Journal of Process Control 24 (2014) 269–277

Contents lists available at ScienceDirect

Journal of Process Control

journal homepage: www.elsevier.com/locate/jprocont

Control oriented modeling and optimization of one dimensional packed bed model of underground coal gasification

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ARTICLE INFO

Article history:
Received 17 June 2013
Received in revised form 1 December 2013
Accepted 2 December 2013
Available online 28 December 2013

Keywords:
Underground coal gasification (UCG)
1-D packed bed model
Sequential quadratic programming (SQP)
and optimization

ABSTRACT

To account for nonlinear nature and huge model uncertainties of underground coal gasification (UCG) process, a robust model based control strategy is to be employed. The available models in the literature do not lend themselves to control applications easily. In this work a control oriented one dimensional (1-D) packed bed model of UCG is developed, which can be used in a closed loop configuration with a robust controller to maintain a desired heating value of the exit gas mixture by manipulating the flow rate of injected gases. The model is also capable of predicting time and space profiles of some important parameters, which include solid temperature, composition of exit gas mixture, rates of different chemical reactions and expected life of the UCG reactor in response to different operating conditions and coal properties. Most of these parameters are either impossible or very expensive to measure. There is uncertainty in some coal properties which is addressed by optimizing few input parameters using sequential quadratic programming (SQP) algorithm, a nonlinear optimization technique. The model results are compared with actual field trials which show a good agreement for the calorific value of exit gas.

1. Introduction

Fossil fuels (coal, natural gas and oil) cover 84% of World's energy demand, of which the share of coal is 28% [1]. The advantages of coal over other fossil fuels are its relative abundance, and its low and stable cost [2]. Thar coal field, situated in southern part of Pakistan contains 175 billion tons of lignite coal [3]. By considering type of coal, depth and thickness of coal seam and location of water aquifers under the surface of earth, UCG project Thar has launched a project of UCG in Block-V of Thar coalfield to address the energy crisis of the country.

Fig. 1 illustrates the process of UCG in a simplified manner. Before the start of process, two wells (inlet and outlet) are drilled from surface to the coal seam, and a link is established between the drilled wells to allow the flow of gas through coal bed. After link establishment, coal seam is ignited and a mixture of gases is injected into the inlet well. The inlet gas consists of air/O_2 or air and H_2O. The gasifier is divided into three zones: oxidation zone, reducing zone and drying and pyrolysis zone. In oxidation zone, char oxidation reaction takes place which increases the temperature of the UCG reactor. In reduction zone, the important gasification reactions take place which generate the desired syngas (a mixture of CO and H_2). In drying and pyrolysis zone, the coal seam is initially dried and then pyrolysed. The estimated temperature ranges for different zones is also depicted in Fig. 1. The product gases including syngas, come out of the outlet well. The syngas can be used as a fuel for combined cycle turbines (CCT) for electricity generation using Integrated Gasification Combined Cycle (IGCC) power plants [5] or as a chemical feedstock [2,6].

Four different types of mathematical models of UCG are found in the literature: channel model, packed bed model, coal block model and process model [2]. In channel model, injection and production wells are physically linked by a horizontal borehole. The coal is gasified at the perimeter of the channel [7]. This type of method is used for the high rank coal, which has very poor permeability e.g. anthracite. Magnani and Farouq Ali [7,8] developed two channel models of UCG, which represent the system dynamics in one and two space dimensions, respectively. In packed bed modeling technique a link is established between inlet and outlet wells either by reverse combustion linking (RCL) or by fracturing the coal seam using pressurized air or chemical explosives [9]. The resultant high permeability zone is ignited and then gasified by suitable inlet gases [10]. This technique is used for low and medium rank coals, e.g. lignite and sub-bituminous, which have relatively higher permeability than anthracite. Winslow [11], Thorsness and Rosza [12], Khadse et al. [6] and Perkins and Sahajwalla [13] considered UCG

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http://dx.doi.org/10.1016/j.jprocont.2013.12.001

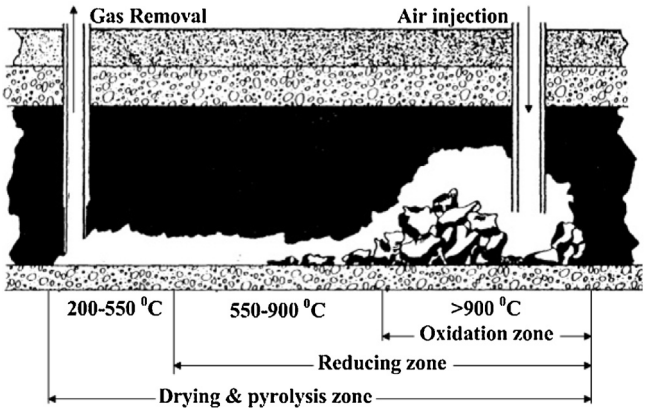

Fig. 1. Schematic of UCG process [4].

process as a packed bed reactor. The coal block modeling technique considers coal seam as a wet slab of coal, which is initially dried and then gasified. Perkins and Sahajwalla [14] have considered coal block model for UCG process. Process models calculate the cavity growth of the UCG reactor with time in a three dimensional (3-D) space, Beizen [15] considered this type of modeling. Solution of all the models evolve in both time and at least one space dimension except for channel models. In channel models the solution is function of space only. These models are only used for quantitative description of UCG process, none of these models have been used for UCG process control.

The control of UCG is an emerging area of research and is so for limited to the laboratory scale UCG setups. In literature, only the model free control of lab scale UCG rig is found [16,17], and there is no evidence of model based control of UCG process. In our earlier work [18], a simplified time domain model of UCG was developed and then a robust model based sliding mode control [19] strategy was successfully implemented on the developed model. The simplified model ignored some important aspects of the UCG process and therefore fell short of predicting the actual UCG phenomena. In the current work, limitations of the simplified model have been addressed and the results of the current model have a better resemblance with the actual field trials.

The primary objective of this research work is to develop a control oriented mathematical model for UCG process, which can assist the actual field trials and in the subsequent control of the process. In this work an already existing model of [20] is adapted with some modifications in model structure and solution strategy. The model is capable of predicting the chemical composition of the product gas as a function of the injected gas composition and rate as well as how it might vary with coal properties. The input stoichiometric coefficients for coal pyrolysis reaction are also optimized in order to compensate for the uncertainty in some coal properties. The optimization is performed by using a constrained nonlinear optimization technique, based on SQP algorithm. The heating value of the model is compared with field trials in order to validate the model. The model can also be used in a feed back configuration with a robust controller, which manipulates the flow rate of injected gas mixture to maintain a desired calorific value of exit gas, as discussed in [18]. The employed optimization technique only compensates for uncertainties in coal parameters, which are used to calculate stoichiometric coefficient matrix. There are a lot of other uncertainties and disturbances due to model assumptions and in situ conditions respectively, which can be mitigated by using robust control algorithms.

The rest of the article is arranged as: The reactor model of UCG is discussed in Section 2. Section 3 explains the solution strategy for solving the model equations. In Section 4 capabilities of the solved model are discussed. Results of the solved model and field trials are compared in Section 5, and the paper is concluded in Section 6.

2. UCG reactor model

This section discusses 1-D packed bed model of UCG, which is adapted from [20]. The salient features and assumptions considered for syngas model are listed below:

- Model of syngas consists of eight gas species: CO, CO_2, H_2, H_2O, CH_4, N_2, O_2, and tar (a pseudo specie used to close the stoichiometry of coal pyrolysis [20]) and two solid species: coal and char.
- Equations for energy and mass balances (derived from laws of conservation of energy and mass, respectively) of gas and solid species are written separately for syngas model.
- 1-D assumption is made for mass and energy balances of gas and solid species. This approximation ignores some important multidimensional effects like heat losses and cavity growth of UCG reactor, but it makes the model simple.
- A set of nine chemical reactions is used to describe the chemical kinetics of the process.
- Heat source generated from chemical reactions is written separately for solid and gas phases, which neglects detailed interaction at the point of reaction between the two phases.
- All the conductive transport is lumped in solid phase, neglecting all the accumulation terms in gas phase, this approximation is actually the part of quasi-steady state assumption. According to this assumption convective inter phase and heat source terms for chemical reactions dominate the accumulation terms at all points in the system. This assumption is valid due to low density of gas phase as compared to solid phase, and also due to the large differences in the characteristic time of both phases.
- Coal seam is assumed to be a porous medium, and Darcy's law is used as momentum balance for gas phase.

2.1. Mathematical equations

2.1.1. Solid phase mass balance

The mass balance equation for solids explains the effect of different chemical reactions on the rate of change of solid density:

$$\frac{\partial}{\partial t}\rho_i = M_i \sum_{j=1}^{9} a_{s_{ij}} R_j \tag{1}$$

where ρ_i is the density of ith solid (kg/m^3), a_{sij} is the stoichiometric coefficient of ith solid specie in jth chemical reaction (a_{sij} is positive for products and negative for reactants), R_j is rate of jth chemical reaction (mol/m^3/s), M_i is the molecular weight of solid component i (kg/mol) and t is variable for time (s).

The chemical reactions along with associated reaction rates are given in Appendix A.3

2.1.2. Solid phase energy balance

Eq. (2) shows that how does solid temperature change with time due to heat transfer through conduction (between adjacent coal layers) and convection (inter phase heat transfer caused by the movement of gases), and heat of chemical reactions:

$$\frac{\partial T_s}{\partial t} = \frac{\frac{\partial}{\partial x}\left[(1-\phi)k\frac{\partial T_s}{\partial x}\right] + h_T(T - T_s) - H_s}{C_s} \tag{2}$$