive forces under isothermal conditions, employing two distinct cubic equations of state and a generalized equation of state.

### 2. Procedure and Methodology

To carry out this study, a logical algorithm was developed for solving a sequence of equations essential for determining properties such as volume, compressibility factor, entropy, internal energy, enthalpy, Gibbs free energy, and Helmholtz free energy for a binary gas mixture. These calculations were performed under predefined conditions of temperature, composition, and pressure.

The algorithm incorporates a comprehensive database, facilitating the exploration of diverse gas mixtures with varying compositions and the assessment of concentration effects on the compressibility factor within a specified pressure range under isothermal conditions. Additionally, it permits an examination of the impacts of molecular size and attractive/repulsive forces on the behavior of the compressibility factor, irrespective of the equation of state or correlation utilized. Figure 1 illustrates the algorithm created.

For the implementation of this algorithm, a software program was developed using Microsoft Excel, creating a thermodynamic calculator with a user-friendly graphical interface. This interface enables adjustment of input parameters, evaluation of output conditions, and correlation of various types of equations of state, thereby enhancing comprehension of the parametric interactions involved in the evaluated cases.

The thermodynamic calculator investigated the cubic Van Der Waals equation, the Soave-Redlich-Kwong (SKW) equation of state and the generalized Virial-type equation truncated to its third term.

This exploration was conducted to assess the parametric attributes associated with each equation, elucidating the physical and molecular interactions within the system, and their impact on the mixing behavior.

### 2.1 Resolution Method

To derive the compressibility factor and molar volume using the cubic equations outlined in this study, the first step involved determining the constants 'a' and 'b' for each equation. These constants were calculated through the correlations provided by Equations (5), (6), (13), and (16), respectively, as specified in the Van der Waals and Soave Redlich-Kwong equations.



Figure 1. Proposed algorithm for determining the thermodynamic parameters of gas mixtures.

Subsequently, armed with the known operating conditions in terms of pressure (P) and temperature (T), the equations were restructured into a cubic equation format, with the molar volume (Vm) serving as the variable of interest.

Upon structuring the cubic equation, the Newton Raphson method was employed to ascertain the mixture's volume using the Taylor series expansion. In this context, the maximum volume identified corresponds to the volume of the gas under examination. This value was employed in determining the compressibility factor (Z), as supported by Equation (24).

$$Z = \frac{P}{V_m RT}$$

(24)

Maxwell's relations were employed to compute the energy variation within the system. This process entailed utilizing the definitions stemming from the equations of thefirst and second laws of thermodynamics. The outcomes obtained through these calculations provided valuable insights into the behavior of these parameters within the systems under investigation.

# 3. Results and Discussions

The thermodynamic calculator, developed in the context of this study, systematically investigates the parametric behavior of a mixture consisting of carbon dioxide (Co2) and methane (CH4) under the prescribed initial conditions, as detailed and specified in Table 1.

Components	Composition (%)	Temperature (K)	Pressure (Bar)	
CO <sub>2</sub>	68	206.15	15	
$CH_4$	32	296.15	15	

Table 1.  $CO_2$  and  $CH_4$  mixture conditions used in this article.

The algorithm proposed (Figure 1) served as a foundation for the development of the Thermodynamic Calculator (Figure 2), which was utilized for data input and solution display for the specified problem. Under the operational conditions employed, the molar volumes and compressibility factors were determined under the prescribed conditions.

Furthermore, the behavior of the compressibility factor was assessed over a predefined pressure range (0 to 1000 bar), utilizing the three aforementioned equations of state. The acquired data exhibited notable similarity, yielding an average compressibility factor of 0.944 for the three equations, resulting in an average deviation of merely 0.5% from this computed average.

An analysis of the compressibility factor profile indicated analogous qualitative patterns: attractive forces were substantial up to 500 bar, with repulsive forces assuming greater significance beyond this pressure range. Conversely, when employing the cubic Van der Waals equation of state, attractive forces exhibited reduced significance, while repulsive forces became more pronounced. This discrepancy can be attributed to the absence of parameters related to molecular size in the Van der Waals equation.

At lower pressures, molecules are generally distanced from one another in these scenarios, with negligible intermolecular forces at play, causing the fluid to behave akin to an ideal gas (Z=1). As pressure increases, molecules draw closer together, and attractive intermolecular forces dominate. Consequently, the gas's volume decreases more significantly than it would if no intermolecular attraction forces were present, resulting in Z < 1.

Conversely, at very high pressures, molecules approach each other to an extent where repulsive forces become dominant, causing a more substantial increase in volumethan expected in the absence of intermolecular repulsive forces, leading to Z > 1. While a value of Z=1 is attained at high pressures in all cases, it does not correspond to ideal gas behavior [9], [11], and [12].



Figure 2. Thermodynamic calculator interface.

The examination of the results presented in Figure 2 and Table 1 unveils a level of molecular disarray characterized by the entropy change ( $\Delta S$ ). This observed molecular disarray emanates from the reduced operational pressures and temperatures taken into account under the assessed operating conditions. These factors significantly impact the stochastic movement of the molecules. A similar pattern is discerned when analyzing the changes in internal energy ( $\Delta U$ ) and Helmholtz free energy ( $\Delta A$ ), both of which exhibit negative values, as recorded in Table 2, acquired at 296.15 K and 15

Table	2. Inermo	aynami	c energi	es evalu	iatea in	inis pa	per.
Equation	Temperature (K)	Pressure (Bar)	ΔS (J/mol.K)	ΔU (J/mol)	ΔH (J/mol)	∆G (J/mol)	ΔA (J/mol)
VDW	296.15	e 150	-4.81	-1432.64	1468.56	2901.2	-1545.81
SRK		13.0	-5.20	-1539.16	1583.21	3122.37	-1418.72

Table ? Thermachingmis energies 1 , 1. .1 .

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The analysis of enthalpy ( $\Delta$ H) and Gibbs Free Energy ( $\Delta$ G), which represent the energies associated with the system, provides insights into non-spontaneous processes. This analysis supports the molecular behavior of the system, which is influenced by both attractive and repulsive forces between the system molecules. It elucidates the disparities in values between the Van der Waals (VDW) and SoaveRedlich-Kwong (SRK) equations.

Numerical results derived from these equations reveal a deviation of approximately 7%. This deviation is noticeable when comparing data from these two equations, with the cubic Soave-Redlich-Kwong equation demonstrating greater accuracy. This enhanced accuracy is attributed to its consideration of the molecular size as a dominant factor in dictating the thermodynamic behavior of gas mixtures.

### 3.1. Non-ideality Analysis

The deviation from gas ideality can be observed through the analysis of the compressibility factor (Z), which is a dimensionless measure describing the behavior of a gas concerning its pressure and volume. According to Elechi et al. [9], when the compressibility factor (Z) deviates from the ideal gas standard, the gas or gas mixture exhibits non-ideal behavior.

Figure 3 illustrates the behavior of the compressibility factor (Z) as a function of pressure (P) for the cubic Van Der Waals, Soave-Redlich-Kwong, and generalized Virial-type truncated equations of state at a temperature of 296.15 K.



Figure 3. Behavior of the compressibility factor as a function of pressure mixture of 32% CH<sub>4</sub> and 68% CO<sub>2</sub>.

The operational conditions employed for the Z calculations (Figure 3) are elucidated within Table 1. The scrutiny of Figure 3 unveils that when subjected to elevated pressures, the methane (CH4) and carbon dioxide (CO2) gas amalgamation demonstrates non-ideal gas behavior, characterized by the preeminence of repulsive intermolecular forces.
Conversely, under reduced pressures, attractive forces hold sway, marked by their heightened efficacy in the intermolecular collisions between CH4 and CO2 molecules, manifesting as a counterintuitive phenomenon at lower pressures.

Furthermore, an examination was conducted to assess the pressure-volume relationship of the studied gas mixture. This analysis indicated that within the high-pressure regime, spanning from 600 to 1000 bar, negligible fluctuations in volume were observed with incremental pressure increments within the stipulated range. Conversely, a conspicuous volume fluctuation was noted within the pressure range of 0 to 300 bar. This phenomenon is attributable to the increased intermolecular spacing induced by compression, leading to pronounced volume alterations within the system. Notably, for all three equations of state examined, a confluence in volume behavior as a function of system pressure was ascertained across the considered pressure spectrum.



Figure 4. Volume profile as a function of pressure for a mixture of 32% CH<sub>4</sub> and 68% CO<sub>2</sub>.

Nevertheless, the ideal gas model exhibited more pronounced deviations within the pressure range of 100 to 400 bar, possibly owing to its inherent gas properties.Figure 4 presents an analysis of gas mixing, entailing the blending of two gases comprising 32% and 68% fractions of CH4 and CO2, respectively. These studies were conducted to gain deeper insights into the mixing phenomena across various compositional ratios.

# 3.2 Influence of Composition on the Compressibility Factor

For the analysis of the influence of the gas mixture composition, CH4 and CO2, data from the Soave-Redlich Kwong equation were utilized due to the qualitative similarity in the behavior of the three equations studied and the incorporation of the acentric factor into this correlation.

Thus, the effects of mixture concentration were investigated, with an examination of systems containing pure CH4 and the progressive increment of CO2, up to maximum CO2 purity. This analysis was conducted under isothermal conditions at 296.15K, as indicated in Figure 5.

In general, it is observed that the compressibility factor of pure CH4 is higher than that of pure CO2, indicating a greater prevalence of attractive forces in CO2 gas compared to CH4 gas.

Conversely, repulsion forces become more significant when analyzing the behavior of CH4 gas, predominating above 300 bars. This phenomenon is also noted for pure Co2gas at pressures exceeding 580 bars.

The 25% CH4 and 75% CO2 mixture exhibits a pronounced influence of attractive forces, surpassing the behavior observed when analyzing the compressibility factor of the individual components, prevailing up to a pressure of 530 bars.

Beyond this threshold, it is observed that this parameter behaves more prominently than that of pure CO2 but less so than pure CH4. The other curves obtained from this evaluation demonstrate mixing effects based on the proportions established in each analysis of this process.



Figure 5. Behavior of Z as a function of pressure for the mixture of  $CH_4$  and  $CO_2$ .

The evaluation depicted in Figure 5 illustrates the behavior of an ideal gas mixture comprising CO2 and CH4 at varying proportions as the system pressures approach zero. As pressure increases, the effects of attractive forces become increasingly apparent, irrespective of the gas fractions' composition within the mixture.

Conversely, when pressures exceed 400 bar, the influence of repulsive forces becomes dominant across all compositions considered and persists throughout the entire range of operating conditions investigated in this study. For all cases analyzed, a transition point is discernible, marking the shift from attraction to repulsion phenomena. This transition point is characterized by a calculated compressibility factor equal to 1 (one), indicating a departure from the conditions of an ideal

# 3.3 Validation of State Equations

The consistency of the data derived from the state equations employed in this study was validated through a comparison with experimental data obtained by Hwang et al. [13]. This comparison was conducted for two distinct cases, with a focus on the specific weight of the gas mixture. In the first case, the data was extracted from experiments conducted at a temperature of 225K, utilizing a mixture composed of 9.826% CO2 and 90.174% methane, respectively. In the second case, experiments were performed under different thermal conditions, specifically at 350K, while maintaining the same composition ratios for the components.

The results for the first case are presented in Figure 6, where a noteworthy approximation between the experimental data and the Soave-Redlich-Kwong (SRK) model data is observed, with an average deviation of 2.27%.

On the other hand, the comparison between experimental data and Van der Waals data in these analyses exhibited an average deviation of 11.59%. In this scenario, smaller deviations in specific mass values were observed for pressures exceeding 100 bar.

Regarding the data derived from the generalized Virialtype equation truncated to its third term (EEG), within the pressure range assessed in this study, the deviation was 10.68% when comparing experimental data with GEEderived data.



pressure for the mixture of  $CH_4$  and  $CO_2$  with 225 K.

In the second case, when comparing experimental data with state equation data at 350 K, a significant approximation was observed for all cases evaluated, as depicted in Figure 7. Nevertheless, the Van der Waals equation displayed an average deviation of 3.69%, whereas the Soave-Redlich Kwong (SRK) and EEG exhibited deviations of 1.78% and 1.74%, respectively.



Figure 7. Behavior of specific weight as a function of pressure for the mixture of  $CH_4$  and  $CO_2$  with 350 K.

The results presented in Figure 7 demonstrate a high degree of consistency when utilizing state equations to evaluate the thermodynamic profiles of gas mixtures, particularly when employing the SRK equation.

On the other hand, both the EEG and SRK equations rely on the acentric factor, a parameter associated with molecular size, as a crucial determinant for assessing the thermodynamic characteristics of gas mixtures.

# 4. Conclusions

Based on the results obtained in this study, the following conclusions can be drawn:

a) Real gases exhibit ideal gas behavior as system pressures approach zero.

b) The influence of gas mixtures can be assessed by examining the behavior of compressibility factors. These factors depend on the fractions of each component in the mixture and the specific type of gas involved in the process.

c) The equations of state analyzed in this study demonstrate compatibility with the analysis of gas mixing behavior. They account for both attractive and repulsive forces between constituent molecules within the system and consider the size of molecules as predominant factors influencing the thermodynamic behavior of gases.

d) The behavior of gases can be characterized by examining the relationship between pressure and

volume. Under high pressures, significant changes in system volume are not observed due to the strong interaction between system molecules, resulting in their close proximity and alterations in the system's physical state.

e) Experimental data corroborate the equations studied in this work, with the best consistency observed when employing the SRK equation within the evaluated temperature and pressure range.

f) At low pressures, the impact of pressure on the system's volume becomes significant, primarily due to the increased distance between constituent molecules within the system under investigation.

# Nomenclature:

P: pressure of the gas (bar); V: molar volume of the gas (cm3/mol); Vm: molar volume of the gas mixture (cm3/mol); T: temperature of the system (K); R: universal gas constant; am and bm: mixture constants of state equations; PA and PB: attractive and repulsive pressure; SRK: Soave-Redlich-Kwong cubic equation; VDW: Van Der Waals cubic equation; PC: critical pressure (Bar); TC: critical temperature (Kelvin); a and b: pure constants of state equations; W: acentric factor: Z: compressibility factor; Tr: reduced temperature; PVT: pressure, volume and temperature;  $\Delta S$ : variation of entropy (Joule/(mol K));  $\Delta U$ : variation of internal energy (Joule/mol);  $\Delta A$ : variation of Helmholtz free energy (Joule/mol);  $\Delta$ H: variation of enthalpy (Joule/mol);  $\Delta G$ : variation of Gibbs Free Energy (Joule/mol).

# Acknowledgements:

The authors of this paper express sincere appreciation for the collaboration of the Post-Graduation Coordination and the Undergraduate Coordination of the Chemical Engineering Program at ISPTEC for their unwavering dedication and support in the development of this research.

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