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Mass Transfer Problem with Saturation Limit on Graph

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Abstract—**This paper contains main results of the research of mass transfer problem in porous medium with saturation limit on graphs. The equation that describes this problem is based on the one-dimensional Richards-Klute equation with additional mass balance equations. Among the results are existence theorem, stability result and effective numerical method for solving equation.**

Keywords—mathematical modeling; Richards-Klute equation; numerical methods; graphs.

I. Introduction (Heading 1)

Mass transfer process in porous medium with saturation limit is one of the most important processes which appear in the fields of agriculture and man-made disaster modeling. It is usually described by one-, two- or three-dimensional Richards-Klute equation [1,2]. For modeling of the mass transfer process in the system of pipes it is also possible to obtain the Richards-Klute equation on graph [3]. All of these equations are quasilinear elliptic-parabolic partial differential equations. Because of this, main instrument to solve these equations are numerical methods. They can be based on finite element method, finite volume method and finite difference method. They can also be modified using implicit/explicit time schemes and different forms of the Richards-Klute equation [4, 5].

Due to the properties of the equation, numerical methods for finding approximate solution require a large number of calculations, main part of which are calculations required to solve linear systems on each time step. Fast and accurate numerical method designed for specific type of the Richards-Klute equation is one of the most important tools for obtaining a more efficient way to model the mass transfer process.

II. Richards-Klute Equation on Graph

Let's consider graph $G = (V,E)$ embedded in three-dimensional space. The edges $e\in E$ of this graph can be interpreted as the pipes in the irrigation system, and the vertices $v\in V$ are the connections of these pipes. Then let's consider the Richards-Klute equation on graph G [3]. This equation is based on the one-dimensional Richards-Klute equation on each edge, continuity conditions of solution in vertices and mass balance equations in vertices.

$$C_e \frac{\partial h}{\partial t} = \frac{\partial}{\partial x}\cdot\left(K_e\left(\frac{\partial h}{\partial x}+g_z\right)\right), x\in[0,L_e], \quad (1)$$

$$h(v) = h(\delta_e), e\in Inc(v), \quad (2)$$

$$\sum_{e\in Inc(v)} q_e(\delta_e) = 0. \quad (3)$$

Here t is time [s], h is a pressure head [m] (unknown), C_e and K_e are the characteristics of the porous medium in the pipe e, g_z is the gravity impact and its value depends on the direction of the pipe in the gravity field, L_e is length of the pipe, $\delta_e = 0$ or L_e depending on which end of e is incident to v, $Inc(v)$ is a set of edges which are incident to vertex v, q_e is a positive flux through the boundary δ_e of the edge e.

For modeling the mass transfer process on the graph, we also must add initial condition on pressure head on all edges and boundary conditions of first or second kind on some of the vertices. By doing this, we obtain a system of equation which is called Richards-Klute equation on graph.

Equations (1)-(3) can be easily transformed to system of linear algebraic equations for numerical methods. Equations on edges (1) can be discretized in the same way as one-dimensional Richards-Klute equation. Continuity conditions (2) simply transform into equations between nodes of different adjacent edges. Mass balance equation (3) for every vertex v can be discretized in the following way.

$$\begin{gathered}\sum_{i=1}^{m_N}\frac{1}{\Delta x_i}K_i^{N_i-\frac{1}{2}}\left(\frac{h_{i,N_i-1}^{j+1}-h_v^{j+1}}{\Delta x_i}+g_{i,z}\right)\\ -\sum_{i=1}^{m_0}\frac{1}{\Delta x_i}K_i^{\frac{1}{2}}\left(\frac{h_{i,1}^{j+1}-h_v^{j+1}}{\Delta x_i}+g_{i,z}\right)=0,\end{gathered} \quad (4)$$

where m_0 is number of edges incident to v, for which $\delta_e = 0$, m_N is number of edges incident to v, for which $\delta_e = L_e$, j is current and $j+1$ is the next time step, Δx_i is the spatial step, $g_{i,z}$ and K_i are calculated at the corresponding point of edge e_i.

III. EXISTENCE AND STABILITY RESULTS

There is classic result of existence of the weak solution of one-, two- and three-dimensional Richards-Klute equations presented in [6]. It is based on some conditions on properties of porous media and initial and boundary functions. These conditions can be modified for Richards-Klute equation on graph [7]. Using these modified conditions, one can prove the next result.

Theorem 1. Under the conditions listed in [7] there is a weak solution of Richards-Klute equation on graph.

To obtain stability result, we need to add one more condition.

$$\left|K(h_1) - K(h_2)\right| \le c\left|h_1 - h_2\right|, \qquad (5)$$

where c is constant. Then we can prove the stability result.

Theorem 2 [7]. Let H_1 and H_2 are solutions of Richards-Klute equation on graph at time T with initial conditions h_1 and h_2 respectively. And let $\theta(h)$ is a function between pressure head and saturation level ($\partial\theta/\partial h=C(h)$). Then

$$\sum_{e\in E}\int_e \left|\theta\left(H_1\right) - \theta_2\left(H_2\right)\right| de \le \sum_{e\in E}\int_e \left|\theta\left(h_1\right) - \theta\left(h_2\right)\right| de. \qquad (6)$$

IV. NUMERICAL METHOD

Using (4) and standard discretization methods for equations (1)-(2) we can transform the Richards-Klute equation on graph to the system of linear algebraic equations. Thus, modeling process is just solving obtained system for every time step.

Matrix of the obtained system on fixed time step has the following properties:

- it is sparse;
- it is symmetric;
- it is diagonally dominant.

These properties allow us to use fast numerical methods for sparse matrices to solve linear system (like Seidel method or conjugate gradient method). But if graph is a simple path, the Richards-Klute equation on graph can be transformed into the one-dimensional Richards-Klute equation and then the direct Thomas method can be used. At the same time, if graph is a simple cycle, then modified Thomas method [8] can be used. Based on original and modified Thomas methods one can build direct numerical method for solving Richards-Klute equation on graph [9].

Let's consider graph *G'* which represents nodes of the discretization of the graph *G* and which is related to linear system in the following way.

$$a_{ij} \ne 0 \Leftrightarrow i \in Adj(j), \qquad (3)$$

where *Adj(j)* is a set of nodes that are adjacent to node j in graph *G'*. Then the modified Thomas method for graphs is just repeating following 3 steps:

- find the longest simple path (cycle) in *G'*;
- solve linear subsystem for found path (cycle) using original (modified for cycles) Thomas method considering all matrix coefficients which connect nodes from found path (cycle) and other nodes of *G'*;
- exclude nodes of found path (cycle) from graph *G'* and exclude corresponding linear equations from system.

As long as one makes these three steps the linear system size gets smaller, so we can say that after finite number of steps, which depends only on properties of graph *G*, one can transform original system to small system, size of which also depends only on properties of graph *G*, but not on the spatial discretization parameters or number of vertices of graph *G'*. This method is also direct and stable, because it is based on direct and stable original and modified for cycles Thomas methods.

V. CONCLUSIONS

A mass transfer process in porous media with saturation limit is described using Richards-Klute equation. Using additional mass balance equations the Richards-Klute equation on graph is obtained. Existence and stability result are given. A direct stable numerical method for solving linear systems for finding approximate solution of the Richards-Klute equation on graph was built.

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