A Non-standard Finite Difference Method for a Class of Nonlinear Reaction-Diffusion Equations with Variable Coefficient

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Abstract

We introduce a non-standard finite difference method to approximate solutions of a class of nonlinear reaction-diffusion equations with variable coefficient. These equations describe the growth, decay, colony and mutual transformation processes of biomass. So, these solutions of model must be bounded and non-negative. Due to obtain the exact solutions is very difficult task, whence, it is high significant that designing numerical techniques to approximate them. Our FDM are quite efficient for ensuring that their boundedness and non-negativity. All these examples have showed that our non-standard FDM can ensure the solution automatically bounded, as long as some conditions are satisfied.

Keywords: Nonlinear, Reaction-diffusion equations, FDM, Convergence, Stability,Non-negative, Bounded.

1. Introduction

It is well known that nonlinear reaction-diffusion equations has been widely applied in physics, biochemistry, biological sciences, environmental sciences, and many other fields of science. However, it is impossible to get their analytical solutions. Hence, it is very significant to develop high-performance numerical algorithms for this kind of equations. Researchers have developed various models to study mechanisms and courses of bacterium biofilm's formation by applying nonlinear reaction-diffusion equation. In the study of biofilm, Eberl etc. presented many type biofilm models, such as single biofilm model, coupling of biofilm model and complex biofilm model etc.[1]-[3]. Many numerical methods including finite difference method, finite volume method etc. are applied to solve this kind of equations[4]-[9]. In this paper, a positivity-preserving non-standard FDM are presented solving the numerical solutions of a class of biofilm model which are constructed by Eberl etc.. The method is powerful to producing an accurate solution, approximating the positive and bounded solutions of biological film model.

2. Mathematical model

In this work, we study three type bio-film models which are governed respectively by the following equations.

$$\frac{\partial u}{\partial t} = \nabla \cdot (D(u)\nabla u) + ru \qquad u \in \Omega \times [0, T] \tag{1}$$

From a biological point of view, the partial differential Eq.(1) is the simplest bio-film model which characterizes the growth, decay, colony process of single species bacteria[1], the partial differential Eqs.(2) is a coupling bio-film model which characterizes the laws of mutual transformation process between the nutrient mass and bio-mass[2], the system of PDEs (3) characterizes the laws of interaction among different bacteria, between a colony of bacteria and a surrounding substrate of nutrients[3].

$$\begin{cases} \dfrac{\partial s}{\partial t} = d_1 \nabla^2 s - k_1 \dfrac{su}{k_4 + s} \\ \dfrac{\partial u}{\partial t} = d_2 \nabla \cdot (D(u) \nabla u) - k_2 u + k_3 \dfrac{su}{k_4 + s} \end{cases} \tag{2}$$

$$\begin{cases} \dfrac{\partial s}{\partial t} = \nabla \cdot (D(M) \nabla s) - \dfrac{\mu}{Y_H} \dfrac{Bs}{k_s + s} + k_L \dfrac{k_s B}{k_s + s} + k_E \dfrac{k_s E}{k_s + s} \\ \dfrac{\partial B}{\partial t} = \nabla \cdot (D(M) \nabla B) + \mu \dfrac{Bs}{k_s + s} - k_L \dfrac{k_s B}{k_s + s} - k_I \dfrac{k_s B}{k_s + s} \\ \dfrac{\partial I}{\partial t} = \nabla \cdot (D(M) \nabla I) + k_I \dfrac{k_s B}{k_s + s} \\ \dfrac{\partial E}{\partial t} = \nabla \cdot (D(M) \nabla E) + Y_E \dfrac{\mu Bs}{k_s + s} - k_E \dfrac{k_s E}{k_s + s} \\ M(X,t) = B(x,t) + I(X,t) + E(X,t) \end{cases} \tag{3}$$

for every $(X,t) \in \Omega \times R^+$, here, $R^+ = \{t > 0 \mid t \in R\}$ and Ω denotes an open, bounded and connected subset of R^d ($d = 1,2,3$), where the biomass grows, $\partial\Omega$ is the boundary of Ω , and $\overline{\Omega} = \Omega \cup \partial\Omega$ is the closed domain where the biomass growth problem is set. Here, ∇ and $\nabla \cdot$ represent, respectively, the spatial gradient operator and the spatial divergence operator. In single and coupling bio-film models, unknown u is the concentration of biological normalized with respect to a maximum value and parameter r is the growth rate of biomass. In couple and complex bio-film models, s is the concentration of nutrient normalized with respect to a maximum value. Furthermore, the unknown function $M(X,t)$ is the total biological mass density of system at $(X,t) \in \Omega \times R^+$ and there are three types of biomass concentrations that are tracked: living biomass denoted by $B(X,t)$, inert or dead biomass denoted by $I(X,t)$, and the extra-cellular polymeric substances (EPS) denoted by $E(X,t)$, all of them normalized with respect to a maximum value.Obviously, s , B , I , E and M are all bounded and limited in interval $[0,1)$ for every $(X,t) \in \Omega \times R^+$. We assume that all these parameters of Eq.(2) and (3) are positive and are obtained by experiment, such that μ , d_1 , d_2 ,etc. The real function $D(u)$ is the nonlinear diffusion coefficient that must reflect the dynamics of the biological evolution (the growth, decay and colony of the biological), and is, in general, a function of biomass, hence it is a source of the non-linearity.

The form of the diffusion coefficient is given as a function of the biomass itself:

$$D(u) = \delta \frac{u^\alpha}{(1-u)^\beta} \tag{4}$$

where $\delta > 0$, $\alpha \geq 1$ and $\beta \geq 1$.

In general, systems (1), (2) and (3) need satisfy some appropriate initial conditions on Ω and are imposed some boundary conditions on $\partial\Omega$, these boundary conditions may be homogeneous Neumann or Dirichlet boundary conditions.

3. Numerical method

Let a, b, c and d be real numbers, such that $a < b$ and $c < d$, and let M, N and K be positive integers. Let $\Omega = (a,b) \times (c,d)$ be an open rectangle domain in R^2. The regular grids can now defined as,

$$x_i = (i-1)\Delta x, i = 1, \cdots, M+1, \text{ and } \Delta x = (b-a)/M;$$

$$y_j = (j-1)\Delta y, j = 1, \cdots, N+1, \text{ and } \Delta y = (d-c)/N;$$

$$t_k = (k-1)\Delta t, k = 1, \cdots, P+1 \text{ and } \Delta t = T/P,$$

where, i, j, k, M, N and P are all positive integers. When $\Delta x = \Delta y$, we denote the ratio of mesh size as

$$R = \frac{\Delta t}{\Delta x^2} = \frac{\Delta t}{\Delta y^2}$$

For every $i \in \{1, 2, \cdots, M+1\}$, $j \in \{1, 2, \cdots, N+1\}$ and $k \in z^+$, let $u_{ij}^k, s_{ij}^k, B_{ij}^k, I_{ij}^k$, E_{ij}^k and M_{ij}^k be the approximation to $u(x,y,t), s(x,y,t)$, $B(x,y,t)$, $I(x,y,t)$, $E(x,y,t)$ and $M(x,y,t)$ at point (x_i, y_j, t_k),respectively. $D_{i,j}^k$ expresses the value of $D(u_{i,j}^k)$ or $D(M_{ij}^k)$.

For every $k \in z^+$, we give the following standard one order differential operator and non-standard differential operators:

$$\delta_x f_{i,j}^k = \frac{f_{i+1,j}^k - f_{i,j}^k}{\Delta x} \approx \frac{\partial f}{\partial x}\Big|_{(x_i, y_j, t_k)} \tag{5}$$

$$\delta_x^2 f_{i,j}^k = \frac{f_{i+1,j}^k - 2f_{i,j}^{k+1} + f_{i-1,j}^k}{\Delta x^2} \approx \frac{\partial^2 f}{\partial x^2}\Big|_{(x_i, y_j, t_k)} \tag{6}$$

$$\delta_y^2 f_{i,j}^k = \frac{f_{i,j+1}^k - 2f_{i,j}^{k+1} + f_{i,j-1}^k}{\Delta y^2} \approx \frac{\partial^2 f}{\partial y^2}\Big|_{(x_i, y_j, t_k)} \tag{7}$$

$$\begin{aligned}\delta_{Dx}^2 f_{i,j}^k &= \frac{1}{2}\Big(\frac{(D_{i+1,j}^k - D_{i,j}^k)(f_{i+1,j}^k - f_{i,j}^{k+1})}{\Delta x^2} + \frac{(D_{i-1,j}^k - D_{i,j}^k)(f_{i-1,j}^k - f_{i,j}^{k+1})}{\Delta x^2}\Big) \\ &\approx (D'(f)(\frac{\partial f}{\partial x})^2)\Big|_{(x_i, y_j, t_k)}\end{aligned} \tag{8}$$

$$\begin{aligned}\delta_{Dy}^2 f_{i,j}^k &= \frac{1}{2}\Big(\frac{(D_{i,j+1}^k - D_{i,j}^k)(f_{i,j+1}^k - f_{i,j}^{k+1})}{\Delta y^2} + \frac{(D_{i,j-1}^k - D_{i,j}^k)(f_{i,j-1}^k - f_{i,j}^{k+1})}{\Delta y^2}\Big) \\ &\approx (D'(f)(\frac{\partial f}{\partial y})^2)\Big|_{(x_i, y_j, t_k)}\end{aligned} \tag{9}$$

Under these assumptions, equations (1), (2) and (3) have following discrete forms[5]-[6]:

$$\delta_t u_{i,j}^k = (\delta_{Dx}^2 + \delta_{Dy}^2) u_{i,j}^k + D(u_{i,j}^k)(\delta_x^2 + \delta_y^2) u_{i,j}^k + r u_{i,j}^k \tag{10}$$

$$\begin{cases} \delta_t s_{i,j}^k = d_1(\delta_x^2 + \delta_y^2) s_{i,j}^k - k_1 \dfrac{s_{i,j}^k u_{i,j}^k}{k_4 + s_{i,j}^k} \\ \delta_t u_{i,j}^k = d_2((\delta_{Dx}^2 + \delta_{Dy}^2) s_{i,j}^k + (\delta_x^2 + \delta_y^2) s_{i,j}^k) - k_2 u_{i,j}^k + k_3 \dfrac{s_{i,j}^k u_{i,j}^k}{k_4 + s_{i,j}^k} \end{cases} \tag{11}$$

$$\begin{cases} \delta_t s_{i,j}^k = (\delta_{D^M x}^2 + \delta_{D^M y}^2) s_{i,j}^k + D(M_{i,j}^k)(\delta_x^2 + \delta_y^2) s_{i,j}^k - \dfrac{\mu}{Y_H} \dfrac{B_{i,j}^k s_{i.j}^k}{k_s + s_{i,j}^k} + k_L \dfrac{k_s B_{i,j}^k}{k_s + s_{i,j}^k} + k_E \dfrac{k_s E_{i,j}^k}{k_s + s_{i,j}^k} \\ \delta_t u_{i,j}^k = (\delta_{D^M x}^2 + \delta_{D^M y}^2) u_{i,j}^k + D(M_{i,j}^k)(\delta_x^2 + \delta_y^2) u_{i,j}^k + \mu \dfrac{B_{i,j}^k s_{i,j}^k}{k_s + s_{i,j}^k} - k_L \dfrac{k_s B_{i,j}^k}{k_s + s_{i,j}^k} - k_I \dfrac{k_s B_{i,j}^k}{k_s + s_{i,j}^k} \\ \delta_t I_{i,j}^k = (\delta_{D^M x}^2 + \delta_{D^M y}^2) I_{i,j}^k + D(M_{i,j}^k)(\delta_x^2 + \delta_y^2) I_{i,j}^k + k_I \dfrac{k_s B_{i,j}^k}{k_s + s_{i,j}^k} \\ \delta_t E_{i,j}^k = (\delta_{D^M x}^2 + \delta_{D^M y}^2) E_{i,j}^k + D(M_{i,j}^k)(\delta_x^2 + \delta_y^2) E_{i,j}^k + Y_E \dfrac{\mu B_{i,j}^k s_{i,j}^k}{k_s + s_{i,j}^k} - k_E \dfrac{k_s E_{i,j}^k}{k_s + s_{i,j}^k} \\ M_{i,j}^k = B_{i,j}^k + I_{i,j}^k + E_{i,j}^k \end{cases} \tag{12}$$

4. Numerical examinations

Example 4. 1 We choose parameters: $r = 0.3$, $\delta = 10^{-4}$, $\alpha = \beta = 4$, $\Delta x = \Delta y = 0.02$ and $\Delta t = 10^{-4}$. The problem domain is $[0,1] \times [0,1]$. The corresponding initial condition is given by

$$\begin{aligned} u0(x,y,0) = {} & 0.68 e^{-60((x-0.2)^2 + (y-0.2)^2)} + 0.65 e^{-50((x-0.8)^2 + (y-0.8)^2)} \\ & + 0.80 e^{-30((x-0.2)^2 + (y-0.8)^2)} + 0.78 e^{-35((x-0.8)^2 + (y-0.2)^2)} \\ & + 0.82 e^{-20((x-0.5)^2 + (y-0.5)^2)} \end{aligned} \tag{13}$$

The homogeneous Neumann boundary conditions are imposed at all the grid points on the four edges of the boundary of Ω. The results are plotted in Fig. 1.

From Fig. 1, it can be observed that the bio-film density continuously grow, and its colony spreads over the problem domain with the increase of time. This is because the biomass growth rate r is set larger than zeros. Eventually, biological density reaches a stable state that is almost close to the peak value 1 at time $t = 3$.

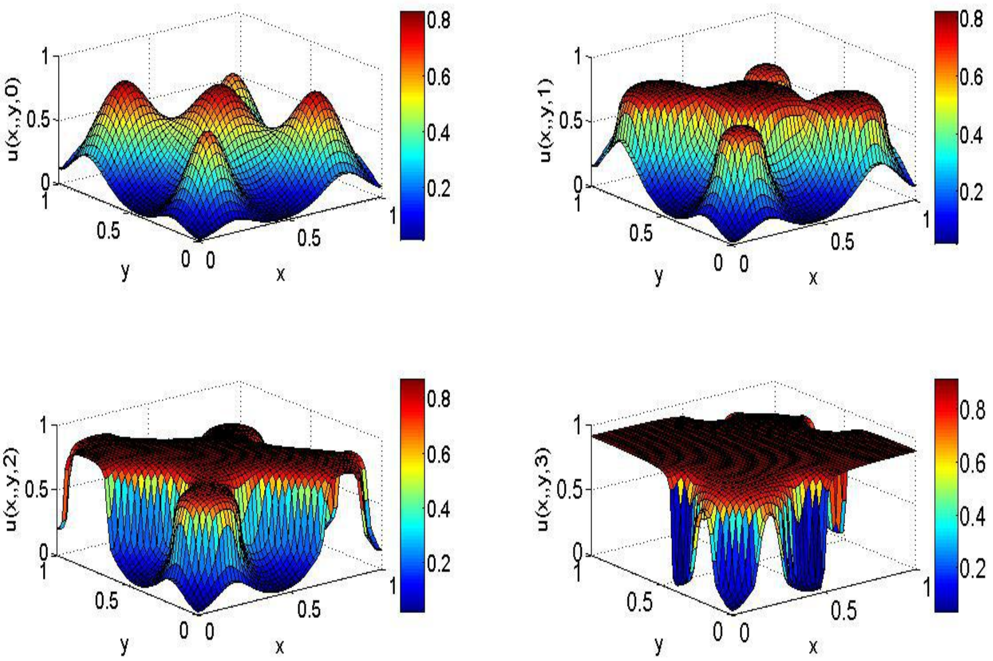

Fig. 1 Graphs of the approximate solutions of single species bio-film system (1) versus x and y at times 0,1,2 and 3.

Example 4. 2 Let $d_1 = 0.015$, $d_2 = 0.005$, $k_1 = 0.65$, $k_2 = 0.2$, $k_3 = 0.85$, $k_4 = 0.1$, $\alpha = \beta = 2$, $\delta = 1$ and $\Omega = (0,1) \times (0,1)$. The corresponding initial conditions are given by

$$
\begin{aligned}
s_0 &= 1 \\
u_0 &= 0.68e^{-60((x-0.3)^2+(y-0.3)^2}) + 0.65e^{-50((x-0.8)^2+(y-0.8)^2)} \\
&\quad + 0.80e^{-30((x-0.5)^2+(y-0.8)^2}) + 0.78e^{-35((x-0.65)^2+(y-0.4)^2)}
\end{aligned}
\tag{14}
$$

The homogeneous Neumann boundary conditions are imposed all grid points on the boundary of Ω. The results are plotted in Fig. 2, using $\Delta t = 0.0004$， and $= \Delta x = \Delta y = 0.02$.

In Fig. 2, it can be observed that the bio-film density continuously grows and colony spreads at initial stage. This is because the bio-film decay rate k_2 is small than the maximum specific growth rate k_3. But the bio-film density will decay with the nutrient consumption. By comparing with the distribution graph of left column and column at time 1, 2 and 3, we can find the left and right graph are highly complementary to each other.

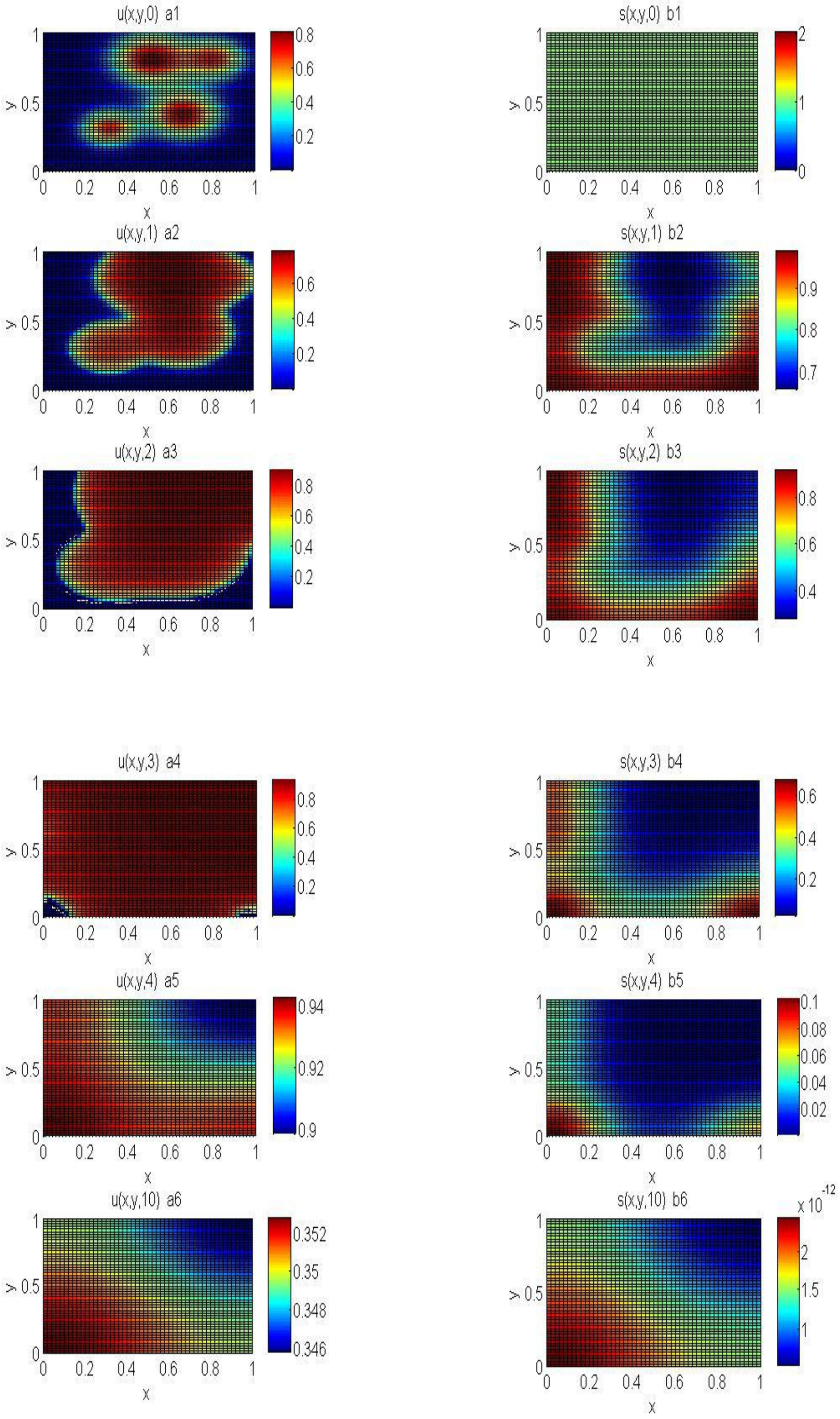

Fig. 2 Graphs of the approximate solutions of the coupling bio-film system (2) versus x and y at times 0,1,2,3,4 and 10.

Example 4. 3 Let $\mu = 0.08$, $Y_H = 0.04$ **,** $Y_E = k_E = 0.04$, $k_s = 0.2$, $k_I = 0.03$, $k_L = 0.08$, $\alpha = \beta = 2$ and $\Omega = (0,1)$. The corresponding initial conditions are given by

$$
\begin{aligned}
s_0 &= 1 \\
B_0 &= 0.56e^{-60(x-0.32)^2} + 0.62e^{-100(x-0.75)^2} \\
I_0 &= 0.38e^{-80(x-0.2)^2} + 0.28e^{-60(x-0.7)^2} \\
E_0 &= 0.1
\end{aligned}
\tag{15}
$$

The homogeneous Neumann boundary conditions are imposed all grid points on the boundary of Ω. The results are plotted in Figure 1, using $\Delta t = 0.0001$， and $\Delta = 0.01$.

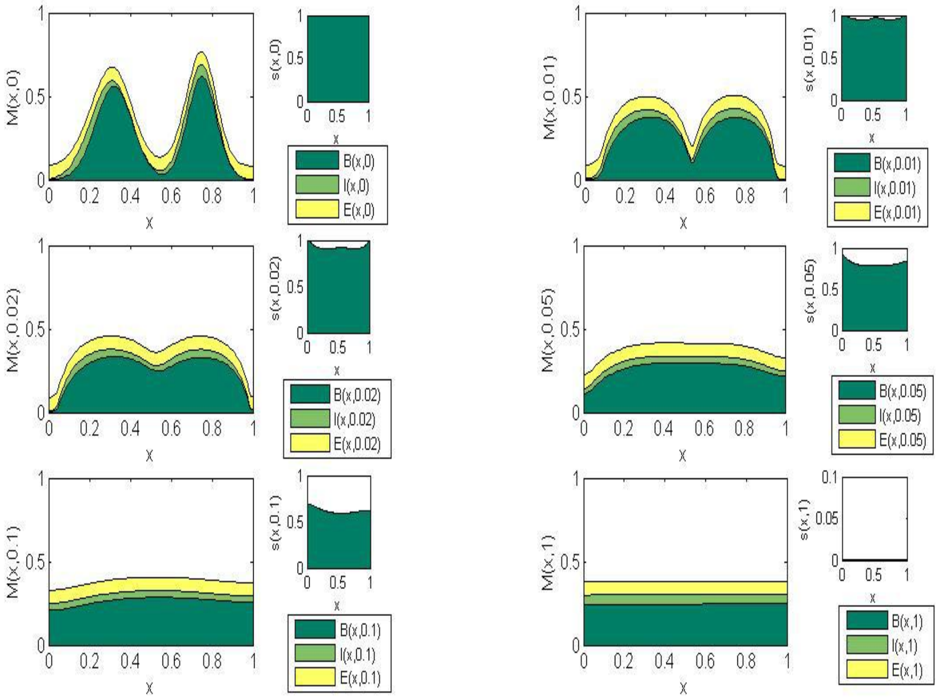

Fig. 3 Graphs of the approximate solutions of the complex bio-film system (3) versus x at times 0,0.01,0.02,0.05,0.1 and 1.

Fig. 3 gives the approximate solutions of system (3) at six different times. Every graph provide the status of the total biomass M, which include active biomass B ,inert biomass I and extra-cellular poly-metric substances E. In each case, the corresponding graph of nutrient consumption also be plotted in right of total biomass M.

5. Conclusions

Applying our method solve three type of nonlinear biofilm models can ensure that numerical solutions are non-non-negative, bounded, and more important is it can also successfully eliminate the ill effects (such as the oscillation of numerical solutions) which is rooted in diffusion coefficient with singularity when biomass density approaches its maximum value at 1.

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Biography

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