Fuel Processing Technology 140 (2015) 188–197

Contents lists available at ScienceDirect

Fuel Processing Technology

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

Research article

Modeling of contaminant migration through porous media after underground coal gasification in shallow coal seam

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ARTICLE INFO

Article history:
Received 11 May 2015
Received in revised form 26 August 2015
Accepted 30 August 2015
Available online 19 September 2015

Keywords:
Underground coal gasification
Mass transport
Transport parameters
Transport phenomena modeling

ABSTRACT

The migration rates of representative underground coal gasification (UCG) related products and contaminants through porous surroundings of a georeactor in a shallow coal seam in gaseous and liquid phases were studied in this work. The proposed comprehensive model, taking into account mass transport phenomena both in gaseous and liquid phase, was based on the real data obtained during the UCG field-scale study carried out at the Experimental Mine "Barbara" in Poland in the framework of the RFCS Project HUGE (2007–2010). The mass transport from the reaction zone was modeled by means of constitutive equations, in gas phase permeation, in liquid phase advection, axial dispersion, diffusion, and adsorption. The applied input values of parameters were based on results from previous pilot experiments. The effects of pore size, porosity, tortuosity, and reaction conditions on the migration rate were individually evaluated and taken into account. The contamination risk for aquifers and potential leakage of poisonous gases and their environmental impact were assessed and thoroughly discussed. It was found that porosity, pore diameter and tortuosity, which belong to the key transport parameters, play a major role in overall permeation transport of gaseous contaminants compared with physical characteristics—pressure and temperature. Migration rates of UCG-related contaminants in the liquid phase are significantly slower compared with the gaseous phase.

1. Introduction

Underground coal gasification (UCG) is considered an alternative method for the extraction of energy from coal which is otherwise considered unattainable by mining for economical or environmental reasons. Moreover, the UCG process has several benefits compared to surface coal gasification, such as lower capital investment costs or no handling of coal [1-3]. During the UCG process the oxidizing stream of air/steam, often enhanced by oxygen, is injected into a coal seam, where the coal undergoes a controlled combustion reaction. Consequently, the reaction mixture is piped away up to the surface and, after cleaning, is used as a syngas for production of electric power, liquid hydrocarbons, synthetic natural gas, hydrogen and other valuable chemical products [4-6].

The UCG process also offers important environmental advantages compared to conventional methods of coal recovery owing to no discharge of tailings and reduced emissions of sulfur, ash, mercury and tar [7]. However, there are certain environmental risks of the UCG process that require careful evaluation. It is evident that the underground gasification cavity can be a possible source of both gaseous and liquid pollutants such as, for example, mono- and polycyclic aromatic hydrocarbons, phenolics, heterocyclic nitrogen compounds, heavy metals, ammonia, sulfides or cyanides [7-12].

The risk of environmental pollution from UCG depends on the migration of contaminants from the reaction zone. The substances mentioned above can be released into the underground environment (porous medium), depending on its transport properties, the UCG process parameters, and local hydrogeological conditions. Contamination of underground aquifers and potential leakage of poisonous and explosive gases into the environment, including surface leakages, are considered to be the most serious environmental concerns related with UCG processes. The contamination risk exists both during UCG operation and after cessation of the process. Concerning the latter case, possible after-effects can still be observed long after the interruption of the UCG process.

One of the first studies of the contaminants associated with the UCG process came from U.S. experiments, mainly regarding the Hanna and Hoe Creek trials [10]. In the scope of those experiments, groundwater pollution was tested and evaluated before, during and after gasification. A wide range of contaminants was found in the surrounding area of the UCG reaction zone. The authors concluded that UCG at shallow depths could represent a significant risk for groundwater in the surrounding strata.

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http://dx.doi.org/10.1016/j.fuproc.2015.08.033
0378-3820/

Nomenclature

B_{mix}	effective permeability coefficient
c	solute concentration
c_S	pore volume compressibility
d_p	pore diameter
D	diffusion coefficient
D_x	the longitudinal dispersion coefficient
E	dispersion coefficient
K_d	Henry's law using the adsorption coefficient
p/p_0	relative pressure value
K_H	coefficient of hydraulic conductivity
N_{mix}^{perm}	permeation molar mixture flux
p	total pressure
q_A	advective flux
q_E	dispersive flux
q_V	volumetric flow rate per unit volume
S	mass of adsorbed contaminants on inner surface of stratum
S_{sp}	specific storage coefficient aquifer
t	time
v_x	interstitial pore fluid velocity
y_i $(i = 1,2,...,n)$	mole fraction
$\langle r \rangle$	mean value of pore radii
$\langle r^2 \rangle$	mean value of squared radii
ε	porosity
ψ	third transport model parameter
ρ_b	bulk density of stratum
τ	tortuosity
μ_{mix}	dynamic mixture viscosity

A field scale underground coal gasification trial carried out at the Experimental Mine "Barbara" [13] demonstrated that gasification in shallow coal seams can cause some operational problems (e.g. gas leakages from the georeactor). As a result of these operational problems, a potential negative environmental impact of the gasification products can occur due to the migration of toxic contaminants out of the reaction zone, which in turn can adversely affect the surrounding environment of the georeactor. Based on the aforementioned semi-technical experiment performed in "Barbara" it was recognized that a comprehensive description of transport phenomena of the UCG-related products would aid in determining the risk of possible threats to the environment. Therefore, the general aim of this study is focused on the identification of the potential impact of the UCG process operated in shallow coal seams on the underground environment, caused by the transport of liquids and/or gases through the surrounding soil mass.

2. Experimental

The porous media surrounding UCG georeactor generally form very complex systems. The soil mass is typically formed of different kinds of soils (sand, silt, loam, etc.) with various porosity and, therefore, also with different permeability. Moreover, a lot of cracks, crevices and faults make the porous surroundings of the georeactor more permeable. The simulation study concerning the migration rates of contaminants during the UCG process described in this paper is based on conditions of the real georeactor which was located in the Experimental Mine "Barbara" in Mikołów, Poland, during a field-scale, in-situ UCG experiment within the project Hydrogen Oriented Coal Gasification for Europe [14]. For the purpose of this study, a porous surrounding medium (porosity) was assumed to be isotropic and continuous.

2.1. Model of gas transport in porous media

The mean transport-pore model (MTPM) [15] was applied to describe the stratum and coal pore structure, both comprised in a georeactor. The considered conception assumes that a decisive part of the mass transport takes place through cylindrical transport-pores with the mean value of their radii $\langle r \rangle$. The integral mean value of squared radii, $\langle r^2 \rangle$, is utilized as the second model parameter. The third model parameter, ψ, represents the ratio of soil porosity, ε, and tortuosity, τ, i.e. $\psi = \varepsilon/\tau$.

The UCG process is generally performed under higher pressure and temperature. For these conditions of the UCG process we found [16] that the permeation of gases plays a dominant role (compared to the gas diffusion) in the overall transport of gaseous products from the reaction zone into both the production well and the surrounding porous medium. Total pressure gradient $\partial p/\partial x$ represents the driving force of permeation transport of reaction gaseous mixture

$$N_{mix}^{perm} = -\frac{B_{mix}}{RT}\frac{\partial p}{\partial x} \tag{1}$$

where N_{mix}^{perm} denotes the permeation molar flux of the reaction mixture B_{mix} represents the effective permeability coefficient that depends on the total pressure p according to:

$$B_{mix} = \frac{\langle r^2 \rangle \psi}{8\mu_{mix}} p \tag{2}$$

where μ_{mix} denotes the dynamic mixture viscosity calculated according to Wilke method [18]. The correlation between transport through the porous medium and the gasification processes taking place in the UCG reactor was evaluated based on designed constitutive Eq. (1). This relation reflects the mass flux of reaction products through a porous medium (surrounding strata and coal). The mass balance of gaseous mixture penetrating in porous medium is described as follows

$$\varepsilon \frac{\partial p}{\partial t} = \frac{\partial}{\partial x} N_{mix}^{perm} \tag{3}$$

The solution of this partial differential Eq. (3) for semi-infinite porous medium was found [17] in the form of series expansion:

$$\frac{p}{p_0} = \xi_0(\xi - \xi_0)\left\{1 - \frac{1}{4}\left(1 - \frac{\xi}{\xi_0}\right) + \frac{1}{72}\left(1 - \frac{\xi}{\xi_0}\right)^2 + \frac{2}{1017}\left(1 - \frac{\xi}{\xi_0}\right)^3 + \frac{5}{18432}\left(1 - \frac{\xi}{\xi_0}\right)^4 + \ldots\right\} \tag{4}$$

The constant boundary $p(0,t) = p_0$ and initial conditions $p(x,0)$ must be taken into account and $\xi_0 = 0.80798$. Dimensionless variable $\xi = x/\sqrt{4B_{mix}t}$ is function of time t and space location x. The permeation flux of reaction mixture vanishes on the front limited by relative pressure value $p/p_0 = 0$ at $\xi > \xi_0$. It is assumed that the chemisorption of the reaction mixture on the stratum does not take place and components are mutually nonreactive.

The calculation of the reaction component concentration penetrating through the porous medium surrounding an underground georeactor was accomplished using Matlab®, R2014a, The Matworks, Inc., USA.

2.2. Contaminant migration through soil mass

The experimental mine "Barbara" is located in southern Poland within the administrative area of Mikolów City. The location both of Barbara mine and georeactor site is depicted in Fig. 1. The layout of the elements in the underground part of the installation is given in Fig. 2. The average depth of the coal deposit was approximately 30 m