# NUMERICAL SOLUTION OF THE COUPLED BOD-DO EQUATIONS BY USING HALF SWEEP EXPLICIT GROUP ITERATIVE METHOD

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## ABSTRAK

PENYELESAIAN BERANGKA BAGI PERSAMAAN PEMBEZAAN PASANGAN *BOD-DO* DENGAN MENGGUNAKAN KAEDAH KUMPULAN TAK TERSIRAT SAPUAN SEPARUH

Dalam realiti, pemodelan alam sekitar untuk kualiti air, dapat dibentuk dengan satu atau lebih persamaan pembezaan separa dalam pemodelan matematik. Kertas kerja ini bertujuan untuk menguji keberkesanan kaedah Kumpulan Tak Tersirat Sapuan Separuh (KTTSS) dibandingkan dengan kaedah Gauss-Seidel dalam menyelesaikan persamaan pembezaan separa dalam model yang dipaparkan. Untuk pengesahan, beberapa eksperimen berangka dilaksanakan untuk menganalisis keberkesanan kaedah KTTSS dalam konteks bilangan lelaran, jumlah masa yang diambil untuk mendapatkan penyelesaian, dan ralat maksimum.

**ABSTRACT**

The real world phenomena, for example in this dissertation, the environmental modeling of water quality, are always described in mathematical model with one or more partial differential equations. This research is to study the effectiveness of the 2 Points Half-Sweep Explicit Group (2HSEG) Iterative scheme compared to the classical Gauss-Seidel (GS) iterative scheme. The GS iterative scheme is used to solve the system of linear equations generated from the discretization process of the finite difference method (FDM). For validation, several numerical experiments were conducted in order to analyse the effectiveness of the HSEG methods in terms of number of iterations, computational time and generated maximum error.

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## LIST OF SYMBOLS

| | |
|---|---|
| $t$ | time, measured in unit seconds (s) |
| $x$ | distance, measured in unit meters (m) |
| $u$ | average river velocity, $m/s$ |
| $D$ | longitudinal dispersion coefficient, $m^2/s$ |
| $L_1$ | BOD concentration, $mg/L$ |
| $k_3$ | BOD removal rate due to combined effects of sedimentation and decay, $s^{-1}$ |
| $L_a$ | BOD addition rate due to other processes, $mg/(Ls)$ |
| $C_1$ | DO concentration, $mg/L$ |
| $k_1$ | BOD deoxygenating rate constant, $s^{-1}$ |
| $k_2$ | reaeration rate constant, $s^{-1}$ |
| $C_s$ | saturation DO concentration, $mg/L$ |
| $L_0$ | initial BOD concentration in river, $mg/L$ |
| $A$ | mean BOD input concentration at upstream boundary, $mg/L$ |
| $B$ | amplitude of BOD variation of input at upstream boundary, $mg/L$ |
| $\omega$ | BOD loading frequency, $s^{-1}$ |
| $C_0$ | initial DO concentration in river, $mg/L$ |
| $a$ | mean DO input concentration, $mg/L$ |
| $b$ | amplitude of DO variation of input at upstream boundary, $mg/L$ |
| $\omega_1$ | DO loading frequency, $s^{-1}$ |
| $k_d$ | deoxygenation rate (per day) |
| $k_r$ | reaeration rate (per day) |
| $D(t)$ | oxygen deficit in the stream (the difference between the saturation and the actual DO level) |
| $L(t)$ | stream BOD remaining at time $t$ |
| $BOD_a$ | BOD deficit concentration at time $t=0$ |
| $D_0$ | initial DO deficit concentration at time, $t=0$ |

| | |
|---|---|
| $\rho$ | corresponding to 1 and 2, represent the Full-Sweep and Half-Sweep cases respectively |
| i | used to denote the spatial location of mesh point within the grid network |
| j | used to denote the temporal layer of mesh point within the grid network |
| $\Delta t$ | differences in time between $t_{j+1}$ and $t_j$ |
| $\Delta x$ | differences in time between $x_{i+1}$ and $x_i$ |
| $\delta_x$ | central difference scheme towards spatial derivatives |
| $\frac{\partial u}{\partial x}$ | first order derivatives towards a function $u$ of $x$ |
| $\frac{\partial u}{\partial t}$ | first order derivatives towards a function $u$ of $t$ |
| $\frac{\partial^2 u}{\partial x^2}$ | second order derivatives towards a function $u$ of $x$ |
| $\frac{\partial^2 u}{\partial t^2}$ | second order derivatives towards a function $u$ of $t$ |
| $u_{i,j}$ | finite difference approximation terms towards a specific derivatives of function $u$ where the subscript i and j are defined as above, $u(x_i,t_j)$ |
| $x_{i\pm n}$ | $x_i \pm n\Delta x$ |
| $N$ | the size of a matrix |

# CHAPTER 1

# INTRODUCTION

## 1.1 BACKGROUND

This chapter will cover the most fundamental idea of this research. First, a brief description of the background of the problem statement will be included, including the sources of the problem and some of the field knowledge. Second, the numerical method, which will be applied in this research, will also be discussed. But the detail part of the numerical methods will only be included in Chapter 2. Next the objectives that this research needs to achieve will be stated also.

### 1.1.1 Water Quality Model In River

Water quality modeling techniques have been used as a tool to understand how the water quality conditions relate to environment, by providing us to study or to analyse the system in mathematical aspect. A water quality model usually consists of a set of mathematical equations. In order to narrow the scope of this research, this research will only consider water quality modeling in river.

Rivers have been used consistently as the principal pathway for disposing of wastewater, industrial, domestic, and agricultural. Water quality modeling originally focused on river and stream pollution, by the means attempt to simulate changes in concentration of pollutants as they move through the river. The majority changes are caused by the relationship between biochemical oxygen demand (BOD) concentration and dissolved oxygen (DO) concentration (James, 1993). The continuous discharge of wastewater that contain significant amounts of biodegradable organic matter which have high BOD levels into rivers will result an exertion in oxygen demand which it will consume significant amounts of oxygen, therefore depletes the dissolved oxygen concentration in river.

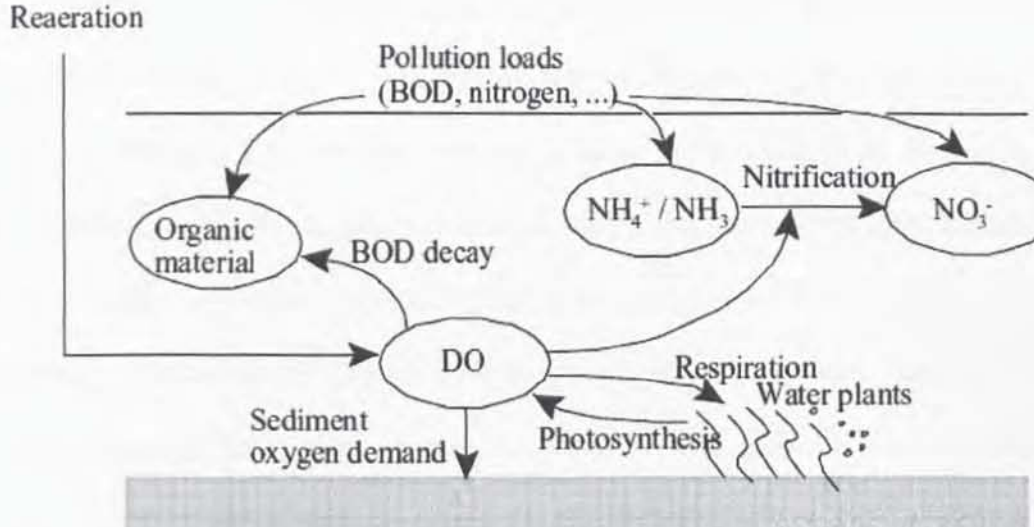


**Figure 1.1** Various important processes that involved in modeling DO concentration.

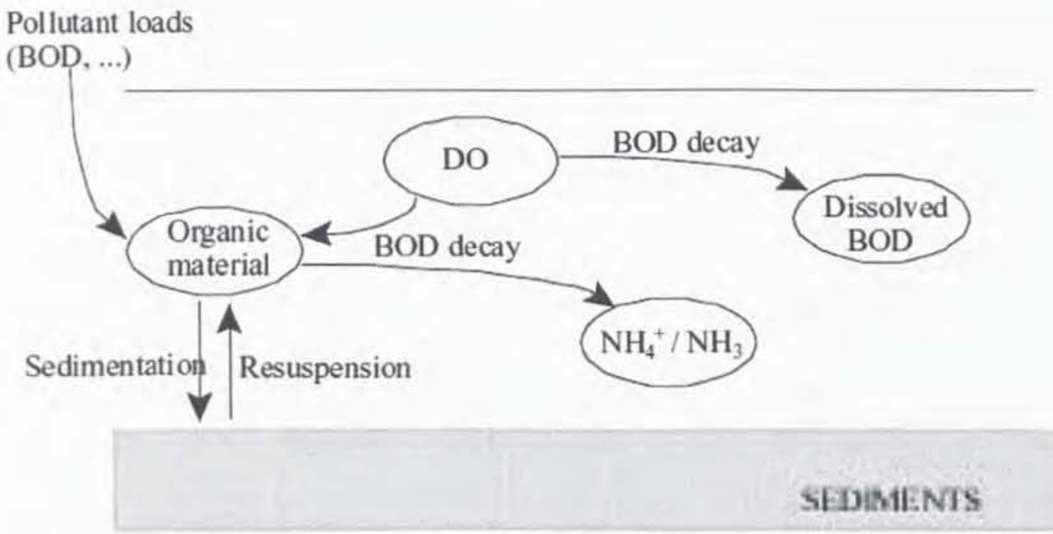


**Figure 1.2** Various important processes that involved in modeling BOD concentration.

Some of the important processes involved in modeling the DO-BOD relationship in river are shown in schematic way in Figure 1.1 and 1.2 (Radwan *et al.*, 2003). In Figure 1.1, oxygen in the aquatic environment is produced by photosynthesis of algae and plants and consumed by respiration of plants, animals and bacteria, BOD degradation process, sediment oxygen demand (SOD) and oxidation. Oppositely, it is re-aerated through interchange with the atmosphere. While in Figure 1.2, degradation of the organic matters expressed as BOD give rise to a consumption of oxygen and BOD is also a sources of nutrients ($NH_4$-N) which also consume oxygen (Radwan *et al.*, 2003).

### 1.1.2 Problem Formulation

Consider a water quality model where BOD concentration and DO concentration in a river vary sinusoidal (Adrian & Alshawabkeh, 1997). This phenomenon is governed by a coupled BOD-DO transport equation, which are given as follows (Dresnack & Dobbins, 1968):

$$\frac{\partial L_1}{\partial t} + u\frac{\partial L_1}{\partial x} = D\frac{\partial^2 L_1}{\partial x^2} - k_3 L_1 + L_a \tag{1.1}$$

$$\frac{\partial C_1}{\partial t} + u\frac{\partial C_1}{\partial x} = D\frac{\partial^2 C_1}{\partial x^2} - k_1 L_1 + k_2(C_s - C_1) \tag{1.2}$$

where

$t$ = time, $s$;

$x$ = distance, $m$;

$u$ = average river velocity, $m/s$;

$D$ = longitudinal dispersion coefficient, $m^2/s$;

$L_1$ = BOD concentration, $mg/L$;

$k_3$ = BOD removal rate due to combined effects of sedimentation and decay, $s^{-1}$;

$L_a$ = BOD addition rate due to other processes, $mg/(Ls)$;

$C_1$ = DO concentration, $mg/L$;

$k_1$ = BOD deoxygenating rate constant, $s^{-1}$;

$k_2$ = reaeration rate constant, $s^{-1}$; and

$C_s$ = saturation DO concentration, $mg/L$.

The coupled partial differential equations are subjected to the following conditions:

Initial condition for (1.1): $L_1(x,0) = L_0$; (1.3)

Boundary conditions for (1.1): $L_1(0,t) = A + B\cos(\omega t)$; (1.4)

$$\lim_{x\to\infty} L_1(x,t) \to \frac{L_a}{k_3}; \tag{1.5}$$

Initial condition for (1.2): $C_1(x,0) = C_0$ (1.6)

Boundary conditions for (1.2): $C_1(0,t) = a + b\cos(\omega_1 t)$; (1.7)

$$\lim_{x\to\infty} C_1(x,t) \to C_s - \frac{k_1}{k_2}\frac{L_a}{k_3} \tag{1.8}$$

where

$L_0$ = initial BOD concentration in river, $mg/L$;

$A$ = mean BOD input concentration at upstream boundary, $mg/L$;

$B$ = amplitude of BOD variation of input at upstream boundary, $mg/L$;

$\omega$ = BOD loading frequency, $s^{-1}$;

$C_0$ = initial DO concentration in river, $mg/L$;

$a$ = mean DO input concentration, $mg/L$;

$b$ = amplitude of DO variation of input at upstream boundary, $mg/L$;

$\omega_1$ = DO loading frequency, $s^{-1}$.

To further simplify our problem statement, substitution technique are applied by introducing new functions which are defined as (Adrian & Alshawabkeh, 1997)

$$L(x,t) = L_1(x,t) - \frac{L_a}{k_3}; \tag{1.9}$$

$$C(x,t) = C_s - \frac{k_1}{k_2}\frac{L_a}{k_3} - C_1(x,t) \tag{1.10}$$

The governing linear homogenous partial differential equations for $L(x,t)$ and $C(x,t)$ become

$$\frac{\partial L}{\partial t} + u\frac{\partial L}{\partial x} = D\frac{\partial^2 L}{\partial x^2} - k_3 L \tag{1.11}$$

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = D\frac{\partial^2 C}{\partial x^2} - k_1 L + k_2 C \tag{1.12}$$

subject to the following conditions:

Initial condition for (1.11): $L(x,0) = \bar{L_0}$; (1.13)

Boundary conditions for (1.11): $L(0,t) = \bar{A} + B\cos(\omega t)$; (1.14)

$\lim_{x\to\infty} L(x,t) \to 0$; (1.15)

Initial condition for (1.12): $C(x,0) = \bar{C}_0$ (1.16)

Boundary conditions for (1.12): $C(0,t) = \bar{a} - b\cos(\omega_1 t)$; (1.17)

$\lim_{x\to\infty} C(x,t) \to 0$ (1.18)

where

$$\bar{L_0} = L_0 - \left(\frac{L_a}{k_3}\right); \tag{1.19}$$

$$\bar{A} = A - \left(\frac{L_a}{k_3}\right); \tag{1.20}$$

$$\bar{C} = C_s - \left(\frac{k_1}{k_2}\right)\left(\frac{L_a}{k_3}\right) - C_0 \text{; and} \tag{1.21}$$

$$\bar{a} = C_s - \left(\frac{k_1}{k_2}\right)\left(\frac{L_a}{k_3}\right) - a. \tag{1.22}$$

In this context, numerical technique called finite difference approach will be used to discretize the simplified coupled BOD-DO partial differential equations (1.11) and (1.12) and then by using iterative method to solve the system of linear equations generated. Finally, by using substituting techniques simultaneously along with equations (1.9) and (1.10), the solution to equations (1.1) and (1.2) can be obtained.

### 1.1.3 Numerical Method In Solving Partial Differential Equations

In order to solve the partial differential equations, there are two methods which can be applied, namely analytical and numerical method. Analytical methods such as separation of variables, D'Alembert General Solution Method for solving first order PDE in terms of arbitrary function, Integral Transform including General Fourier Series Transform, Laplace Transform and Standard Transform, Method of Characteristic and Green's Function Solution Method are used to solve specific types PDEs. However there is no such a general method that can use to solve any types of PDEs. Often it's very difficult to find the analytical solution for PDEs. But instead of using only single analytical method, combination of various methods is usually needed to get the solution (Evans *et al.*, 1999; Haberman, 2004).

Numerous numerical methods such as finite difference method (FDM), finite element method (FEM), finite volume method (FVM), boundary method, spectral approximation method and so on are used for solving the partial differential equations. Figure 1.3 (McDonough, 2001) below shows the graphical visualization of the solution domain discretization by using FEM, FDM and spectral approximation schemes.

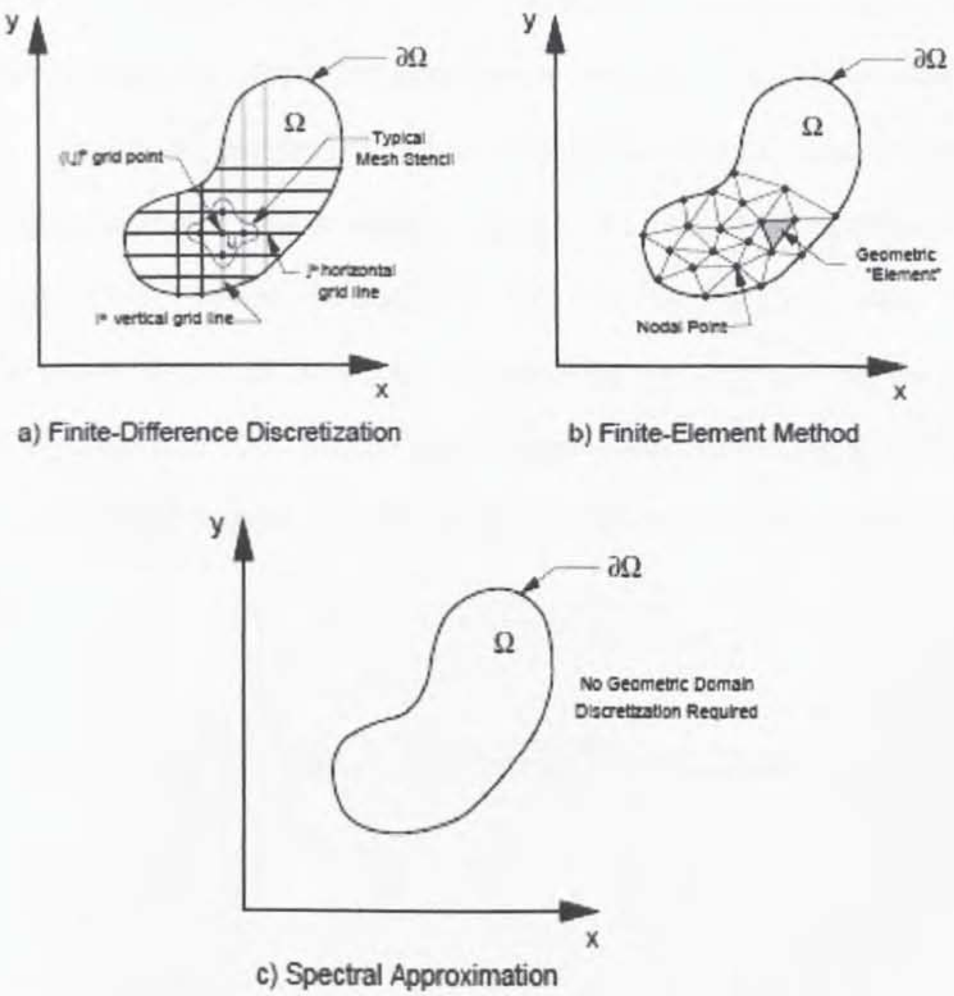


**Figure 1.3** Visual representations of various numerical methods for solving partial differential equations.

FDM and FEM are the most common approaches that are used to convert a set of partial differential equations (PDEs) that constitute a mathematical model, into system of algebraic linear equations that constitute a discrete model. The solution domain is discretized into cells to provide FDM and FEM spatial and temporal grid. Iterative method or direct method is then applied to solve the system of linear equations (Mansell *et al.*, 2002).

The early pioneers of the finite difference solution techniques were Runge in 1908 and Richardson in 1913. FDM were first used to analyze heat diffusion as well as solve stress analysis problems. Since the early 1900s, FDM has been applied to a number of different situations in engineering problems including open channel flow (Hammond, 2004). FDM is constructed by first discretize the PDEs using Taylor series expansion to provide difference approximation for derivatives in the set of PDEs. For example, the Theta Method which is a generalization of 3 classical schemes that are used in FDM to solve one-dimensional parabolic type PDEs, is giving by this equations:

$$\frac{u_{i,j+1}-u_{i,j}}{\Delta t}=\alpha\left(\frac{(1-\theta)(u_{i+1,j}-2u_{i,j}+u_{i-1,j})}{(\Delta x)^2}+\frac{\theta(u_{i+1,j+1}-2u_{i,j+1}+u_{i-1,j+1})}{(\Delta x)^2}\right) \tag{1.24}$$

Subscripts $i$ and $j$ denote the spatial location of nodes and time level within grid network respectively. Obviously it can be seen that $\theta=1$ gives the fully implicit method (backward-difference scheme) which is unconditionally stable, with the spatial derivative is approximated solely at the advanced time level $t_{j+1}$. $\theta=0$ gives the fully explicit method (forward-difference scheme) which is not computationally efficient and not so stable unless very small value of $\Delta t$ and $\Delta x$ are used, with the spatial derivative is approximated solely at the old or current time level $t_j$; and $\theta = 0.5$ gives the Crank-Nicolson (CN) method (central-difference scheme) which is both computationally efficient and unconditionally stable, with the spatial derivatives occurred midway between time level $t_{j+1}$ and $t_j$ (McDonough, 2001; Burden & Faires, 1993; Mansell *et al.*, 2002).

FEM approximates the unknown function in PDEs by using a simpler known function, often a polynomial or piecewise polynomial function, choosing it to satisfy the original PDEs approximately. The implementation of FEM is first divide the problem domain into small regions, often of triangular or (in 3-dimensions) tetrahedral shape. On each of these sub-regions a multidimensional polynomial is used to approximate the solution and various degree of smoothness of the approximate solution are achieved by requiring constructions to guarantee continuity of prescribed number of derivatives across element boundaries. FEM provides distinct advantage over FDM by approximating irregular geometrical regions. Compared to FDM, FEM result in more accurate solution but more complicated implementation than FDM (McDonough, 2002; Gerald & Wheatley, 2003; Mansell *et al.*, 2002).

Besides the most widely used methods like FDM and FEM, other methods such as FVM is often used in computational fluid dynamics; spectral method, spectral element method and boundary element method which are related to FEM, and are particularly applicable for a very restricted class of problems. In order to enhance the

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