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GRADIENT METHODS FOR IDENTIFICATION OF POINT SOURCE POWER IN POROUS MEDIUM

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ГРАДІЄНТНІ МЕТОДИ ІДЕНТИФІКАЦІЇ ПОТУЖНОСТІ ТОЧКОВОГО ДЖЕРЕЛА В ПОРИСТОМУ СЕРЕДОВИЩІ

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Abstract. The article is dedicated to several gradient based methods for solving a two-dimensional humidification problem, described by Richards equation. Several assumptions are made: water is assumed incompressible, external pressure and temperature are constant. The initial state and desired function are known, while the optimal source power should be calculated. Kirchhoff transformation is applied to the initial equation to simplify the stated problem. Time and space coordinates are scaled to get linear dimensionless equation, which can be easily discretized over space and time. Numerical methods are applied to rewrite and solve the system. Also gradient methods are applied for cases, where it is possible to define the optimization functional for every allowed source power.
Keywords: Mathematical simulation, Control, Optimization, Richards–Klute equation.

Анотація. Стаття присвячена кільком градієнтним методам розв'язання двовимірної задачі зволоження, що описується рівнянням Річардса-Клюта. Зроблено кілька припущень: вода вважається нестисливою, зовнішній тиск і температура постійні. Початковий стан і бажана функція відомі, а оптимальну потужність джерела слід розрахувати. Для спрощення поставленої задачі до початкового рівняння застосовано перетворення Кірхгофа. Координати часу та простору масштабуються, щоб отримати лінійне безрозмірне рівняння, яке можна легко дискретизувати в просторі та часі. Для переписування та розв'язування системи застосовуються чисельні методи. Також градієнтні методи застосовуються для випадків, коли можна визначити функціонал оптимізації для кожного дозволеного джерела потужності.
Ключові слова: математичне моделювання, керування, оптимізація, рівняння Річардса–Клюта.

1. Introduction

Moisture transfer in porous medium is often described by Richard equation, which is nonlinear and hard for complete analysis depending on moisture conductivity and diffusion [1, 2]. Still for some cases it is possible to apply Kirchhoff transformation to simplify it and make transition to a problem with scaled values. As an alternative, iterative methods and their combinations for the Richards equation can be used [3].

For the resulting system of equation, variation algorithm, consisting of direct problem, conjugate problem and new source power approximation can be applied [4]. The optimization problem is formulated as minimization of modular difference between received humidity using chosen source powers and the desired humidity at the last time step. Existence and uniqueness of the optimal source power and an approach to get the initial approximation, were discussed for similar problems in [5, 6].

To solve the linear system for direct and conjugate equations explicit and implicit methods were used [7–9]. In case of explicit method, the amount of time steps is larger to gain convergence, but calculations are relatively simple. In case of implicit scheme, Gaussian Elimination Method was used to get exact solutions and Jacobi method as an alternative. All three approaches showed alike results.

Richards equation in its initial form has been discussed for a long time because of its complexity. A review of advances and challenges while solving Richards equation can be found in [10, 11]. For the problem stated for variably saturated flow in heterogeneous layered porous media, in [12] a numerical method to compute a solution of Kirchhoff-transformed Richards equation is discussed.

An extension of the Richards equation at [13], where non-equilibrium effects like hysteresis and dynamic capillarity are incorporated, is demonstrated through analysis of the water pressure and the saturation. Parameters describing pore structure are investigated in [14] using image based modeling. A three-dimensional, X-ray computed tomography image stack of a soil sample is used here to get computational mesh and solution of related equation leads to obtaining the up-scaled parameters in Richards equation.

A catalog of effective models which are validated by numerical computations model for describing flow in an unsaturated porous medium containing a fracture is obtained in [15]. Here both the flow in the fracture as well as in the matrix blocks are governed by Richards' equation coupled by natural transmission conditions. In [16] a nonlinear solver, based on variable switching, for the resolution of the Richards equation is proposed. Implementation includes a fictitious variable allowing to describe both the saturation and the pressure.

Free software library AMGCL is used [17] to speed up the process of obtaining solutions, compared to finite element and finite volume methods. Up to 79% reduction of the computational running time was achieved without losing accuracy. Seven models with different soils and geometries were tested, and the analysis of these tests showed, that AMGCL causes a speedup in all models with 20,000 or more nodes. However, the numerical overhead of AMGCL causes a slowdown in all models with 20,000 or fewer nodes.

Several implicit and semi-implicit temporal discretization techniques are studied in [18] with second-order accuracy. To obtain a linear system for the semi-implicit schemes, extrapolation formulas and/or semi-implicit Taylor approximations for the temporal discretization of nonlinear terms are used. To analyze efficiency and robustness of the different schemes, numerical convergence study and a series of numerical tests are performed. A great combination of collecting data using modern technology and Richards equation is demonstrated in [19]. P-band radar remote sensing applied during the Airborne Microwave Observatory of Subcanopy and Subsurface (Air-MOSS) mission has shown great potential for estimation of root zone soil moisture. In this paper, a physically-based soil moisture profile model containing three free parameters is derived, based on a solution to Richards' equation for unsaturated flow in soils.

In [20] a multi-scale method for simulating a dual-continuum unsaturated flow problem is studied for the case of complex heterogeneous fractured porous media. After time discretization, Picard iteration procedure is used to deal with non-linearity for linearization of the homogenized Richards equations. At each Picard iteration, some degree of multi-scale still remains from the intermediate level, so researchers utilize the generalized multi-scale finite element method (GMsFEM) combining with a multi-continuum approach, to upscale the homogenized system to a macroscopic (coarse-grid) level.

Idea of method, alike to [21] is used to find the solution of minimization problem using values, known at fixed source power combinations. Then more tests are performed if necessary in sub areas, where results are currently the best.

2. Process description and its model

Consider a two-dimensional problem, described by the following equation [1]:

$$\frac{\partial \omega}{\partial t} == \frac{\partial}{\partial x}\left[K_x(\omega)\frac{\partial H}{\partial x}\right] + \frac{\partial}{\partial y}\left[K_y(\omega)\frac{\partial H}{\partial y}\right] + \sum_{m=1}^{M} Q_m\left(t\right)\delta\left(x - x_m, , y - y_m\right),$$

$$(x, y, t) \in \Omega_0 \times (0, T]\,.$$

In this formula H stands for hydraulic head, K is a moisture conductivity function, ω describes humidity, t refers to time, y represents vertical space coordinate taken positive downwards and x represents horizontal space coordinate. This equation can be applied to homogeneous and heterogeneous medium. Our approach describes concentrated sources of water, in the current research boundary conditions are:

$$\omega|_{x=0} = \omega_0;\ \ \omega|_{x=L_1} = \omega_0, \omega|_{y=0} = \omega_0;\ \ \omega|_{y=L_2} = \omega_0,$$

Let us assume that $K_x\left(\omega\right) = k_1 k\left(\omega\right)$ and $K_y\left(\omega\right) = k_2 k\left(\omega\right)$, where $k_1$and k_2 are filtration coefficients along axes Ox, Oy, and $k(\omega)$ stands for humidity function for the ground. To make a transition to an equivalent dimensionless equation, some more scaling variables are used:

$$\beta_2 = 0,5, \beta_1 = \sqrt{\frac{k_2}{k_1}}\beta_2, \alpha = \frac{\langle D_x \rangle}{\beta_2^2}, \xi = \frac{beta_1}{L_1}x, \zeta = \frac{\beta_2}{L_2}y, \tau = \alpha t.$$

Here $\langle D_y \rangle$ is the average value of the Kirchhoff's potential $D_y(\omega) = K_y(\omega)\frac{d\psi}{d\omega}$ represents diffusion along y axis, will be: $\Theta = \frac{4\pi k_1}{Q^* k_2 \beta_2}\int_{\omega_0}^{\omega} D_y(\omega)\, d\omega)$, where Q^* is a vector parametric scale multiplier, Ω are dimensionless analogue to Ω_0.

As a result, we can make a transition to linearized problem

$$\frac{\partial\Theta}{\partial\tau} = \frac{\partial^2\Theta}{\partial\xi^2} + \frac{\partial^2\Theta}{\partial\zeta^2} - -2\frac{\partial\Theta}{\partial\zeta} + 4\pi\sum_{m=1}^{M} q_m(\tau)\,\delta(\xi - \xi_m, \zeta_i - \zeta_m),$$

$$(\xi, \zeta, \tau) \in \Omega \times (0,1].$$

The boundary conditions over new axes can be written as:

$$\Theta|_{\xi=0} = \Theta_0, \Theta|_{\xi=1} = \Theta_0, \Theta|_{\zeta=0} = \Theta_0, \Theta|_{\zeta=1} = \Theta_0,$$

$$(\xi, \zeta, \tau) \in \Gamma \times (0,1].$$

At the start of simulation, the initial condition will be:

$$\Theta(\xi, \zeta_0) = \Theta_0,$$

$$(\xi, \zeta) \in \Omega.$$

To make such transition, several conditions are required:

- The relation between $\Theta(\omega)$ and $K_y(\omega)$ is linear:

$$D_y^{-1}(\omega)\frac{dK_y(\omega)}{d\omega} = \ell = const.$$

- Linearization is achieved by assuming

$$\frac{\partial\omega}{\partial t} = \frac{Q^* k_2 \beta_2}{4\pi k_1}\frac{1}{D_y(\omega)}\frac{\partial\Theta}{\partial t} \approx \frac{k_2\beta_2^3 Q^*}{4\pi k_1}\frac{\partial\Theta}{\partial t}.$$

3. Control and optimization

For the control problem we will use an approach offered in [4] so that we can apply results on existence and uniqueness of the solution [5]. Consider the optimal control belongs to Hilbert space.

Measurements of the target state at the last time step φ are given as a known function. The task is to minimize the deviation between the reached state according to current approximation and the target state.

By determining $0 < \alpha < min\left(h^2, \tau\right)$ as a regularization parameter according to possible measurement errors, the smoothing functional will be:

$$J(q) = \int_{\Omega} (\Theta(\xi, \zeta; q) - \varphi(\xi, \zeta))^2\, d\Omega + \alpha\|q\|^2 \to \min_q.$$

The iterative variation algorithm proposed in [4] consists of three stages. As for the conjugated operator, it is tested and explained by P. N. Vabishevich [7].

1. Solve the state problem

$$\frac{\partial \Theta^n}{\partial \tau} - \frac{\partial^2 \Theta^n}{\partial \xi^2} - \frac{\partial^2 \Theta^n}{\partial \zeta^2} + 2\frac{\partial \Theta^n}{\partial \zeta} = 4\pi \sum_{m=1}^{M} q_m(\tau)\,\delta(\xi - \xi_m, \zeta - \zeta_m),$$

$$0 < \tau \ \leq 1, \Theta^0 = \Theta(\xi, \zeta, 0) = 0.$$

2. Solve the conjugate problem

$$-\frac{\partial \Psi^n}{\partial \tau} - \frac{\partial^2 \Psi^n}{\partial \xi^2} - \frac{\partial^2 \Psi^n}{\partial \zeta^2} - 2\frac{\partial \Psi^n}{\partial \zeta} = 2\left(\Theta^n - \varphi^n(\tau)\right),$$

$$0 \leq \tau < 1, \Psi^n = \Psi(\xi, \zeta, 1) = 0.$$

3. Define the new approximation for the optimal control

$$\frac{q_m^{p+1} - q_m^p}{\hat{\tau}_{p+1}} + \Psi_m^0 + \hat{\alpha} q_m^p = 0, p = 0, 1 \ldots$$

This approach was effective and is described in other our works, so as alternative gradient methods are tested for the optimization problem. The simplest can be described by the following algorithm.

Gradient descent method

1. Solve the state problem for the current power approximation (analytic or numerical solution).
2. Calculate the derivatives and current direction.

$$Dir = \left(\left(-\frac{\partial J(q)}{\partial q_1}\right)|_{q=q^i}, \left(-\frac{\partial J(q)}{\partial q_2}\right)|_{q=q^i}\right), \ldots, \left(-\frac{\partial J(q)}{\partial q_n}\right)|_{q=q^i}.$$

3. Adding variable QQ as universal source power step and rewriting the functional as depending from QQ, direction vector and current points (i-th) leads to optimization along a specific direction:

$$J(q_1, \ldots, q_n) = J\left(q_1^i + QQ * \left(-\frac{\partial J(q)}{\partial q_1}|_{q=q^i}\right) \ldots, \left(-\frac{\partial J(q)}{\partial q_n}|_{q=q^i}\right)\right).$$

4. As a result, the functional will be a quadratic functional with known coefficients and we can find the optimal point by finding its derivative by QQ and the point where it is equal or near zero. After that, the found solution $\widetilde{QQ}$ is used to get the next optimal source power approximation.
5. Define the new approximation for the optimal control:

$$q_1^{i+1} = q_1^i + \widetilde{QQ} * \left(-\frac{\partial J(q)}{\partial q_1}|_{q=q^i}\right) \ldots q_n^{i+1} = q_n^i + \widetilde{QQ} * \left(-\frac{\partial J(q)}{\partial q_n}|_{q=q^i}\right).$$

Finally, the found solution is tested. In case $J\left(q_1^{i+1}, \ldots, q_n^{i+1}\right) \leq \varepsilon$, where epsilon is chosen according to calculation error, the calculation ends. Otherwise the process goes back to modeling with a new source power at step.

Conjugate gradient descent

1. Solve the state problem for the current power approximation (analytic or numerical solution).
2. Calculate the derivatives and current direction.

   Adding variable QQ as universal source power step and rewriting the functional as depending from QQ, direction vector and current points (i-th) leads to optimization along a specific direction. Then Find the optimal point by finding its derivative and the point where it is equal or near zero.
3. Next, scaling multiplier is calculated. After that, the found solution $\widetilde{QQ}$ is used to get the next optimal source power approximation.
4. Define the new approximation for the optimal control.

   Finally, the found solution is tested. In case $J\left(q_1^{i+1}, ..., \dots, q_n^{i+1}\right) \leq \varepsilon$, where epsilon is chosen according to calculation error, the calculation ends. Otherwise we repeat step 1 with a new source power approximation and calculate (which is step 2 for the following cycle)

$$Mult_1 = \frac{\sum_{j=1}^{n}\left(\left(-\frac{\partial J(q)}{\partial q_j}\Big|_{q=q^i}\right)^2\right.}{\sum_{j=1}^{n}\left(\left(-\frac{\partial J(q)}{\partial q_j}\Big|_{q=q^i+1}\right)^2\right.},$$

$$NewDir = \left\{-\frac{\partial J\left(q\right)}{\partial q_j}\Big|_{q=q^{i+1}}\right\}_{j=1}^{n}.$$

   Steps 3 and 4 in the cycle are exactly same but for the new power approximation. The process is finished when accuracy criterion is fulfilled, or after a fixed amount of iterations.

Pyjavskyj type method

Let us assume that every source power is limited $[0, Q_{max}]$. Then all the interval for every source can be equally divided into parts, and resulting points should be tested.

1. Solve the state problem for the current power approximation (analytic or numerical solution).
2. Calculate the optimization functional in general format as result of modeling if possible, if not – use modeling each time instead. For each source divide the possible source power interval into equal pieces and test each combination. Compare the results to find one or several sub regions with best values of optimization functional.

$$J\left(q_1^{i_1}, \dots, q_n^{i_n}\right), 0 \leq q_1^{i_1} \leq q_1^m, \dots, q_1^{i_n} \leq q_1^m.$$

4. For the chosen sub regions, divide them again and find smaller parts with best values, then compare all results. This process can be finished according to accuracy, division number or sub region linear size

achieved. Best found combination of source powers to minimize the functional is the solution.

4. Solving the example task

In the research, a two-dimensional linearized according to [2] problem is solved. The target function values are equal to results of modeling phase with q equal to 10. The initial approximation for source power can be taken near zero. For the direct and conjugate problems explicit scheme leads to the following equation:

$$\frac{\Theta_{ij}^{n+1}-\Theta_{ij}^{n}}{\widetilde{\tau}}=\frac{\Theta_{i+1,j}^{n}-2\Theta_{ij}^{n}+\Theta_{i-1,j}^{n}}{h^2} - \frac{\Theta_{i,j+1}^{n}-2\Theta_{ij}^{n}+\Theta_{ij-1}}{h^2}+4\pi\widetilde{q},$$

$$-\frac{\Psi_{ij}^{n+1}-\Psi_{ij}^{n}}{\widetilde{\tau}}=\frac{\Psi_{i+1,j}^{n}-2\Psi_{ij}^{n}+\Psi_{i-1,j}^{n}}{h^2} - \frac{\Psi_{i,j+1}^{n}-2\Psi_{ij}^{n}+\Psi_{ij-1}}{h^2}+\frac{\Psi_{i,j+1}^{n+1}-\Psi_{i,j-1}^{n+1}}{h}+2\left(\Theta_{ij}-\varphi_{ij}\right).$$

Here the first equation starts from the known state at the start $\Theta_{ij}^{0};\ i,j=0,\dots,\hat{N},\ N=\left[\frac{1}{h}\right]$. The source power $\widetilde{q}$ depends on the placement of sources, it is constant over time and equal to zero if the source is not there.

Combined with boundary conditions, where humidity is fixed, a system of equations is solved. In case of explicit scheme, these equations are transformed into iterative process of calculating new values using known values on previous time step. Initial distribution is known for direct problem, so each next time step is easily calculated. Conjugate equations are solved in opposite direction. Starting from the last time step $\Psi_{ij}^{N}=0,\ i,j=0,...,\hat{N}$, calculations lead to the first one. As a result, variation algorithm can be applied.

However, for the considered methods only direct problem should be solved. All necessary values can be obtained from solving direct problem and, if possible, defining the quality functional for abstract source powers. Then an iterative method is applied to improve the result, using either the functional or modeling for new source power approximations.

So instead of solving 2 systems of equations only one is enough on each iteration.

In order to reduce the amount of calculations and show ideas of three offered options, the area is divided into equal parts with calculation point indexes 0...5 over each axis.

Ten using symbolic calculations at Maple, it is possible to define the system of polynomials describing humidity at each point of a system. Here two sources are taken in order to describe the situation.

The first source is located at point with indexes, equal to 1 on both axes, the second one with power 10 is located at the point with indexes (3,3). Desired function is built as result of modeling with $q_1=5$ and $q_2=10$.

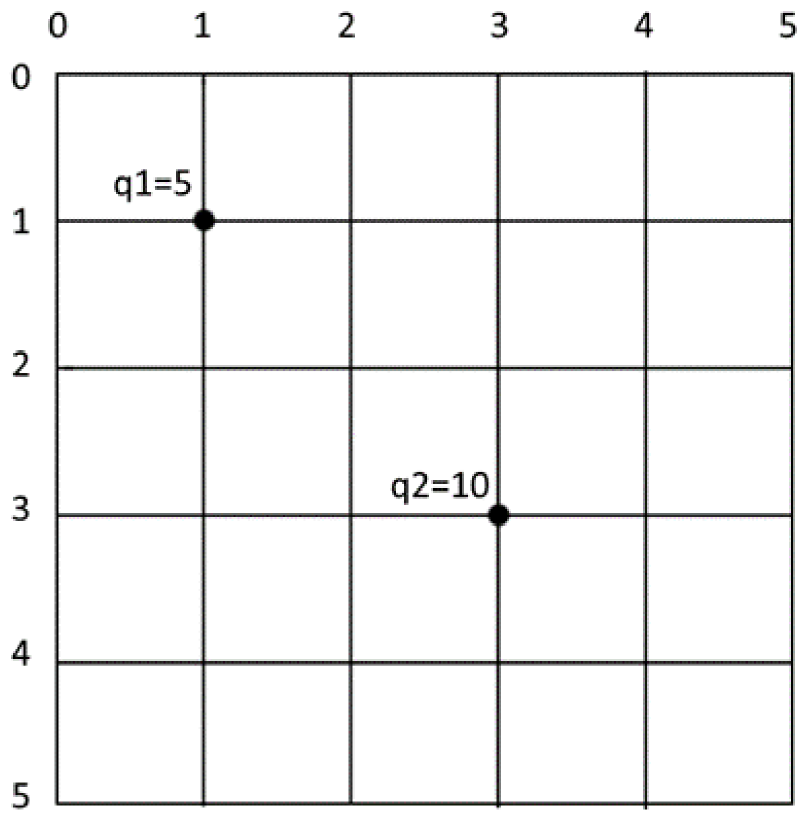

Fig. 1. Demonstration test with 2 sources

For this test, the optimization functional with unknown source power values can be written as:

$$\sum_{i=0}^{5}\sum_{j=0}^{5}\left(\Theta_{ij}\left(q_1^{optimal}, q_2^{optimal}\right) - \Theta_{ij}\left(q_1^{approximal}, q_2^{approximal}\right)\right)^2.$$

Here $\Theta\left(q_1^{optimal}, q_2^{optimal}\right)$ represents desired function and is known as result of modeling with a given source power combination. Using calculations and modeling with abstract source power $\Theta\left(q_1^{approximal}, q_2^{approximal}\right)$ it is possible to write a formula describing the functional. This formula can be simplified in case high accuracy of calculations is guaranteed – otherwise solution can be complex because of calculation error, leading to non-zero functional on all possible source power combinations. If that happen, we take real part of the solution.

$$9,337 + 0,003\pi^2 q_1^2 + 0,007\pi^2 q_2^2 + 0,003\pi^2 q_1 q_2 - 0,203\pi q_1 - 0,493\pi q_2.$$

Now it is possible to calculate derivatives along each axe and use gradient methods. First of all, let us find the anti-gradient vector for the functional to see the proportion according to (6).

$$Dir = \left(\left(-\frac{\partial J\left(q\right)}{\partial q_1} \right) |_{q=(0,0)}, \left(-\frac{\partial J\left(q\right)}{\partial q_2} \right) |_{q=(0,0)} \right).$$

Then, using these values for the proportion (7), we may rewrite the functional along chosen direction as:

$$JJ\left(QQ\right) = 0,933 + 0,021 \cdot \pi^2 \cdot QQ^2 - 0,893 \cdot \pi \cdot QQ.$$

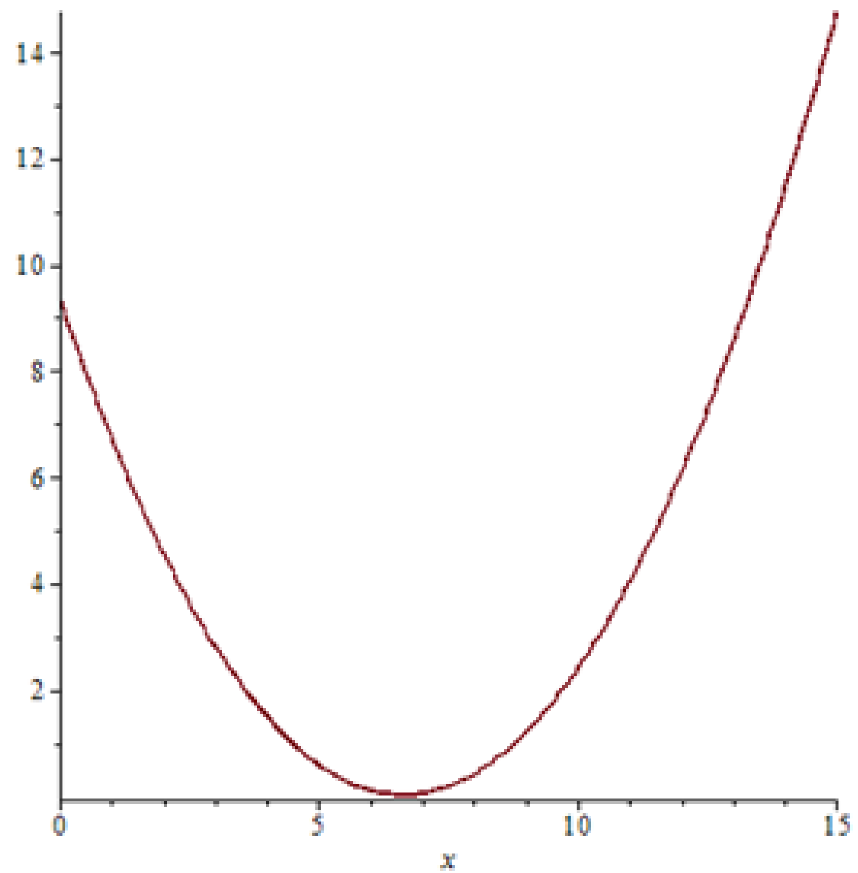

Fig. 2. Functional along the chosen direction.

Its derivative is $JJ\ prime\left(QQ\right) = 0,043 \cdot QQ - 0,893 \cdot \pi$, which gives us a general solution $QQ = 6,64$ at current step. To calculate it, we use current approximation and scaled multipliers (8), so $q_1 = 4,23, q_2 = 10,28$. These values are then used to calculate the next direction if necessary. Here the process was stopped, because functional reached 0.0188 value, which is less than $0,04 = h^2$ (error according to discretization step). That's the result, achieved with Method 1 and Method 2.

As for Method 3, let us assume that both source powers are between 0 and 15. Then we can calculate values of functional at each combination of source powers k, l in 0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15. As a result, the following values of optimization functional were received (here they are grouped according to same value of one source):

$$\sum_{i=0}^{5}\sum_{j=0}^{5}\left(\Theta_{ij}(5,10)-\Theta_{ij}(0,0)\right)^2,$$
$$\ldots$$
$$\sum_{i=0}^{5}\sum_{j=0}^{5}\left(\Theta_{ij}(5,10)-\Theta_{ij}(15,10)\right)^2,$$
$$\sum_{i=0}^{5}\sum_{j=0}^{5}\left(\Theta_{ij}(5,10)-\Theta_{ij}(0,15)\right)^2,$$
$$\ldots,$$
$$\sum_{i=0}^{5}\sum_{j=0}^{5}\left(\Theta_{ij}(5,10)-\Theta_{ij}(15,15)\right)^2.$$

So, obviously the best achieved result was achieved $q_1 = 5$, $q_2 = 10$. That's the exact solution, so no further calculations are required. In case accuracy is not good enough, one or several best sub areas (with minimal sum of 4 elements – values of optimization functional, defining the sub area) are chosen, divided into equal parts and tested. The amount of sub areas is chosen manually and should take into account the form of plot describing optimization functional.

To sum up, results for all options fulfill the requested accuracy for optimal source power.

5. Discussion

This article describes several approaches to the problem, based on anti-gradient direction. The direct problem (modeling with fixed source power) is mostly solved numerically to calculate humidity for a given source power. However, if it is possible to calculate distribution for abstract source power (for example using Maple software), that distribution can be used to combine the results at each discretization point into a functional, which describes quality of solution for a given source power combination.

For cases when it is possible to formulate the functional, instead of repetitive modeling, direct value insertion can be done which is much faster. By calculating the functional derivative and determining direction according to anti-gradient, a multidimensional problem is transformed into one dimensional with a much easier solution. After that direction is calculated again to improve the result. Methods 1 and 2, described above, fit this approach and calculate values with allowed functional error.

For cases when it is hard to formulate the functional or find its derivative, Method 3 works nicely by dividing the area into the smaller parts, removing potentially useless (with worst simulation results at limitation points) and eventually resulting into a set of small areas with best results. The stop condition for this case may be either accuracy of solution, or size of subareas. The mentioned above methods can be applied to more sources and smaller discretization step, here only an example is demonstrated to make the idea clear.

6. Conclusion

The proposed algorithm can be applied for nonlinear problems with respect to transition limitations and buried sources with low or zero humidity values on borders. The general idea of the combination is to apply Kirchhoff transformation and scale the space and time values leading to the new quasi-linear equation. Then variation algorithm is applied to get the optimal source power. It consists of direct problem, conjugate problem and the new approximation step.

To solve the algorithm's problems numerical approaches are used with proper discretization. Received values are used to construct optimization functional in general form, depending on source power. Then gradient methods are applied to find the optimal solution.

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