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Calculation of phase transformation of groundwater when evaluating its efficiency as a mobile heat-transfer agent

S. V. Zholudiev

Dnipropetrovsk National University named after Oles Honchar, e-mail: ggf2009@ukr.net

The article is devoted analytic evaluation of energy efficiency as high groundwater intermediate movable carrier phase in the presence of heterogeneity.

Groundwater significantly affect the thermal conditions of the geological environment as carry on only the substance but also diffusion and convective heat.

Evaluation of the energetic efficiency of groundwater as a mobile heat-transfer agent should be performed with consideration of the phase non-uniformity of the geological environment, i.e. the presence of liquid and gas components. Fluid (in this case, groundwater) significantly affects the thermal regime. When the water-bearing horizons are being filtrated, the ground water transfers not only substances dissolved in it, but also transfers heat energy. As with the migration of substances, the transfer runs in a convectional and diffusive way.

Considering groundwater filtration area reduces heating medium in the presence of high-temperature sources (underground gasification and combustion of coal deposits, industrial thermal pollution). So it reduces speed and cooling medium for removing high-temperature source.

Further refinement of paintings thermal state of the geological environment in the account of the possible phase transitions groundwater (so-called "Stephen’s task").

To solve it in the presence of thermal groundwater (evaporation-condensation) proposed solution, which is similar to known solutions "solidification - melting." It is based on the account of heat loss in the crystallization zone, according to the state diagram solution or melt.

The results of the calculation indicate the change in the heat field character of the generator over time. The areas of increase in the curve’s slope correspond to the transition zone of condensation. At the upper boundary of the phase conversion area, we see the first area of rapid temperature fall. The diameter of the gas zone does not exceed five meters (on average 3 - 4 m).

Taking into consideration phase conversions and the transition zone improves the accuracy of thermal image of the object. The temperature regime, calculated separately for the water vapor, binary fluid and water, with the resultant curve gives an overview of the deviation of results obtained using standard methods of calculation from those obtained by the proposed methods.

The obtained results of environmental temperature change resulting from the operation of an underground gas-generator, which are based upon a calculation using familiar equations of heat-conductivity, coincide with the data obtained from the locality and may be used for the calculation of heat regimes of underground burning.

Keywords: phase inhomogeneity, underground coal, underground coal gasification, intermediate rolling coolant, heat, Stephen’s task.

Урахування фазових перетворень підземних вод під час оцінювання енергетичної ефективності рухомого проміжного теплоносія

С. В. Жолудєв

Дніпропетровський національний університет імені Олеся Гончара, e-mail: ggf2009@ukr.net

Висвітлена можливість аналітичного оцінювання енергетичної ефективності високотемпературних підземних вод як проміжного рухомого теплоносія за наявності фазової неоднорідності.

Підземні води істотно впливають на тепловий режим геологічного середовища, оскільки переносять не тільки речовини, а й дифузивну та конвективну теплову енергію.

Урахування фільтрації підземних вод знижує область прогріву середовища за наявності високотемпературних джерел (підземні газифікації та спалювання вугільних покладів, промислове теплове забруднення). Так само
Introduction. Evaluation of the energetic efficiency of groundwater as a mobile heat-transfer agent should be performed with consideration of the phase non-uniformity of the geological environment, i.e. the presence of liquid and gas components. Fluid (in this case, groundwater) significantly affects the thermal regime. When the water-bearing horizons are being filtrated, the ground water transfers not only substances dissolved in it, but also transfers heat energy. As with the migration of substances, the transfer runs in a convectional and diffusive way.

Presentation of the general material. The considered filtration of groundwater decreases the area of heating of the space surrounding a burning coal seam to 10 m, the speed of cooling is much higher, and the initial thermal regime practically recovers in six months. The area of heating of surrounding rocks in general does not exceed the first few meters (on average 5-7 m), which corresponds to the data from the literature on experimental measurements of temperatures in real conditions of stations with underground coal gasification and underground coal burning (Figure 1). According to the studies by the Institute of Physics of the Earth, the containing rock’s heating interval in the temperature of underground generator is not more than 1-2 m from the combustion source (Silin-Bekchurin at all, 1960). More recent studies, conducted by VNIIPodzemgaz in the Podmoskowny coal basin, registered the heating of rocks up to 100°C at a distance of 4-6 m from coal, and the total radius of thermal influence of a generator at 12-15 m. Similar results were obtained by the Laboratory of Hydro-geological Problems named after F. P. Savarensky in the studies led by A. I. Silin-Bekchurin and E. V. Kreynin (Kreynin, 1960).

Figure 1. Comparison of temperature regime with generator in operation, calculated with consideration of influence of groundwater filtration and without it.

Taking into account the established conditions of thermal fields, the following parameter should be considered: variation of environmental temperature depending upon change of phase condition of groundwater. Theory of thermal physics considers these processes as a Stefan problem and uses different modifications of traditional numerical computation methods for solving it (Belyaev at all, 1992. Barenblatt at all, 1972. Bulyandra, 2001).

Before choosing a particular method, one should evaluate its practicability in a particular situation. Having analyzed different methods, we can state that apart from the difficulty and awkwardness of calculation, they have one more disadvantage, which is significant in the considered situation. During underground gasification and combustion, the water in the surrounding area is both in a liquid and in gaseous state (water vapor). Although there is no clear differentiation of phases, there is some transitional zone, where water can be in a liquid and gaseous state (gas cut fluid or binary compound). The size of this zone and the extent of its influence cannot be neglected. The most widely used methods do not permit this fact to be incorporated into the calculation, otherwise the calculating process will become significantly more complicated. Therefore, we propose taking into account the heat of phase conversion.
There are many numerical methods for solving a Stefan problem, which are based on approaches which change the mathematical model and make it easier for numerical realization (Smirnov, 1975. Misnar, 1968. Gerashchenko, 1983). The equation of heat conduction describes the distribution of temperatures during each phase of a multi-phase body

\[ \rho(T) c(T) \frac{\partial T}{\partial t} = \text{div} (\lambda(T) \text{grad} T) + q_v, \]  

(1)

Where \( \rho, c, \lambda \) - density, specific heat and coefficient of thermal conductivity; \( q_v \) – intensity of internal heat source.

In the case of two phases (a case of higher number of phases does not cause any significant differences), we shall designate the magnitudes related to the phase, for which \( T < T_{ph} \) by index 1, and the magnitudes related to the phase, for which \( T > T_{ph} \) by index 2. Then

\[ \rho(T) = \rho_1(T), \text{ при } T < T_{ph}, \text{ и } \rho(T) = \rho_2(T), \text{ при } T > T_{ph}; \]

\[ c(T) = c_1(T), \text{ при } T < T_{ph}, \text{ и } c(T) = c_2(T), \text{ при } T > T_{ph}; \]

\[ \lambda(T) = \lambda_1(T), \text{ при } T < T_{ph}, \text{ и } \lambda(T) = \lambda_2(T), \text{ при } T > T_{ph}. \]

Consideration of conditions on the phase front and changing (2) with (1) can be made by factoring function.

\[ H = \int_{0}^{T} c_i(\xi) \rho_i(\xi) d\xi + H_{ph} \gamma(T - T_{ph}), \]  

(3)

Where \( \gamma(\xi) = 1, \text{ with } \xi\geq0, \text{ and } \gamma(\xi) = 0, \text{ with } \xi<0. \)

As a result

\[ \frac{\partial H}{\partial t} = \text{div} (\lambda(T) \text{grad} T) + q_v, \]  

(4)

Differentiation (4) according to \( \tau \) considering that \( H \) – complicated function and \( d\gamma(\xi)/d\xi = \delta(\xi) \) is Dirac's delta function, gives

\[ \rho(T)[c(T) + L \delta(T - T_{ph})] \frac{\partial T}{\partial t} = \text{div} (\lambda(T) \text{grad} T) + q_v, \]  

(5)

This equation unites expression (1) with condition (2) on phase surface.

It is known that function \( H(T) \) with \( T = T_{ph} \) experiences discontinuity of the first type with sudden change \( H(T_{ph} + 0) - H(T_{ph} - 0) = H_{ph} = pL \), and its derivative according to \( T \) is directed to infinity. That is why using difference schemes for (4) does not achieve acceptable practical results. The same occurs with (5). In order to eliminate these shortcomings, smoothening of different functions at some final interval of temperature was conducted. Smoothening of functions (5) is better for numeric realization by finite-difference methods, as given below.

As we see in (5), with \( (T) \) and \( L\delta(T - T_{ph}) \) are factored into the equation in a similar way; \( L\delta(T - T_{ph}) \) are involved in the equation in the same way; \( L\delta(T - T_{ph}) \) is a concentrated heat capacity (on the surface \( T \) in \( T_{ph} \)). Let us replace delta function by...
approximate delta-like, or “smeared” delta-function
\( \delta(T - T_{ph}, \Delta) \) \( \geq 0 \), where \( \Delta \) — magnitude of half-interval, \( \delta(T - T_{ph}, \Delta) \) is different from zero. This smoothing is equivalent to a replacement on the interval \( (T_{ph} - \Delta, T_{ph} + \Delta) \) of discontinuous function \( \gamma(T - T_{ph}) \) by continuous function \( \gamma'(T - T_{ph}, \Delta) \) so that \( \gamma'(T - T_{ph},\Delta) = \delta(\xi, \Delta) \). In other words, smoothing is made by factoring a parameter of so-called “smoothened” or “efficient” heat capacity \( c_{eff}(T) = c(T) + \Delta \delta (T - T_{ph}, \Delta) \), which should be chosen in such a way that changing of enthalpy on the interval \( [T_{ph} - \Delta, T_{ph} + \Delta] \) remains the condition

\[
c_{eff} = c(T), \quad \text{with } T < T_{ph} - \Delta ,
\]

\[
c_{eff} = c(T) + \Delta \delta (T - T_{ph}, \Delta), \quad \text{with } T_{ph} - \Delta \leq T \leq T_{ph} + \Delta ,
\]

\[
c_{eff} = c_2(T), \quad \text{with } T > T_{ph} + \Delta
\]

And the equation

\[
\int_{T_{ph} - \Delta}^{T_{ph} + \Delta} c_{eff}(T) \rho(T) \, dT = \rho \Delta + \int_{T_{ph} - \Delta}^{T_{ph} + \Delta} c_1(T) \rho_1(T) \, dT + \int_{T_{ph} - \Delta}^{T_{ph} + \Delta} c_2(T) \rho_2(T) \, dT ,
\]

Or a condition of normalizing for delta-like function should be fulfilled

\[
\int_{T_{ph} - \Delta}^{T_{ph} + \Delta} \delta(T - T_{ph}, \Delta) \, dT = 1 , \tag{8}
\]

At the same interval \( [T_{ph} - \Delta, T_{ph} + \Delta] \), smoothing of the heat capacity coefficient \( \lambda(T) \) is made. As a result, it leads to a problem with boundary conditions, which formally coincides with a problem of heat conductivity without phase conversions

\[
\rho(T) c_{eff}(T) \frac{\partial T}{\partial T} = \text{div} (\lambda(T) \text{ grad } T) + q_v , \tag{9}
\]

For solving this problem, different iteration schemes can be used, because now there are no specific elements in the conditions. Such formulation does not depend either upon the number of calculations or upon the number of phases.

Significant difficulties occur while choosing the magnitude \( \Delta \), because the width of interval of “smoothening” significantly affects the results. An incorrect choice of magnitude \( \Delta \) can cause unacceptable errors. If the width of the “smoothening” interval and steps of difference scheme is chosen arbitrarily, a situation can occur, when the interval \( [T_{ph} - \Delta, T_{ph} + \Delta] \) will contain one-two coordinate blocks or none. It is obvious, that in this case the heat release during phase conversions is not taken into consideration at all. In this sense, the zone of “smoothening” should be wide enough to “include” a few coordinate blocks. Also, the increase of \( \Delta \) also decreases the accuracy of the calculations. The optimum variant is simultaneous decrease of \( \Delta \) and of the magnitude of the coordinate steps. Contemporary requirements for the accuracy of solving the problems with phase conversions force require the use of coordinate schemes which have about ten and more coordinate blocks in the zone of “smoothening” (for one-dimensional problems) (Oradovskaya, 1982. Farlou S., 1985).

The solving of the problem “evaporation – condensation” we used an analogy with the familiar solving of the problem “solidification – melting”, which is based upon heat release in the zone of crystallization in accordance with diagram of the condition of the solution and alloy. These approaches are quite similar and are considered in more detail.

The stating of the Stefan problem includes the condition of flat phase boundaries with no local boundaries, where an equilibrium temperature of phase conversion is maintained. However, observations of phase conversion processes indicate the existence of some type of two-phase zone, which is a composition similar to gas cut fluid with some concentration of gaseous impurities. Therefore, considering the distance from the combustion source, three zones could be highlighted (Figure 2): zone of gaseous phase (I), two-phase zone of
condensation (transition zone) (II), zone of liquid phase (III).

The boundaries of the transition zone are defined by the temperature at the beginning (Tₐ) and at the end (Tₐ) of condensation (Figure 3).

Concentration of a gaseous element within this zone changes with a gradual decrease from dominant (under the temperatures near Tₐ) to isotherm Tₐ.

Relative quantity of liquid phase within two-phase zone, which is in a state of equilibrium with water vapor at the temperature T is found by the ratio

\[ \psi = \frac{V_{g} \cdot c_{l}}{V_{l} \cdot c_{g}} = \frac{c_{g} \cdot c_{l}}{c_{g} - c_{l}} = \psi(T), \quad (10) \]

Where V₁ and Vₐ – magnitudes of liquid and two-phase zone, respectively;

\( c_{g}, c_{l}, c_{t} \) – specific heat of gaseous, transition and liquid zones, respectively.

The existence of a two-phase zone causes the heat of phase conversion \( L \) to be released within the volume of the two-phase zone, and not on some surface. Therefore, the calculation of heat released during phase conversion can be made by factoring a function of heat source \( q(T) \) into the equation of heat conductivity (9) at the interval of temperatures \([T_{g}, T_{f}]\) (\( q(T) = \psi(T) \)).

\[ \rho(T) c(T) \frac{\partial T}{\partial \tau} = \text{div} (\lambda(T) \text{ grad } T) + q(T), \quad (11) \]

When solving (11), the same difficulties occur as in (9), but after using ratio \[ \frac{\partial \psi}{\partial \tau} = \frac{\partial \psi}{\partial \Omega} \frac{\partial \Omega}{\partial \tau} \]
and factoring efficient heat capacity \( c_{eff}(T) = c_{ph}(T) \cdot L \)
at the interval of temperatures \([T_{g}, T_{f}]\) (with \( T > T_{s} \)), where \( c_{eff} = c_{g} \), and with \( T < T_{f} - c_{eff} = c_{l} \), we come to (10) to (11), which coincides in form with (9)

\[ \rho(T) c_{eff}(T) \frac{\partial T}{\partial \tau} = \text{div} (\lambda(T) \text{ grad } T), \quad (12) \]

The magnitude \( \frac{\partial \psi}{\partial \tau} \), which is called the tempo of condensation, can be calculated analytically, if the lines of phase conversion of binary fluid \( L_{1}(T) \) and \( L_{2}(T) \) are expressed as lines which are parallel to one another. In this case, the condensation tempo is expressed as an equation

\[ \frac{\partial \psi}{\partial \tau} = \frac{1}{T_{s} - T_{f}}, \quad (13) \]

Using this method, we calculated the temperature regime change over time with movement away from the gasification source, considering phase conversions of ground water and conditions of thermal environment resulted from the conversions. We chose 374.15°C (so-called “critical temperature”) and 100°C for the beginning and the end of condensation. It can be assumed that in certain conditions, the water will be in a state of equilibrium with water vapor at this particular interval of temperature. The increase of temperature above the critical temperature causes oversaturated vapor, when water cannot be in a liquid state; and the decrease of temperature below the boiling point leads to total condensation. Thus, a transitional zone is realized in practice, which includes a binary mixture of liquid and gas – highly gasified liquid. The parameters of the calculation were as follows: \( L = 1930 \) kj/kg (at a temperature of 200 °C), \( c_{l} = 4.2 \) kj/kg×K (average value for temperature below 100 °C), \( c_{ph} = 2.0 \) kj/kg×K (for water vapor at temperatures 200-300 °C), \( c_{g} = 2.208 \) kj/kg×K (for water vapor at temperatures 500-600 °C), \( \lambda_{l} = 0.683 \) W/m×K, \( \lambda_{ph} = 1.229 \) W/m×K (at a temperature of 300 °C), \( \lambda_{g} = 1.536 \) W/m×K (at a temperature of 400 °C), \( \rho_{g} = 0.598 \) kg/m³ (provisionally for water vapor...
The temperature of the combustion source and surrounding environment – 1,000 °C and 20 °C, the period of the underground gas-generator’s operation - 180 days. Density ρt changes depending on

\[ \rho_t = \frac{\rho}{1 + \beta t} \]  

Where ρ and ρt – density of substance, respectively, at temperatures of 20 °C and some (t); β - coefficient of cubic extension of substance (for water at a temperature of 100 °C equals 5.87 x 10⁻⁴).

The parameters of calculation were taken for typical conditions: heat radius influence of the generator equals 20 m (i.e. the distance to the nearest generator is 40 m) (Figure 1), the temperature of the combustion source – 1,000°C, temperature of the surrounding environment is 20°C. The period of operation of the generator is half a year, followed by cooling. The coefficient of heat-conductivity for containing rocks was calculated according to the formula (a = λ/Cₚ), where the coefficient of heat conductivity for sandy-clayey and carbonaceous rocks equals 0.5...3.5 W/m×°C, Cₚ – coefficient of volumetric heat-capacity of sandy seam, equals 3,0...3,7 x 10⁶ j/(kg×°C) (Koshkin at all, 1980. Vargaftik, 1963. Vukalovich at all, 1969. Kozdoba, 1992).

The calculation used a constant value of ground water filtration speed, typical for conditions of the highly water-bearing containing rocks of the Dnipro brown coal basin v = 3.0 m/24 hours (Berman, 1989. Enohovich, 1989).

The results of the calculation presented in Figure 4 indicate the change in the heat field character of the generator over time. The areas of increase in the curve`s slope correspond to the transition zone of condensation. At the upper boundary of the phase conversion area, we see the first area of rapid temperature fall. The diameter of the gas zone does not exceed five meters (on average 3 - 4 m). The inflection of curve at the lower boundary is also seen clearly, but its value is not strongly significant due to the relative remoteness from the source and due to much lower fluctuations of temperatures.

**Conclusions.** Taking into consideration phase conversions and the transition zone improves the accuracy of thermal image of the object. Figure 5 compares the temperature regime, calculated separately for the water vapor, binary fluid and water, with the resultant curve which indicates the conversion between the phases. This graphic gives an overview of the deviation of results obtained using standard methods of calculation from those obtained by the proposed methods.

![Figure 4. Change in environmental temperature in relation to phase conversion of water depending on the distance from the combustion source.](image)

![Figure 5. Comparison of temperature regime of ground water in different phase conditions.](image)

The obtained results of environmental temperature change resulting from the operation of an underground gas-generator, which are based upon a calculation using familiar equations of heat-conductivity, coincide with the data obtained from the locality and may be used for the calculation of heat regimes of underground burning.

**References**

Silin-Bekchurin A.I., Bogoroditskiy K.F., Kononov V.I., 1960. Rol podzemnyih vod i drugih prirodnyih faktorov v protsesse podzemnoy gazifikatsii ugl'ya [The role of water and another natural factors in the process of underground coal gasification]. Proceedings Laboratory of hydrogeological problems named after F.P. Savarenskiy, vol. XXIII. Publishing USSR Academy of Sciences, Moscow, 126 p. (in Russian).
Kreynin E. V., Revva M. S., 1960. Podzemnaya gazifikatsiya ugley [Underground coal gasification]. Kemerov’s Book Publishing 83 p. (in Russian).

Belyaev N. M., Ryadno A. A., 1992. Matematicheskie metody teploprovodnosti: Uchebnoe posobie [Mathematical methods of heat transferee]. Vischa shkola, Kyev. 415 p. (in Russian).

Barenblatt G. I., Entov V. M., Ryzhik V. M., 1972. Teoriya nestatsionarnoy filtratsii zhidkosti i gaza [Theory of no stationary filtering of liquids and gas]. Nedra, Moscow. 288 p. (in Russian).

Bulyandra O. F., 2001. TehnIchna termodinamIka: PIdr. dlya energ. spets. VNZIv [Technical Thermodynamics. Handbook for energy spec. in Universities]. TehnIka, Kyev. 320 p. (in Ukrainian).

Smirnov B. V., 1975. Ispolzovanie modelirovaniya dlya prognoza inzhenerno-geologicheskikh usloviy razrabotki mestorozhdeniy poleznyih iskopaemyih [Using modeling for the prediction of engineering and geological development of mineral resources]. Nedra, Moscow, 100 p. (in Russian).

Minsar A., 1968. Teploprovodnost tverdyih tel, zhikostey, gazov i ih kompozitsily [Heat transferee of solid bodies, liquids, gases and their compositions]. Mir, Moscow, 464 p. (in Russian).

Teploperedacha i prikladnaya gidrodinamika [Heat transfer and fluid dynamics Applied]. Ed. Gerashchenko O.A., 1983. Naukova dumka, Kyev, 200 p. (in Russian).

Oradovskaya A. E., 1982. Migratiya veschestva i tepla v podzemnih vodah [Migration of substance and heat in the underground water]. Hydroreolohycheskkye research abroad, Nedra, Moscow, p. 33 – 74. (in Russian).

Farlou S., 1985. Uravneniya s chastnyimi proizvodnymi dlya nauchnyih rabotnikov i inzhenerov [equation with partial derivatives for the Scientific workers and engineers]. Mir, Moscow, 384 p. (in Russian).

Koshkin N. I., Shirkevich M. G., 1980. Spravochnik po elementarnoy fizike: [Spravochnik] [Handbook on elementary physics [Directory]. Nauka, Moscow, 208 p. (in Russian).

Vargaftik N. B., 1963. Spravochnik po teplofizicheskim svoystvam gazov i zhidkostey: [Spravochnik][Handbook on heat physical properties of gases and liquids [Directory]. Fiz.- mat. Lit. Publishing, Moscow, 708 p. (in Russian).

Vukalovich M. P., Ryivkin S. L., Aleksandrov A. A., 1969. Tablitsyi teplofizicheskikh svoystv vodyi i vodyanogo para: [Spravochnik][Tables of heat physical properties of water and water steam [Directory]. Standards Publishing, 407 p. (in Russian).

Kozdoba L. A., 1992. Vyichislitelnaya teplofizika [Calculable heat physics]. Naukova dumka, Kyev, 224 p. (in Russian).

Berman R., 1989. Teploprovodnost tverdyih tel [Heat transferee of solid bodies]. Mir, Moscow1979. – 286 p. (in Russian).

Enohovich A. S., 1989. Spravochnik po fizike i tehnikе [Spravochnik] [Handbook on the physics and technique [Directory]. Prosveschenie, Moscow, 224 p. (in Russian).

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