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河流水质模型求解的Chebyshev正交多项式方法

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摘　要: 提出一种考虑弥散时Streeter-Phelps一维稳态河流水质模型Chebyshev正交多项式的近似解法. 通过对稳态河流水质模型的非线性高阶微分方程式分析, 采用Chebyshev正交多项式对各阶微分和弥散系数D进行近似描述, 得到稳态河流水质模型的近似表达式. 针对近似模型给出了误差指标, 并采用最小二乘对近似式中的未知参数进行估计; 同时, 对算法的总精度进行了讨论. 仿真结果表明, 该方法的精度高于多种微分方程数值计算方法(如龙格-库塔), 不仅可以提高生化需氧量的计算精度, 而且能够大大提高溶解氧浓度计算结果的准确性.

关键词: 水质模型; 正交多项式; 数值计算
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Shifted Chebyshev polynomials for the solution of storm-water quality model

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Abstract: A solution scheme of Streeter-Phelps model of one-dimensional storm water quality is presented. Through analyzing high-order differential equations of steady storm-water quality model, shifted-Chebyshev polynomials are used to approximate a series of differentials of BOD parameter and diffusion-coefficient D. A approximate solution of steady storm water quality model is developed. To get the coefficient vector of shifted-Chebyshev polynomials, least square method is introduced. Simulation results show that the approach can give more accurate estimates of BOD and DO than the ordinal methods.

Key words: model of water quality; orthogonal polynomials; numerical computation

1　引　　言

对于较长河段或河流进行水质规划时, 常常需要使用一维水质模型. 在所有一维模型中, 应用最多的是BOD-DO耦合模型. 该模型能较为真实地反映实际, 因此对水污染控制具有普遍的重要性. 几十年来, 人们一直对最具代表性的Streeter-Phelps模型进行了研究[1,2]. 当复氧系数与水流速度的比值很小时, 实际分析时可以不考虑弥散作用[3]; 然而, 当复氧系数与水流速度比值不可忽略时, 在对水质分析时, 必不可免地要面临高解非线性系统求解问题. 对此, 国内外很多学者给出了一系列逼近方法, 但计算过于复杂且对求解算法的收敛性和计算精度讨论较少[4~7]. 为保证求解的收敛性和工程精度, 本文给出了一种正交级数逼近方法.

2　河流水质模型

一维稳态河流水质模型可用生化需氧量(BOD)和溶解氧(DO)两组方程来表达:

$$\begin{cases} u\dfrac{\partial L}{\partial x} = D\dfrac{\partial^2 L}{\partial x^2} - K_1 L, \\ u\dfrac{\partial O}{\partial x} = D\dfrac{\partial^2 O}{\partial x^2} - K_1 L + K_2(O_s - O). \end{cases} \tag{1}$$

式中: L 和O 分别为水中BOD和溶解氧浓度

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$[ML^{-3}]$, D 为弥散系数$[L^{2}T^{-1}]$, K_1 和 K_2 分别为耗氧与复氧系数$[T^{-1}]$, u 为断面平均流速$[LT^{-1}]$, O_s 为水中饱和溶解氧浓度$[ML^{-3}]$.

当 $K_2/u^2 \ll 1$ 时, 式(1) 可近似求解[3], 而对于其他情形, 式(1) 求解比较困难. 为此, 本文作如下处理:

因弥散系数 $D = O_s - O$, 由式(1) 可得

$$L = -\left(D\frac{\partial^2 D}{\partial x^2} - u\frac{\partial D}{\partial x} - K_2 D\right)\Big/K_1, \tag{2}$$

$$\frac{\partial L}{\partial x} = -\frac{1}{K_1}\left(\frac{\partial D}{\partial x}\frac{\partial^2 D}{\partial x^2} + D\frac{\partial^3 D}{\partial x^3} - u\frac{\partial^2 D}{\partial x^2} - K_2\frac{\partial D}{\partial x}\right), \tag{3}$$

$$\frac{\partial^2 L}{\partial x^2} = -\frac{1}{K_1}\left[\left(\frac{\partial^2 D}{\partial x^2}\right)^2 + 2\frac{\partial D}{\partial x}\frac{\partial^3 D}{\partial x^3} + D\frac{\partial^4 D}{\partial x^4} - u\frac{\partial^3 D}{\partial x^3} - K_2\frac{\partial^2 D}{\partial x^2}\right]. \tag{4}$$

将式(2)～(4) 代入式(1), 得

$$\frac{u}{K_1}\left(\frac{\partial D}{\partial x}\frac{\partial^2 D}{\partial x^2} + 2D\frac{\partial^3 D}{\partial x^3}\right) + \left(1 + \frac{K_2}{K_1}\right)D\frac{\partial^2 D}{\partial x^2} = \frac{u^2}{K_1}\frac{\partial^2 D}{\partial x^2} + \left(1 + \frac{K_2}{K_1}\right)u\frac{\partial D}{\partial x} + K_2 D + \frac{D}{K_1}\left[\left(\frac{\partial^2 D}{\partial x^2}\right)^2 + 2\frac{\partial D}{\partial x}\frac{\partial^3 D}{\partial x^3} + D\frac{\partial^4 D}{\partial x^4}\right]. \tag{5}$$

由式(5) 可见, 水质模型求解必须涉及高阶非线性问题.

3 模型的级数逼近

为简化问题, 将水中BOD 和溶解氧浓度$\frac{\partial^4 D}{\partial x^4}$展成Chebyshev 正交级数, 并将Chebyshev 正交多项式定义为

$$T_i(z) = \cos(i\cos^{-1}z),\quad i = 0, 1, 2, \cdots;\ -1 \leqslant z \leqslant 1. \tag{6}$$

为便于应用, 令

$$x = \beta(1 - z)/2, \tag{7}$$

将 x 的取值区间扩展到$[0, \beta]$. 于是得到如下的Chebyshev 正交多项式的递推形式:

$$\begin{cases} T_0(x) = 1, \\ T_1(x) = 1 - 2x/\beta, \\ T_2(x) = 8(x/\beta)^2 - 8(x/\beta) + 1, \\ \vdots \\ T_{i+1}(x) = 2T_1(x)T_i(x) - T_{i-1}(x). \end{cases} \tag{8}$$

令

$$\frac{\partial^4 D}{\partial x^4} \approx \sum_{i=1}^{n} d_i f_i(x) = [d_1\ d_2 \cdots d_n][f_1(x)\ f_2(x) \cdots f_n(x)]^{\mathrm{T}} = \mathbf{d}^{\mathrm{T}}\mathbf{f}. \tag{9}$$

式中: $\mathbf{f} = [T_0(x)\ T_1(x) \cdots T_N(x)]^{\mathrm{T}}$, $\mathbf{d}$ 为待确定常数(成为参数向量).

这样, 各阶导数和 D 分别为

$$\frac{\partial^3 D}{\partial x^3} \approx \mathbf{d}^{\mathrm{T}}\int_0 \mathbf{f}\,\mathrm{d}x + \frac{\partial^3 D}{\partial x^3}\Big|_{x=x_0} = \mathbf{d}^{\mathrm{T}}\mathbf{H}\mathbf{f} + \frac{\partial^3 D}{\partial x^3}\Big|_{x=x_0} = \mathbf{d}^{\mathrm{T}}\mathbf{H}\mathbf{f} + A_3, \tag{10}$$

$$\frac{\partial^2 D}{\partial x^2} \approx \mathbf{d}^{\mathrm{T}}\mathbf{H}^2\mathbf{f} + \frac{\partial^3 D}{\partial x^3}\Big|_{x=x_0}(x - x_0) + \frac{\partial^2 D}{\partial x^2}\Big|_{x=x_0} = \mathbf{d}^{\mathrm{T}}\mathbf{H}^2\mathbf{f} + A_2, \tag{11}$$

$$\frac{\partial D}{\partial x} \approx \mathbf{d}^{\mathrm{T}}\mathbf{H}^3\mathbf{f} + \frac{1}{2}\frac{\partial^3 D}{\partial x^3}\Big|_{x=x_0}(x - x_0)^2 + \frac{\partial^2 D}{\partial x^2}\Big|_{x=x_0}(x - x_0) + \frac{\partial D}{\partial x}\Big|_{x=x_0} = \mathbf{d}^{\mathrm{T}}\mathbf{H}^3\mathbf{f} + A_1, \tag{12}$$

$$D = \mathbf{d}^{\mathrm{T}}\mathbf{H}^4\mathbf{f} + \frac{1}{6}\frac{\partial^3 D}{\partial x^3}\Big|_{x=x_0}(x - x_0)^3 + \frac{1}{2}\frac{\partial^2 D}{\partial x^2}\Big|_{x=x_0}(x - x_0)^2 + \frac{\partial D}{\partial x}\Big|_{x=x_0}(x - x_0) + D_0 = \mathbf{d}^{\mathrm{T}}\mathbf{H}^4\mathbf{f} + A_0. \tag{13}$$

式中

$$A_3 = \frac{\partial^3 D}{\partial x^3}\Big|_{x=x_0},$$

$$A_2 = \frac{\partial^3 D}{\partial x^3}\Big|_{x=x_0}(x - x_0) + \frac{\partial^2 D}{\partial x^2}\Big|_{x=x_0},$$

$$A_1 = \frac{1}{2}\frac{\partial^3 D}{\partial x^3}\Big|_{x=x_0}(x - x_0)^2 + \frac{\partial^2 D}{\partial x^2}\Big|_{x=x_0}(x - x_0) + \frac{\partial D}{\partial x}\Big|_{x=x_0},$$

$$A_0 = \frac{1}{6}\frac{\partial^3 D}{\partial x^3}\Big|_{x=x_0}(x - x_0)^3 + \frac{1}{2}\frac{\partial^2 D}{\partial x^2}\Big|_{x=x_0}(x - x_0)^2 + \frac{\partial D}{\partial x}\Big|_{x=x_0}(x - x_0) + D_0,$$

$$\mathbf{H} = \beta\begin{bmatrix} 1/2 & -1/2 & 0 & \cdots \\ 1/8 & 0 & -1/8 & \cdots \\ -1/6 & 1/4 & 0 & \cdots \\ -1/16 & 0 & 1/8 & \cdots \\ \vdots & \vdots & \vdots & \ddots \\ \dfrac{-1}{2(m-1)(m-3)} & 0 & 0 & \cdots \\ \dfrac{-1}{2m(m-2)} & 0 & 0 & \cdots \end{bmatrix} \rightarrow$$

$$
\leftarrow \begin{bmatrix}
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
\vdots & \vdots & \vdots \\
\frac{1}{4(m-3)} & 0 & \frac{-1}{4(m-1)} \\
0 & \frac{1}{4(m-2)} & 0
\end{bmatrix},
$$

$$m = 4, 6, \cdots.$$

对于水中BOD 的求解, 可将式(9)～(13) 代入式(2) 中直接得到, 即

$$L = [(d^T H^4 f + A_0)(d^T H^2 f + A_2) - u(d^T H^3 f + A_1) - K_2(d^T H^4 f + A_0)]/K_1. \quad (14)$$

4　等价逼近式和计算方法

将式(9)～(13) 代入式(5) 中可得

$$\frac{u}{K_1}[(d^T H^3 f + A_1)(d^T H^2 f + A_2) + 2(d^T H^4 f + A_0)(d^T H f + A_0)] + \left(1 + \frac{K_2}{K_1}\right)(d^T H^4 f + A_0)(d^T H^2 f + A_2) = \frac{u^2}{K_1}(d^T H^2 f + A_2) + \left(1 + \frac{K_2}{K_1}\right)u(d^T H^3 f + A_1) + K_2(d^T H^4 f + A_0) + \frac{1}{K_1}(d^T H^4 f + A_0)\{[(d^T H^2 f + A_2)]^2 + 2(d^T H^3 f + A_1)(d^T H f + A_3) + (d^T H^4 f + A_0)d^T f\}. \quad (15)$$

为便于分析, 式(15) 可表示为

$$d^T P_2 d + d^T P_1 + P_0 - \frac{1}{K_1} d^T H^4 f\, d^T Q_2 d = 0. \quad (16)$$

式中

$$Q_2 = H^2 f f^T (H^2)^T + 2H^3 f f^T H^T + H^4 f f^T,$$

$$P_2 = \frac{u}{K_1}[H^3 f f^T (H^2)^T + 2H^4 f f^T H^T] + \left(1 + \frac{K_2}{K_1}\right)H^4 f f^T (H^2)^T - \frac{A_0}{K_1}Q_2 - \frac{1}{K_1}H^4 f\,(2H^2 f A_2 + 2H^3 f A_3 + 2H f A_1 + f A_0)^T,$$

$$P_1 = \frac{u}{K_1}(H^3 f A_2 + H^2 f A_1 + 2H^4 f A_3 + 2H f A_0) - \frac{u^2}{K_1}H^2 f + \left(1 + \frac{K_2}{K_1}\right) \times (H^4 f A_2 + H^2 f A_0) - K_2 H^4 f - \frac{1}{K_1}H^4 f\,(A_2 A_2 + 2A_1 A_3) - \left(1 + \frac{K_2}{K_1}\right)u H^3 f - \frac{A_0}{K_1}(2H^2 f A_2 + 2H^3 f A_3 + 2H f A_1 + f A_0),$$

$$P_0 = \frac{u}{K_1}(A_1 A_2 + 2A_0 A_3) + \left(1 + \frac{K_2}{K_1}\right)A_0 A_2 - \frac{u^2}{K_1}A_2 - \left(1 + \frac{K_2}{K_1}\right)u A_1 - K_2 A_0 - \frac{A_0}{K_1}(A_2 A_2 + 2A_1 A_3).$$

于是, 式(5) 表示的高阶非线性微分方程问题便转化为式(16).

定义

$$e = \Psi(d^T P_2 \hat{d} + d^T P_1 + P_0 - d^T H^4 f\, d^T Q_2 d / K_2). \quad (17)$$

将式(17) 在 d 的估计值处展开成泰勒级数, 可得

$$e = \Psi(\bullet) + (d - \hat{d})^T \frac{\partial \Psi(\bullet)}{\partial \hat{d}} + \frac{1}{2}(d - \hat{d})^T \left[\frac{\partial \Psi(\bullet)}{\partial \hat{d}} \frac{\partial \Psi(\bullet)}{\partial \hat{d}^T} + \frac{\partial^2 \Psi(\bullet)}{\partial \hat{d}\, \partial \hat{d}^T}\right](d - \hat{d}) + \gamma(\hat{d}). \quad (18)$$

式中: $\Psi(\bullet) = \Psi(\hat{d}^T P_2 \hat{d} + d^T P_1 + P_0 - \hat{d}^T H^4 f\, d^T Q_2 \hat{d} / K_1)$, $\hat{d}$ 为 d 的估计值, $\gamma(\hat{d})$ 为余项.

当指标函数取为 $J = \int e^2 dx$ 时, 使 J 达到最小的 $\hat{d}$ 可按最小二乘方法估计. 未知参数向量的迭代估计式为

$$d - \hat{d} = \left\{\int \left[\frac{\partial \Psi(\bullet)}{\partial \hat{d}} \frac{\partial \Psi(\bullet)}{\partial \hat{d}^T} + \frac{\partial^2 \Psi(\bullet)}{\partial \hat{d}\, \partial \hat{d}^T}\right]\right\}^{-1} \times \int \left[\frac{\partial \Psi(\bullet)}{\partial \hat{d}}\right] \Psi(\bullet)\, dx. \quad (19)$$

式(19) 中的偏导数为

$$\frac{\partial \Psi(\bullet)}{\partial d^T} = 2P_2 d + P_1 - (H^4 f\, d^T Q_2 d + 2d^T H^4 f Q_2 d)/K_1, \quad (20)$$

$$\frac{\partial^2 \Psi(\bullet)}{\partial d\, \partial d^T} = 2P_2 - \{2(H^4 f) \otimes d^T Q_2) + 2(d^T H^4 f)Q_2 + 2[f^T (H^4)^T] \otimes (Q_2 d)\}/K_1. \quad (21)$$

5　仿真研究及应用

为进一步说明上述方法的有效性, 对式(19) 的迭代算法进行仿真验证. 设有一均匀河段中平均流

速 u = 12 km/d, L_0 = 55.897 6 mg/l, $O_s - O_0$ = 1.960 4 mg/l, K_1 = 0.51 d^{-1}, K_2 = 1.15 d^{-1}. 选取采样周期(步长) 为 0.02, 计算点数 = 500. 为说明计算误差, 首先根据实际测量的统计分析, 给定函数 $D = O_s - O$; 然后, 再通过式(2) 得到 L 的真值. 这样, 便可直接得到此条件下有关方法的实际误差.

图 1 给出了采用本文方法所得的 $x \sim (O_s - O)$ 和 $x \sim L$ 拟合曲线(其中: 实线为计算值, 虚线为理论值). 由图 1 可见, 采用本文的逼近方法可获得比较准确的拟合结果. 本方法已成功地用于延安市延河水的水质判定, 取得了良好的效果.

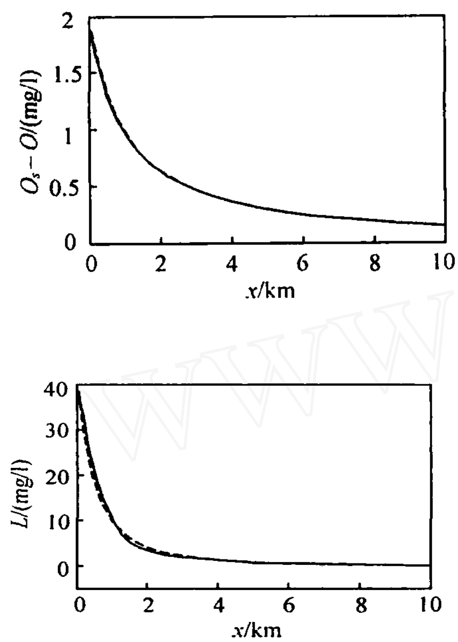

图 1 按 Chebyshev 正交级数逼近的结果

6 结 语

为减少考虑弥散时 Streeter-Phelps 一维稳态河流水质模型求解方法的误差, 本文给出了以 Chebyshev 正交多项式为基础的求解方法. 根据 Chebyshev 正交多项式近似模型, 采用最小二乘估计对近似式中的未知参数进行估计. 仿真结果表明, 该方法的精度高于多种微分方程数值计算方法(如龙格-库塔), 不仅可以进一步提高 BOD 的计算精度, 而且能大大提高溶解氧浓度计算结果的准确性. 理论和实际应用结果都表明, 本文方法可用于一维稳态河流水质的预测和检测结果的分析.

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