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EXACT ANALYTICAL SOLUTIONS FOR NON-STEADY HEAT TRANSFER PROBLEMS AND THEIR ROLE IN VERIFICATION OF MODELS FOR THERMO-HYDRO-MECHANICAL PROCESSES IN DEEP GEOLOGICAL RADIOACTIVE WASTE REPOSITORIES

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Numerical simulation of complex underground facilities, such as deep geological radioactive waste repositories, requires coupled assessment of thermo-hydro-mechanical and, possibly, other processes. Therefore, obtaining robust estimates for the temperature field is considered as a crucial task. Computer codes used for modelling require verification on the problems that have exact analytical solution. Furthermore, these problems should reflect characteristic features of modelled objects. For heat transfer problems, these features primarily involve spatial and temporal distribution of heat sources. In this paper, the exact analytical solutions for non-steady 3D heat transfer equation are obtained for the medium with constant thermal properties and exponentially decreasing point, linear and planar heat sources. In terms of verification purposes these configurations sufficiently well fit with actual problems solved in safety analysis of deep geological repositories for radioactive waste. Presented solutions can be used to verify computer codes with numerical solution of heat transfer equation or similar numerical models, such as diffusion, Brownian movement, etc.

Keywords: *radioactive waste, deep geological repository, computer code verification, non-steady heat transfer equation, exact analytical solutions.*

Introduction

To date, large amounts of high-level waste (HLW) have been accumulated both in Russia and abroad. A number of specific aspects should be considered in the development of relevant HLW final disposal solutions, in particular, of deep disposal facilities for radioactive waste (DDF RW). High heat output should be considered as one of these aspects. Large volumes of radionuclides and the need for ensuring their robust isolation for a long time, namely, over tens of thousands of years, require extensive research to be done to demonstrate the safety of such disposal facilities [1—4]. DDF RW evolution is determined by numerous coupled processes: thermal, mechanical, hydrological, chemical, biological and other, thus, its modelling should be implemented in a comprehensive manner suggesting that mutual impact of different phenomena is accounted for. This fact has been evidenced by international experience [5]. Moreover, thermal phenomena largely determine the occurrence of other processes, since the temperature impacts the transport properties of the medium, the speed of chemical reactions and the way these reactions take place, distribution of mechanical stresses in the materials, and so on. In turn, heat transfer in deep geological repository and host rocks is determined, for example, by convection of the pore water and heat sources or heat sinks both associated with heat release from radioactive waste and chemical reactions. Thus, today evolution of complex underground facilities is being evaluated with the use of computational tools involving thermo-hydro-mechanical-chemical (THMC) models suggesting different degrees of interfacing [6]. In some cases, the impact of biological processes is also accounted for, for example of those resulting in the alteration of material's transport and mechanical properties [7]. It should be noted that complete coupling of all these processes in a single calculation haven't been implemented to date, for example, [6] discusses some case studies where a maximum of three models is simultaneously coupled (THM, THC).

Currently developed computer code FENIA (Finite Element Nonlinear Incremental Analysis) [8, 9] also accounts for the coupling of three models: thermal, hydraulic and mechanical (THM). In this case, equations for energy conservation (thermal conductivity) and equilibrium (mechanics) are solved sequentially at each time step. Thus, current state of the calculated temperature field is always applied in the mechanics model. The reverse effect associated with the impact of mechanical processes on the thermal state is negligible and is not taken into account in the code.

There are two ways enabling to couple the hydraulic model with a thermal one. The first one suggests that a simplified hydraulic model implemented in FENIA code is interacting with a thermal one similarly to the mechanical one: current temperature field is applied at each time step. However, relevant feedback is also taken into account: at the next step, updated values for the medium's thermal properties (heat capacity, thermal conductivity) being dependent on the water content are used. The second case suggests that hydraulic processes are being modeled by an external calculational tool — the GeRa code [9]. In this case, more complex hydraulic models are used, but the data exchange takes place via external interfaces of computer codes. In this case, synchronization at each time step is impossible, respectively, information exchange between different codes is rarer. Similarly, other computer codes can be used, for example, those simulating chemical reactions.

All the above mentioned facts indicate that the results from the solution of a thermal problem are used as input data for a number of other models. Thus, without detracting the merits of other processes, robust assessment of temperature field is considered as a key task in demonstrating the safety of DDF RW. At the same time, due to the complexity of the geological environment, supplemented by relevant features of engineered safety barriers, on the one hand, and the structure of the excavations used for RW emplacement, on the other, calculation of DDF RW thermal state even without being coupled with other models should be viewed as a non-trivial task.

Therefore, immediate application of analytical solutions for heat transfer equation to forecast the evolution of DDF RW thermal state is practically impossible, and software tools (computer codes) implementing numerical simulation methods are required.

Applying analytical solutions for computer code verification

Nevertheless, the importance of accurate analytic solutions should not be underestimated, since such software should be verified prior to its application. In this paper verification means checking the implementation of numerical methods for tasks implying exact analytical solution in accordance with a concept suggesting separate consideration of verification (analytical problems) and validation (experimental data, etc.) processes [11]. Samarskiy A. A., Member of the Academy of Sciences, once stated that [12] "oftentimes it's hard to estimate properties an algorithm used to solve gas dynamics problems theoretically. Therefore, when analyzing the quality of numerical schemes, various a priori judgments should be supplemented by a posteriori research playing a major role. Testing schemes and algorithms by applying particular "exact" solutions (tests) should be primary viewed as such. For this purpose, some simplified concepts of the original problem are being calculated. These may not provide a complete physical picture of the process, but allow a simple (for example, analytical) solution. Comparison of the results of calculations with known solutions allows us to judge on the accuracy of the scheme, the rate of convergence and etc. Therefore, construction of exact test solutions, in particular, self-similar ones, is a necessary element in a general program aimed at constructing numerical algorithms."

Obviously, such an approach should be applied to other numerical algorithms as well, and to the algorithms solving heat transfer equations in particular. Moreover, theoretical studies exploring the convergence of numerical schemes are valid only if the size of the computational cell tends to zero and cannot guarantee the accuracy of the results in case of finite cell size. Only comparisons with exact solutions allow to estimate the proximity of the numerical solution to the solution of the original differential equations in case of finite size computational cells, which are always used in solving complex practical problems. Therefore, obtaining accurate analytical solutions, especially those to a certain extent reflecting current physical state associated with the practical task being under consideration, is viewed as a most important part in the development of numerical algorithms and relevant software products. This has been reflected in regulatory provisions, namely NP-100-17 [13] stating that: "Adequacy, reliability and accuracy of mathematical models, applied calculation methods and calculation schemes should be justified by comparing numerical solutions with analytical ones obtained using other models, the adequacy, reliability and accuracy of which has been evaluated".

Below are overviewed the specific aspects that should be taken into account when analytical problems are stated applicable to the verification of computational tools designed to simulate deep repository's thermal state. First of all, it should be noted that the problem considered is non-stationary, since the heat release from radioactive waste varies with time. Vitrified waste involves various isotopes and, as a result, may be characterized with complex heat-release time dependence. However, in accordance with the radioactive decay law, for verification purposes this dependence can be considered as an exponential one. Stationary heat conduction problem suggests the availability of exact analytical solutions (see, for example, [14]) for various spatial configurations of the heat source. However, general solution for a non-stationary problem should be a complex one [15]. Furthermore, authors of the paper have no information on the analytical solutions for exponentially decaying sources. Semi-analytical solution derived by D. P. Hodgkinson and described in [16] can be considered as a greatest progress achieved to date in this area. However, this solution requires numerical integration, therefore, for verification purposes it can only be used with certain reservations, as all the above-mentioned arguments concerning the accuracy of the pattern, convergence rate, and other relevant items are associated both with the solution itself and the result obtained from computer code application.

This paper overviews a number of problems with an exponentially decaying heat source that can be used to verify computational codes simulating the dynamics of DDF RW thermal state suggesting exact analytical solutions derived by the authors.

Single insulating container (IC) with heat-generating HLW surrounded by a sufficiently large volume of host rock can be approximately considered as a point heat source. Indeed, IC characteristic size amounts to several meters. At the same time if such IC is disposed of alone, for example, as part of an experiment in an underground research laboratory (URL), it may be surrounded by tens of meters of rock. Thus, we can approximately state that this problem suggests modeling of a three-dimensional temperature field coming from a point heat source with an exponential decrease in heat generation. This and all the following case studies suggest that the rock is assumed to be homogenous, as a medium with heterogeneities described by linear or piecewise constant spatial dependence can be easily reduced to a homogeneous one by changing the variables. More complex spatial dependences result in a considerable complication of the problem enabling to obtain an analytical solution.

Unlike URL case, DDF RW designs consider some series of IC and not a single IC. For example, disposal in long horizontal galleries being several tens of meters long is considered in Belgium and France [17]. Another option considered, deep boreholes or combination of boreholes and horizontal galleries [9]. With HLW container diameter of about a meter, a single gallery or borehole can be considered as a heat source with heat release uniformly distributed along a line. Due to large length of the section occupied by waste, effects occurring near the ends of the sections can be largely neglected. Thus, the following problem applicable for verification purposes can be stated as modeling two-dimensional temperature field for an infinite (linear) heat source along a straight line with an exponential decrease in heat generation.

In some cases, DDF RW on the whole can be considered as a heat generation source. For example, KBS-3 project implemented in Sweden and Finland involves HLW containers emplaced into separate wells located at the same horizon. When describing the thermal state of the host rocks at a substantial distance above or below DDF RW, a set of HLW containers can be approximately considered as a heat-generating plane. Thus, one more verification problem can be defined as a problem suggesting simulation of a one-dimensional temperature field for a heat source distributed over a plane. The heat decay will be also assumed to be exponential.

Exact analytical solutions suggesting the use of a unified approach based on generalized solution of the heat equation were obtained for these three problems.

Unsteady temperature field of an exponentially decaying source

General case

General case suggests that the solution of non-stationary heat-transfer equation for a medium with constant physical properties in n-dimensional space R_n, $\mathbf{x} = (x_1, \ldots, x_n)$ with initial condition:

$$\frac{\partial T}{\partial t} - a^2 \Delta T = q(t, \mathbf{x}),$$
$$T\big|_{t=0} = T_0(\mathbf{x}) \quad (1)$$

is stated using the following equation [15]

$$T(\mathbf{x},t) = \int_0^t \int_{R^n} \frac{q(s,\xi)}{\left[2a\sqrt{\pi(t-s)}\right]^n} \exp\left(-\frac{|\mathbf{x}-\xi|^2}{4a^2(t-s)}\right) d\xi ds +$$
$$+ \frac{1}{\left[2a\sqrt{\pi t}\right]^n} \int_{R^n} T_0(\xi) \exp\left(-\frac{|\mathbf{x}-\xi|^2}{4a^2 t}\right) d\xi. \quad (2)$$

In (1) $q(t,\mathbf{x}) = \frac{Q(t,\mathbf{x})}{\rho c}$, $Q(t,\mathbf{x})$ — stands for heat generation rate, ρ — rock density, c – heat capacity, $a^2 = \lambda/(\rho c)$ — heat conductivity, $\Delta = \sum_{i=1}^{n} \frac{\partial^2}{\partial x_i^2}$ — Laplace operator. If homogeneous initial conditions are considered $T_0(\mathbf{x}) = T_0$ = const, equation (1), after the following substitution is done: $T(\mathbf{x},t) = u(\mathbf{x},t) + T_0$, can be reduced to an equation with zero initial condition.

$$\frac{\partial u}{\partial t} - a^2 \Delta u = q(t, \mathbf{x}),$$
$$u\big|_{t=0} = 0. \quad (3)$$

Solution of the equation (3) will depend only on the first summand located in the right part of equation (2).

$$u(\mathbf{x},t) = \int_0^t \int_{R^n} \frac{q(s,\xi)}{\left[2a\sqrt{\pi(t-s)}\right]^n} \exp\left(-\frac{|\mathbf{x}-\xi|^2}{4a^2(t-s)}\right) d\xi ds. \quad (4)$$

Analytical solutions for a centered source (plane, straight line and point)

From (4) solutions can be obtained being relevant for the cases $n = 1, 2, 3$ (plane, straight line and point source respectively) to study the thermal field around heat-generating RW. Figures 1—3 present the considered configurations generally describing the shape of the temperature distributions.

For a heat source concentrated on a plane $z = 0$, heat will propagate along z axis, and the problem can be assumed to be one-dimensional ($n = 1$, $x_1 = z$, $\mathbf{x} = (z)$, Figure 1). For a heat source concentrated on a straight line (axis z), heat will be propagating within a plane being orthogonal to this axis ($n = 2$, $x_1 = x$, $x_2 = y$, $\mathbf{x} = (x, y)$, Figure 2). For a point source, heat will be propagating in all directions, and the problem should be viewed as a three-dimensional one ($n = 3$, $x_1 = x$, $x_2 = y$, $x_3 = z$, $\mathbf{x} = (x, y, z)$, Figure 3). In this case, we consider the source centered in the zero-point, $\mathbf{x} = (0, 0, 0)$.

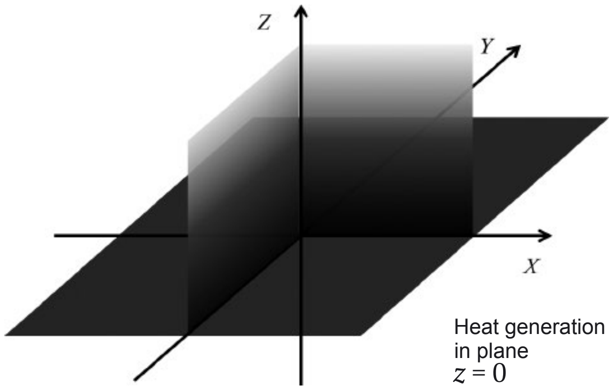

Figure 1. Problem involving a heat-generating plane (n = 1)

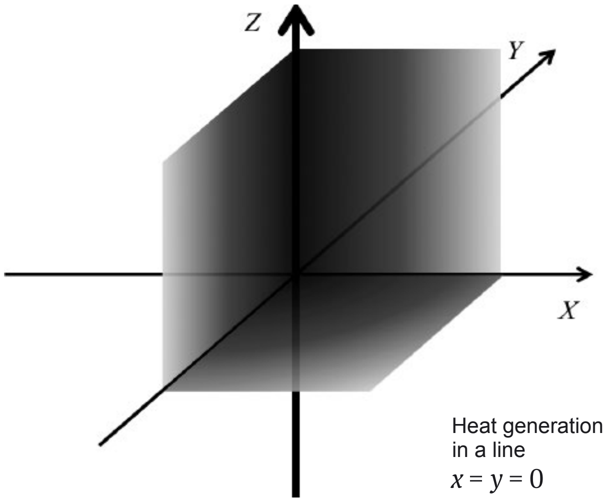

Figure 2. Problem involving a heat-generating line (n = 2)

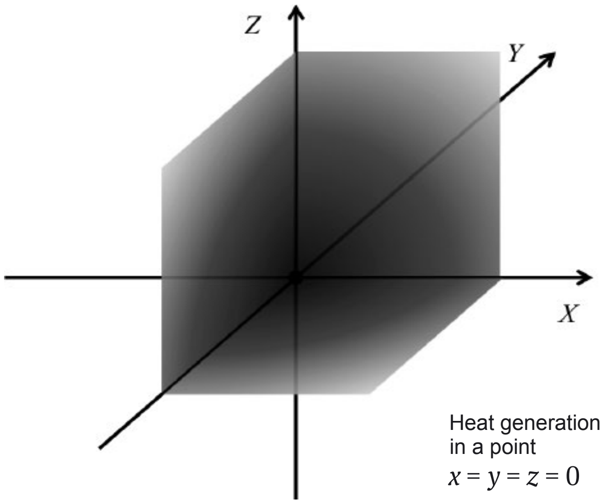

Figure 3. Problem involving a heat-generating point source (n = 3)

For a decaying heat source, the following equation was considered:

$$q(t,\mathbf{x}) = q_0 \exp(-pt)\delta(\mathbf{x}). \quad (5)$$

It should be noted that source term member of equation (3) in the form of (5) describes all cases $n = 1, 2, 3$, and has the following dimension [q] = W/m^{3-n}.

By substituting (5) into (4), the following equation can be derived:

$$u(\mathbf{x},t) = \int_0^t \int_{R^n} \frac{q_0 \exp(-ps)\delta(\xi)}{\left[2a\sqrt{\pi(t-s)}\right]^n} \exp\left(-\frac{|\mathbf{x}-\xi|^2}{4a^2(t-s)}\right) d\xi ds =$$

$$= q_0 \int_0^t \frac{\exp(-ps)}{\left[2a\sqrt{\pi(t-s)}\right]^n} \exp\left(-\frac{|\mathbf{x}|^2}{4a^2(t-s)}\right) ds. \quad (6)$$

The following substitution $t - s \to bs'$ in (6) results in:

$$b = \frac{|\mathbf{x}|^2}{4a^2}, \; r = |\mathbf{x}|. \quad (7)$$

After non-dimensional values $h = pb$, $c = t/b$ are introduced, expression (6) will take the form as follows:

$$u(\mathbf{x},t) = q_0 \int_0^c \frac{\exp(-p(t-bs'))}{\left[2a\sqrt{\pi bs'}\right]^n} \exp\left(-\frac{1}{s'}\right) b ds' =$$

$$= \frac{q_0 \exp(-pt) b^{1-n/2}}{\left[2\sqrt{\pi}a\right]^n} \int_0^c \frac{1}{s^{n/2}} \exp\left(hs - \frac{1}{s}\right) ds. \quad (8)$$

For further calculations the value of exp(hs) in (8) is decomposed into a Maclaurin series, thus, the integral from (8) can be expressed as follows:

$$\int_0^c \frac{1}{s^{n/2}} \exp\left(hs - \frac{1}{s}\right) ds = \int_0^c \frac{1}{s^{n/2}} \sum_{i=0}^{\infty} \frac{(hs)^i}{i!} \exp\left(-\frac{1}{s}\right) ds =$$

$$= \sum_{i=0}^{\infty} \frac{h^i}{i!} \int_0^c s^{i-n/2} \exp\left(-\frac{1}{s}\right) ds. \quad (9)$$

Following another substitution $s \to \frac{c}{s'}$, the integral under the summation symbol in (9) can be expressed through the following exponential integral $E_n(x) = \int_1^{\infty} \frac{\exp(-xs)}{s^n} ds$ being considered as a special function that can be calculated based on available GSL and boost libraries.

$$\int_0^c s^{i-n/2} \exp\left(-\frac{1}{s}\right) ds = -\int_1^{\infty} \left(\frac{c}{s}\right)^{i-n/2} \exp\left(-\frac{s}{c}\right) d\left(\frac{c}{s}\right) =$$

$$= c^{i+1-n/2} \int_1^{\infty} \frac{\exp\left(-\frac{s}{c}\right)}{s^{i+2-n/2}} ds = c^{i+1-n/2} E_{i+2-n/2}\left(\frac{1}{c}\right). \quad (10)$$

Substituting (10) into (9) and the result obtained into (8), and also revealing the expressions for h, c constants, the final solution can be derived:

$$u(\mathbf{x},t) = \frac{q_0 \exp(-pt) b^{1-n/2}}{\left[2\sqrt{\pi}a\right]^n} \sum_{i=0}^{\infty} \frac{h^i}{i!} c^{i+1-n/2} E_{i+2-n/2}\left(\frac{1}{c}\right) =$$

$$= \frac{q_0 \exp(-pt) b^{1-n/2} c^{1-n/2}}{\left[2\sqrt{\pi}a\right]^n} \sum_{i=0}^{\infty} \frac{(pt)^i}{i!} E_{i+2-n/2}\left(\frac{1}{c}\right) =$$

$$= \frac{q_0 \exp(-pt) t^{1-n/2}}{\left[2\sqrt{\pi}a\right]^n} \sum_{i=0}^{\infty} \frac{(pt)^i}{i!} E_{i+2-n/2}\left(\frac{r^2}{4a^2 t}\right). \quad (11)$$

Separately can be obtained the final solutions for all of the three cases (n = 1, 2, 3). For a source concentrated on a plane (n = 1):

$$u(z,t) = \frac{q_0 \exp(-pt)\sqrt{t}}{2\sqrt{\pi}a} \sum_{i=0}^{\infty} \frac{(pt)^i}{i!} E_{i+3/2}\left(\frac{z^2}{4a^2 t}\right). \quad (12)$$

For a source concentrated on a line (n = 2):

$$u(x,y,t) = \frac{q \exp(-pt)}{4\pi a^2} \sum_{i=0}^{\infty} \frac{(pt)^i}{i!} E_{i+1}\left(\frac{x^2+y^2}{4a^2 t}\right). \quad (13)$$

For a source concentrated in a point (n = 3):

$$u(x,y,z,t) = \frac{q_0 \exp(-pt)}{\left[2\sqrt{\pi}a\right]^3 \sqrt{t}} \sum_{i=0}^{\infty} \frac{(pt)^i}{i!} E_{i+1/2}\left(\frac{x^2+y^2+z^2}{4a^2 t}\right). \quad (14)$$

In case of three-dimensional modeling, it is also possible to obtain a solution suggesting that the temperature is expressed by so-called error function. Transformation of the equation (6) by setting n = 3 in it and introduction of (7) results in the following equation:

$$u(\mathbf{x},t) = \int_0^t \frac{q_0 \exp(-ps)}{\left[2a\sqrt{\pi(t-s)}\right]^3} \exp\left(-\frac{r^2}{4a^2(t-s)}\right) ds =$$

$$= \frac{2q_0}{(2a)^2 \left(\sqrt{\pi}\right)^3 r} \int_0^t \exp\left(-ps - \frac{r^2}{4a^2(t-s)}\right) d\frac{r}{2a\sqrt{t-s}}. \quad (15)$$

The following $\frac{r}{2a\sqrt{t-s}} \to s' \Rightarrow s = t - \frac{r^2}{2a^2 s'^2}$ substitution in (15) provides the following equation:

$$u(\mathbf{x},t) = \frac{2q_0}{(2a)^2 \left(\sqrt{\pi}\right)^3 r} \int_{r/2a\sqrt{t}}^{\infty} \exp\left[-p\left(t - \frac{r^2}{4a^2 s^2}\right) - s^2\right] ds =$$

$$= \frac{q_0 \exp(-pt)}{4a^2 \pi r} \frac{2}{\sqrt{\pi}} \int_{r/2a\sqrt{t}}^{\infty} \exp\left[\frac{pr^2}{4a^2 s^2} - s^2\right] ds =$$

$$= \frac{q_0 \exp(-pt)}{4a^2 \pi r} \frac{2}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{pr^2}{4a^2}\right)^n \int_{r/2a\sqrt{t}}^{\infty} \frac{1}{s^{2n}} \exp\left[-s^2\right] ds. \quad (16)$$

A recurrence relation can be obtained for the integral in (16):

$$\int_{r/2a\sqrt{t}}^{\infty}\frac{1}{s^{2n}}\exp\left(-s^2\right)ds=-\frac{1}{2n-1}\int_{r/2a\sqrt{t}}^{\infty}\exp\left(-s^2\right)d\frac{1}{s^{2n-1}}=$$

$$=-\frac{1}{2n-1}\left[\exp\left(-s^2\right)\frac{1}{s^{2n-1}}\Big|_{r/2a\sqrt{t}}^{\infty}+\int_{r/2a\sqrt{t}}^{\infty}\frac{2}{s^{2n-2}}\exp\left(-s^2\right)ds\right]=$$

$$=\frac{1}{2n-1}\left[\left(\frac{r^2}{4a^2t}\right)^{-n+1/2}\exp\left(-\frac{r^2}{4a^2t}\right)-2\int_{r/2a\sqrt{t}}^{\infty}\frac{1}{s^{2n-2}}\exp\left(-s^2\right)ds\right]. \quad (17)$$

Below equation can be obtained by setting $I_n=\frac{2}{\sqrt{\pi}}\int_{r/2a\sqrt{t}}^{\infty}\frac{1}{s^{2n}}\exp\left(-s^2\right)ds$, equal to

$$I_{n+1}=\frac{1}{2n+1}\left[\frac{2}{\sqrt{\pi}}\left(\frac{r^2}{4a^2t}\right)^{-n-1/2}\exp\left(-\frac{r^2}{4a^2t}\right)-2I_n\right],$$

$$n=0,1,2,\ldots \quad (18)$$

With I_0 standing for a function referred to as error integral.

$$I_0=\frac{2}{\sqrt{\pi}}\int_{r/2a\sqrt{t}}^{\infty}\exp\left(-s^2\right)ds=\operatorname{erfc}\left(\frac{r}{2a\sqrt{t}}\right). \quad (19)$$

Thus, the following expression can be derived for (16):

$$u(\mathbf{x},t)=\frac{q_0\exp(-pt)}{4a^2\pi r}\sum_{n=0}^{\infty}\frac{I_n}{n!}\left(\frac{pr^2}{4a^2}\right)^n. \quad (20)$$

The derived solution can be implemented using standard C++ libraries. Thus, its software implementation does not require the development of additional procedures for numerical integration.

It should be noted that slow decrease in heat generation when $p\to 0$ in the expression for the time dependence for heat generation rate (5) and rather short time periods considered, source power can be approximately considered as a constant one. In this case, we can restrict ourselves to the first member in the series:

$$u(\mathbf{x},t)=\frac{q_0}{4\pi a^2 r}\operatorname{erfc}\left(\frac{r}{2a\sqrt{t}}\right). \quad (21)$$

When obtained solutions are used for an exponentially decaying heat source to verify the computational tools, one should keep in mind that these solutions have a special point at $r=0$. Therefore, for r values being close to zero, the numerical simulation may require some small spatial and temporal discretization.

Conclusion

It’s clear that in the solutions obtained some specific aspects of actual RW disposal facilities such as final size of waste matrices, the complex structure of engineered safety barriers, heterogeneity and anisotropy of the host rock and other are not accounted for, describing to some extent idealized cases. Nevertheless, they reflect the basics associated with RW emplacement in DDF. Therefore, they can be used to test the basic possibility of modeling basic DDF RW configurations using software tools.

The solutions obtained were embodied into the software tool developed [18] and used to verify thermal models for FENIA computer code. Verification results were presented in [19], thus, they were not further discussed in this paper. However, it should be noted that comparison of the FENIA output data with analytical solutions revealed their good consistency. Calculations were performed implying the initial heat generation values, its decay rate and heat conductivity of the host rock being considered realistic for the DDF RW.

These analytical solutions can be also used to verify other calculation tools implementing numerical solution of heat transfer equations. In particular, these can be models of diffusion, Brownian motion, or their analogues being considered in other areas, for example, in economics [20].

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