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Full Length Article

A process model for underground coal gasification – Part-I: Cavity growth

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HIGHLIGHTS

- UCG process is divided in two phases based on growth pattern of the cavity.
- Proposed a compartment model for phase-I based on virtual RTD studies using CFD.
- Integrated non-ideal flow patterns with spalling and detailed kinetics of the given coal.
- Model predictions are in agreement with the results of lab-scale UCG experiments.

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ABSTRACT

In underground coal gasification (UCG), a cavity is formed in the coal seam due to consumption of coal. The irregular-shaped cavity consists of a spalled-rubble on the cavity floor, a cavity roof and a void zone between the two. Depending on the cavity growth pattern, UCG process can be divided into two distinct phases. In phase-I, coal/char near injection well gets consumed and cavity grows in a vertical direction and hits the overburden. Phase-II starts thereafter, in which the cavity grows in the horizontal direction toward the production well. This paper presents an unsteady-state model for gas production during phase-I for a coal under consideration for UCG. The non-ideal flow patterns in the cavity are determined using computational fluid dynamics (CFD). The CFD results and residence time distribution (RTD) studies show that the complex UCG cavity can be reduced to a computationally less time consuming compartment model consisting of a radial plug flow reactor (PFR) followed by a continuous stirred tank reactor (CSTR). The developed compartment model incorporates reaction kinetics, heat-transfer, mass-transfer, diffusional limitations and thermo-mechanical failure effects for the coal of interest. The model is tested on a lab scale UCG; it can predict the location of reaction and drying fronts, profiles of solid and gas compositions, exit gas calorific value and cavity growth rates. Further, the model predictions show an excellent match with the cavity growth rate and exit gas quality observed during laboratory-scale UCG-like experiments on the coal of interest. Therefore, the model can potentially be used to determine feasibility of UCG for any other coal for the known kinetics and spalling parameters.

1. Introduction

Underground coal gasification (UCG) is a process of *in-situ* conversion of coal into combustible gases. The process involves vertical drilling of injection and production wells up to the bottom of the coal seam and connecting them with a horizontal highly-permeable linkage [1]. The reactants injected are air or oxygen, with or without steam. The products of the process include CO, CO_2, H_2, CH_4, H_2O and tars. Stringent criteria for selection of UCG site can eliminate the possibility of pollution of nearby water aquifer [2]. The contamination hazard for aquifers and its environmental impact have been assessed and discussed thoroughly in literature [3].

UCG process for any coal seam occurs in two distinct phases, characterized by the direction of cavity growth and the state of the cavity. In the first phase, cavity grows vertically till it hits the overburden and in the second phase, it grows horizontally, toward

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Nomenclature

Acronyms

CCS	Carbon Capture and Sequestration
CFD	Computational Fluid Dynamics
CRIP	Controlled Retracting Ignition Point
CSTR	Continuous Stirred Tank Reactor
DAE	Differential–Algebraic Equation
LVW	Linked Vertical Wells
PFR	Plug Flow Reactor
RPM	Random Pore Model
RTD	Residence Time Distribution
UCG	Underground Coal Gasification
VRM	Volumetric Reaction Model
WGS	Water Gas Shift

Symbols

A_c	cross sectional area (m^2)
A_{roof}	area of roof surface (m^2) changes with time
C_g	gas concentration (kmol/m^3)
C_p	specific heat (kJ/kmol/K for gas and kJ/kg/K for solids)
D_{eff}	effective diffusivity (m^2/s)
E	activation energy (J/mol)
ΔH	heat of reaction (kJ/kmol)
F_g	gas flow rate (kmol/s)
F_w	rate of water influx (kmol/s)
H	enthalpy (kJ/kmole)
K_{per}	permeability of rubble (m^2)
M	molecular weight (kg/kmol)
N	order of reaction
V	volume (m^3)
P	pressure (kPa)
Q_g	gas flow rate in rubble (m^3/sec)
R	gas constant (kJ/kmol/K)
R_C	lumped rate based on chemical reaction and internal resistance (kmol/m^3/sec)
R_j	jth reaction (kmol/m^3/sec)
R_M	rate of mass transfer of limiting reactant (kmol/m^3/sec)
R_T	total rate (kmol/m^3/sec)
T	temperature (K)
V_c	volume of PFR (m^3)
V_{cav}	volume of cavity = volume of (rubble + void) (m^3)
X	solid conversion
a_{ij}	stoichiometric coefficient of ith gas species in jth reaction
$a_{s,ij}$	stoichiometric coefficient of ith solid species in jth reaction
u_g	gas velocity (m/s)
h_T	heat transfer coefficient in between gas and bed of particles (kW/m^3/K)
h_{Tcav}	heat transfer coefficient from void to wall transfer (kW/m^2/K)
k_{eff}	effective conductivity (kW/m/K)
$k_{y,cav}$	mass transfer coefficient from void to wall transfer (m/s)
k_0	specific rate constant (sec^{-1} (kmole/m^3)$^{-N}$ K$^{-\alpha}$)
t	time (sec)
υ_{df}	velocity of drying front (m/s)
α	temperature exponent in reaction kinetics
ε_r	radiation emissivity
ρ	solid density (kg/m^3)
σ	Stefan Boltzmann constant (kW/m^2/K^4)
μ	viscosity of gas mixture (Pa sec)
τ	residence time in CSTR (sec)
υ	flow rate in CSTR (m^3/sec)
Φ	porosity
Ψ	structural parameter for RPM

Subscripts

g	gas phase
s	solid phase
0	inlet to the cavity
c	cross-section
r	values at roof
w	water influx or water
d	drying
i	species index
j	reaction index
tr	top of rubble
in	inlet of CSTR
cav	cavity
$roof$	cavity roof
vap	vaporization
df	drying front
T	volume of total coal seam (at the end of wet zone)
L	liquid phase
dry	dry zone
wet	wet zone

the production well. This paper focuses on the initial vertical growth during phase-I as shown in Fig. 1. This figure is not to the scale and the actual distance between the two wells can be very long compared to the height of the coal seam.

The process involves several phenomena including non-ideal flow patterns, multiple chemical reactions, water intrusion, spalling and heat and mass-transfer effects [1]. Because of the complexity of the UCG process and inability to visualize the underground cavity, process model can play a very important role. The model can provide useful inputs at the design stage for determining the capacity of a pair of wells and should be able to predict the effects of unforeseen events such as water intrusion or sudden spalling. Several modeling efforts are reported in the literature and reviews can be found elsewhere [1,2]. Available models can be classified into packed bed models [4–6], channel models [7–10], coal block models [11–13] and process models [14–17]. However, first three classifications have idealized flow patterns and therefore they cannot adequately include effect of actual flow patterns on product gas composition. On the other hand, most of the process models are based on assumptions which are difficult to verify or they neglect important features to save computational time. The process model developed by Biezen [14] is limited by assumptions related to heat transfer including constant reactor temperature. CFD based process models [15,17] are limited by huge computational loads for simulating actual underground gasifier. This leads to a need of a comprehensive yet computationally less intensive process model for UCG. This study provides a complete modeling solution for UCG process by using compartment modeling approach for both the phases of UCG. This paper focuses on modeling the initial vertical growth during phase-I only. Another process model for phase-II of UCG is presented in the second part of this paper. A model is developed and solved by taking inputs from the experimental data on kinetics, spalling and physical parameters for an Indian lignite. The predictions of cavity growth are based on unsteady-state models for the three zones (rubble, void and roof) in the cavity.