Gasification of Heavy Fuel Oils: A Thermochemical Equilibrium Approach

M. Vaezi[1], M. Passandideh-Fard[2], M. Moghiman[3], and M. Charmchi[4]

[1,2,3] Mechanical Engineering Department, Ferdowsi University of Mashhad, Mashhad, Iran
[4] Mechanical Engineering Department, University of Massachusetts-Lowell, USA

ABSTRACT

Combustion of heavy fuel oils is a major source of production of particulate emissions and ash, as well as considerable volumes of SO_X and NO_X. Gasification is a technologically advanced and environmentally friendly process of disposing heavy fuel oils by converting them into clean combustible gas products. Thermochemical equilibrium modeling is the basis of an original numerical method implemented in this study to predict the performance of a heavy fuel oil gasifier. The model combines both the chemical and thermodynamic equilibriums of the global gasification reaction in order to predict the final syngas species distribution. Having obtained the composition of the produced syngas, various characteristics of the gasification process can be determined; they include the $H_2{:}CO$ ratio, process temperature, and heating value of the produced syngas, as well as the cold gas efficiency and carbon conversion efficiency of the process. The influence of the equivalence ratio, oxygen enrichment (the amount of oxygen available in the gasification agent), and pressure on the gasification characteristics is analyzed. The results of simulations are compared with reported experimental measurements through which the numerical model is validated. The detailed investigation performed in the course of this study reveals that the heavy oil gasification is a feasible process that can be utilized to generate a syngas for various industrial applications.

1. INTRODUCTION

The main source of energy in modern civilization is achieved by utilization of hydrocarbon fuels, including heavy fuel oil. In spite of the available state-of-the-art technologies in the refining industry that can reduce significantly the volume of refinery bottom products [1], heavy fuel oils are still produced and play an important role in providing energy worldwide [2]. Heavy oil is any petroleum-based fuel which contains the undistilled residue obtained during the distillation process of crude oil. It is a thick, syrupy, black, tar-like liquid which may become semi-solid in cooler temperatures and is often called bunker fuel oil (bunker C), furnace fuel oil, or No.6 fuel oil [3-5].

The high sulfur content of heavy fuel oils results in their combustion to produce considerable volumes of SO_X; pollutants that are the main causes of acid rains and responsible for low-temperature corrosion process [6]. Due to such shortcomings, many research efforts have been concentrated on improving the available methods for utilization of heavy fuel oils. Gasification is a technologically advanced and environmentally friendly process of disposing heavy fuel oils by converting them into usable gas products [7].

Gasification and combustion originate from two different concepts. Combustion process is performed using excess air to thermally decompose feed material into products dominantly comprised of CO_2, H_2O, SO_x, and NO_x. In contrast, gasification process takes the advantage of an oxygen/air starved environment to convert feedstock into more valuable, environmentally friendly product: a combustible synthetic gas (syngas) mainly consisting of H_2, CO, CH_4, H_2S, and NH_3. Gasification consistently exhibits much lower level of air emissions and corrosive effects than competing technologies, such as combustion and incineration [8]. The produced syngas can be used as a raw material for the synthesis of chemicals, liquid fuels (in conjunction with Fischer-Tropsch technology), or other gaseous fuels such as hydrogen [9]. In addition, the gasification technology may be combined with a power plant system to make an Integrated Gasification Combined Cycle (IGCC) that can provide efficiency well above 50% [1, 10].

The many advantages of gasification over combustion make it feasible to review the possibilities of syngas production as an alternative technology for utilizing heavy fuel oils with their high sulphur/metal contents, while simultaneously not exceeding the environmental red lines.

In spite of considerable investigations being conducted on gasification of solid fuels [11-12], only a limited number of studies on gasification of liquid fuels are available in the literature most of which concentrated on black liquor gasification [13]. Ashizawa et al. [14] made an experimental study on gasification process of Orimulsion[TM] (registered trademark of BITOR Ltd.), which is a bitumen-in-water emulsified fuel comprised of approximately 30% water and 70% bitumen [15] (www.orimulsion.com). They employed a 2.4 tons/day research-scale gasifier in order to investigate the gasification characteristics of Orimulsion[TM]. The considered gasifier was equipped with several unique measuring devices, such as heat flux probes, optical gas analyzer, etc. Their results included a range of performance indicators, such as the syngas calorific value and cold gas/carbon conversion efficiency. Recent modeling efforts on gasification include the application of thermochemical equilibrium approach through the gasification of biomass materials [12, 16]. These models are based on the minimization of Gibbs free energy [16] or equilibrium constants [12].
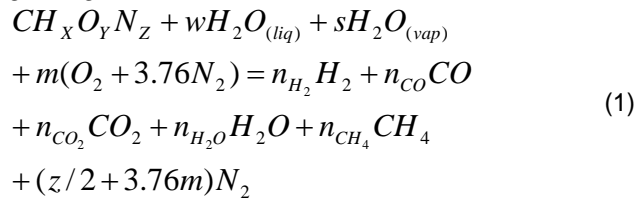
In this paper, a zero dimensional model is developed for simulating a gasification process of heavy fuel oils; the model takes the advantage of

thermochemical equilibrium approach based on equilibrium constants. The combination of the laws of conservation of energy in an open system, conservation of atomic species, and the laws of chemical equilibrium provides a novel numerical algorithm that can be used in predicting the composition of syngas, and investigating the effect of important variables such as gasification pressure on gasification characteristics, e.g., H_2:CO ratio. To validate the model, the results of simulations are compared with those of the experiment performed by Ashizawa et al. [14]. The results of the model are generated in a format that may be employed in the design/optimization of actual heavy fuel oil gasifiers.

2. MATHEMATICAL MODELING

In this study, a thermochemical equilibrium approach is employed to develop a numerical model for predicting the performance of a downdraft heavy fuel oil gasifier. The main assumptions of the model are as follows. The residence time of the reactants is supposed to be high enough to reach chemical equilibrium [17]; all carbon in feedstock is assumed to be gasified and, therefore, the formation of char is neglected; the syngas is comprised of H_2, CO, CO_2, H_2O, CH_4 and N_2; and the gasifier is considered to be adiabatic.

To develop the numerical model, the chemical formula of the feedstock is defined as $CH_xO_yN_z$. The global gasification reaction can be written as:

$$CH_XO_YN_Z + wH_2O_{(liq)} + sH_2O_{(vap)}$$
$$+ m(O_2 + 3.76N_2) = n_{H_2}H_2 + n_{CO}CO$$
$$+ n_{CO_2}CO_2 + n_{H_2O}H_2O + n_{CH_4}CH_4 \quad (1)$$
$$+ (z/2 + 3.76m)N_2$$

Concentrations of H_2S and NH_3 are negligible [14] and, therefore, are not considered in the simulation. w in Eq.1 is the molar quantity of water per one kmol of heavy fuel oil and can simply be obtained as:

$$w = \frac{M_{HFO} \times WC}{M_{H_2O} \times (1 - WC)} \quad (2)$$

For a fuel with a chemical formula of $C_\alpha H_\beta O_\gamma N_\zeta$, the stoichiometric air/fuel ratio can be calculated based on the following relation [18]:

$$Sto = \alpha + \frac{1}{4}\beta - \frac{1}{2}\gamma \quad (3)$$

During the gasification process, the feedstock is subjected to partial pyrolysis under sub-stoichiometric conditions, therefore, m (equivalence ratio) is assumed to be a fraction of the calculated stoichiometric air (30% - 60%).

For the development of an equilibrium model, the number of independent reactions has to be determined by applying the phase rule, as described by Tassios [19]. In the case where no solid carbon remains in the equilibrium state, as in the present model, only two independent reactions need to be considered. Ashizawa et al. [14] introduced water-gas shift reaction

together with steam reforming as dominant gasification equations in their experiments on liquid fuel gasification. We use the same equations in this study because as mentioned before, the reported measurements of Ashizawa et al. will be used to validate the developed model. The two equations are:

Water - gas shift reaction :
$$CO + H_2O \leftrightarrow CO_2 + H_2 \quad (4)$$
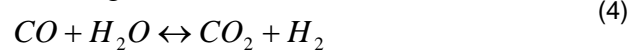
Steam reforming (Methane decomposition)
$$: CH_4 + H_2O \leftrightarrow CO + 3H_2 \quad (5)$$
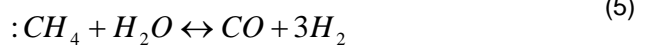
The equilibrium constants of the above reactions generate two of five equations required to obtain unknown species of the produced syngas (H_2, CO, CO_2, H_2O, and CH_4). The remaining three equations are formulated by balancing each chemical element consisting of carbon, hydrogen, and oxygen. The equilibrium constants for the gasification processes can be written based on the following [20]:

$$K = \prod_i (x_i)^{v_i} \left(\frac{P^\circ}{n_{total}}\right)^{\sum_i v_i} \quad (6)$$

Based on this equation, the equilibrium constants for the water-gas shift and the steam reforming reactions are calculated as follows:

$$K_1 = \frac{(n_{CO_2})(n_{H_2})}{(n_{CO})(n_{H_2O})} \quad (7)$$

$$K_2 = \frac{4(n_{CH_4})(n_{H_2O})}{P^\circ(n_{CO})(n_{H_2})^3} \quad (8)$$

The values of the equilibrium constants, which are mere functions of temperature, can be calculated using the Gibbs free energy [18]:

$$\ln K = \frac{-\Delta G_T^\circ}{\tilde{R}T} \quad (9)$$

The dependence of ΔG° (the standard Gibbs function of formation) on temperature can be written as follows [21]:

$$\frac{d(\Delta G^\circ / RT)}{dT} = \frac{-h_f^\circ}{\tilde{R}T^2} \quad (10)$$

The amounts of h_f° (the enthalpy of formation) and ΔG° of common combustion products can be found in combustion/chemical engineering books/handbooks [18,20,21].

Heat of formation of complicated molecular structures such as heavy fuel oil is calculated using their calorific value (HHV) and dry, ash-free ultimate analysis [18]. Channiwala et al. [22] presented a single correlation for estimating the calorific value from dry-based ultimate analysis of liquid fuels as follows:

$$HHV = 0.3491C + 1.1783H + 0.1005S$$
$$- 0.1034O - 0.0151N - 0.0211A \quad (11)$$

The above correlation is used to calculate the calorific value of the heavy fuel oil and estimate its heat of formation.

Substituting Eq.9 in Eq.10 leads to:

$$\frac{d \ln K}{dT} = \frac{h_f^\circ}{\tilde{R} T^2} \qquad (12)$$

Since the heat of formation is a function of temperature, Eq.12 can be integrated as follows:

$$\ln K = \int \frac{h_f^\circ}{\tilde{R} T^2} dT + I \qquad (13)$$

where h_f° is linked to temperature, based on the following equation [21]:

$$\frac{h_f^\circ}{\tilde{R}} = \frac{J}{\tilde{R}} + (\Delta A)T + \frac{(\Delta B)}{2}T^2 + \frac{(\Delta C)}{3}T^3 - \frac{(\Delta D)}{T} \quad (14)$$

Here J is a constant and ΔA, ΔB, ΔC, and ΔD are the coefficients for determining the specific heat. Considering the definition of Gibbs function from Eq.9 and substituting Eq.14 into Eq.13 to perform the integration finally results in:

$$\Delta G^\circ = J - RT \left(\begin{array}{c} (\Delta A)\ln T + \frac{(\Delta B)}{2}T \\ + \frac{(\Delta C)}{6}T^2 + \frac{(\Delta D)}{2T^2} + I \end{array} \right) \qquad (15)$$

Equations 13 to 15 will be used to find the equilibrium constant for any reaction temperature. Having obtained the value of h_f°, the knowledge of specific heat is sufficient to determine the constant J using Eq.14 at the reference temperature of 298.15K. Similarly, the constant I is determined using Eq.15 at the same temperature where the value of ΔG° is known. Having known the I and J constants, together with h_f° and ΔG°, we can use Eq.13 in order to determine the equilibrium constant K. As an example, the equilibrium constant for steam reforming reaction is obtained as follows:

$$\ln K_2 = \frac{22752325}{T} - 7.951 \ln T$$
$$+ 4.354 \times 10^{-3} T - 0.3606 \times 10^{-6} T^2 \qquad (16)$$
$$- \frac{0.0485 \times 10^5}{T^2} + 24.954$$

To improve the model accuracy, the equilibrium constants are multiplied by certain factors obtained from a comparison between calculated results and those of the experiments performed by Ashizawa et al. [14]. Jarungthammachote et al. [23] used the same approach in their model.

The temperature of the gasification zone also needs to be determined in order to calculate the equilibrium constants. For this reason, an enthalpy balance is performed on the gasification process. If the temperature in the gasification zone is T and that of the

inlet is assumed to be 298K, the enthalpy balance for this process can be written as:

$$\sum_{j=react} n_j (h_{f,j}^\circ + \Delta h_{T,j}^\circ) = \sum_{i=prod} n_i (h_{f,i}^\circ + \Delta h_{T,i}^\circ) \qquad (17)$$

where Δh_T°, which represents the difference in the enthalpy of any given state and that of the reference state, can be approximated by:

$$\Delta h_T^\circ = \int_{298}^{T} \overline{C}_p(T) dT \qquad (18)$$

where $\overline{C}_p(T)$ is the specific heat at constant pressure that can be obtained by available empirical correlations for petroleum liquid fuels [24] and gasification products [21], respectively, as:

$$\overline{C}_p(T_{fuel}) = 0.76 + 0.000335(T_{fuel}) \qquad (19)$$

$$\overline{C}_p(T) = C_1 + C_2 \left[\frac{C_3/T}{\sinh(C_3/T)} \right]^2$$
$$+ C_4 \left[\frac{C_5/T}{\sinh(C_5/T)} \right]^2 \qquad (20)$$

When the equilibrium constants are defined, a system of equations will be obtained that need to be solved. Because of the non-linear nature of some of the equations, the implicit Newton–Raphson method is used where the solution is obtained by an iterative procedure. This enhanced strategy ensured solution convergence. The procedure starts with an initial guess for the gasification temperature. Equilibrium constants are then calculated and the set of equations are subsequently solved to obtain the syngas composition which in turn is used to determine the new gasification temperature. This iterative procedure continues until the gasification temperature does not change within a certain limit (much less than 1 K) in successive iterations.

3. RESULTS AND DISCUSSION

In this section, first we present a model validation of the simulation results for a case for which experimental results were available in the literature. Next, a parametric study of the important operating parameters is performed.

3.1 MODEL VALIDATION

To validate the model, the extra-heavy oil (Orimulsion™) used by Ashizawa et al. [14] is selected for which measurements are available. The physical properties and chemical composition of Orimulsion™ are very close to those of heavy fuel oils [15]. This fact has been used by many researchers who conducted experiments to compare the combustion/pollution characteristics of Orimulsion™ with those of heavy oils [25-26]. Operating conditions selected for the simulation performed to validate the model, were exactly the same as those of the experiments. The preferred criteria in order to quantify the amount by which numerical results differ from experimental values is the root mean square

error ($\sqrt{\sum_{i=1}^{N}(Experiment_i - Model_i)^2 / N}$) which is the root square of the variance and summarizes the overall error [27].

The results of the model for the composition of the syngas and its corresponding calorific value are presented in Table 1 along with the measurements. A graphical representation of this table is also shown in Fig. 1. As observed from both Table 1 and Fig. 1, the model predictions agree well with those of the experiments. This comparison validates the model and its underlying assumptions. It is observed that for H_2 and CO, the proposed equilibrium model shows a slight over prediction. For CH_4, however, the model under predicts the experimental value. This was expected as reported in all equilibrium modeling [23,28]. In the numerical model, the equilibrium constant of the steam reforming reaction tends to infinity at the elevated temperatures of the reduction zone [12]; therefore, the predicted CH_4 concentration in the syngas will be small. In a real gasifier, devolatilization of fuel gives higher contents of CH_4 and heavier hydrocarbons (e.g., C_xH_y), which do not react completely with equilibrium concentrations of CO, CO_2, and H_2 [29]. Therefore, an equilibrium state is not established and higher methane content is detected in the measurements.

Table 1. Comparison between numerical results and measurements [14] for syngas produced from Orimulsion[TM].

Operating Conditions [14]				
Equivalence ratio		0.4		
Gasification pressure		18.75[a] atm		
Gasification agent		oxygen		
Syngas from Orimulsion[TM]				
	Experimental		Numerical	
H_2	39.4	vol%	39.77	vol%
CO	38.7	vol%	39.83	vol%
CO_2	8.67	vol%	8.9	vol%
H_2O	11.85	vol%	11.34	vol%
CH_4	0.08	vol%	0.01	vol%
Others (considered as N_2)	0.38	vol%	0.15	vol%
HHV[b]	9.5 – 10.5 MJ/m^3		10.1	MJ/m^3
RMS error	0.54			

a) Maximum operating pressure reported
b) The extent where the calorific value ranges

3.2 PARAMETRIC STUDY

Having validated the model, it was used to simulate the gasification process for a widely used commercial heavy fuel oil. The physical/chemical properties of this fuel are given in Table 2. The results of the simulations for a typical gasification process along with the corresponding operating conditions are presented in Table 3.

A parametric study was performed for the effects of equivalence ratio, enrichment of oxygen in air, and operating pressure. A number of different criteria, which are frequently quoted for gasification processes, are employed to investigate the effect of each parameter while holding the others constant. These criteria includes: syngas composition and its calorific value, gasification temperature, cold gas efficiency (CGE) and carbon conversion efficiency (CCE).
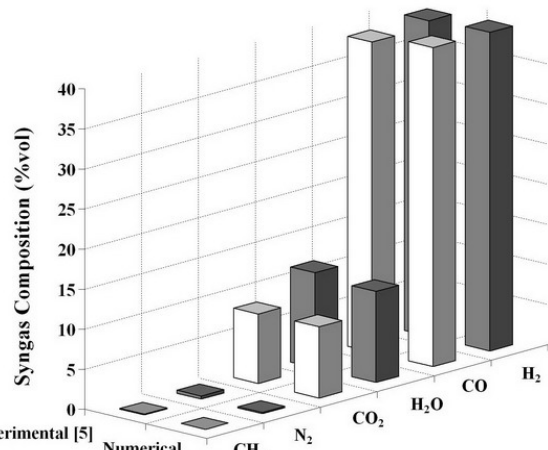

Fig. 1. Graphical comparison between numerical and experimental results for the composition of syngas produced from Orimulsion[TM]

Table 2. Properties of the heavy fuel oil selected for the simulation [30-32]

Physical properties		
Flash point	> 60	°C
Pour point	< 30	°C
Boiling point	> 260	°C
Auto-ignition point	400	°C
Density	0.95	g/ml @ 15°C
Viscosity	2400	mPa.s @ 30°C

Chemical properties					
Proximate analysis			Ultimate analysis (Dry)		
Water content	0.3	wt%	carbon	86.25	wt%
Ash	0.1	wt%	hydrogen	11.05	wt%
Total-sulfur	2.2	wt%	oxygen	0.0	wt%
HHV	43.2 MJ/Kg		nitrogen	0.4	wt%
			sulfur	2.2	wt%
			ash	0.1	wt%

Table 3. The operating conditions of a typical gasification process along with the results of the simulation.

Operating Conditions		
Equivalence ratio	0.4	
Gasification pressure	10.0	atm
Gasification agent	oxygen	
Air inlet temperature	298.0	K
Fuel inlet temperature	400.0	K
Results		
H_2	39.968	vol%
CO	53.852	vol%
CO_2	2.783	vol%
H_2O	3.275	vol%
CH_4	0.006	vol%
N_2	0.116	vol%
HHV	11.9	MJ/m^3

3.2.1 EQUIVALENCE RATIO

The effect of equivalence ratio - the ratio of virtual air/oxygen to stoichiometric air/oxygen – on the syngas composition, gasification temperature and its calorific value, and cold gas and carbon conversion efficiencies are shown in Figs. 2 to 4. All calculations were performed at a 10 atm pressure with an air inlet temperature of 400 K considering pure oxygen as the gasification agent; the equivalence ratio ranged between 0.32 and 0.7.

The syngas species distribution presented in Fig. 2 shows that an equivalence ratio of 0.32 corresponds to an ideal gasification process where the only species produced are those of H_2, CO, and CH_4. For this condition, the syngas consists of 34.7% H_2 and 57.5% CO by volume. The CO_2 and H_2O species made a negligible contribution to the syngas mixture with 0.021% and 0.015%, respectively. As the equivalence ratio is increased, the process approaches a combustion region with a tendency to produce more CO_2 and H_2O as such that for an equivalence ratio of 0.7 the volume percent of CO_2 and H_2O rises to 24.2 and 28.7, respectively. As expected, with increasing the equivalence ratio, the gasification temperature is also increased as displayed in Fig. 3. Thus, the CH_4 dissociates to H_2 [12] and as a result the CH_4 content of the syngas drops sharply until its concentration becomes nearly zero for an equivalence ratio of 0.37 (see Fig. 2). Figure 3 also shows the variation of the syngas calorific value against the equivalence ratio. Up to an equivalence ratio of 0.37, in spite of the increase of H_2, the calorific value of the syngas is decreased sharply. This can be attributed to the decrease of CH_4 with a high calorific value equal to three times that of H_2. Beyond an equivalence ratio of 0.37, the reduction of both H_2 and CO concentrations is the reason for the decrease of the syngas calorific value. The figure shows that the syngas calorific value that can be obtained using the gasification process can be as high as 15 MJ/m^3. This amount for the syngas is a noticeable value considering that the minimum calorific value required for a gas in order to be used in gas engines and gas turbines according to [33-34] is approximately 3.0 MJ/m^3 and 6.0 MJ/m^3, respectively.

Figure 4 presents the influence of the equivalence ratio on the CGE and CCE. As observed, for a wide range of variation of the equivalence ratio (less than 0.65), a CGE higher than 70% can be achieved. Regarding the CCE, as the equivalence ratio is increased (i.e., the gasification process approaches combustion) less carbon of feedstock is burnt out to satisfy the endothermic nature of gasification reactions; consequently, the volume of carbon gasified into gaseous products increases, which in turn results in the CCE to be increased. The figure also shows a sharp increase of the CCE below a certain value of equivalence ratio; the same variation is reported from experiments performed by Ashizawa et al.[14].

3.2.2 OXYGEN ENRICHMENT

From a technical viewpoint, there is a fundamental choice of gasifying the heavy fuel oil with air and gasifying with oxygen. On paper there is not much to choose between the two. The decreased size of the gas production unit and treating equipment and of the steam cycle for an oxygen-blown system almost exactly compensates the additional investment cost of the air separation unit. Similarly, the operating cost savings achieved by not compressing all the nitrogen in the air to the gasification pressure more or less balances the energy requirement of the oxygen plant.
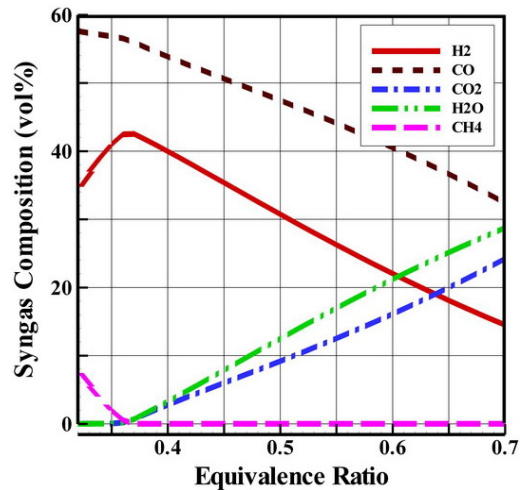

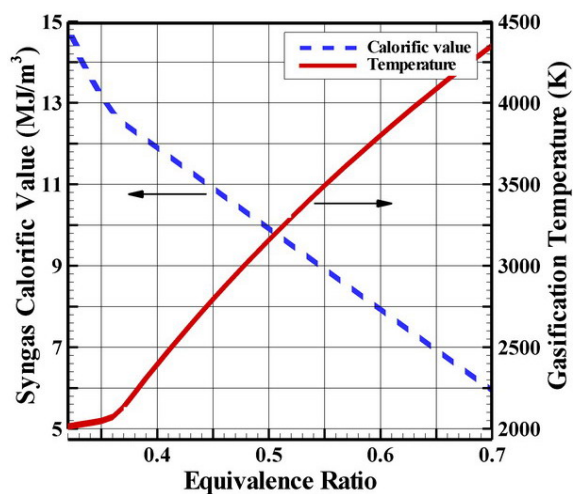**Fig. 2.** Effect of equivalence ratio on syngas composition

Fig. 3. Effect of equivalence ratio on the syngas calorific value and gasification Temperature
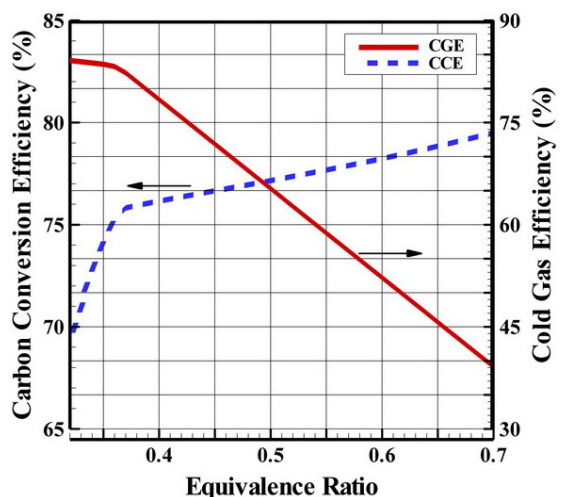

Fig. 4. Effect of equivalence ratio on gasification efficiency

The significant effects of increasing oxygen available in the gasification agent can be seen in Figs. 5 and 6. The results were obtained using an equivalence ratio of 0.37 (the optimum value based on the discussion given in previous section), a gasification pressure of 10 atm, and an air inlet temperature of 298 K. The oxygen enrichment varied from 21% (equivalent

to the amount of oxygen available in the atmospheric air) to 100% (pure oxygen); this covers a wide variety of gasification processes including the gasification with air, oxygen-rich air, and pure oxygen.

The influence of oxygen enrichment on the syngas composition is given in Fig. 5. As seen from the figure, the gasification with air produces a syngas with low hydrogen content (less than 20% by volume). As the amount of oxygen is increased, the H_2 and CO contents of the syngas are also increased as such that for an oxygen enrichment value of 100% the H_2 content of the syngas increases to a considerable value of 42.5%. This variation can be explained as follows. The increase of oxygen enrichment means less amount of N_2 content available in the gasification agent which in turn translates in less carbon being combusted to produce CO_2 in order to maintain the heat balance. As a result, the more carbon contributes to the gasification process leading to a higher concentration of useful syngas (H_2+CO).

Figure 6 shows that when the oxygen content of the gasification agent is increased, the syngas calorific value and gasification temperature are noticeably increased. The calorific value varies from an amount of 6 MJ/m^3 for 21% of oxygen (air) to 12.5 MJ/m^3 for 100% of oxygen, and the gasification temperature from 1300 K to 2135 K. The main reason for these variations is the amount of heat required to raise the N_2 (which acts as a thermal sink) from its inlet temperature of 298 K to the gasification temperature.

The effect of oxygen enrichment on gasification efficiency is displayed in Fig. 7. As the oxygen enrichment increases from 21% to 30%, the CGE increases as much as 1.3%. More increase of the oxygen enrichment, however, has no significant effect on the CGE; the same result is reported by Mathieu et al. [35]. Figure 7 also shows a decrease of the CCE with increasing the oxygen enrichment. As mentioned above, the reduction of the rate of combustion of carbon burnt out in the gasifier, results in the volume of carbon gasified to decrease, therefore, the CCE reduces.
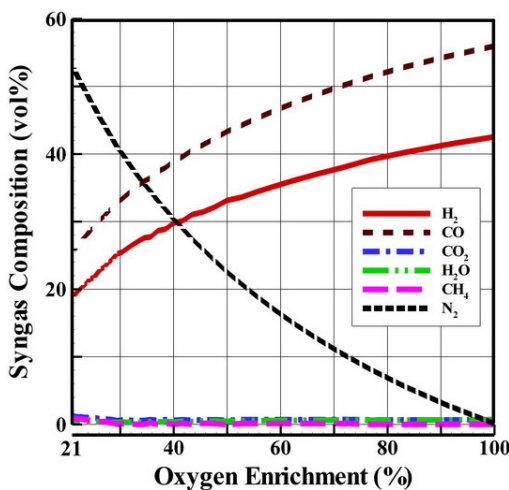

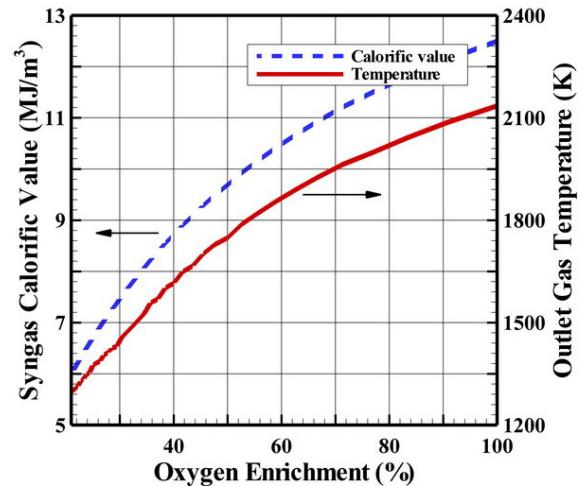**Fig. 5.** Effect of oxygen enrichment on syngas composition

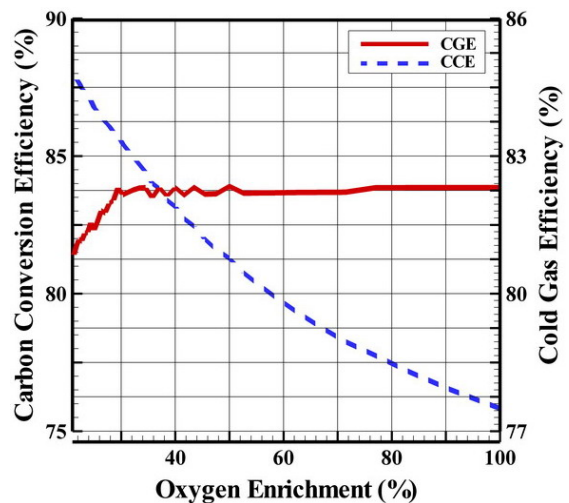**Fig. 6.** Effect of oxygen enrichment on the syngas calorific value and gasification temperature

Fig. 7. Effect of oxygen enrichment on gasification efficiency

3.2.3 GASIFICATION PRESSURE

The effects of pressure variations on composition of syngas, its calorific value, and the gasification temperature are also investigated. While the pressure ranged from atmospheric pressure to 80 atm, the equivalence ratio (0.37), gasification agent (air), and air preheating temperature (298 K) were kept unchanged.
Figure 8 gives the syngas composition as a function of gasification pressure. The diagram is plotted logarithmically, due to the miniature changes in species concentrations. It is observed that the amount of CO and H_2 decrease slightly as the pressure increases. The CH_4, CO_2, and H_2O contents, however, grow with increasing pressure. This trend, reported in the literature for other feedstocks [35-36], can be explained in accordance with Le Chatelier's principle [37].

The effect of gasification pressure on the syngas calorific value and gasification temperature are presented in Fig. 9. Although increasing pressure reduces the rate of production of CO and H_2, the syngas calorific value does not decrease due to the increasing generation of CH_4. As observed from Fig. 9, the gasification temperature starts rising as the gasification pressure increases. This is because the

endothermic behavior of the process dilutes with increasing pressure, which is expected as all the reactions responsible for conversion of char into gaseous product reverse at higher pressures in accordance with Le Chatelier's principle [12]. A close inspection of the detailed results obtained from the simulations show that the gasification efficiency (both CCE and CGE) is not sensitive to the pressure changes. Increasing pressure from 10 atm to 80 atm reduced the CGE by a maximum of 1.06%. The increase of CH_4 concentration, which compensates the decrease of H_2 and CO, results in such behavior. As observed, the gasification pressure has no significant effects on gasification characteristics. In reality, however, the gasification under pressure is economically preferred over pressurizing the syngas in downstream equipments such that all modern processes are operated at a pressure of at least 10 atm and up to a maximum 100 atm [38].

Finally, the effect of operational conditions, consisting of equivalence ratio, oxygen enrichment, and gasification pressure, on syngas H_2:CO ratio is plotted in Fig. 10. The syngas quality is usually characterized by the H_2:CO molar ratio, typically around 0.4-0.7:1.
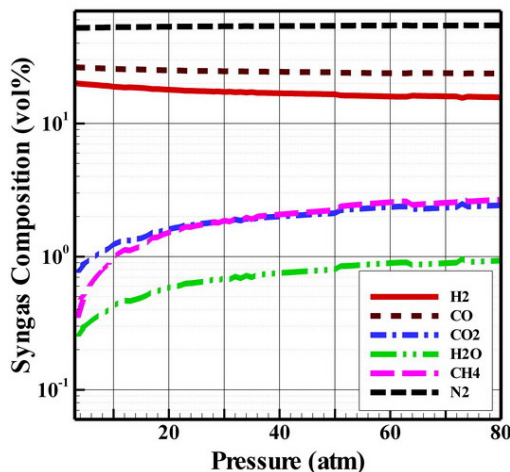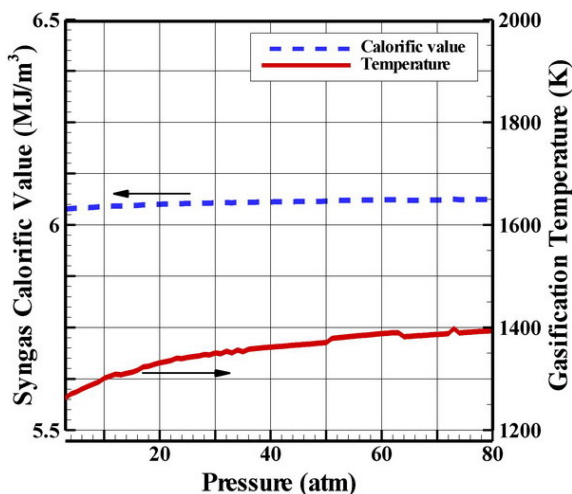

Fig. 10. Effects of equivalence ratio, oxygen enrichment, and gasification pressure on syngas H_2:CO ratio

As it can be observed in Fig. 10, an equivalence ratio of 0.37 represents the maximum H_2:CO ratio (i.e., 0.76). Beyond a value of 0.37, the greater the equivalence ratio, the lower the H_2:CO ratio is obtained. Increasing the oxygen enrichment increases the amount of both H_2 and CO with nearly the same rate (see Fig. 5); as a result, the H_2:CO ratio remains constant. Figure 10 also shows that the increase of gasification pressure from atmospheric pressure to 80 atm results in a small reduction of $H2$:CO ratio from 0.75 to 0.65.

4. CONCLUSION

A numerical algorithm based on thermochemical equilibrium approach was developed for the simulation of the heavy fuel oil gasification process. The model can predict the produced syngas species distribution and gasification characteristics under actual operating conditions. The model was validated by a comparison of the numerical results with those of the measurements. Through a parametric study, it was shown that the gasification of heavy fuel oil at a low equivalence ratio of 0.32, makes it possible to obtain a syngas with a considerable calorific value of about 15 MJ/m^3. A syngas with such heating value is suitable for applications like gas turbines that consume high calorific value gases. Taking the advantage of pure oxygen as gasification agent results in producing a high calorific value and hydrogen-rich syngas with hydrogen content of 42.5% by volume and H_2:CO ratio of about 0.76. A syngas with such a high H_2:CO ratio can be used in the methanol synthesis process and in the production of pure hydrogen for fuel cell applications. The parametric study also revealed that the gasification pressure had no significant effects on gasification characteristics.

The simulations performed in the course of this study suggest that the heavy oil gasification is a feasible process that can be utilized to generate a syngas for various industrial applications. The developed numerical model can be employed for the design and optimization of such gasifiers.
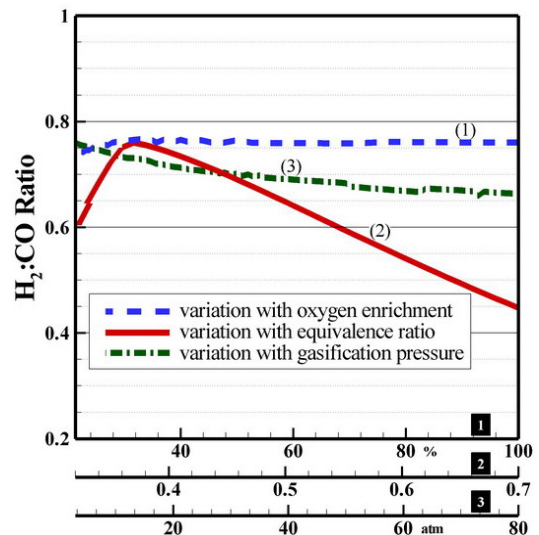

Fig. 8. Effect of gasification pressure on syngas composition

Fig. 9. Effect of gasification pressure on the syngas calorific value and gasification temperature

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