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Solution of inverse problems in contaminant transport

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Abstract: We discuss the inverse problem for contaminant transport in porous media. The nonlinear adsorption in equilibrium and nonequilibrium mode is included. The corresponding mathematical model of convection-diffusion-adsorption type with dominant convection is numerically approximated by time stepping and operator splitting method. An efficient numerical method is developed with small numerical dispersion to solve the direct problem and applied to the solution of ill-posed inverse problem. We focus to the determination of sorption isotherms and kinetic rate of adsorption. The Lagrange method (via the adjoint system) is used to construct the gradient of the corresponding cost functional with respect to the parameters under determination. The method is applied to the dual-well setting and some numerical experiments are presented.

Key Words: contaminant transport, inverse problems, sorption isotherme, Lagrange method

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1 Introduction

Precise mahtematical models for contaminant transport with adsorption are available and a big effort has been done to develop efficient numerical methods. Nonlinear adsorption, e.g. of Freundlich, or Langmuir type, can create sharp fronts in the solution. Moreover, dominant convection can lead to numerical instabilities which require the application of some "up-wind" methods. These in turn lead to numerical dispersion which shadows the sensitivity on the model data. This is the main reason to use the operator splitting method which allows us to control the transport part with small numerical dispersion. Time stepping allows us to use a micro time step in solving the adsorption part, since the time scaling for transport and diffusion significantly differs from the one during adsorption. The obtained numerical results support our approach.

2 Mathematical model

Contaminant transport with diffusion and adsorption is modelled in (see [1]) as follows

$$\partial_t b(u) + \operatorname{div}(\bar{v}.u - D\nabla u) = -\varrho \partial_t S, \tag{1}$$

in $x \in \Omega \subset R^d,\ t \in (0,T) := I,\ (d = 2,3)$ coupled with

$$\partial_t S = \kappa(\psi_n(u) - S), \tag{2}$$

and the boundary conditions

$$u = C_0(t) \text{ on } \partial\Omega_1;\ (\bar{v}.u - D\nabla u).\nu = 0 \text{ on } \partial\Omega_2; \tag{3}$$

$$-D\nabla u = 0 \text{ on } \partial\Omega_3.$$

where $\partial\Omega_i \subset \partial\Omega$ $(i = 1,2,3)$ are nonintersecting. The initial condition is

$$u(x,0) = 0, \quad S(x,0) = 0. \tag{4}$$

Here, u is the concentration of contaminant, $\bar{v}$ is the velocity of the groundwater, ψ_n is the sorption isotherm (for nonequilibrium adsorption), κ is the kinetic rate of adsorption, S is the mass of adsorbed contaminant per unit mass of the porous medium and ϱ is the bulk density of porous medium. The function $b(u)$ is of the form $b(u) = u + \varrho\psi_e(u)$ where ψ_e is the sorption isotherm in equilibrium mode. It corresponds to the case $\kappa \to \infty$ and consequently $S = \psi$ with $\psi \leftrightarrow \psi_e$. Thus, our system (1),(2) represents transport of contaminant with adsorption in equilibrium and nonequilibrium mode.

The most common sorption isotherms are (Freundlich, Langmuir)

$$\psi(s) = as^b,\ a, b > 0;\ \psi(s) = \frac{as}{1 + bs}.$$

Furthermore, D is the dispersivity tensor

$$D_{ij} = \{(D_0 + \alpha_T|v|)\delta_{ij} + \frac{v_i v_j}{|v|}(\alpha_L - \alpha_T)\},$$

where D_0 is the molecular diffusion, δ_{ij} the Kronecker symbol and $\alpha_L,\ \alpha_T$ are longitudinal and transversal dispersion coefficients, respectively. The functions $\psi_e,\ \psi_n$ and parameter κ are to be determined. We shall look for ψ_e and ψ_n in a special class of smooth functions $\psi_n \to \psi_n(s, \lambda)$, $\psi_e \to \psi_e(s, q)$ where $\lambda \in R^s,\ q \in R^r$ are parameters underlying to determination. For the determination of unknown vector parameter $p = (q, \lambda, \kappa)$ we shall use the additional measurements of the concentration evolution $u_*(x, t)$ on the outflow part of the boundary (breakthroughcurve BTC), which response to the inflow concentration $C_0(t)$. We construct the cost functional $F(p, u)$ by means of which we measure the descrepancy between the solution $u = u(x, t, p)$ and $u_*(x, t)$. We have

$$\mathcal{F}(u, p) = \int_0^T \int_{\partial\Omega_3} \bar{v}.\nu(u - u_*)^2 dxdt. \qquad (5)$$

Now, the solution of the inverse problem consists of the determination of optimal $p^0 = (\lambda^0, q^0, \kappa^0)$ such that the functional F attains its minimum in p^0. Then the required isotherms are $\psi_n := \psi_n(s, \lambda^0),\ \psi_e := \psi_e(s, p^0)$.

3 Numerical approximation

To solve our convection-diffusion-adsorption problem, we use time stepping and operator splitting in which, along any small time interval, the problem is split into: transport , diffusion and adsorption problems. Let $\tau = T/n$ be a time step and $u_i \approx u(x, t_i),\ t_i = i\tau$ for $i = 1, ..., n$. First, we realize transport along (t_{i-1}, t_i) with the initial value u_{i-1}. We indicate the result by $u_i^{1/3} = T^i(\tau)u_{i-1}$, where $T^i(\tau)u_{i-1}$ corresponds to the solution of the transport equation

$$\partial_t b(\phi) + \ div\ (\bar{v}\phi) = 0, \qquad (6)$$

with the inflow condition $\phi_T(x, t) = C_0(t)$ and the initial condition $\phi_T(x, t_{i-1}) = u_{i-1}$. Then we denote $u_i^{1/3} = \phi_T(x, t_i)$. The diffusion operator $D^i(\tau)$ generates the solution of the diffusion equation along (t_{i-1}, t_i)

$$\partial_t b(\phi) + \mathrm{div}(D\nabla\phi) = 0 \qquad (7)$$

with boundary condition $D\nabla\phi.\nu = 0$ on $\partial\Omega$ and with initial condition $\phi_D(x, t_{i-1}) = u_i^{1/3}$. Then, we define $u_i^{2/3} = D^i(\tau)u_i^{1/3} = D^i(\tau)T^i(\tau)u_{i-1}$. The adsorption part is realized by the operator $R^i(\tau)$ solving the following system of ODE

$$\partial_t b(\phi) + \frac{\varrho}{\theta_0}\partial_t S = 0, \quad \partial_t S = \kappa(\phi - S), \qquad (8)$$

with the initial conditions $\phi_R(x, t_{i-1}) = u_i^{2/3}$, $S(x, t_{i-1}) = S_{i-1}$. Then we set

$$u_i = R^i(\tau)D^i(\tau)T^i(\tau)u_{i-1}, \quad S_i = S(x, t_i).$$

The convergence of this approximation is based on the results in [3, 5] .

3.1 Numerical approximation of (6)

We use implicite Godunov type higher order approximation. In the case of Freundlich, or Langmuir sorption isotherms the function $b(s)$ is concave which makes construction of an entropy solver for the corresponding Rieman problems easier. In our application to the steady state velocity field generated in the dual-well setting, the velocity is parallel to one of the axes when using bipolart transformation. Then the solution can be obtained in semianalytical form -see [4].

3.2 Numerical approximation of (7)

We use the finite volume approximation and solve the resulting nonlinear algebraic system by a Newton iteration method. In the case of larger time steps we can use alternatively the relaxation method -see [8, 7].

3.3 Numerical approximation of (8)

Integrating (8) we obtain

$$b(\phi(t))+S(t) = c \equiv b(u_{i-1})+S_{i-1} \quad \forall t \in (t_{i-1}, t_i).$$

$$S(t) = S_{i-1}e^{-\kappa t}+$$
$$\kappa \int_{t_{i-1}}^{t} e^{-\kappa(t-s)}\psi(\phi(s))\; ds,\; t \in (t_{i-1}, t_i)$$

and hence, after elimination of S, we solve the resulting nonlinear integral equation by time discretization with a micro time-step $\tau_i < \tau$. We approximate the unknown function $\psi_n(\phi(t))$ by a piecewise linear function by means of ϕ_k on micro-time levels $t_{i-1} + k\tau_i$. Then, successively for $k = 1, ...k_i,\; k_i\tau_i = \tau$ we determine $\phi_k = \phi_k(x)$ using Newton-iterations - see [6]. Then we set

$$R^i(\tau)\phi(x, t_{i-1}) := \phi_{k_i}(x) \approx \phi(x, t_i).$$

3.4 Construction of gradient for (5)

Our solution of inverse problem is based on iterations (Conjugate gradient, De Broyden, Levenberg-Marquardt) requiring construction of gradient. When we have to determine only a few parameters of the model, the gradient can be constructed numerically. When more parameters are under determination this can be very costly since our direct problem is complex and time consuming. In that case the Lagrange method via the solution of an adjoint problem (which is linear) is more efficient. We construct the solution Ψ of the adjoint system

$$\partial_u b(u, q)\partial_t\Psi + \bar{v}.\nabla\Psi + div\ (D\nabla\Psi) \tag{9}$$
$$-\varrho\kappa\partial_u\phi(u, \lambda)(\Psi - \eta) = 0,$$

where

$$\eta(x, t) = \kappa \int_{t}^{T} e^{\kappa(t-s)}\Psi(x, s)ds,\; i.e.$$

$$\frac{d}{dt}\eta = \kappa(\eta - \Psi), \eta(T) = 0. \tag{10}$$

with the boundary and initial conditions

$$\Psi(x, t) = 0 \text{ on } \partial\Omega_1,\; D\nabla\Psi.\nu = 0 \text{ on } \partial\Omega_2 \tag{11}$$

$$(\bar{v}\Psi+D\nabla\Psi).\nu = 2\bar{v}.\nu(u-u_*) \text{ on } \partial\Omega_2; \Psi(x, T) = 0$$

Then, we transform the time variable $\tau \leftrightarrow T - t$, $\bar{\Psi}(x, \tau) = \Psi(x, T - t)$ and note that (9) is then a linear parabolic problem for $\bar{\Psi}$. Then the gradient of the functional (5) is of the form

$$\nabla_q\mathcal{F} = \int_0^T \int_\Omega \nabla_q b(\bar{u}, q)\partial_t\bar{\Psi}dxdt+ \tag{12}$$
$$\int_\Omega \nabla_q b(u_0, q)\bar{\Psi}(x, T)dx$$

$$\nabla_\lambda\mathcal{F} = -\varrho\kappa \int_0^T \int_\Omega \nabla_\lambda\psi_n(\bar{u}, \lambda)(\bar{\Psi} - \bar{\eta})dxdt \tag{13}$$

$$\partial_\kappa\mathcal{F} = -\varrho \int_0^T \int_\Omega \psi_n(\bar{u}, \lambda)(\bar{\Psi} - \bar{\eta} - \bar{\xi})dxdt \tag{14}$$

with

$$\frac{d}{dt}\xi = \kappa(\xi + \eta - \Psi),\text{ with } \xi(T) = 0. \tag{15}$$

4 Application to dual-well

To obtain realistic model data, the real in-situ measurements are required. The most common is the dual-well setting in an acquiffer under the Dupuit-Forchheimer assumption (the vertical component of the flow can be neglected). The local steady-state flow generated by injection-extraction wells significantly simplifies the original problem and the measurements of the flow field as an input data for (1). The flow in the accquiffer is horizontal with uniform thickness H and bounded below by impermeable boundaries. The wells are assumed to be fully penetrating and the injection-extraction is uniformly distributed over the depth of the well- for the details -see [2]. In this case our domain $\Omega = \mathbf{R}^2 \setminus B_{r_1}(-d, 0) \cup B_{r_2}(d + c, 0)$ where $B_{r_1}(-d, 0)$ is the extraction well with radius r_1 centered at the point $(-d, 0)$ and B_{r_2} is the injection well. In the injection well a tracer is injected with the known concentration $C_0(t)$ and its time evolution response is measured (breakthrough curve - BTC) at the extraction well. This is the only source for our callibration. The steady state flow is governed by

$$\Delta\Phi = 0 \qquad \text{in } \Omega,\; \vec{v} = -\frac{1}{h_{\text{eff}}\theta_0}\nabla\Phi,$$

where $\vec{v}$ is the corresponding velocity field. Here, the flow potential is defined by

$$\Phi(x, y) = khH-(1/2)kH^2,\text{ if } \Phi(x, y) > (1/2)kH^2$$

in the confined zone, and for the unconfined zone by

$$\Phi(x,y) = (1/2)kh^2, \text{ if } \Phi(x,y) < (1/2)kH^2,$$

where k is the hydraulic conductivity, h is the head (measured from the bottom of the acquifer), θ_0 is the porosity and $h_{\text{eff}} = \min(h,H)$. The curve $h(x,y) = H$ separates the confined and unconfined zones. Due to the symmetry of the flow, we can cosider Ω as the upper half plane ($y > 0$). The flow problem can be significantly simplified when using bipolar transformation (see [9]) that transforms Ω into a rectangle $\tilde{\Omega} = (0,\pi) \times (v^{(1)}, v^{(2)})$ with coordinates (u,v):

$$x = \frac{\delta}{2}\frac{\sinh v}{\cosh v - \cos u}, \quad y = \frac{\delta}{2}\frac{\sin u}{\cosh v - \cos u},$$

where the value δ can be determined from

$$z = 2{r_1}^2M^2 + {r_1}^4 - 2\,{r_1}^2{r_2}^2 + {r_2}^4 - 2\,{r_2}^2M^2 + M^4$$

$$d = \frac{1}{2}\sqrt{\frac{z}{M^2}}, \ \delta = 2\sqrt{d^2 - r_1^2}, \ c = M - 2d.$$

Here the equipotential curves of Φ in Ω create the horizontal lines in $\tilde{\Omega}$ (parallel with the u-axis) and the streamlines, which are orthogonal to them, create the vertical lines, parallel with the v-axis (conformal mapping). Then $\tilde{\Phi}(u,v) = \Phi(x,y)$ depends only on the v variable and $\tilde{\Phi}(v) = Av + B$ where A, B are to be determined from the boundary conditions. As to the values $v^{(1)}$ and $v^{(2)}$, they are obtained from

$$\sinh v^{(1)} = -\delta/(2r_1), \qquad \sinh v^{(2)} = \delta/(2r_2).$$

The coefficients A and B are obtained from the boundary conditions

$$Av^{(1)} + B = \Phi_1, \qquad Av^{(2)} + B = \Phi_2.$$

Problem (1) can be transformed into the form (see [2])

$$\partial_t b(C) = g\{\partial_u(a\partial_u C) + \partial_v(b\partial_v C)\} + G\partial_v C - \varrho\partial_t S, \tag{16}$$

where g, a, b and G are known functions depending on u and v:

$$\begin{aligned} g &= \frac{4\chi^2}{\gamma^3\theta_0 h_{eff}(v)}, \ \chi = \cosh v - \cos u, \\ a &= D_0\gamma\theta_0 h_{eff}(v) + 2\alpha_T\chi A \\ b &= D_0\gamma\theta_0 h_{eff}(v) + 2\alpha_L\chi A, \ G = A\gamma g, \end{aligned}$$

and where α_L, α_T are the longitudinal and transversal dispersion coefficients, respectively.

The transformed boundary conditions are

$$C(u, v^{(1)}, t) = C_0(t) \ \text{ on } \Gamma_1 \tag{17}$$

$$\partial_u C = 0 \text{ on } \Gamma_2 \cup \Gamma_4, \quad \partial_v C = 0 \ \text{ on } \Gamma_3, \tag{18}$$

where $\Gamma_1 := (0,\pi) \times \{v = v^{(2)}\}$, $\Gamma_2 := \{0\} \times (v^{(1)}, v^{(2)})$, $\Gamma_3 := (0,\pi) \times \{v^{(1)}\}$ and $\Gamma_4 := \{\pi\} \times (v^{(1)}, v^{(2)})$, together with the homogeneous initial condition $C((u,v),0) = 0$.

The advantage of this transformation can be demonstrated on the corresponding transformed equation (using the splitting method)

$$\partial_t b(\phi) - G(u,v)\partial_v\phi = 0, \tag{19}$$

which is a one dimensional problem in v (u can be taken as constant in space disctretization strip $u \in (u_{i-1}, u_i)$). Then, the corresponding solution can be constructed in a semianalytical form (see [4], [7]).

5 Inverse problem in $\tilde{\Omega}$

For the inverse problem we shall measure the time evolution of the concentration $C^{(1)}(t)$ in the extraction well depending on the concentration evolution $C_0(t)$ in the injection well. In fact, we can measure the average concentration

$$C_p^{(1)}(t) = \frac{\int_{\delta B_{r_1}(-d,0)} (\nabla_\nu\Phi) C_p(\sigma,t)\, d\sigma}{\int_{\delta B_{r_1}(-d,0)} (\nabla_\nu\Phi)\, d\sigma}$$

which in $\tilde{\Omega}$ takes the form

$$C_p^{(1)}(t) = \frac{1}{\pi}\int_0^\pi C_p(u, v^{(1)}, t) du.$$

Our cost functional now takes the form

$$\mathcal{F}(p, C_p) = \int_0^T (C_p^{(1)}(t) - \hat{C}^{(1)}(t))^2\, dt$$

with the gradient given by formulas (12), (13), (14) and (10),(15), where $\bar{\Psi}$ is the solution of the corresponding adjoint (parabolic) problem

$$\nabla_q b(\bar{C}, q)\partial_\tau\bar{\Psi} + A\gamma\partial_v(g\bar{\Psi}) - \partial_v(D\partial_v(g\bar{\Psi})) + \varrho\kappa\nabla_\lambda\phi(\bar{C},\lambda)(\bar{\Psi} - \bar{\eta}) = 0, \tag{20}$$

for $D_0 = \alpha_T = 0$, with the boundary conditions

$$\bar{\Psi} = 0 \text{ on } \Gamma_1; \quad b\partial_v(g\bar{\Psi}) - A\gamma g\bar{\Psi} =$$

$$\frac{1}{\pi^2}\int_0^\pi (C(u, v^{(1)}, \tau) - C^*(\tau))du \text{ on } \Gamma_3$$

with the homogeneous initial condition $\Psi(u, v, 0) = 0$, where $\bar{\Psi}(u, v, \tau) = \Psi(u, v, T-\tau) \equiv \Psi(u, v, t)$.

6 Numerical experiments

For the direct and inverse problems, we shall consider $H = 15m, d = 5m, \varrho_1 = r_2 = 15cm, \theta_0 = 0.2$ and $k = 10^{-5}$ m/s $= 0.864$ m/day. We solve a direct problem with nonlinear transport, where we inject the tracer with concentration $C_0 = 1$ during 2 days and then we stop the injection. We consider $\psi_e(C) = C^{0.75}$, $\alpha_L = 0.1$ and $\alpha_T = D_0 = 0$. We solve the problem on a space grid with 80×400 nodes and the upper bound for the time step is 0.04.

In Fig. 1, we illustrate the dependence of the BTC (average contaminant concentration versus time) on the sorption rate coefficient κ. We take $\psi_n(C) = C^{0.75}$. In Fig. 2, we show BTC for $\kappa = 0.1$ and $\psi_n(C) = C^q$ for different q. Qualitatively similar results are obtained with $\psi_e(C) = C^q$ for various q.

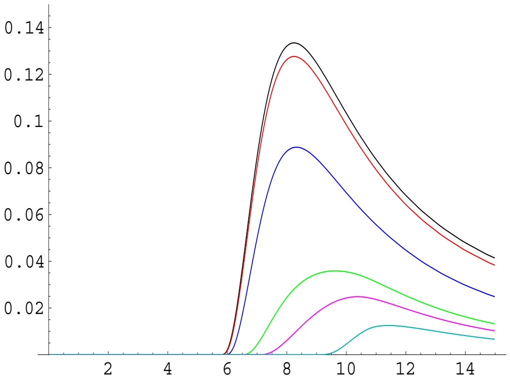

Figure 1: BTC for $\kappa = 10^{-5}$ (black), 0.01, 0.1, 0.5, 1.0, 10.0 (cyan)

Table 1: Determination of κ

step	κ	*res*
1	0.516459	0.873973
2	0.128196	0.0158943
3	0.106859	0.00104487
4	0.100622	8.86792e-06

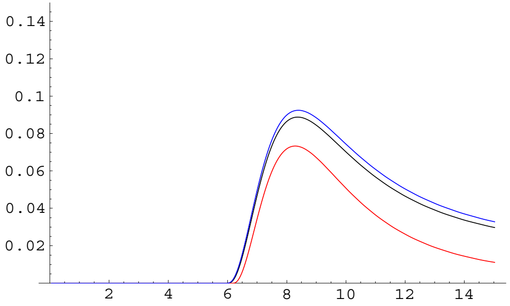

Figure 2: BTC for $\psi_n = C^q$ with q=0.9 (blue), 0.75 (black), 0.3 (red)

For the inverse problems we generate $\hat{C}^{(1)}(t)$ by solution of direct problem. In Table 1 we determine κ ($\kappa = 0.1$) starting from the value $\kappa = 1$. In Table 2 we determine $\psi_n = aC^b$, $(a = 1, b = 0.75)$ starting from $a = 1.2$, $b = 0.3$.

Table 2: Determination of ψ_n

step	*b*	*a*	*res*
1	0.305428	1.12444	0.142267
2	0.315242	1.02182	0.100131
3	0.339558	0.881168	0.0550554
4	0.408132	0.770948	0.0273729
5	0.531708	0.774542	0.013951
6	0.63673	0.862957	0.00449045
7	0.6995	0.935394	0.000934897
8	0.72977	0.973005	0.000157976
9	0.742355	0.989535	2.34244e-05
10	0.747188	0.996101	3.23506e-06

The numerical dispersion can be demonstrated in the case $\alpha_L = \alpha_T = D_0 = 0$ (only transport). The numerical dispersion in transport part can be significantly reduced using adaptive mesh refinement. We consider a problem with only transport and equilibrium adsorption (nonlinear transport) and with step input. In that case the solution is reduced to 1D transport along strips between streamlines. In the next pictures we consider Ω with the wells situated in the points $(-5, 0), (5, 0)$. In Fig. 3, we show the solution obtained using a fixed space grid with 400 points in each strip and in Fig. 4 we can see the solution obtained using and adaptive grid with 200 fixed points and 10 extra moving points placed around the solution's front. The exact solution obtains only the values $\{0, 1\}$ when $C_0(t) \equiv 1$. The space betveen concentration isoclines in Fig.

3 corresponds to the smearing of the shock (the concentration there attains the values from $(0, 1)$. This numerical dispersion is still much better in comparison with the used "up wind" method.

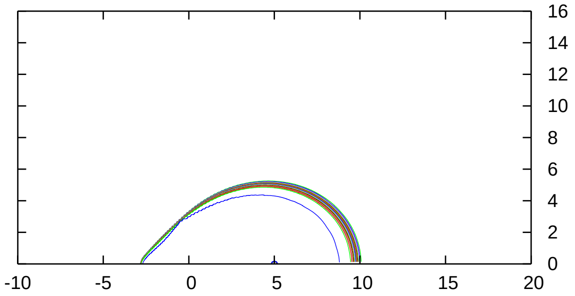

Figure 3: Solution of a 2D nonlinear transport problem with fixed grid shown after 6 days

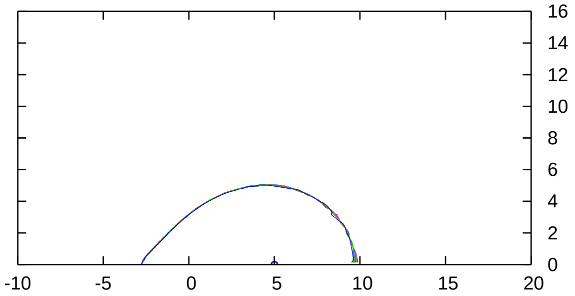

Figure 4: Solution of a 2D nonlinear transport problem with adaptive space grid shown after 6 days

7 Conclusions

The pricise and efficient numerical method for contaminant transport with adsorption in dual-well flow is presented. Due to the low numerical dispersion the method can be used in solving the inverse problems to determine the equilibrium and non-equilibrium sorption isotherms and kinetic rate of adsorption. The method has been successfully applied in [2] to the determination of hydraulic permeability and longitudinal dispersion coefficients. The method is applicable under the following assumptions: the flow in the acquifer is horizontal (Dupuit-Forheimer); acquifer is homogeneous with the uniform thickness and impermeable ground; the wells are fully-penitrating; the injection-extraction (of water and solute) are uniformly distributed over the depth.

The additional numerical experiments supporting the used method will be included in an extended version of te WSEAS international Journal.

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