Gasification of Two Untapped Resources: El-Lajjun Oil Shale and Municipal Solid Waste (MSW)

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Abstract

This work explains a numerical model for the gasification of El-Lajjun oil shale and municipal solid waste (MSW) inside an air-fed atmospheric gasifier. The fuels were first characterized at the Waste-2-Energy Lab at Masdar Institute with thermo-gravimetric analyzer (TGA) for the proximate analysis, Flash 2000 for the ultimate analysis, and bomb calorimeter (Parr 6100) for the heating value determination. The model is based on the Langrangian-Eulerian approach whereby the solid phase particles are tracked with the Langrangian approach and the surrounding gas phase is tracked by the Eulerian phase. The model takes into account the turbulent flow for the continuous phase (SST k-ω model), gas phase gasification (species transport model), devotalization (Kobayashi two competing rate model), heterogeneous char reaction (multiple surface reaction model), particle dispersion by turbulent flow (stochastic discrete random walk model), radiation (P1), and particle distribution (Rosin Rammler model). The variations in the mole fraction of the product gas and temperature along the centerline of the gasifier was studied. While the mole fraction of carbon dioxide and water reduced along the centerline with increasing residence time, the mole fraction of the carbon monoxide and hydrogen rose along the centerline of the gasifier for both cases. Based on this study, the oil shale was shown to have an ash content of 60.88%, which indicates that it may require a low cost separation process of the ash and moisture from the feedstock, or tapping into the sensible heat of the ash, for it to be competitive for gasification.

Introduction

Two major feedstocks are not well utilized and sometimes cause problems in the world today. On one hand, huge amount of generated municipal solid wastes (MSW) are destined to be dumped into landfills worldwide. For example, over 5 million tons of solid waste was generated in Abu Dhabi alone in 2009 [1]. These solid wastes often end up in landfills, which causes lots of havoc. Landfills generates landfill gases that have a global warming potential of almost 21 times that of carbon dioxide. Apart from this, landfills occupy spaces that could be utilized for other purposes and harbor dangerous animals and disease agents. On the other hand, there are large reserves of oil shale, which aggregates to about 790 billion cubic meters worldwide [2]. The Green River deposits in the western part of United States, the Tertiary deposits in Australia, and the El Lajjun deposits in Jordan are some of the world

deposits that generate several million barrels of oil shale. These two feedstocks can be converted into synthetic gases of high economic value through their oxidation in limited amount of oxidant in a pathway known as gasification.

Some studies have examined the gasification effects on oil shale and MSW. Jaber [3] studied the effect of bed temperature and fluidizing gas type on the gas composition, quantity, and calorific value of the syngas during the gasification of Ellujun oil shale samples in a continuous feed fluidized bed reactor. In another work, Jaber et al. [4] investigated the influence of temperature on the gasification of oil shale in a continuous-fed fluidized bed reactor, using carbon dioxide as the fluidizing gas. Ingel et al. [5] studied the use of concentrated solar energy for gasifying oil shale with the solar central receiver at Weizmann Institute of Science. Xiao et al. [6] investigated the gasification characteristics of MSW in a fluidized bed gasifier at temperatures between 550-700° C. Thereafter, the melting characteristics of the fly ash generated was conducted within 1100-1460° C in a fixed bed furnace. Wang et al. [7] studied the steam gasification of MSW with NiO on modified dolomite (NiO/MD) catalyst in order to obtain a hydrogen rich synthetic gas.

The objective of this study is to investigate the entrained flow gasification behavior of Ellajun oil shale and MSW using ANSYS Fluent. The gasification numerical model is based on the drop tube experimental facility at Masdar Institute. The investigation starts with material characterization of the feedstocks in order to determine their suitability for gasification and provide essential data for the numerical model, which is based on the Lagrangian-Eulerian scheme. The model takes into account the turbulent flow for the continuous phase (realizable k- ε model), gas phase gasification (species transport model), devotalization (Kobayashi two competing rate model), heterogeneous char reaction (multiple surface reaction model), particle dispersion by turbulent flow (stochastic discrete random walk model), radiation (P1), and particle distribution (rosin rammler model). The model will aid in determining specific characteristic of each feedstock under the same conditions.

Material Characterization

Proximate Analysis

The thermo-gravimetric or proximate analysis is an essential tool in gasification process, which helps to break down the feedstock into moisture, volatile, fixed carbon, and ash. The decomposition process was conducted with a DSC/TGA Q600 thermal analyzer. These data (Figures 1 and 2; Table 1) are required in order to model the gasification process.



Figure 1. Proximate analysis of the El Lajjun oil shale



Figure 2. Proximate analysis of the MSW

Table 1. The proximate analysis of El Lajjun oil shale and municipal solid waste

Proximate Analysis	El Lajjun Oil Shale (Wt %)	Municipal Solid Waste(Wt %)
Moisture	1.62	7.56
Volatile	22.19	53.61
Fixed Carbon	15.30	22.38
Ash	60.88	16.45

Ultimate Analysis

The ultimate analysis is based on the determination of the elemental composition of the fuel. The elemental composition of any carbonaceous material in terms of the mass percentages of C, H, O, N, S components can be determined using FLASH Elemental Analyzer.

Determination of the elemental content composition is very important in gasification as it helps to determine the equivalence ratio of the fuel. The ultimate analysis data for the feedstocks are as depicted in Table 2.

Ultimate Analysis	El Lajjun Oil Shale (Wt %)	Municipal Solid Waste (Wt %)
Carbon	19.17	45.32
Hydrogen	1.96	5.68
Nitrogen	0.39	1.14
Oxygen	14.41	31.13
Sulfur	3.19	0.28
Ash	60.88	16.45

Table 2. The ultimate analysis of El Lajjun oil shale and municipal solid waste

Bomb Calorimetry

The bomb calorimeter helps to determine the heating value of the feedstocks to be gasified. The equipment used for this analysis was the Parr 6100 bomb calorimeter. The heating value obtained for the El Lajjun oil shale and MSW are 7.82MJ/kg and 17.57MJ/kg, respectively.

Model Development

The assumption of instantaneous equilibrium and equal diffusivity may be too generic for numerical solid feedstock conversion under gasification conditions. Hence, the numerical investigation for this gasification study is based on global reaction kinetics to more accurately describe the multi-physics, multi-scale, multi-phase model. The gasification process, which is based on the Langrangian-Eulerian approach (used due to the low volume loading in EFGs), is modeled with the consideration of four events. The Langrangian-Eulerian approach tracks the particles as they move in space and takes the gas phase as the whole control volume. As the particle is injected into the gasifier, residual moisture content in the feedstock is evaporated during passive heating. The volatile content is then released in a process known as devolatilization or pyrolysis. The volatiles and other gaseous species then undergo homogeneous reactions, but the char is consumed through heterogeneous reactions. While the particle was monitored over space, the continuum approach was used for the gas phase. The multi-physics, multi-scale model was developed to describe the details of the different physical and chemical processes occurring in the drop tube reactor (DTR) through key sub-models and their coupling. The mesh structure was developed with the GAMBIT meshing tool (Figure 3).



Fig. 3. The 2-D and 3-D mesh structure

The numerical model is based on the drop tube experimental facility at Masdar Institute (Figure 4). The specifications of the drop tube are listed in Table 4.

Parameter	Value
Length Tube B	1540 mm
Outer Diameter Tube B	75 mm
Inner Diameter Tube B	66 mm
Heated Length	750 mm
Power Rating	4.6 kW
Material Tube B	APM
Maximum Temperature	1400 K

Table 4. Drop tube specifications



Figure 4. Schematic representation of the drop tube experimental set-up

Gas Phase Analysis

The fluid phase was modeled with the Eulerian concept where a control volume—the DTR is being monitored. The conservation of mass, momentum, energy and species were ensured based on the equations in Table 5 respectively. The closure problem for the Reynolds stresses in the momentum equation was solved according to equation 5, and the gas phase turbulence was modeled with the k- ω shear stress transport model as represented in equations 6-8.

Quantity	Conservation Equation	
Mass	$\frac{\partial}{\partial x_i}(\rho u_i) = S_{p,m}$	(1)
Momentum	$\frac{\partial}{\partial x_j} \left(\rho u_i u_j \right) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left[\mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_l}{\partial x_l} \right) \right] + \frac{\partial}{\partial x_j} \left(-\rho \overline{u_i' u_j'} \right) + S_{p,mom}$	(2)
Energy	$\frac{\partial}{\partial x_i}(\rho u_i h) = \frac{\partial}{\partial x_i} \left[\lambda \frac{\partial T}{\partial x_i} \right] + S_{rad} + S_h + S_{p,h}$	(3)
Species	$\frac{\partial}{\partial x_i}(\rho u_i Y_i) = \frac{\partial}{\partial x_i}(\rho D Y_i) + S_{Yi} + S_{p,Yi}$	(4)
Reynolds Stresses	$-\rho \overline{u_i' u_j'} = \mu_t \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \left(\rho k + \mu_t \frac{\partial u_l}{\partial x_l} \right)$	(5)
Turbulent KE	$\frac{\partial}{\partial x_i}(\rho k u_i) = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + G_k - Y_k + S_k$	(6)
Specific Dissipation of Turbulent KE	$\frac{\partial}{\partial x_i}(\rho\omega u_i) = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_\omega} \right) \frac{\partial \omega}{\partial x_j} \right] + G_\omega - Y_\omega + D_\omega + S_\omega$	(7)
Turbulent Viscosity	$\mu_t = \alpha^* \frac{\rho k}{\omega}$	(8)

Table 5 List	of the	equations	for the	ase	nhase	nrocesses
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The kinetics for the homogeneous reactions and their chemical equations are described in Table 6.

	Table 6.	Kinetic	data for	the	homogeneous	reactions	[8-9]
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Reaction	Activation Energy (<i>E_a</i>)	Pre-Exponential Factor (A)	N
$CH_4 + \frac{1}{2}O_2 \rightarrow CO + 2H_2$	1.25×10^{8}	4.4×10^{11}	0
$H_2 + \frac{1}{2}O_2 \to H_2O$	1.67×10^{8}	6.8×10^{15}	-1
$CO + \frac{1}{2}O_2 \rightarrow CO_2$	1.67×10^{8}	2.24×10^{12}	0
$CH_4 + H_2 O \rightarrow CO + 3H_2$	1.25×10^{8}	3×10^{8}	0
$CO + H_2O \rightarrow CO_2 + H_2$	8.37×10^{7}	2.75×10^{9}	0

Particle Phase Analysis

In this model, and for entrained flow gasifiers in general, the discrete Lagrangian frame of reference is used to track each spherical particles of diameter distribution given by Rosin-Rammler. This approach is valid since its fundamental loading assumption is that the volume fraction of the solid phase must be less than 10% [10]. The conservation of mass, momentum and energy of the particles are given in the equations in Table 7.

Quantity	Conservation Equation	
Mass	$\frac{dm_p}{dt} = \frac{dm_{C-O_2}}{dt} + \frac{dm_{C-CO_2}}{dt} + \frac{dm_{C-H_2O}}{dt} + \frac{dm_{pyrolysis}}{dt} + \frac{dm_{vapor}}{dt}$	(9)
Momentum	$\frac{du_p}{dt} = F_D(u - u_p) + \frac{g_i(\rho_p - \rho)}{\rho_p} + F_i$	(10)
Drag	$C_D = a_1 + \frac{a_2}{Re_p} + \frac{a_3}{Re_p^2};$	(11)
	$Re_p = \frac{\rho d_p u - u_p }{\mu};$	
	$F_D = \frac{18\mu}{\rho_p d_p^2} \frac{C_D R e_p}{24}$	
Energy	$Q_{G} = \frac{dm_{C-O_{2}}}{dt}H_{C-O_{2}} + \frac{dm_{C-CO_{2}}}{dt}H_{C-CO_{2}} + \frac{dm_{C-H_{2}O}}{dt}H_{C-H_{2}O}$	(12)
	$m_p c_p \frac{dT_p}{dt} = h_p A_o (T - T_p) + \frac{\varepsilon_p A_o}{4} (G - 4\sigma T_p^4) + Q_G$	
Nusselt Number	$Nu = \frac{h_p d_p}{k_g} = 2.0 + 0.6 Re_p P r^{\frac{1}{3}}$	(13)

Table 7. List of the equations for the particle phase processes

The char gasification process consists of three reactions namely: $char-O_2$, $char-CO_2$ and $char-H_2O$. The first reaction is exothermic and releases heat into the reactor. However, the last two reactions are endothermic and require a lot of heat for them to proceed, as is apparent in their activation energy values in Table 8.

Reaction	Activation Energy, <i>E_a</i> (J/mol)	Pre-Exponential Factor (A)	Ν	
$C + \frac{1}{2}O_2 \to CO$	9.23×10^{7}	2.3	1	
$C + \overline{CO}_2 \rightarrow 2CO$	1.62×10^{8}	4.4	1	
$C + H_2 O \to CO + H_2$	1.47×10^{8}	1.33	1	

Table 8. Kinetic data for the heterogeneous reactions [11]

Results and Discussions

Model Validation

The validity of the results of every point on the contour depends mainly on the rigor of the constraint for the validation of the experimental data. The more the model results agree with the experimental values, the more the fidelity in the model. Hence, the numerical model has been validated with experimental data obtained from the drop tube experimental set-up at Masdar Institute. The model results predict the experimental values reasonably well under both non-reactive and reactive conditions as depicted in Figures 5-6. The experimental values were obtained with the drop tube facility at Masdar Institute.



Figure 5. Axial temperature validation with experimental data for non-reactive flow



Figure 6. Axial temperature validation with experimental data for reactive flow

Effect of Gasification of Oil Shale and MSW

One of the most important issues as regards the use of gasification is its fuel flexibility capability. Hence, this study had been conducted to observe the behavior of entrained flow gasifiers to oil shale and MSW. The contour profile of the temperature (Figure 7) showed that the temperature in the gasifier during the conversion of the MSW is generally higher as compared to that of the oil shale. This is due to the higher volatile content in the MSW. Volatile matter are known to undergo exothermic reactions, which generate a lot of heat.



Figure 7. Contour profile of the temperature: MSW (left), oil shale (right)

The mole fraction of the oxidant along the gasifier confirmed that the reactor is under gasification conditions (Figure 8). The mole fraction of the oxidant along the gasifier showed that the oxygen content finished along the reactor for both feedstocks. However, the oxidant finished earlier for the oil shale. This can be accounted to the lower oxygen content in the oil shale.



Figure 8. Contour profile of the oxygen mole fraction: MSW (left), oil shale (right)

The mole fraction of the volatile (Figure 9) showed that more volatile matter was released for the MSW as compared to the oil shale. This is evident from the fact that MSW (53.61%) contains more volatile than oil shale (22.19%).



Figure 9. Contour profile of the volatile mole fraction: MSW (left), oil shale (right)

Conclusions

El Lajjun oil shale and MSW have been analyzed for their material characteristics at the Waste-2-Energy Lab. at Masdar Institute. The result showed that El Lajjun oil shale has a high quantity of ash (60.88%) and oxygen (14.41%), which in turn affected its gasification behavior. However, the MSW yielded a lower amount of ash (16.45%) but produced more volatile matter (53.61%) and oxygen (31.13%). A predictive model has been developed for the gasification of El Lajjun oil shale and MSW. The model has been validated with MI drop tube experimental data. This model allows for the observation of specific gasification behavior of each of the feedstocks. Based on this study, the oil shale was shown to have an ash content of 60.88%, which indicates that it may require a low cost separation process of the ash and moisture from the feedstock, or tapping into the sensible heat of the ash, for it to be competitive for gasification.

Future works would involve the utilization of large eddy simulation to study the gasification of these two feedstocks. With the large eddy simulation, the turbulence can be more appropriately captured. In addition, the effect of ash minerals on the gasification of high ash feedstocks would be studied.

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