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CFD Modeling of Co-Gasification of Waste Tires Mixed with Indigenous Coal

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--ABSTRACT--

Co-gasification of coal and waste product is an excellent method to produce syngas. In the current study, co-gasification of the mixture of coal and waste tires were utilized as a source material for syngas production. These materials were selected due to the easy availability in the local region. Concentric tube entrained flow gasifier model was used for the gasification of source materials. The impact of kinetic and diffusion rates was investigated using Three-dimensional computational fluid dynamics model. The Euler–Lagrange technique was applied for the development of entrained flow Coal/Tire gasifier through Commercial computational fluid dynamics code ANSYS FLUENT VR 14. The movement of the particles was estimated using discrete phase model, moreover the gas phase was treated as the continuous phase with a standard k–e turbulent model to predict the behavior of gas phase flow. The homogenous and heterogeneous reaction rates calculations were predicted using Finite rate/Eddy dissipation model. Oxygen was used as a gasifying agent coal, tire and mixture of both materials with varying ratios were used as a feed stock. The results showed that syngas production efficiency was <36% in the case of pure coal and tire feedstock. Moreover, at 70% Coal and 30% Tire mixture the maximum syngas production efficiency was found to be 32.60%. The oxygen/carbon (O/C) ratio plays an important role in the co-gasification process. The O/C ratio above 0.8 favored combustion reactions and enhanced mole fraction of carbon dioxide (CO2) and in syngas composition. In contrast the co-gasification reactions became dominant below 1.2 O/C ratio, thereby resulting enhanced mole fraction of CO and H2 in syngas composition.

KEYWORDS: Computational fluid Dynamics, co-gasification, entrained flow gasifier, syngas

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I. INTRODUCTION

During last few decades the Fossil fuels remained the primary source of energy among the developed and developing countries. It is estimated that, the world natural gas and oils reservoirs will no longer be available in next 40–50 years[1]. Whereas, the coal reserves found around the world higher than oil and gas, which are predicted to be remain more than one decade. In addition, the use of coal for energy production has risen serious health and environmental concern due to the emission of the carbon dioxide, SO_x, and NO_x. Thus, due to these reasons it is essential to develop a method to effectively use the coal. Further coal, waste tire could also be utilized for energy production[2,3]. It is estimated that about 1.5 billion tires globally produced every year, which is projected to be increased to 4 billion per year. A recent study assessed that waste tires are being used in different application such as fuel 52%, 12% crumb rubber in construction and 14% is discarded in landfills [4]. However, the disposal of waste tires in ground has recognized as harmful impacts on the environment. There are several options to for waste tire usage, however, till to date limited research has been conducted. The conversion of waste tires into various fuels through thermo chemical, biochemical and extraction processes has been reported [5,6]. For syngas production, the coal and waste tire gasification are carried out in reactors commonly known as gasifier. The syngas quality significantly depends upon the different factors such as design of gasifier as well as fuel properties [7]. Moreover, essential parameters such as particle size, moisture content, temperature, pressure, equivalence ratio (ER), and gasifying medium also affect the quality of produced gas [8,9]. Consequently, it is important to understand all the chemical and physical changes occurring during co-gasification of coal and waste tire for the optimization of gasification process [10].Amongst many gasifying models, the Entrained flow gasifiers (EFG) is broadly used due to the high carbon conversion efficiencies and short residence time[11]. A recent study suggested that concentric tube entrained flow gasifiers (CT-EFG) showed enhances performance efficiency because of the oxidizing agent and robust mixing design of the feed mixture. The syngas obtained from the thermo chemical conversion of coal and waste tire may provide an alternative energy source for the production of electricity hydrogen, and heat generation[8]. The syngas produced during the co-gasification is mainly composed of CO and H_2[12,13]. Several researchers have reported that the quality of the produced syngas is significantly depend on the composition of the combustion materials [14,15].However, the literature on the co-gasification of coal and waste tires seems insufficient. In addition, no previous data is available for parametric investigations of coal and waste tire co-gasification using a CT-EFG. Thus, this study aimed to explore the behavior of co-gasification process using various coal and waste tire feedstock's mixtures ranging from (0-100 %) at different oxygen/carbon ratios (O/C) and its effect on the syngas quality.

II. MATERIALS AND METHODS

Development of CFD model: Initially CFD geometry of (CT-EFG) model was developed using ANSYS work bench design modeler 14.0 software. Afterwards, the suitable governing equations were chosen for estimating the co-gasification processes within the CFD model.

Computational domain: The co-gasification process using the coal and waste tire in the CT-EFG was investigated as shown in figure 1. Figure 2 illustrate the mesh structure, the geometry of the an EFG was modified as previously reported by [16]. The geometry and meshing both were developed using Ansys workbench mesh 14. The coal, waste tire feed mixture fed to the CT-EFG through the central tube, while the oxygen as a gasifying agent was injected into an outer ring which is concentric with the inner tube as illustrate in figure 1.

Governing equations and assumptions: In gasifier several processes occurring simultaneously e.g., heat transfer, mass transfer, homogenous, and heterogeneous chemical reactions. The similar hypothesis of CT-EFG was adopted as reported in a recent study of [17]Coal and waste tires are co-gasified and the inorganic matter (ash) melts to produce slag. Since the melting of Ash and production of slag is a complex process, thus ash and its associated slugging /melting are not included in the CFD model. Energy equation, Navier–Stokes steady state and time-averaged were solved along with the standard k–e turbulence model [16]. Table 1 shows all the governing equations (1-9) with their related constants.

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Table – 1 List of governing equations

Governing equations

$$Continuity\ \frac{\partial}{\partial x_i}(\rho u_{ij}) = \frac{\Delta m_p}{m_{p,0}}\dot{m}_{p,0} \quad (1)$$

$$Momentum\ \frac{\partial}{\partial x_i}(\rho u_i u_j) = -\frac{\partial p}{\partial x_j} + \frac{\partial}{\partial x_i}\left(\tau_{ij} - \overline{pu'_\iota u'_J}\right) + \sum\left[\frac{18\mu C_D Re}{\rho_p d_p^2 24}(u_p - u)\right]\dot{m}_p \Delta t \quad (2)$$

$$Energy\ \frac{\partial}{\partial x_i}(\rho c_p u_i T) = \frac{\partial}{\partial x_i}\left(\lambda\frac{\partial T}{\partial x_i} - \rho c_p \overline{u'_\iota T'}\right) - \sum_j \frac{\Delta H_j^0}{M_j}\bar{R}_J \quad (3)$$

$$Species\ \frac{\partial}{\partial x_i}(\rho u_i y_j) = \frac{\partial}{\partial x_i}\left(\rho D\frac{\partial Y_j}{\partial x_i} - \overline{\rho u'_\iota Y'_J}\right) + Sr + \bar{R}_\iota \quad (4)$$

Turbulence model

$$kinematic\ viscosity\ \mu_t = \rho C_\mu k^2/\varepsilon \quad (5)$$

$$kinetic\ energy\ \frac{\partial}{\partial x_i}(\rho u_i k) = \frac{\partial}{\partial x_i}\left[\left(\mu + \frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_i}\right] + G_k - \rho\varepsilon \quad (6)$$

$$Dissipation\ rate\ \frac{\partial}{\partial x_i}(\rho u_i \varepsilon) = \frac{\partial}{\partial x_i}\left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_i}\right] + C_{1_\varepsilon} G_k \frac{\varepsilon}{k} - C_{2\varepsilon} G_k \rho \frac{\varepsilon^2}{k} \quad (7)$$

$$Heat\ conductivity\ \rho c_p \overline{u'_\iota T'} = -\lambda\frac{\partial T}{\partial x_i} = -C_p \frac{\mu_t}{Pr_t}\frac{\partial T}{\partial x_i} \quad (8)$$

$$Diffusion\ coefficient\ \rho u'_i \overline{Y'_J} = -\rho D\frac{\partial Y}{\partial x_i} = -\frac{\mu_t}{SC_t}\frac{\partial Y}{\partial x_i} \quad (9)$$

C_μ	$C_{1\varepsilon}$	$C_{2\varepsilon}$	σ_k	σ_ε	Pr_t	Sc_t
Constant 0.09	1.44	1.92	1.0	1.3	0.85	0.7

Chemical reactions : The co-gasification involving several chemical reactions. At high temperature the decay of feed mixture into char, volatiles, and ash takes place as demonstrated by Wen et al and given in equation (10).

$$fuel \rightarrow \alpha_1 CH_4 + \alpha_2 H_2 + \alpha_3 CO + \alpha_4 CO_2 + \alpha_5 H_2O + \alpha_6 Char + \alpha_7 Ash \sum \alpha i = 1 \quad (10)$$

At the initial stage of feed mixture, the de-volatilization process pre-dominates among the other reactions[18]. The two-step de-volatilization model could be used to describe the volatile evolved during the process as given by equation (11) for low temperature and equation (12) for high temperature respectively[19].

$$Fuel \overset{K1}{\rightarrow} (1 - Y_1) \times Char_1 + Y_1 \times Volatile \qquad (11)$$

$$Fuel \overset{kh}{\rightarrow} (1 - Y_h) \times Char_h + Y_h \times Volatile \qquad (12)$$

Where Y shows the stoichiometric coefficient.
Moreover, the volatile reaction kinetics can be described through the equation 13-15 respectively.

$$dV/dt = (k_1 Y_1 + K_h Y_h) \qquad (13)$$
$$K_1 = A_1 exp(-E_{a,l}/RT_p) \qquad (14)$$
$$K_1 = A_h exp(-E_{a,h}/RT_p) \qquad (15)$$

Where T_P is the temperature of feed mixture; Vis the mass of fraction of volatiles; A represent the pre-exponential factor; k shows the reaction rate constant and Ea is the reactions activation energy respectively. The value of Kl; Kh; E_h; E_l; Y_h and Y_l can be found elsewhere [19]. The co-gasification of char form during devolatilization process is shown by the following reaction equation (16-18).

$$C + \tfrac{1}{2}O_2 \overset{k1}{\rightarrow} CO \quad \triangle H^0 = -111 MJKmol^{-1} \qquad (16)$$
$$C + CO_2 \overset{K2}{\rightarrow} 2CO \quad \triangle H^0 = +111 MJKmol^{-1} \qquad (17)$$
$$C + H_2O \overset{k3}{\rightarrow} CO + H_2 \quad \triangle H^0 = +131 MJKmol^{-1} \qquad (18)$$

In addition, in the case of gas phase the chemical reaction, the specific relevant reactions are giving by the equation (19-21) [20].

$$H_2 + \tfrac{1}{2}O_2 \overset{k4}{\rightarrow} H_2O \quad \triangle H^0 = -242 MJKmol^{-1} \qquad (19)$$
$$CO + \tfrac{1}{2}O_2 \overset{k5}{\rightarrow} CO2 \quad \triangle H^0 = -283 MJKmol^{-1} \qquad (20)$$
$$CO + H_2O \overset{k6}{\rightarrow} CO_2 + H_2 \quad \triangle H^0 = -41.1 MJKmol^{-1} \qquad (21)$$

Feed mixture composition, operating parameters, and performance indicators: The feed mixture utilized in the co-gasifier includes coal, waste tires and their mixture with different ratios. The proximate and ultimate analyses test of chosen samples was conducted through a TGA model SDT-Q600 with standard method (ASTM D-7582–12) as shown in Table 2. Moreover, the elemental analyses were performed using ASTM D3176 method, the detail procedure can be found elsewhere. The percentage of sulfur, nitrogen, hydrogen, and carbon were determined by Vario MAX elementary analyzer. The ER, and oxygen to carbon ratio (O/C) are essential for effective process of co-gasification[21]. The calculation formula for O/C ratio is given by the equation 22.

$$\frac{\mathrm{O}}{\mathrm{C}}\mathrm{ratio} = \mathrm{m_{Oxygen}} \ / \ \mathrm{m_{carbon}} \ \mathrm{Stiochiometric} \qquad (22)$$

The law of conversation of mass can be used for the stoichiometric calculation of O/C ratio $\mathrm{m_{Oxygen}} \ / \ \mathrm{m_{carbon}}$. The stoichiometric reactions of different fuels and waste tire mixture ratio with oxygen can be obtained through the following reaction as given by equation stoichiometric reactions of fuels with oxygen could be as per reactions (equation23-27).

100 % Coal

$$C_{0.76}H_{4.21}O_{0.40}N_{0.0478}S_{0.1390} + 1.37O_2 \rightarrow 0.76CO_2 + 2.10H_2O + 0.0239N_2 + 0.1390SO_2 \qquad (23)$$

100 % Tire

$$C_{1.74}H_{2.65}O_{0.05}N_{0.0065}S_{0.0142} + 2.39O_2 \rightarrow 1.74CO_2 + 1.32H_2O + 0.0032N_2 + 0.0142SO_2 \qquad (24)$$

50 % Coal/ 50 % Tire

$$C_{1.43}H_{3.12}O_{0.16}N_{0.0191}S_{0.0530} + 2.19O_2 \rightarrow 1.43CO_2 + 1.56H_2O + 0.0095N_2 + 0.0530SO_2 \qquad (25)$$

60 % Coal/ 30 % Tire

$$C_{1.37}H_{3.22}O_{0.18}N_{0.0219}S_{0.0610} + 2.15O_2 \rightarrow 1.37CO_2 + \quad 1.61H_2O + 0.0109N_2 + 0.0610SO_2 \qquad (26)$$

70 % Coal / 30 % Tire

$$C_{1.22}H_{3.46}O_{0.23}N_{0.0279}S_{0.0797} + 2.05O_2 \rightarrow 1.22CO_2 + \quad 1.73H_2O + 0.0139N_2 + 0.0797SO_2 \qquad (27)$$

Amongst many parameters of performance evaluation of co-gasification operation, two factors such as conversion efficiency and quality of syngas are most important. Moreover, the behavior of fuel particles in the continuous fluid phase was investigated by using discrete phase model (DPM). In CT-EFG the feed mixture at 300 K temperature was injected to the central tube positioned at the top of the gasifier. Moreover, at the same temperature the oxygen was injected through a ring located outside, which relates to another inner centric tube. This tube enhances the transportation of fees particles. The size of feed mixture particles was kept with the range of 58-252 mm, while the observed average size of particle was 113 mm. The EFG performance significantly depends upon the size of particles thus smaller size of particles were selected. Due to the adiabatic wall of the reactor the slip condition was not taken into the account. In addition, simulation software ANSYS FLUENT VR 14.0 was employed for the numerical study of the coal, waste tires and various feed mixture ratio co-gasification phenomena.

III. RESULTS AND DISCUSSIONS

In this section, effect of varying O/C ratio on the behavior of gasification is covered;

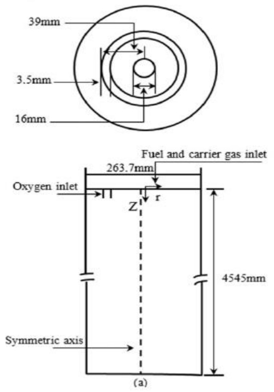
Temperature profile within the gasifier : The Figure 3 shows the temperature profile at different O/C ratios. It can be observed that that temperature is low at lower O/C ratios ranging from 0.8 to 1.0, afterwards it gradually enhanced at upper O/C ratios (> than 1.0). The possible phenomena for this trend of temperature might be related to the fact of gasification reactions (equation 17 and 18) due their endothermic nature thereby reducing the overall temperature of the feed mixture in this O/C range. In contract, the abundant oxygen is available at the upper ranges of O/C, thus the combustion reactions (equation 16, 20 and 21) became dominant than other gasification reaction resulting rise in the temperature following decline in quantity of Syngas production [22]. This observation revealed that at O/C ratio 0.8 to 1.0 favors the reduction reactions, thereby enhancing the production of syngas.

Effect of Oxygen/Carbon ratio on syngas quality: The O/C ratio is an essential factor to be studied during the designing and operation of gasifier. During the CFD modeling the O/C ratio was varied by changing the oxidant flow, whereas fuel flow and feed inlet temperature was kept constant. The figure (4A- E) shows the effect of O/C ratio on the production of syngas. In the case of pure Larkhra coal the maximum mole fraction of CO and H_2 were observed to be 0.18 and 0.192 at 0.8 O/C ratio respectively as shown in figure 4A. However,CO_2 and volatile matter mole fraction at this point were observed to be 0.16 and 0.078 respectively. The increase in O/C ratio, results in gradual decrease of syngas production to a lowest level at maximum test O/C ratio of 1.2.This observation suggested that at lowest O/C ratio favors the gasification reactions in comparison to the combustion reaction equation (16,17,20 and 21)[23].

Likewise, in the case of pure waste tire, the highest mole fraction of CO and H_2were found to be 0.134 and 0.14 at O/C ratio of 0.8 respectively. However, mole fraction of CO_2 and volatile showed the opposite trends such as at O/C ratio of 0.8 the value was found to be 0.25 and 0.16as illustrated in figure 4B. For different mixtures of coal and waste tires shows almost similar trend. Such as in the case of (50 % Coal/ 50 % Tires) the maximum mole fraction of CO and H_2 productions were obtained to be 0.158, 0.16, while lowest mole fraction was found to be 0.056, 0.148 respectively as shown in figure 4 C. Similarly, in the sample containing (60 % Coal/ 40 % Tires) resulted the maximum and minimum mole fraction of CO and $H_2$was measured to be 0.16, 0.17 and 0.059, 0.15 respectively as depicted in figure 4D. For trial mixture containing (70 % Coal/ 30 % Tires) the highest and lowest mole fractions of CO and H_2 were calculated to be 0.168, 0.176 and 0.063, 0.157 correspondingly as shown in figure 4E. The mole fraction of CO_2 and volatile matters showed the reverse phenomena in all cases of mixtures, e.g., the fraction of both components enhanced with increase in O/C ratio throughout the maximum tested level.

These resulted suggested that at lowest O/C ratio, from 0.8 to 1.0, favors the gasification reactions (equation 9 and 10). Further increase in O/C ratio from 1.0 to 1.2, the combustion reaction inside the gasifier became dominant (equation 20 and 21). At lower O/C ratio the O_2 content is lower thereby, resulting in incomplete combustion of carbon particle increasing the concentration of CO productions. In contrast, enhanced O_2 concentration generates higher CO_2, due to complete combustion of gaseous hydrocarbons. Thus, the excess amount of O_2 supply did not enhanced the syngas quality in the gasification reaction.

I. FIGURES AND TABLES



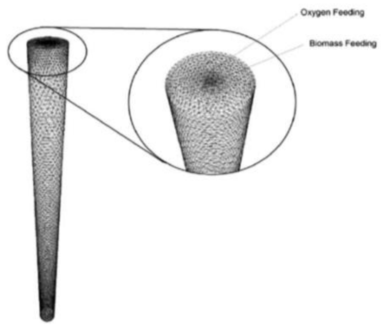


Figure1:The simple geometry of entrained flow gasifier, Figure2: Computational domain of CT-EFG and mesh.

Table 2. Results of Proximate and Ultimate analysis

Proximate analysis Lakhra Coal and Waste Tire Blends					
Coal/Tire mixture %	Moisture	Volatile matter	Fixed carbon	Ash	
100 C+0 T	17.65	27.63	22.39	32.34	
0 C+100 T	0.89	66.68	27.91	4.52	
50 C+50 T	9.19	47.36	25.17	18.28	
60 C+40 T	10.37	44.61	24.79	20.24	
70 C+30 T	12.75	39.04	23.99	24.21	
Ultimate analysis Lakhra Coal and Waste Tire Blends					
Coal/Tire mixture %	**C**	**H**	**N**	**O**	**S**
100 C+0 T	65	9.4	1.48	14.28	9.85
0 C+100 T	88.63	7.55	0.26	2.28	1.29
50 C+50 T	79.82	8.23	0.71	6.80	4.44
60 C+40 T	78.22	8.36	0.79	7.60	5.03
70 C+30 T	74.62	8.65	0.97	9.43	6.34

C: coal, T: Tire; C: Carbon; H: Hydrogen; N; Nitrogen; O: Oxygen; S: Sulphur

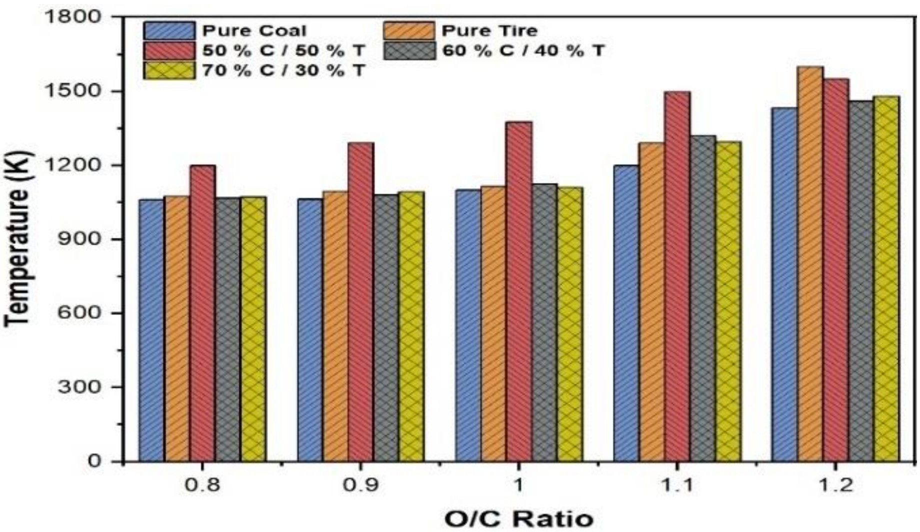


Figure 3. Temperature profile at different O/C ratios

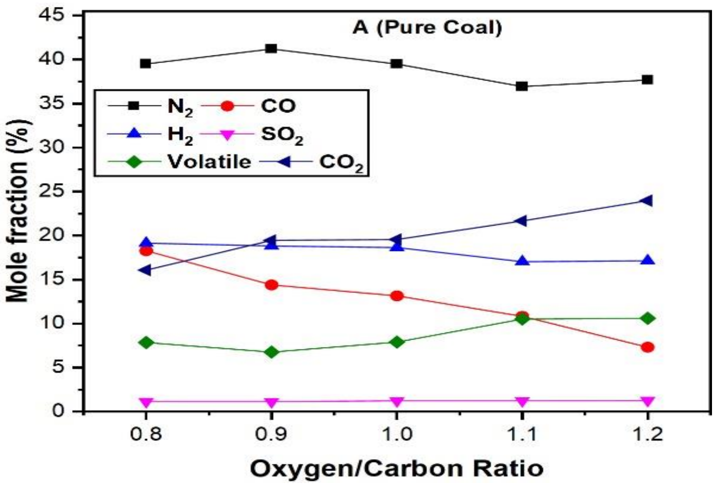


Figure 4 (A) Behavior under varying O/C ratio showing for the case Pure Lakhra coal

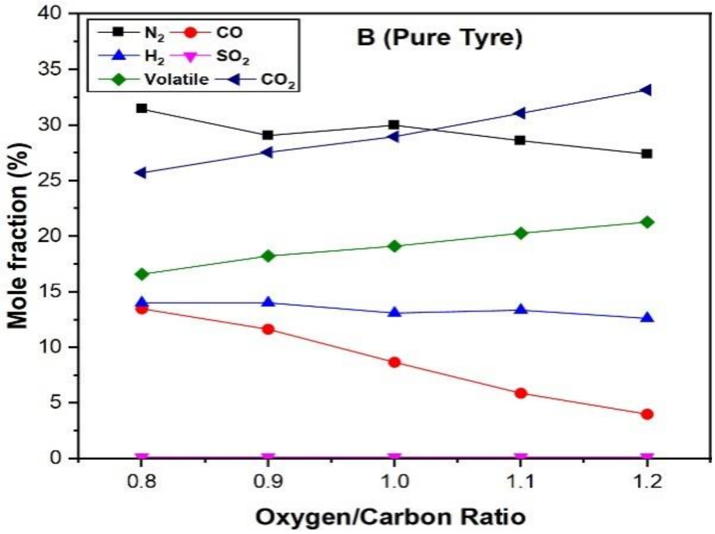


Figure 4 (B) Behavior under varying O/C ratio showing for the case Pure waste tire

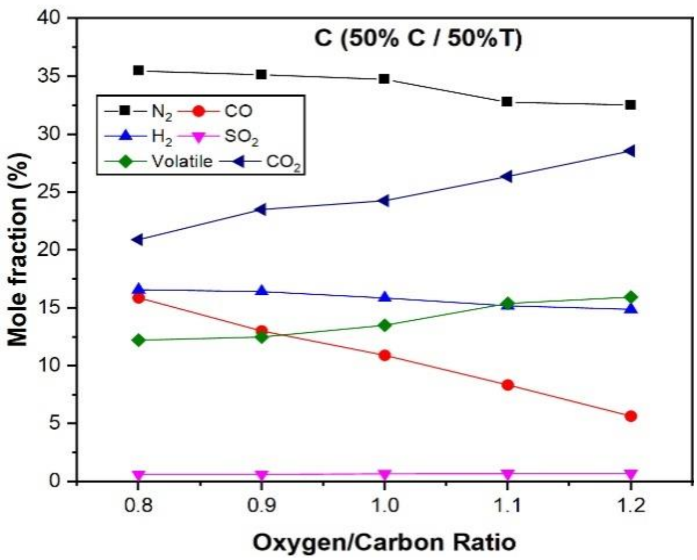


Figure 4 (C) Behavior under varying O/C ratio showing for the case 50 % Coal / 50% Tire

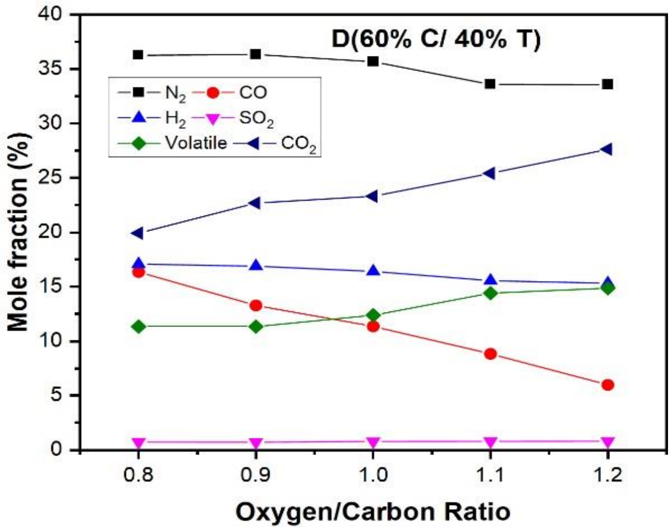


Figure 4. (D) Behavior under varying O/C ratio showing for the case 60 % Coal / 40% Tire

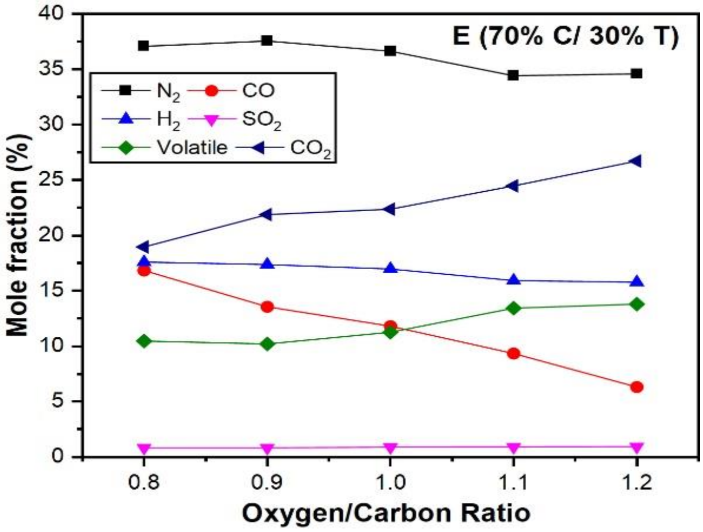


Figure 4. (E) Behavior under varying O/C ratio showing for the case 70 % Coal/ 30% Tire

IV. CONCLUSION

The co-gasification behavior of coal, waste tire and different blends in CT-EFG was studied using CFD simulation method. Moreover, the effect on the syngas composition at various O/C ratios was also investigated. The current model estimated that the effect of varied O/C ratio on temperature, syngas production, and quality in CT-EFG. The results of pure sample of coal showed the maximum mole fraction of CO and H_2 in comparison to the pure waste tire at similar O/C ratio. Moreover, maximum CO_2 mole fraction in case of pure tire feed stock was observed at maximum tested O/C ratios. The mixing blend of coal and waste tire has synergistic effect on total syngas production as compared to pure waste tires. The maximum mole fractions of CO were found in the blend mixture containing higher percentage of coal. These results advance understanding of the waste tire utilization as a source material for energy production and reducing the waste tire as well as economical usage of coal in gasification process. Moreover, the developed CFD model may provide some insight into the simulation of coal and waste tire gasification plants relating to CT-EFG**.**

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