2nd World Congress on
Petrochemistry and Chemical Engineering
October 27-29, 2014 Las Vegas, USA

CFD and Process Simulations of air gasification of plastic wastes in a conical spouted bed gasifier

Dr. Abdallah S. Berrouk
Dr. Chaohe Yang
Mr. Yupeng Du

Outline

- Background
- Process description
- CFD model and analysis
- ERN model and Process simulations
- Results and discussion
- Conclusions

Background

- Total consumption of plastics in both developing and developed countries has dramatically increased in the recent years (200 billions pounds as of 2013)
- Plastics have an LHV of 40 MJ/kg much higher in comparison with biomass (10MJ/kg) or Coal (30 MJ/kg) which are extensively utilized as energy sources
- Current plastic waste treatment technologies are: landfill, mechanical recycling, chemical recycling, and incineration.
- The chemical recycling approach does not only recovers valuable petrochemicals as feedstock, it also produces energy in the form of heat, steam, etc.
- Advantages of conical spouted bed gasifier over fluidized-bed gasifier: vigorous solid circulation pattern; high heat transfer rates; simple design; low segregation, etc.

Background

- Based on the hydrodynamics of the gas–solid flow in CSB, the entire vessel can be divided into four zones: spout, annulus, fountain and freeboard.
- The equivalent reactor network (ERN) methodology seems quite suitable for modeling spouted bed gasifiers.
- CFD-based ERN model is developed through a procedure consisting of three steps.
- CFD model is run that accounts only for the reactor hydrodynamics.
- An image analysis or algorithm is applied to the CFD-generated flow field to create an ensemble of connected zones or compartments.
- Each zone or compartment is considered as an ideal chemical reactor and 0-dimensional or 1-dimensional calculations are run with detailed kinetics.

Background

➢CFD-based ERN models reasonably simplify transport process and avoid calculation divergences of CFD models

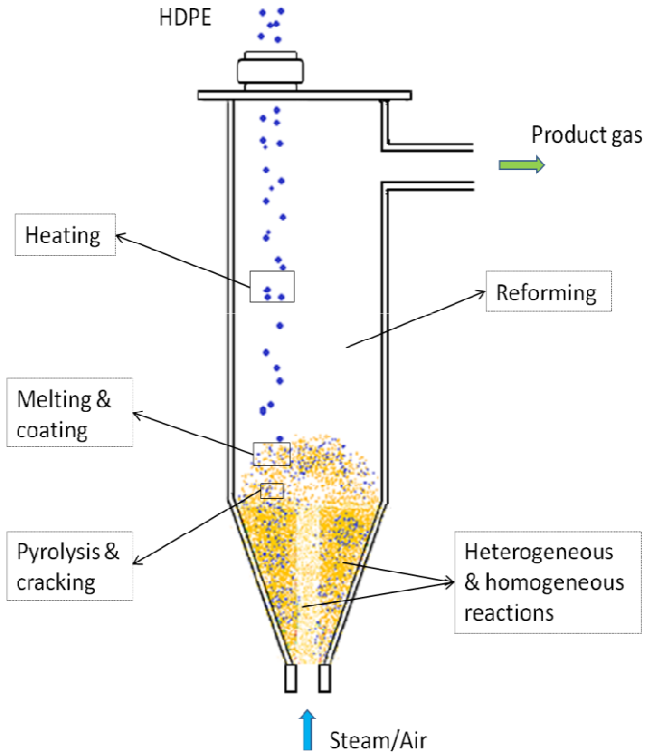
➢This especially true for situations where many kinds of reactants and complicated and non-linear reaction paths are involved in the process.

➢ ERN models perform simulations in very short time generally in the magnitude of several minutes or even fewer on a desktop personal computer compared to multiple days or months on multiple processors for more detailed CFD simulations.

➢ The main objective of the present study is to investigate using CFD-based ERN model air gasification of a plastics waste feedstock that consists of 100% polyethylene in a conical spouted bed reactor.

Process description

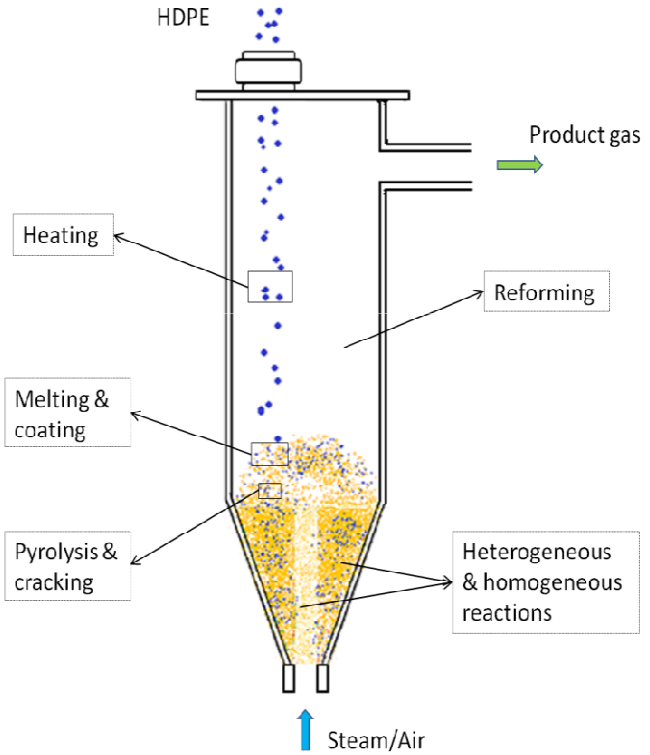
- The gasifying agent (air or steam) is blown upwards from the bottom inlet of the vessel
- PE particles introduced from the top inlet
- PE particles melt and coat on silic sands, release a large amount of volatiles and little amount of char
- Released volatiles are commonly the mixture consisting of many species such as H_2, CH_4, C_2H_4, C_3H_6, and heavier hydrocarbons which are usually termed as primary tars.



Schematic diagram of a spouted bed gasifier (SBG)

Process description

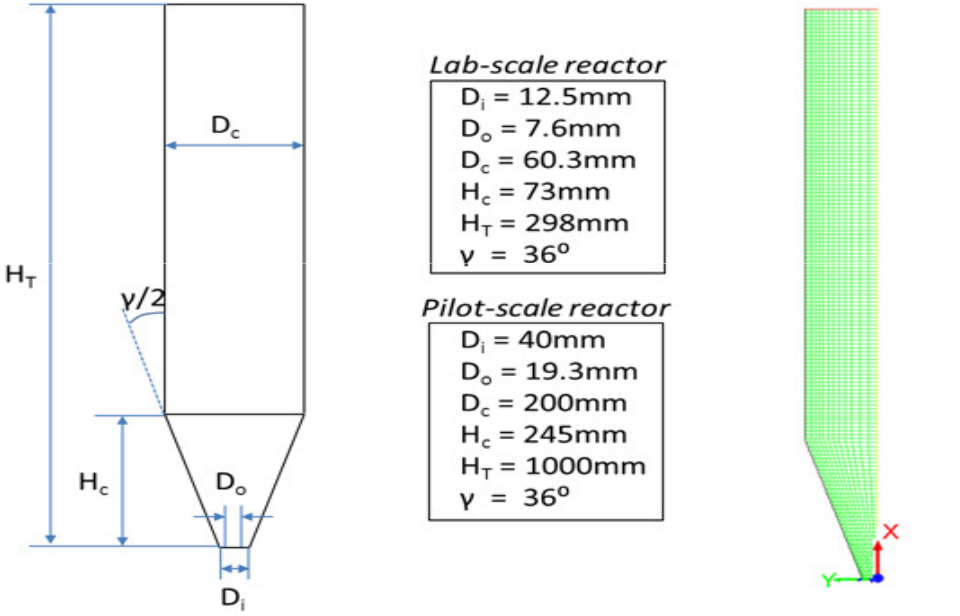
- Heterogeneous reactions and homogeneous reactions takes place in annulus and spout zones
- The difference between the reactions' products in the two zones is dictated by the volume fraction of solid and the contact time with the gasifying agent in both zones.
- Secondary reactions of tars on sands take place in freeboard
- They include stream reforming, dry reforming, oxidation, and cracking reactions.
- The products of the secondary reactions of primary tars are generally non-condensable gases, condensable species (usually termed as secondary tars and char



Schematic diagram of a spouted bed gasifier (SBG)

CFD model and analysis

- The computational domain is a newly-designed conical spouted bed gasifier (SBG) at a laboratory scale
- Mesh consists of regularly-structured quadrilateral elements (7,780 cells) that provide quick convergence and minimal numerical errors
- Two-Fluid Model is used
- Kinetic theory of granular flows (KTGF) is used to close the solid phase equations



(a) The geometry and main dimensions of the vessel (b) The numerical grids

Geometry of the spouted bed and the numerical grid used

CFD model and analysis

- Continuity Equations (k=g, s):

$$\frac{\partial}{\partial t}(\alpha_k \rho_k) + \nabla \cdot (\alpha_k \rho_k \mathbf{v}_k) = 0$$

- Momentum Equations (k=g, s; l=s, g):

$$\frac{\partial}{\partial t}(\alpha_k \rho_k \mathbf{v}_k) + \nabla \cdot (\alpha_k \rho_k \mathbf{v}_k \mathbf{v}_k) = -\alpha_k \nabla p_g + \nabla \cdot \boldsymbol{\tau}_k + \alpha_k \rho_k \mathbf{g} + K_{lk}(\mathbf{v}_l - \mathbf{v}_k)$$

- Turbulence Model (k-ϵ):

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho u_i k) = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right] + G_k + G_b - \rho\varepsilon - Y_M$$

$$\frac{\partial}{\partial t}(\rho \varepsilon) + \frac{\partial}{\partial x_i}(\rho u_i \varepsilon) = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_j}\right] + C_{1\varepsilon}\frac{\varepsilon}{k}\left(G_k + C_{2\varepsilon}\rho\frac{\varepsilon^2}{k}\right)$$

- Stress Equations:

$$\boldsymbol{\tau}_g = 2\mu_g \mathbf{S}_g + \alpha_g \lambda_g \nabla \cdot \mathbf{v}_g$$

$$\boldsymbol{\tau}_s = [-p_s + \alpha_s \lambda_s \nabla \cdot \mathbf{v}_s] + 2\mu_s \mathbf{S}_s$$

CFD model and analysis

- Deformation Rate:

$$\mathbf{S}_k = \frac{1}{2}\alpha_k\left[\nabla v_k + (\nabla v_k)^T\right] - \frac{1}{3}\alpha_k \nabla \cdot \mathbf{v}_k \mathbf{I}$$

- Solid Phase Pressure:

$$p_s = \alpha_s \rho_s \Theta_s \left[1 + 2\alpha_s g_0 (1+e)\right]$$

- Solid Phase Viscosity:

$$\mu_s = \mu_{s,kin} + \mu_{s,col}$$

$$\mu_{s,kin} = \frac{\alpha_s d_s \rho_s \sqrt{\Theta_s \pi}}{6(3-e)}\left[1 + \frac{2}{5}(1+e)(3e-1)\alpha_s g_0\right]$$

$$\mu_{s,col} = \frac{4}{5}\alpha_s \rho_s d_s g_0 \pi (1+e)\sqrt{\frac{\Theta_s}{\pi}}$$

- Granular Temperature Equation:

$$\frac{3}{2}\left[\frac{\partial}{\partial t}(\rho_s \alpha_s \Theta_s) + \nabla \cdot (\rho_s \alpha_s \mathbf{v}_s \Theta_s)\right] = \boldsymbol{\tau}_s : \nabla \mathbf{v}_s - \nabla \cdot (k_{\Theta_s} \nabla \Theta_s) - \gamma - 3\beta\Theta_s$$

- Collisional Energy Dissipation:

$$\gamma = \alpha_s^2 \rho_s g_0 (1-e^2)\frac{12}{d_p\sqrt{\pi}}\Theta_s^{3/2}$$

CFD model and analysis

- Drag Coefficient:

$$K_{sg} = 150\frac{\alpha_s^2 \mu_g}{\alpha_g d_p^2} + 1.75\frac{\alpha_s \rho_g |u_g - u_s|}{d_p}, \quad when\ \alpha_g < 0.8$$

$$K_{sg} = \frac{3}{4} C_D \frac{\alpha_s \alpha_g \rho_g |u_g - u_s|}{d_p} \alpha_g^{-2.65}, \quad when\ \alpha_g > 0.8$$

- Where:

$$C_D = \frac{24}{Re_s}\left[1 + 0.15(Re_s)^{0.687}\right], \quad for\ Re_s \le 1000$$

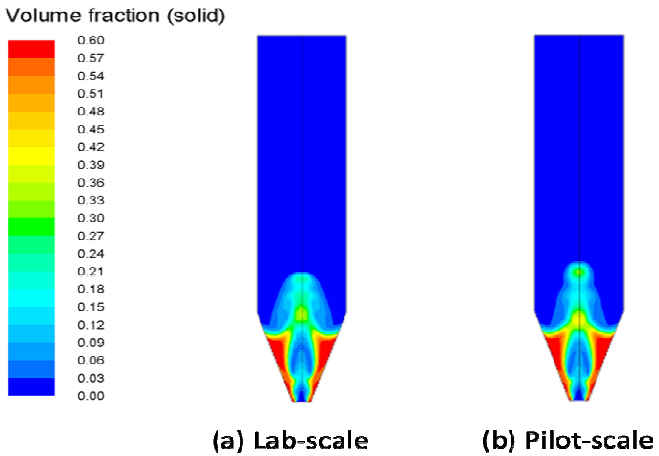
$$C_D = 0.44, \quad for\ Re_s > 1000$$

$$Re_s = \frac{\alpha_g \rho_g d_p |u_g - u_s|}{\mu_g}$$

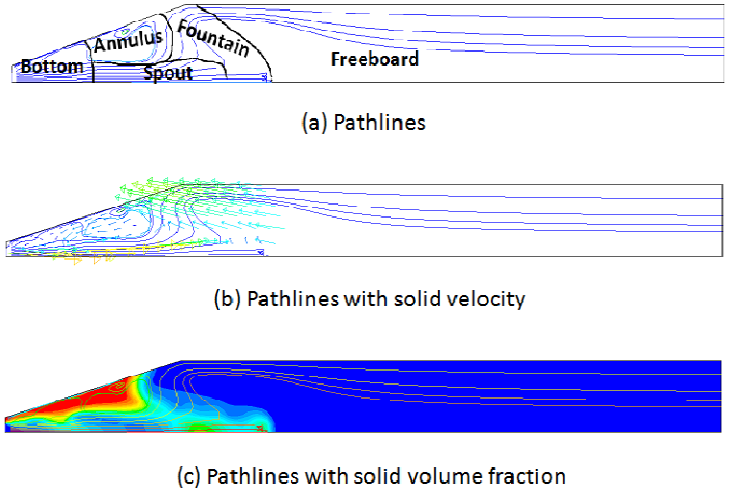
CFD model and analysis

CFD results analysis:

- Figures illustrate flow pathlines, flow pathlines with solid velocity vectors, and flow pathlines with solid volume fraction in the SB.
- The CFD results depict well the four different zones characterizing solid-gas flow in the SB



Time-averaged solid volume fraction at different times

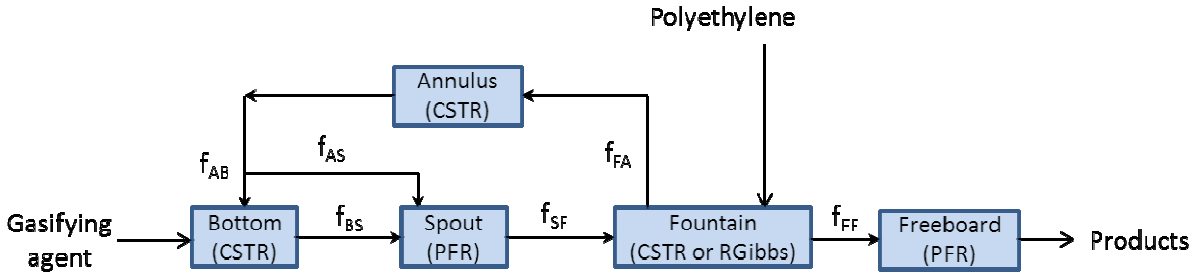


Flow pathlines from inlet of the spouted bed gasifier

CFD model and analysis

CFD results analysis:

1. *Bottom* zone: continuous stirred tank type of reactors (CSTR);
2. *Annulus* zone: CSTR;
3. *Spout* zone: plug flow type of reactor (PFR);
4. *Fountain* zone: either a CSTR or RGibbs reactor;
5. *Freeboard* zone: PFR



A reactor network constructed for spouted bed vessel based on CFD analysis

CFD model and analysis

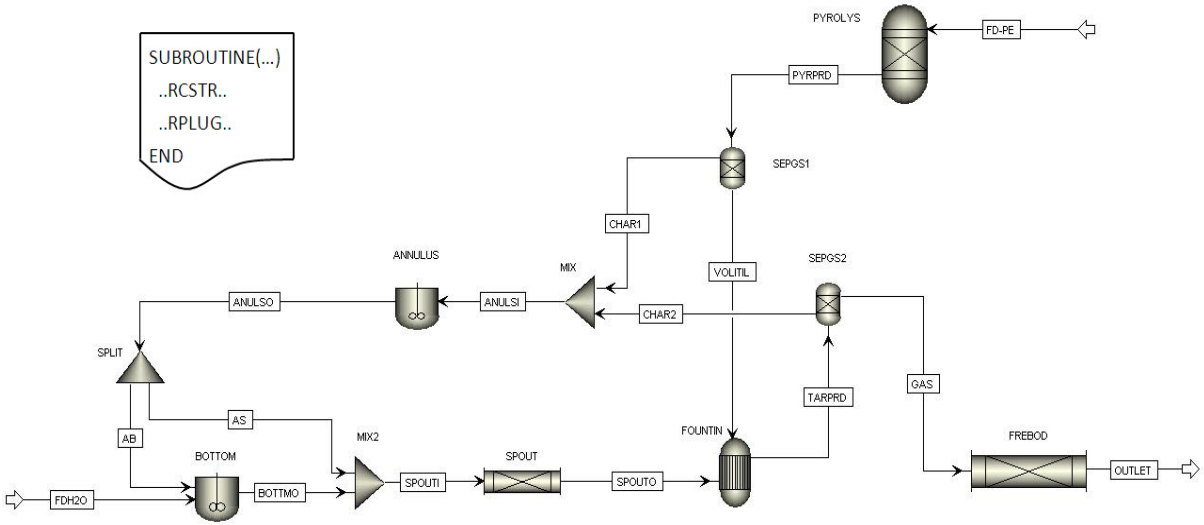
CFD results analysis:

Zone name	Reactors representing the zone	Characteristics of each reactor	Averaged gas volume fraction in each reactor	Fraction of mass flux between connected reactors
Bottom	CSTR	Volume=8.83e-5m^3	0.78	f_{BS}=1.0; f_{gBS}=0.82; f_{gBA}=0.18
Spout	PFR	Length=0.2m; Diameter=0.02m	0.88	f_{SF}=1.0; f_{gSF}=1.0
Annulus	two CSTRs in series	Volume=1.87e-3m^3	0.441	f_{AB}=0.93; f_{AS}=0.07
Fountain	RGibbs	Volume=2.43e-3m^3	0.73	f_{FA}=1.0; f_{gFF}=1.0
Freeboard	PFR	Length=0.7m; Diameter=0.20m	0.999	

Auto-zoning results for ERN model based on the CFD analysis

ERN model and process simulations

- Construction of an equivalent reactor network model (ERN) for the newly-designed conical spouted bed gasifier based on the CFD results.
- The structure of the reactor network is based on the schematic depicted in the Figure below with an added PE pyrolysis reactor and Rgibbs reactor to represent the fountain zone.

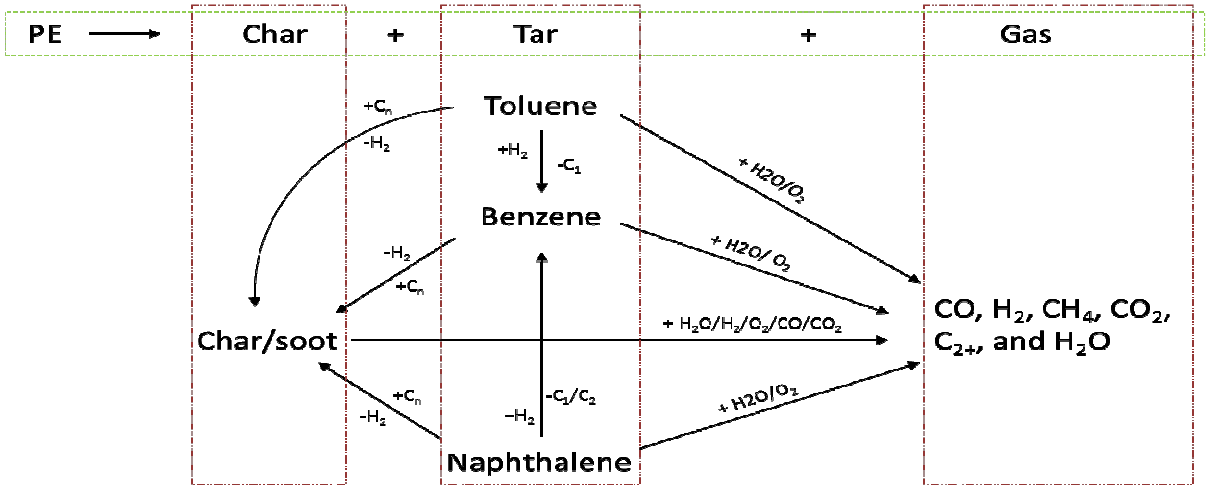


Simulation flowchart

ERN model and process simulations

Reactions:

- *Pyrolysis:* the yields of the gas and tar are ***64.11%wt*** and ***35%wt***, respectively, and the rest are char. The gas consists of ***0.056%wt H_2***, ***0.149%wt CH_4***, and **0.795%wt C_{2+}**(Cozzani's data at 700^{0}C). Benzene, toluene and naphthalene are used to represent PE tar.
- *Gasification* process is described using a simplified reaction scheme



Simplified reaction scheme of polyethylene gasification process

ERN model and process simulations

Reaction number	Stoichiometry	Reaction name	Reference
1	$C_6H_6 + 7.5O_2 \rightarrow 6CO_2 + 3H_2O$	oxidation	Gerun et al.[40]
2	$C_7H_8 + 3.5O_2 \rightarrow 7CO + 4H_2$	oxidation	Su et al.[41]
3	$C_{10}H_8 + 12O_2 \rightarrow 10CO_2 + 4H_2O$	oxidation	Su et al.[41]
4	$pC_mH_n \rightarrow qC_xH_y + rH_2$	thermal cracking	Li et al.[42]
5	$C_7H_8 + 7CO_2 \rightarrow 14CO + 4H_2$	dry reforming	Wu et al.[43]
6	$C_6H_6 + 2H_2O \rightarrow 1.5C + 2.5CH_4 + 2CO$	steam reforming	Su et al.[41]
7	$C_6H_6 + 6H_2O \rightarrow 9H_2 + 6CO$	steam reforming	Coll et al.[44]
8	$C_7H_8 + 7H_2O \rightarrow 11H_2 + 7CO$	steam reforming	Kantarelis et al.[38]
9	$C_{10}H_8 + 10H_2O \rightarrow 14H_2 + 10CO$	steam reforming	Wang et al.[45]
10	$C_7H_8 + H_2O \rightarrow C_6H_6 + CO + 2H_2$	steam dealkylation	Wu et al.[43]
11	$C_7H_8 \rightarrow 4H_2 + 7C$	carbon formation	Srinivas et al.[34]
12	$C_{10}H_8 \rightarrow 4H_2 + 10C$	carbon formation	Li et al.[42]
13	$C_7H_8 + H_2 \rightarrow CH_4 + C_6H_6$	hydrodealkylation	Jess[46]

C_mH_n represents tar, and C_xH_y represents hydrocarbon with smaller carbon number than C_mH_n.

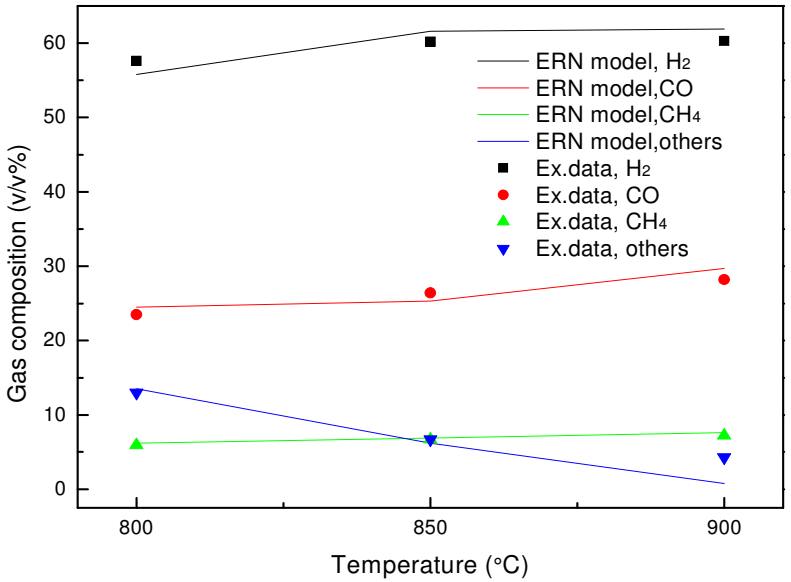
Possible reactions of tar with benzene, toluene, and naphthalene

Results and discussion

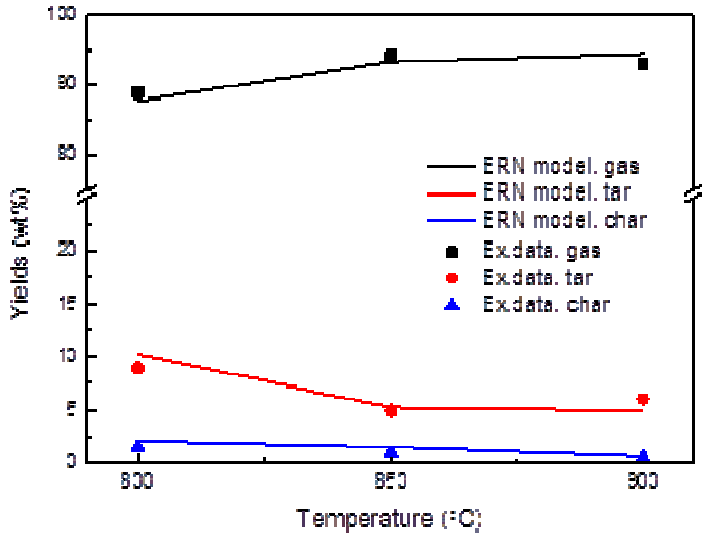
Model validation:

- The Model predictions are compared to the experimental observations of Erkiaga *et al. (Fuel* 2013**,** *109*, 461-469.)

- ERN model predictions of gasification products, including H_2, CO, and CH_4, are in very good agreement with experimental data.



Gas compositions as predicted by ERN model and Erkiaga et al. (2013) experiment for S/P=1.0

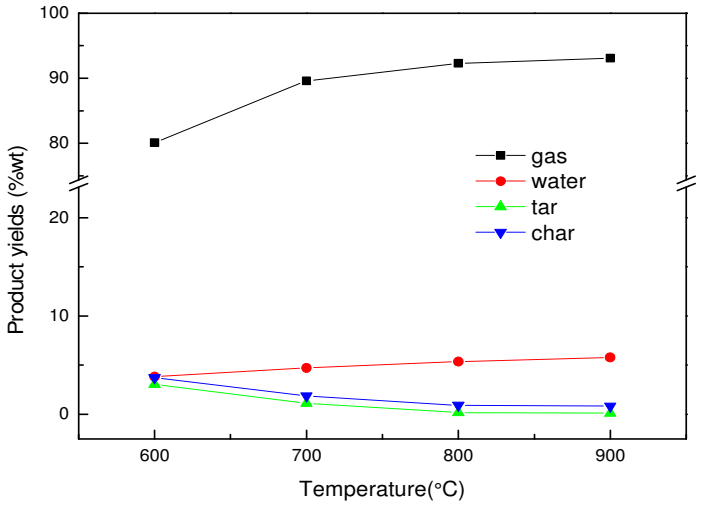


Products yields as predicted by ERN model and Erkiaga et al. experiment for S/P=1.0.

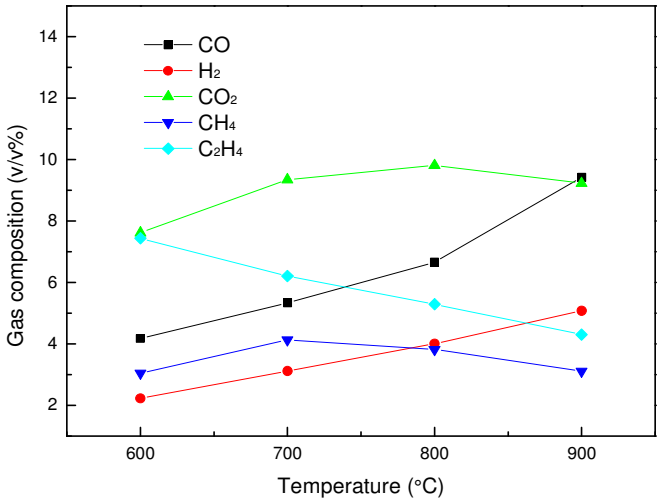
Results and discussion

Effect of Temperature:

A range of 600 ^{0}C to 900 ^{0}C is selected for the purpose of finding out the optimum T for PE gasification process at ER=0.4^{0}C.



Effect of gasification temperature on products yield at ER=0.4

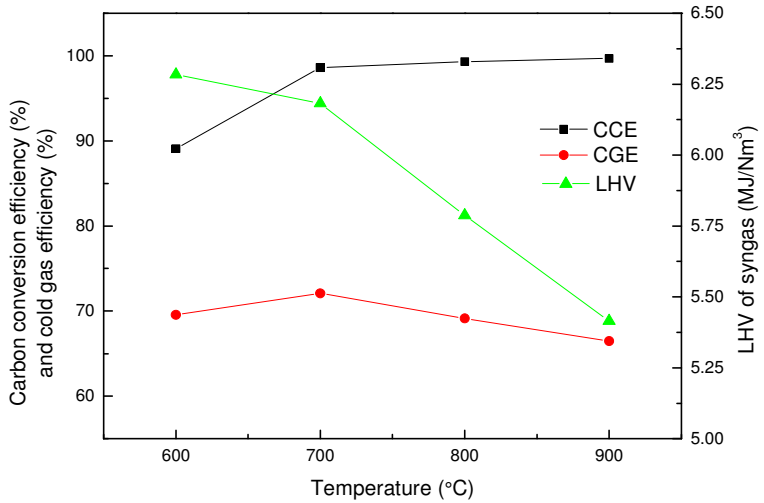


Effect of gasification temperature on syngas composition at ER=0.4

Results and discussion

Effect of Temperature:

$$LHV(MJ\ Nm^{-3}) = (30 \times [CO] - 25.7 \times [H_2] - 85.4 \times [CH_4] - 151.3 \times [C_2H_4]) \times 4.2 \quad 1000$$



Effect of gasification temperature on syngas LHV, CGE, and CCE at ER=0.4

$$CGE = \frac{carbon\ content\ in\ syngas \times syngas\ flow\ rate}{carbon\ content\ in\ PE\ feed \times PE\ flow\ rate} \times 100\%$$

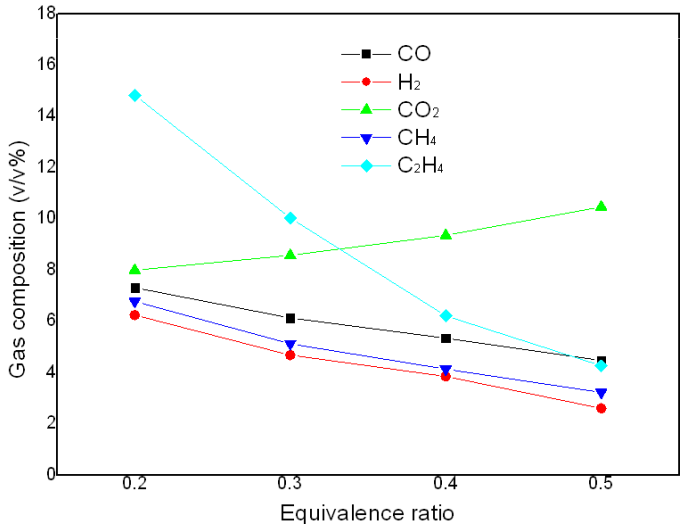
$$CCE = \frac{LHV\ of\ syngas \times syngas\ flow\ rate}{LHV\ of\ PE\ feed \times PE\ flow\ rate} \times 100\%$$

$$ER = \frac{weight\ of\ air \quad weight\ of\ PE}{stoichiometric\ air \quad PE\ ratio}$$

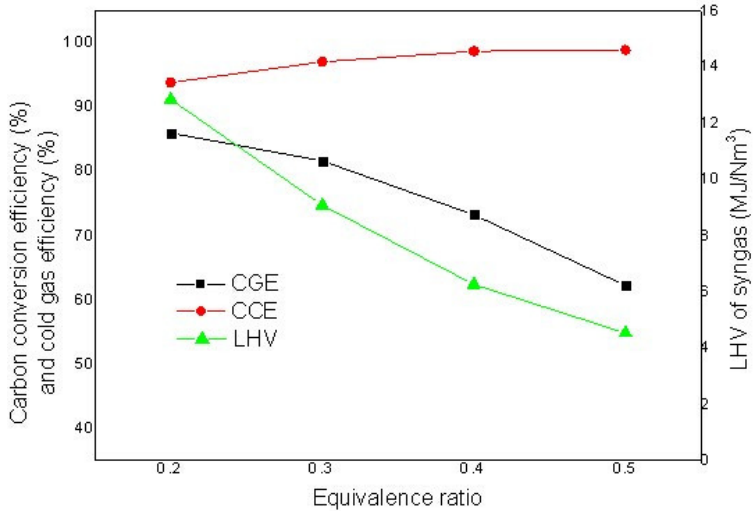
Results and discussion

Effect of Equivalence Ratio:

A range of 0.2 to 0.5 is selected for the purpose of finding out the optimum ER for PE gasification process at T=700^{0}C.



Effect of ER on syngas composition at T=700^{o}C



Effect of ER on syngas LHV, CCE, CGE at T=700^{o}C

Conclusions

- Plastic waste gasification is one of the most promising techniques to use non-decomposable solid waste and to produce syngas.

- CFD-based Equivalent Reactor Network (ERN) model is developed for simulation of polyethylene gasification in a designed pilot-scale conical spouted bed gasifier.

- CFD-based ERN model is established through two steps:
  (i) hydrodynamics simulations using CFD; (ii) the equivalent reactor network is built with gasification reactions taken into account through external FORTRAN modules.

- Model predictions are in very good agreement with experimental data of a lab-scale conical spouted bed gasifier used for steam gasification of polyethylene.

Conclusions

- Developed CFD-based ERN model is used to investigate the effects of gasification temperature and equivalence ratio on the gasification performance of polyethylene in a pilot-scale CSB reactor.
- It is found that the proper values of temperature and ER for air gasification are 700℃ and 0.4, respectively.
- With this operation condition, a value of LHV of 6.2MJ/Nm3, a value of CGE of 72.14% and a value of CCE of 97.3% are recorded
- Present work has demonstrated the capabilities of the developed CFD-based ERN model in simulating polyethylene waste gasification process
- It has also demonstrated the appropriateness of the designed pilot-scale conical spouted bed gasifier to carry out such a process.