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Research of geomigration processes during underground coal gasification and combustion

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Today one of the main problem for areas of intense technological activities related to the production, processing and use of fossil fuels is management and environmental protection. With the current technology development difficult to achieve effective results in terms of further improving the technical and economic performance and in terms of environmental protection. Fundamentally new in the transition to underground coal gasification (UCG) and coal combustion (UCC) is the transition to non-waste technology. The possibility of smoke emission elimination through recycling, directing the underground gasification oxides of sulfur, nitrogen and other toxic components of smoke emissions. In underground water is possible their destruction to non-toxic state. Other harmful for the biosphere chemicals substances (arsenic, strontium) also remain in the underground gas generator. Also in the underground space may direct solid waste for laying out space voids possible reduction surface subsidence and preserve the landscape. Reducing the volume of drilling and laying out space allows you to transfer temporarily useless agriculture territory. Underground space of gas generators with hot rocks can be used for commercial purposes. Utilization of physical warm rocks by pumping cold and getting hot coolant can increase efficiency. But with all the above-mentioned, the environmental justification for building the station of underground coal gasification and coal combustion necessarily involves the analysis and forecast of man-made impact on the geological environment. In terms of the studied region of brawn coal Dnieper basin the prospects of widespread introduction of underground coal gasification and coal combustion technology inherent protection from problem resolution is actively used in the household groundwater from chemical contamination of underground coal combustion, disposal and coolant waste.

Keywords: underground coal gasification, underground coal combustion, geomigrational processes, geotechnical system

Дослідження геоміграційних процесів під час підземних газифікації та спалювання вугілля

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На сучасному етапі розвитку суспільства проблема раціонального використання і охорони довкілля входить в число пріоритетних і особливо гостро вона проявляється в районах інтенсивної техногенної дії, пов'язаної із видобутком, переробкою і використанням горючих корисних копалин. При існуючій технології розробки все важче домогтися ефективних результатів як з точки зору подальшого поліпшення техніко-економічних показників, так і з точки зору охорони природи. Принципово новим при переході на підземні газифікації (ПГВ) та спалювання вугілля (ПСВ) є перехід на безвідходну технологію. Відкривається можливість ліквідації димових викидів шляхом їх рециркуляції, спрямування в підземний газогенератор оксиди сірки, азоту і інших токсичних елементи димових викидів. За наявності вологи можливе їх руйнування до нетоксичного стану. Інші шкідливі для біосфери хімічні сполуки (миш'як, стронцій) також залишаються в підземному газогенераторі. Також в підземний газогенератор можливо спрямовувати тверді відходи для закладки порожнеч виробленого простору, що дозволяє істотно зменшити осідання поверхні і зберегти ландшафт. Скорочення об'єму бурових робіт і закладання виробленого простору дозволяє передавати сільському господарству тимчасово відчужені землі для рекультивції. Підземний простір відпрацьованих газогенераторів з гарячими породами можна використовувати в господарських цілях. Утилізація фізичного тепла порід шляхом закачування холодного і отримання гарячого теплоносія дозволяє підвищити ефективність. Але при всьому вищеперерахованому, екологічне обґрунтування будівництва станції ПГВ і ПСВ обов'язково передбачає і прогностичний аналіз техногенної дії на геологічне середовище. В умовах досліджуваного регіону Дніпровського басейну питання перспектив широкого впровадження технологій ПГВ і ПСВ невід'ємне від вирішення проблеми захисту активно використовуваних в господарстві підземних вод від хімічного забруднення продуктами підземного горіння вугілля, утилізації теплоносія і відходів.

Ключові слова: підземна газифікація, підземне спалювання, геоміграційні процеси, геотехнічна система

Introduction. In the process of underground gasification and coal combustion numerous chemical substances are emitted. They can leave the underground burning zone and move to the subsoil hydrosphere and polluting it in depends on water saturated above coal and sub coal water-bearing horizons. That is why it is necessary to prevent or limit their penetration into water-bearing horizons during and after the operation of underground burning. But at the stage of active operations, the risk of penetration by pollutants remains high. To some extent, this problem can be solved by estimating the possible distribution of pollutants from the area of underground generator.

Presentation of the general material. The literature data provides us with the approximate content of pollutants in the products and wastes of underground gasification and underground coal combustion (table 1), which makes it possible to predict the extent and character of chemical pollution of the groundwater around the underground generator using methods of mathematical modeling.

Theoretical description of geomigrating processes with consideration of hydro-chemical transformations should use methods of thermodynamic modeling. Such approach is used for modeling contamination processes when considering conditions of technogenic pollution, the sources of which are in water-bearing rocks and enter the water supply during changes of thermodynamic condition in groundwater.

The determinant in the study of geomigrational process is mass transfer, which is the process of transferring certain ground water components (migrants). The importance of studying the mass transfer processes is related with high mobility of water solutions in the lithosphere.

Usually, the key component of the ground water filtration flow is convective transfer, which proceeds hydraulically with filtrating water. A single mass flow of convective mass transfer j_k which is the amount of

the migrant which passes convectional through a single area of flow per unit time, will be

$$j_k = C * V, \quad (1)$$

where j_k – the flow of convective mass transfer;

C – migrant concentration;

V – velocity of filtration, related to actual velocity of the current u_0 by correlation $u_0 = V/n_0$, where n_0 – active porosity of a rock.

Also the process of mass transfer includes different forms of dispersion, which cause the scattering of migrants in space. There are considered processes of micro dispersion which take place at inner porous (inner fault) levels, and macro dispersion, which takes place at the levels of aggregates and blocks of rocks.

At the molecular level, micro dispersion is caused, first of all, by the process of molecular diffusion, which creates a flow of migrant, described in Fick's law.

$$j_d = D_m \text{grad} C, \quad (2)$$

where j_d – single mass diffusion flow (the amount of the substance which diffuses through a single area of flow per unit time);

D_m – coefficient of molecular diffusion.

Coefficient of molecular diffusion characterizes the sinuosity of filtration routes in porous environments, and according to experimental data, equals 0.5-0.7 for incoherent sands, and 0.25-0.5 for coherent sands.

According to the results of laboratory studies, the value of the diffusion coefficient for clayey rocks has the order of 10^{-5} m²/day. At the same time, the magnitude D_m can significantly decrease after sealing of rocks, and the magnitude D_m significantly depends upon moisture in incomplete water saturation.

Fick's law in the form (2) is reasonable for isothermal processes and in independent diffusion of components of a solution. Otherwise, more complicated phenomena of non-isothermal multi-component diffusion occur.

Table 1

The content of chemicals in products and waste PGV and PSV [1, 2]

№	Name of substance	The substance content in products and waste, mg/dm ³	Maximum permissible concentration (MPC) of chemical substances, mg/dm ³
1	Ammonia	1,9 – 3,0	2,0
2	Benzene hydrocarbons	1,0 – 2,2	0,5
3	Pyridine bases	0,04 – 0,68	0,2
4	Hydrogen sulfide	0,03 – 0,32	0,003
5	Naphthalene	0,0004 – 0,1	0,01
6	Acetylene	0,000003 – 0,015	0,0015
7	Prussic acid	0,000006 – 0,008	0,0035
8	Phenol	0,0013	0,001

Extension of hydro dispersion (along the flow's direction) is described by Fick's law, where D_m is changed by the coefficient of hydro dispersion extension, which depends on filtration velocity. The results of laboratory tests for homogenous sands show linear dependency of D_l on V .

$$D_l = D_m + \delta_l V, \quad (3)$$

The generalization of experimental data shows the possibility of disordered structure of dependency for sandy-gravel rocks (3).

In the non one dimension flow of transfer, transversal hydro dispersion occurs, which causes transversal flow of the migrant, which is also defined by the Fick's law, where D_m is changed by the coefficient of transversal dispersion D_t . Their rough approximation can be represented as

$$D_t = D_m + \delta_t V, \quad (4)$$

where δ_t – parameter of transversal dispersion, which has typical meaning for close sand, equals $\delta_t = 0.06 - 0.2 \text{ mm}$.

In a homogenous environment, the model of transfer includes description of convective transfer and micro dispersion. The model of convective dispersion uses a scheme of displacement by piston, where it is considered that all areas of water move in each section with the same velocity. In such conditions, let us define the equation for transfer velocity of the dividing edge (front of displacement) of migrant solutions, which divide area of concentrations with C_0 for condition of instant increase in sorption equilibrium (i.e. not considering sorption kinetics), making balance equation of migrant in infinitesimal element of current dl , which is the border section of the migrant solutions for time (t)

$$U = \frac{dl}{dt} = \frac{Q}{\omega} \left(n_0 + \frac{N - N_0}{C - C_0} \right)^{-1}, \quad (5)$$

where Q – debit of the flow on the current line;

N i N_0 – content of sorbed migrant (occluded) per unit volume of rock;

C i C_0 – concentration of the solution;

ω – area of transversal section of the current line.

The equation (5) is solved by integration towards the trajectory current, should be based upon the geofiltration assessments, made for a general case using methods of numerical modeling.

After superposing convectional and dispersive transfer, the total unit mass current j_m will be as follows

$$j_m = j_k + j_d, \quad (6)$$

where j_k is defined with (1), and j_d for micro dispersion is defined by the equation (2), where D_m is

substituted with hydro dispersion coefficient D_l in filtration flow.

Theoretical description of such process was made for one-dimensional transfer in a filtration current with filtration velocity V in direction l written (7) in form

$$j_m = C * V = D_l \frac{\partial C}{\partial l}, \quad (7)$$

Balance equation for a neutral migrant in an infinitesimal element with length ∂l and unit area of transversal section:

$$\frac{\partial j_m}{\partial l} + n_0 \frac{\partial C}{\partial t} = 0, \quad (8)$$

where n_0 – active porosity of a rock.

After substituting expression (7) for j_m , in (8), we will receive differential equation of one-dimensional convective dispersion transfer

$$n_0 \frac{\partial C}{\partial t} + V \frac{\partial C}{\partial l} = D_l \frac{\partial^2 C}{\partial l^2}, \quad (9)$$

Transformed (9), and inserting Laplace-Carson integral transformation $\bar{C} = L(c)$

$$n_0 p (\bar{C} - C_0) + V \frac{\partial \bar{C}}{\partial l} = D_l \frac{d^2 \bar{C}}{dl^2}, \quad (10)$$

where p – parameter of transformation.

Solution (10) in condition $\bar{C} = C_0$ at the edge $l = 0$ of half limited current is as follows

$$\frac{\bar{C} - C_0}{C_0 - C_0} = e^{-al}, \quad a = \sqrt{\left(\frac{V}{2D_l}\right)^2 + \frac{n_0 p}{D_l}} - \frac{V}{2D_l}, \quad (11)$$

Transformation from (11) to original in $C^0 = \text{const}$ gives

$$\bar{C} = \frac{C - C_0}{C^0 - C_0} = 0,5(\text{erfc}\xi + e^{\eta} \text{erfc}\xi^*), \quad (12a)$$

$$\xi = \frac{n_0 l - Vt}{2\sqrt{n_0 D_l t}}, \quad \xi^* = \frac{n_0 l + Vt}{2\sqrt{n_0 D_l t}}, \quad \eta = \frac{Vl}{D_l}, \quad (12b)$$

Calculations according to (12) show that after a certain time after the process had started, three main migration zones are formed:

- the zone of dismissing migrant (with relative concentration $\bar{C} = 1$),
- transitional ($1 > \bar{C} > 0$)
- initial content of the migrant $\bar{C} = 0$.

Another element of equation (12a) is small and can be neglected, so a simplified expression for relative concentration can be used.

$$\bar{C} = 0,5 \operatorname{erfc} \xi, \quad (13)$$

Analysis of solving fundamental task shows the peculiarities of convective and dispersion transfer forms manifestations. The equation (13) shows that, during piston displacement, defined only by convective transfer, where is ($l = l_0 = \frac{Vt}{n_0}$), the position of piston displacement front corresponds to the middle of transitional zone with average concentration between the content which displaces and which is being displaced.

To describe the transversal macro dispersion, it is reasonable to use the model of "sieving" small parts through a net of large grains, which filtrate. Using this model for point transfer of small particles, the division of their concentration in flat flow was defined

$$C = \frac{c_0}{\sqrt{\frac{2\pi x}{d}}} \exp\left(-\frac{y^2}{2xd}\right), \quad (14a)$$

where c_0 – initial concentration;

x i y – coordinates in the direction of sieving (filtration) and perpendicular to it;

d – diameter of grains which filtrate, corresponding to size of blocks.

Let us compare (14a) with the expression obtained by solving the task of convective-dispersion transfer, which provides division of concentration in the flow, which moves with velocity V without extended dispersion, but with transversal dispersion, which is characterized by coefficient D_m , with constant intensity $P = V \cdot d \cdot C_0$ at the beginning of the source's coordinates. Such solution provides the following expression for a migrant's concentration

$$C = \frac{P}{2\sqrt{\pi D_y x V}} \exp\left(-\frac{V y^2}{4 D_y x}\right), \quad (14b)$$

where $D_y = D_m$ – coefficient of transversal dispersion (in the (y) direction).

After comparing equations (14a) and (14b), we can see their similarity, and that they equally coincide if we consider that

$$D_T = \delta_T V, \delta_T = \frac{d}{2}, \quad (15)$$

If the shape of blocks is considered cubic and the diameter of grains is defined by the size of block (for sand clays and loams – 0.1 m, for sands – 1 – 10 m), the magnitude can be connected to diffusion mass transfer. Considering ($f_d = 36$) for cubic blocks, the correlation will be

$$\delta_T = \sqrt[3]{\frac{D_m}{\alpha_d}}, \quad (16)$$

Using these methods, the calculations of horizontal and vertical migration of contaminant components (see table. 1) were made. The parameters of calculation are given in table 2.

There are many methods for calculation of hydro dispersion coefficient, but in this case, initial meanings allow to use Averianov's method

$$D = \frac{Vl}{2 \ln \frac{C_0}{C}}, \quad (17)$$

where V – velocity of ground water, which is calculated

$$V = \frac{K_{\phi} I}{n}.$$

Conclusions. For calculating horizontal mass transfer, we used (12a), (12b) and (17). The results of calculations are given in fig. 1. The significant difference between the results in above coal and sub coal water bearing horizons is related to differences of filtration parameters. The largest radius of pollution was obtained by ammonia, although the difference between initial and maximum permissible concentrations was one of the smallest. At the same time, the difference of concentration of hydrogen sulfide is higher and the pollution radius is one of the smallest. So, the extent of pollution does not depend on the differences of concentrations, and should be defined separately for each contaminant, and defining the true regularities of pollution spreading in a horizontal direction requires additional studies.

For calculation of vertical mass transfer, we used (4.14a), (4.14b) and (4.15). The calculation shows similarity of pollution by all substances. Both water-bearing horizons will have the same spread of

Table 2

Initial data for calculation

№	Name of substance	Above coal horizon	Sub coal horizon
1	Coefficient of filtration, Kf, m / day	3-6	6-12
2	Active porosity	0,175	
3	Flows gradient	0,014	
4	The path length of filtration, L, m	5000	
5	Period of time, t, days	182,5	
6	The diameter of the grains, d, m	10	

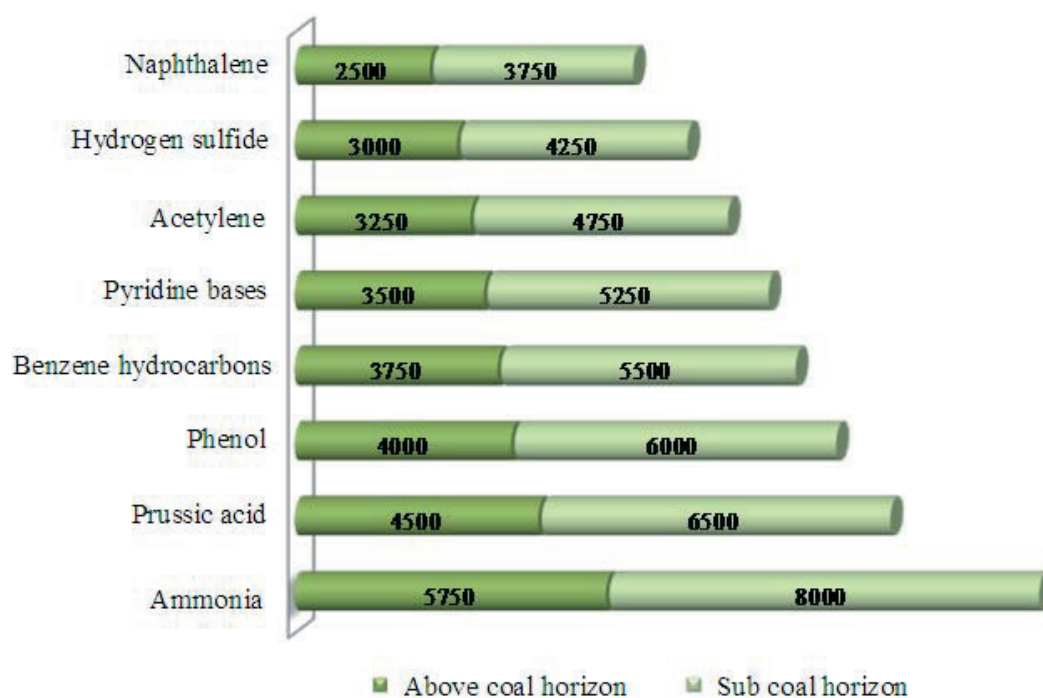


Fig. 1. Diagram of spreading of different pollution contaminants in a horizontal direction

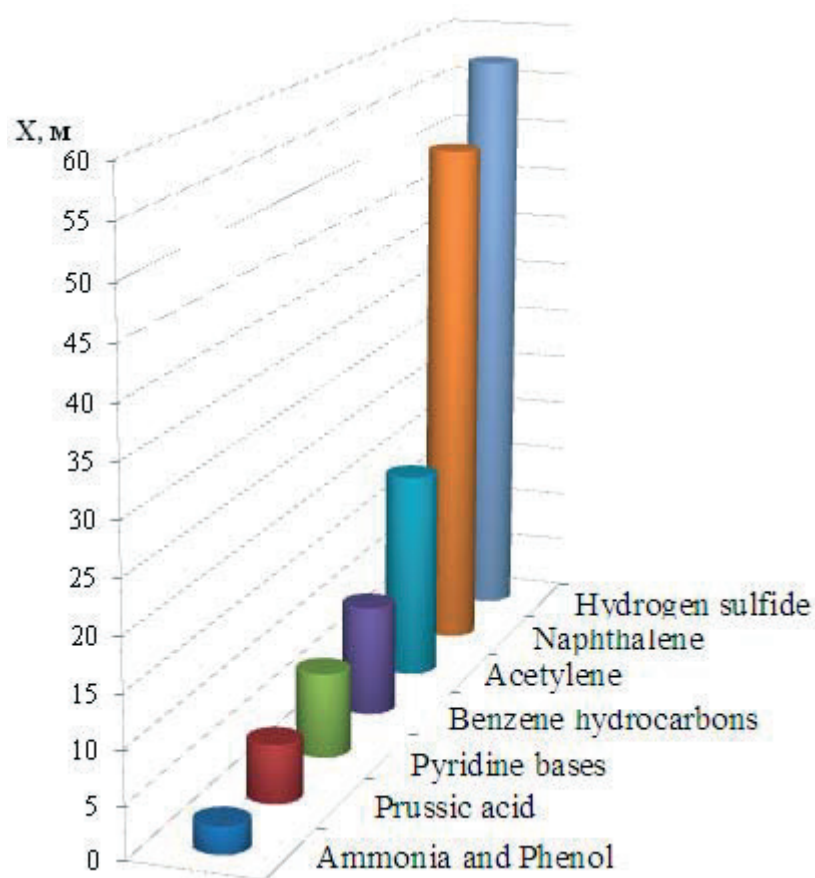


Fig. 2. Diagram of vertical spreading of contaminant substances

pollution spreading with all contaminants. The greatest pollution will be hydrogen sulfide pollution and will equal 57 m in a section, the least (2.5 m) – ammonia and phenol. Such a pattern clearly represents the correlation between the difference of concentration and radius of vertical pollution. The results of calculations are given in fig. 2.

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