A high accuracy scheme of three layers and nine points for Solving the concentration diffusion equation

Yuanyuan Wen, Jianguo Lin, Xue Qiu, Shuting Li, Haiyuan Yu

School of Environmental Science and Engineering, Dalian Maritime University, Dalian 116026, China

*Corresponding author e-mail: 627054905@qq.com

Abstract. A three layers and nine points implicit difference scheme is proposed for solving the one dimensional diffusion equation, using the method of undetermined coefficients and the accuracy is $O(h^4)$. Though the numerical solution and the Von Neumann analysis, the stability condition is proved to be $\tau = \frac{\alpha}{h^2} \leq 0.2235$. The stability condition and accuracy of the scheme are verified by numerical calculation. Compared with the existing three—layers scheme, this paper’s scheme reaches a higher accuracy in case of less nodes. In summary, the scheme mentioned in this paper has academic significance and application value.

1. Introduction

With the rapid development of industry and water transport, the pollutants discharged into water body in great quantities, chemicals and oil spill events such as often happens, the rivers, lakes and oceans ecological environment worsening, seriously affected the water ecological environment and agricultural production, causing great harm to human body health. Thus, further study of pollutants in water body of the behavior and end-result, to develop more effective preventive and emergency measures has the very vital significance.

Diffusion of pollutants in water body mainly includes the two forms——convection and diffusion. This paper only considers the concentration of one dimensional diffusion problem:

\[
\begin{align*}
\frac{\partial C}{\partial t} + \frac{\partial C}{\partial x} & = D \frac{\partial^2 C}{\partial x^2} \\
C(x, 0) & = f(x) \\
C(0, t) = C(L, t) & = 0
\end{align*}
\]

Annotation: $D$ is the coefficient of diffusion term; $C(x, t)$ is concentration; $t$, $x$ are time and space variables respectively

Scholars at home and abroad did a lot of research on the above issues in recent years, such as: The Crank-Nicolson format structured and adjusted by Qiaoling He [1]; The two layers of difference scheme structured by Jiaquan Gao [2]; A semi-explicit differencing scheme of seven points structured by Zelong Chen and Dakai Zhang [3]; Yongqiang Zhan and Chuan-lin Zhang [4] constructed the three...
layer and nine points format, its stability conditions is $\tau = \frac{D}{h^2}$. The accuracy is $o\left(\tau, h^6\right)$; Xiangrong Shan[5] constructed the three layer display difference scheme and the stability condition is $\tau < \frac{1}{2}$, its accuracy is $o\left(\tau, h^6\right)$; A. Hadijidimos [6], Guangwei Yuan and Fengli Zuo[7] are also constructed respectively unconditional stability three-layer format, the precision respectively is $o\left(\tau, h^4\right)$, $o\left(\tau, h^2\right)$.

This paper adopts the method of undetermined coefficients [8], we get the three layers and nine points difference scheme of problem(1) through a series of calculations, its precision can achieve $o\left(\tau, h^6\right)$, stable conditions is $\tau \leq 0.2235$. A numerical example show that the format is very effective, numerical precision and theoretical precision are consistent. Compared with the three layer and high accuracy’s literature [4], this paper’s format has the characteristics of high precision, small amount of calculation.

2. Structure difference scheme

Combined with the problem (1) the characteristics of the diffusion equation, construct the following three-layer nine-node format:

$$
\alpha_1 (c_i^{n+1} + c_{i+1}^{n+1} + c_{i-1}^{n+1}) + \alpha_2 (c_i^n + c_{i+1}^n + c_{i-1}^n) + \alpha_3 (c_i^{n-1} + c_{i+1}^{n-1} + c_{i-1}^{n-1}) + \alpha_4 c_i^{n+1} - \rho = 0
$$

(2)

**Annotation:** $\alpha_1$, $\alpha_2$, $\alpha_3$, $\alpha_4$, $\alpha_5$ are the undetermined coefficient, superscript represents the time horizon, subscript represents the space node.

The eight nodes of type (2) except the point $(i, n)$, in turn on $(i, n)$ based on Taylor series expansion, keep to the item $o\left(\tau, h^6\right)$. Through the equation (1) the time derivative transforms into space derivative, after conversion and the equal of corresponding spatial derivative coefficient, we can get the coefficient $\alpha_1$, $\alpha_2$, $\alpha_3$, $\alpha_4$, $\alpha_5$ of formula (2):

$$
\alpha_1 = \frac{-50400\rho^4 + 12600\rho^3 + 1260\rho^2 - 330\rho + 13}{4(100800\rho^4 - 6300\rho^2 + 313)}
$$

$$
\alpha_2 = \frac{-50400\rho^4 + 63000\rho^3 + 1260\rho^2 + 3450\rho + 313}{2(100800\rho^4 - 6300\rho^2 + 313)}
$$

$$
\alpha_3 = \frac{-2(100800\rho^4 - 6300\rho^2 + 313) + 3}{2(100800\rho^4 - 6300\rho^2 + 313)}
$$

$$
\alpha_4 = \frac{-50400\rho^4 + 63000\rho^3 + 1260\rho^2 - 3450\rho + 313}{2(100800\rho^4 - 6300\rho^2 + 313)}
$$

$$
\alpha_5 = \frac{-50400\rho^4 + 12600\rho^3 + 1260\rho^2 - 330\rho + 13}{4(100800\rho^4 - 6300\rho^2 + 313)}
$$

**Annotation:** $r = \frac{\rho\rho}{h^2}$. And $\alpha_1$, $\alpha_2$, $\alpha_3$, $\alpha_4$, $\alpha_5$ are to be sure, problem (1) can be solved using format (2) by the numerical method, its precision can be achieved $o\left(\tau, h^6\right)$.

3. Stability analysis

Von Neumann stability analysis method is adopted, and combined with numerical calculation the stability of the difference scheme (2) is analyzed.

Making $e^{\rho\tau} - e^{\rho\tau}$ into formula (2), we can get the following:

$$
\begin{align*}
\alpha_1 e^{-i\rho} + \alpha_2 e^{i\rho} + \alpha_3 e^{2i\rho} + \alpha_4 e^{3i\rho} + \alpha_5 e^{4i\rho} = 0
\end{align*}
$$

(3)
Let $\varepsilon = A^{n+1} / A^n$, then the stability of the format (2) is

$$\left| \frac{A^{n+1}}{A^n} \right| \leq 1$$

(4)

According to formula (4) and (3), we can get:

$$\alpha_2 \cos(kh) + \alpha_3 - \alpha_4 \cos(kh) + \alpha_5 = 0$$

Annotation: $0 \leq kh \leq 2\pi$;
Making $2\alpha_1 \cos(kh) + \alpha_2 = a_1$; $2\alpha_3 \cos(kh) + 1 - b; \alpha_5 \cos(kh) + \alpha_4 = c$. There are $ac^2 - bc = 0$;

So the mode of the solution: $|k|_1 = \frac{b - \sqrt{b^2 + 4ac}}{2a}$, $|k|_2 = \frac{b + \sqrt{b^2 + 4ac}}{2a}$

By making the $|k|_1$, $|k|_2$ numerical solution, we can get the contour Figure 1, 2 of $|k|_1$, $|k|_2$ (among them, the abscissa is Angle(kh), ordinate is $r$):

![Figure 1](image-url)
According to Figure 1 and Figure 2, when $0.3 < r < 1$, $|z_1|, |z_2|$ are less than 1. In order to further determine the corresponding stable range of $r$, Figure 2 is amplified locally available Figure 3.

As seen from the above figure, when $0.2235 < r < 0.2235$, $|z_2| < 1$. In general, when $r < 0.2235$, $|z_1|, |z_2|$ are less than 1. The format 2 is stable.

4. Numerical example
Corresponding question (1), making $D = 1$, $L = 1$ and the following initial and boundary conditions:

Boundary condition: $C(x,0) = C(1,0) = 0$ ($t \geq 0$); Initial condition: $C(x,0) = \sin(\pi x)$ ($0 \leq x \leq 1$)
Analytical solution: \( c_{x,t} = e^{-x^2/2\tau} \sin(x/\tau) \) (\( 0 \leq x \leq 1, t \geq 0 \)); Absolute error: \( \Delta n = |c_{x,t} - c_{x,t}^n| \);

\( c_{x,t}^n \) is Numerical solution of each node, \( c_{x,t} \) is the analytical solution of each node.

The following examples are the result of \( t = 0.2 \).

### 4.1. Stability verification and Verify the accuracy

To verify the stability condition, in turn, \( r = 0.5, r = 0.4, r = 0.224, r = 0.224, r = 0.2, r = 0.1 \), through formula (2) making numerical calculation, the results are in the Table 1.

| \( r \) | \( h \) | \( \tau \) | Stability | Maximum absolute error |
|---|---|---|---|---|
| 0.5 | 1.25 e-3 | 1.25 e-3 | unstable | —— |
| 0.4 | 1/20 | 1.0 e-3 | unstable | —— |
| 0.224 | 5.6 e-4 | 5.6 e-4 | —— | —— |
| 0.223 | 5.575 e-4 | 1.33e-10 | stable | 2.23e-12 |
| 0.2 | 5.0 e-4 | 2.5 e-4 | —— | 5.48e-14 |
| 0.1 | 2.5 e-4 | 2.5 e-4 | —— | 5.48e-14 |

The results of Table 1 verifies the conclusion by Von Neumann stability analysis method and combining with the stability of the numerical calculation in this paper: \( r \leq 0.2235 \); formula (2) is stability.

In order to further verify the consistency between the theoretical accuracy and the actual numerical accuracy about the formula (2), Under the condition of satisfy the stability, \( \tau, h \) are selected, and the results are shown in Table 2.

| \( \tau \) | \( h \) | Theoretical accuracy | Maximum absolute error |
|---|---|---|---|
| 10^{-3} | 1/10 | 1e-8 | 1.31e-11 |
| 5*10^{-4} | 1/20 | 3.91e-11 | 2.23e-12 |
| 10^{-4} | 1/40 | 1.53e-13 | 1.74e-14 |

The results of Table 2 show that the numerical accuracy of formula (2) can reach its theoretical accuracy and it is often higher than the theoretical accuracy.

### 4.2. Comparison with the literature [4]

In the three-layer format, the literature [4] has a high numerical calculation precision and a wide range of stability. Therefore, the format of this paper (2) is compared with the following:

1) When \( r = 5*10^{-4}, \hbar = 0.05, r = 0.2 \), which has meet their respective stability conditions, The results are shown in Table 3.

| \( x \) | Literature [4] | The paper |
|---|---|---|
| 0.1 | 2e-9 | 6.9e-13 |
| 0.3 | 3e-9 | 1.8e-12 |
| 0.5 | 4e-9 | 2.2e-12 |
| 0.7 | 3e-9 | 1.8e-12 |
| 0.9 | 2e-9 | 6.9e-13 |

The Table 3 shows that the accuracy of the format (2) in this paper is much higher than literature [4].

2) The stability condition of the format (2) in this paper is \( r \leq 0.2235 \) and the literature [4] is \( r > 1/6 \). When taking the same \( r \), the paper can use the larger \( h \), and the literature [4] can only be selected
relatively small $h$ because of the stability condition. Therefore, this paper has the advantage of small computation. To further illustrate this point, the same $r$ and different $h$ calculations are taken in the condition of satisfying the literature [4] and the stability of this paper, and the results are as shown in Table 4:

|       | $\tau$ | $h$ | $x=0.1$ | $x=0.3$ | $x=0.5$ | $x=0.7$ | $x=0.9$ |
|-------|--------|-----|---------|---------|---------|---------|---------|
| literature [4] | $1.25*10^{-4}$ | 1/20 | 4.0e-9  | 1.1e-8  | 1.6e-8  | 1.5e-8  | 7.0e-9  |
| The paper       |        |      |         |         |         |         |         |
| literature [4] | $5*10^{-4}$  | 1/10 | 2.3e-12 | 6.1e-12 | 7.5e-12 | 6.1e-12 | 2.3e-12 |
| The paper       |        |      |         |         |         |         |         |
| literature [4] | $2.5*10^{-3}$ | 1/5  | 1.2e-10 | 3.2e-10 | 3.9e-10 | 3.2e-10 | 1.2e-10 |
| The paper       |        |      |         |         |         |         |         |

Compared with the literature [4], the numerical accuracy can be guaranteed higher than the literature [4], although the space step in this paper is larger than that in literature [4]. In the guarantee accuracy is not lower than the literature [4] under the premise, this also indicates that the calculation of the format of this paper can be far less than the literature [4].

5. Conclusion
In this paper, a three-layer nine-point implicit difference scheme of concentration diffusion equation is obtained by the method of undetermined coefficients. The accuracy is $\eta(\tau, h)$. The stability of the obtained difference scheme is analyzed by Von Neumann stability analysis and numerical calculation, the stability condition is $r \leq 0.2235$. The stability conditions and their accuracy of the proposed scheme are verified by numerical calculation. Compared with the literature [4] shows that in the case of fewer nodes the format of this paper can still get higher calculation accuracy, in summary, the format of this paper not only has a certain academic significance, but also has a high application value.

References
[1] QiaoLing He etc.Modified C-N Scheme and Stability Analysis of Heat Conduction Equation [J]. Journal of Shandong University of Technology, 2014, 28(4): 21 -24 .
[2] Jiaquan Gao, Guixia He. An unconditionally stable parallel difference scheme for parabolic equations [J]. Applied Mathematics and Computation, 2003,135(2-3): 391-398.
[3] ZeLong Chen, DaKai Zhang. A Family of High Accuracy Implicit Difference Schemes for Solving Parabolic Equations. [J]. Journal of Guizhou University, 2006,23(1): 31-34
[4] YongQiang Zhan, ChuanLin Zhang. A Family of High Accuracy Implicit Difference Schemes for Solving Parabolic Equations [J]. Applied Mathematics and Mechanics, 2014, 35(7): 790-797.
[5] ShuangRong Shan. Three - Layer Display Difference Scheme for Solving Higher Order Parabolic Equations [J]. Journal of Huaqiao University (Natural Science), 2005, 26(3): 240-242.
[6] A. Hadjidimos. A new explicit three level difference scheme for the solution of the heat flow equation [J], BIT Numerical Mathematics. 1969. 9(4): 315-323.
[7] Guangwei Yuan and Fengli Zuo. Parallel difference scheme for heat conduction equations [J]. Intern. J. Computer Math. 2003, 80(8): 993–997.
[8] Liu Lei. The Construction of Parallel Format of Convection - Diffusion Equation And Its Application in Environment [D]. DMU, 2016.