

PHYSICAL-MATHEMATICAL MODEL FOR FIXED-BED SOLID FUEL GASIFICATION PROCESS SIMULATION

Konstantin V. Slyusarskiy^{1,*}, *Alexander G. Korotkikh*¹, and *Ivan V. Sorokin*¹

¹Tomsk Polytechnic University, 634050, Tomsk, Russia

Abstract. Physical-mathematical model for fixed-bed coal gasification process simulation is proposed. The heterogeneous carbon oxidation chemical reactions were simulated via Arrhenius equation while homogeneous reactions in gas phase were calculated using Gibbs free energy minimization procedure. The syngas component concentration field and fuel conversion distribution as well as syngas final temperature and composition were defined for fixed bed gasification of T-grade coal of Kuznetskiy deposit. The optimal fuel residence time and gasifier specific productivity were defined. The prevail reactions in oxidizing and reduction zones together with its height were defined.

1 Introduction

Solid fuel is one of major sources of primary energy in the world nowadays according to BP data [1] and provides nearly 30 % of world generation. While energy consumption is expected to increase by 35 % to 2035 year the share of coal generation is expected to be significant and has a value close to 25 % [1]. Such decrease is seem to appear due to economic and ecological issues connected to coal usage like carbon, sulfur and nitrogen oxide emissions, lower efficiency compared to combined cycle for natural gas and solid particles in flue gases [2].

The solid fuel gasification may solve both these problems. Syngas may be used in combined cycle. Gasification process features allow to decrease nitrogen oxide formation intensity and apply modern gas-cleaning technics [3] which are inefficient with existing direct combustion technology.

Gasification – process of turning fixed carbon from coal into combustible gas – include many chemical reactions and physical processes. That makes it quite difficult to define process outcome at different expoitational conditions. To resolve this problem the physical-mathematical model with macrokinetic limitations was proposed. Based on it the gasification process characteristics were calculated for T-grade bituminous coal of Kuznetskiy deposit.

2 Material characterization

* Corresponding author: konstantinsv@tpu.ru

The T-grade bituminous coal was used to simulate fixed bed coal gasification process. The fuel proximate analysis was carried out using ISO 17246:2010 [4]. The moisture, ash, volatile matter and fixed carbon content values were defined. Ultimate analysis was carried out via Euro EA 3000 CHNOS analyzer. Results presented in Table 1.

Table 1. Proximate and ultimate analysis results for T-grade bituminous coal.

Proximate analysis, wt. %				Ultimate analysis, wt. %				
Moisture	Ash	Volatiles	Fixed carbon	C	H	N	S	O
3	21	20	66	68	4	3	<1	4

Kinetic characteristics of heterogeneous carbon oxidation reactions for T-grade mark coal were taken from literature data [5]. The frequency factor and activation energy values for reactions of carbon interacting with oxygen and carbon dioxide as the most intense reactions are given in table 2.

Table 2. Kinetic constant values for heterogeneous chemical reactions.

Химическая реакция	$C+O_2=CO_2$	$C+CO_2=2CO$
Pre-exponential factor A_0 , 1/c	211	71230
Energy of activation E_a , кДж/моль	21	156

3 Model statement

The fixed bed counter-flow gasification process was modeled. Reactor chamber was presented as a set of consequently connected cylindrical domains with equal height and fuel residence time. The temperature distribution in each domain was considered to be uniform. The rate of heterogeneous chemical reactions were simulated via Arrhenius equation. Considering fuel residence time in each domain to be marked as τ , the total amount of turned into gas phase carbon could be calculated as:

$$w_i = A_0 \exp\left(\frac{-E_a}{R \cdot T_i}\right) (1 - X_i) \tau [OX] \quad (1)$$

there R – gas constant, J/(mole K); T_i – temperature in domain i , K; X_i – fuel conversion value; τ – fuel residence time, s; $[OX]$ – oxidizer molar concentration. Conversion value could be calculated as:

$$X_i = \frac{m_i - m_a}{m_0 - m_a} = X_{i-1} - w_i \quad (2)$$

here m_i – fuel mass after i^{th} domain, kg; m_a – ash mass, kg; m_0 – initial fuel mass, kg.

Because next conversion value depends on previous, to increase calculation preciseness the equation 1 was integrated by time:

$$\int_{X_i}^{X_{i+1}} dX = \int_{t_i}^{t_{i+1}} A_0 \exp\left(\frac{-E_a}{R \cdot T}\right) (1 - X) dt \quad (3)$$

there t is time moment, s.

Considering $t_{i+1} - t_i = \tau$ analytical solution of equation 3 will take the following form:

$$X_{i+1} = 1 - (1 - X_i) \exp\left(-A_0 \exp\left(\frac{-E_a}{R \cdot T}\right) \tau\right) \quad (4)$$

The gas-phase composition was defined by Gibbs free energy minimization procedure with assumption that gaseous mixture in each domain exists in equilibrium by following equation [6]:

$$G = RT \sum_{i=1}^m n_i \left((\mu_i / RT)_i + \ln\left(n_i / \sum_{i=1}^m n_i\right) \right), \quad (5)$$

there n_i – molar amount of i^{th} substance, mole; μ_i – molar potential of i^{th} substance, J/mole, which could be defined as follows:

$$\mu_i = h_i - s_i T + RT \ln(p / p_0), \quad (6)$$

there h_i , s_i – enthalpy and entropy of formation of i^{th} substance at temperature T , J/mole, J/(mole K); p_0 and p – ambient and current pressure in system, Pa.

To follow material balance of system with N substances and M types of atoms the possible solution domain was limited by following set of equations:

$$\sum_{i \in N} a_{ij} n_i = b_j, \quad j \in M, \quad n_i > 0, \quad (7)$$

there a_{ij} – stoichiometric coefficient (number of j -type atoms in molecule i); b_j – total amount of j -type atom in system, mole.

The Gibbs free energy minimization procedure was realized using Lagrange multipliers via steepest descent methods. As long as presence of components with close to zero content has a negative impact on calculation preciseness the number of taken into account substances was decreased to six following: H_2O , CO , CO_2 , H_2 , CH_4 and O_2 . Nitrogen content in air and inorganic matter content in fuel were considered to be chemically passive and were taken into account only in equation of thermal balance.

To define thermal effect of turning system from initial condition into final the Hess law was used:

$$\Delta H_r = \sum n_i^{pr} H_{fi}^{pr} - \sum n_i^f H_{fi}^f, \quad (8)$$

there H_{fi} – enthalpy of formation of i^{th} substance, J/mole; « pr » and « f » indexes refer to reaction products and feed, respectively.

Thermal effect of process could be defined as follows:

$$Q = \Delta H_r + \sum H_i^f m_i - \sum H_i^{pr} m_i, \quad (9)$$

there H_i – i^{th} substance heat of formation, J/kg; m_i – mass of i^{th} substance, kg.

3 Simulation results

Using proposed model the fixed bed gasification process characteristics were defined for T-grade bituminous coal. The initial conditions were 400 °C for gaseous feed and 20 °C for fuel. The coal/steam/air ratio was 1/1/1.5 according to [7]. The residence time of fuel in

gasifier was chosen to supply final conversion 0.9 and was defined to equal to 0.15 min. The temperature and conversion fields were obtained (fig. 1) as well as substance concentration distribution (fig. 2) over reactor height.

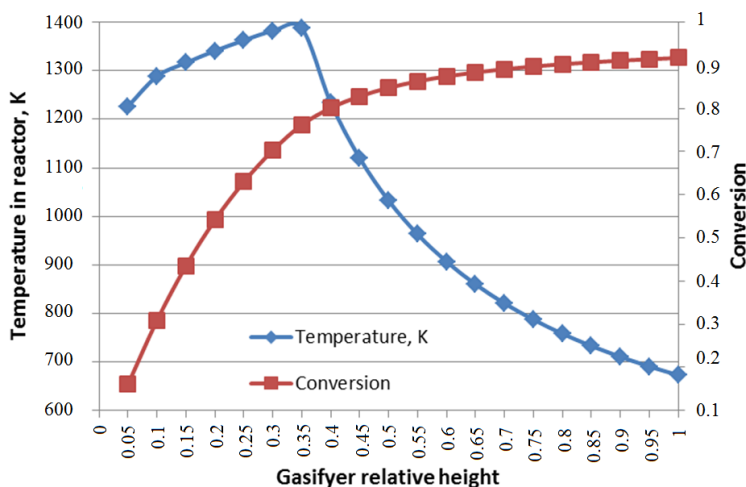


Fig. 1. Syngas temperature and fuel conversion distribution over reactor height.

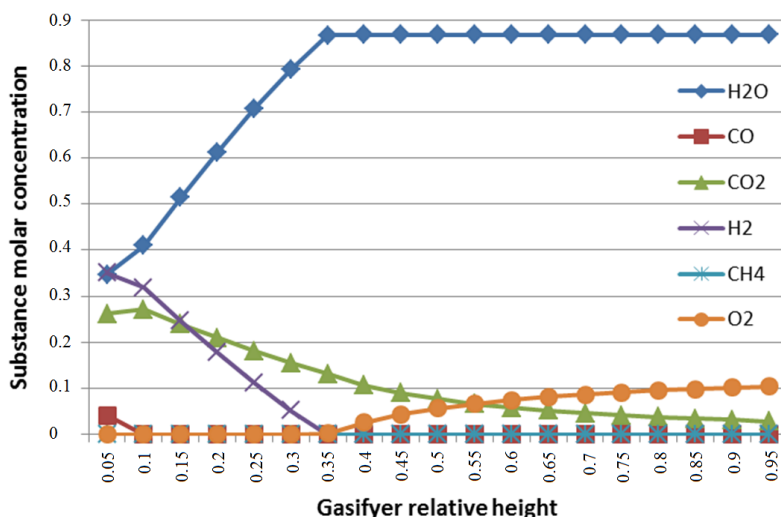


Fig. 2. Syngas component molar concentration over reactor height.

Graph analysis allows to clearly distinguish two reaction zones. The first is characterized by carbon complete oxidation reaction prevailing:



Other substances remain inactive – their concentration does not change. It begins at the 0.35 of gasifier relative height and lasts till the end of process. It is characterized by rapidly increasing temperature and slowly increasing conversion growth rate. It is connected to high temperatures and low conversion values at the beginning of this zone while the

average temperature in this phase is quite low. The syngas calorific value does not change and stays equal to zero.

The second phase is connected to water-gas shift reaction:



As long as this chemical reaction endothermic the temperature decreases during this stage. The carbon dioxide content is keep growing together with hydrogen content. At the very end of this stage the signs of carbon heterogeneous oxidation by water appears:



This resulted into more intense temperature drop and calorific value increasing. The methane content values over the reaction zone was small and could be not taken into account in further calculations.

4 Conclusion

Equilibrium thermodynamics and heterogeneous chemical kinetics combination were used to simulate counter-flow fixed bed gasification process for T-grade bituminous coal of Kuznetskiy deposit. The optimal fuel residence time was defined as well as syngas composition and final temperature. Based on temperature distribution and syngas concentration fields over the reactor height the oxidation and reduction zones were distinguished. Prevailing chemical reaction on each step were defined.

References

1. *British Petroleum Statistical review of World Energy* (Pureprint Group Limited, Uckfield, (2016)
2. A. Zenkov, S. Yankovsky, A. Matveeva, S. Lavrinenko, A. Gromov, MATC Web of Conf. **72**, 01131 (2016)
3. K. Larionov, I. Korjashov, S. Jankovskij, V. Gubin, A. Zenkov, MATEC Web of Conf. **37**, 01030 (2015)
4. ISO 17246:2010 (2010)
5. A. Korotkikh, K. Slyusarskiy, A. Ditts, Rus. J. of Phys. Chem. B. **10**, 576 (2016)
6. D. Svishchev, A. Kozlov, I. Donskoy, A. Ryzhkov, Fuel **168**, 91 (2016)
7. A. Korotkikh, K. Slyusarskiy, I. Sorokin, MATC Web of Conf. **72**, 01104 (2016)