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THE CFD MODELING IN BIOREACTOR TRACER STUDIES

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Abstract: This paper presents the effects of dispersion on predicting longitudinal tracer concentration profiles in an activated sludge bioreactor located at the Wschód Waste-Water Treatment Plant in Gdansk. The aim of this study has been to use the one-dimensional advection-dispersion equation to simulate a non-active substance flow (based on the measured tracer concentration). The simulation results were compared with those obtained in the traditional *tanks-in-series* approach, commonly used in designing biological reactors. The dispersion coefficient was calculated from a statistical formula based on differences in the tracer concentration distributions at two sampling points. The study has shown that the numerical simulation using the one-dimensional tracer migration equation yields better results than the *tanks-in-series* model in predicting longitudinal tracer concentration profiles. This paper is an introduction to the study of reactive substances in activated sludge bioreactors.

Keywords: mathematical modelling, pollutant migration, reactor hydraulics, advection-dispersion equation, tracer studies

1. Introduction

Longitudinal concentration profiles of continuous flow activated sludge reactors can be solved numerically with the advection-dispersion equation (ADE). Several numerical techniques for solving ADE have been successfully applied [1, 2], usually based on the finite difference method (FDM), the finite element method (FEM) or the finite volume method (FVM). The aim of this study, carried out at the Wschód Waste-Water Treatment Plant (WWTP) in Gdansk, was to apply ADE in simulation of flow conditions (based on tracer concentrations at selected points). The results obtained from the simulations were compared with those based on the traditional *tanks-in-series* approach, commonly used in designing biological reactors.

2. Mathematical models of dissolved matter migration

In general, transport of dissolved matter, defined as concentration, c_i, can be described as follows [3]:

$$\frac{\partial c_i}{\partial t} + (\boldsymbol{u}\nabla)c_i = \boldsymbol{D}_{Ti}\Delta c_i + \sum_{j=1}^{m} S_{ij}, \tag{1}$$

where:

c_i – inert tracer concentration (i – dissolved matter, M^1L^{-3}),
t – time (T^1),
$\boldsymbol{u}$ – the vector of velocity (L^1T^{-1}),
∇ – the nabla operator (L^{-1}),
$\boldsymbol{D}_{Ti}$ – the effective diffusion coefficient of substance i (L^2T^{-1}),
Δ – the Laplace operator (L^{-2}),
$\sum_{j=1}^{m} S_{ij}$ – the sum of m source terms ($M^1L^{-3}T^{-1}$).

2.1. One-dimensional model

The equation describing the transport of dissolved matter in an activated sludge reactor is a one-dimensional (1D) ADE:

$$\frac{\partial c_i}{\partial t} + \frac{1}{A}\cdot\frac{\partial(u\cdot A\cdot c_i)}{\partial x} = \frac{1}{A}\cdot\frac{\partial}{\partial x}\left(A\cdot D_{TL}\cdot\frac{\partial c_i}{\partial x}\right) + \sum_{j=1}^{m} S_{ij}, \tag{2}$$

where:

A – the reactor's cross-section area (L^2),
u – velocity along the reactor (L^1T^{-1}),
x – distance along the reactor's axis (L^1),
D_{TL} – the longitudinal dispersion coefficient (variable along the reactor, L^2T^{-1}).

If the sum of source terms $\sum_{i=1}^{m} S_{ii} = 0$, Equation (2) describes the transport of a tracer.

At the same time, the complete-mix and plug-flow model of reactors is the most commonly used in wastewater treatment [4]. In this model, the concentration, c_i, of a non-reactive tracer is distributed uniformly across the cross-sectional area of the control volume. The material balance of this approach for the differential volume element can be written as follows:

$$\frac{\partial c_i}{\partial t}\Delta V = Q\,c_i|_x - Q\,c_i|_{x+\Delta x}, \tag{3}$$

where:

ΔV – a differential volume element (L^3),
Q – the volumetric flow rate (L^3T^{-1}),
x – a point along the reactor's length (L^1),
Δx – differential distance (L^1).

By substituting the differential form for the $Q\,c_i|_x$ and $Q\,c_i|_{x+\Delta x}$ terms and substituting $A\Delta x$ for ΔV, we obtain Equation (3) in the following form:

$$\frac{\partial c_i}{\partial t} = -\frac{Q}{A}\frac{\Delta c_i}{\Delta x}. \tag{4}$$

Equation (4) describes the change of tracer concentration in a single tank about length Δx and volume ΔV. In practice, tanks are used in series (effluent of signal c_i

from the previous tank is the influent to the next tank). This model is known in the literature as the *tanks-in-series* or TIS model. The TIS model is characteristic for fully mixed flows with Poisson distribution.

3. Numerical methods

Equations (2) and (4) were solved using FVM. As finite volume methods are closely related to finite difference methods, FVM can be interpreted as a finite difference approximation to a differential equation. In one-dimension space, FVM is based on subdividing the domain into intervals (finite volumes, grid cells) and approximation to the integral of unknown function $c_i(x,t)$ over each of these volumes. The values of c_i (notated as C) are updated using approximations to the flux through cell edges (see Figure 1).

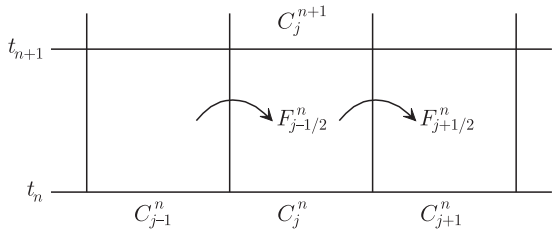

Figure 1. FVM for updating the cell average by fluxes at cell edges

In general, the value of C in FVM [2] can be computed as follows:

$$C_j^{n+1} = C_j^n - \frac{\Delta t}{\Delta x}\left[F_{j+1/2}^n - F_{j-1/2}^n\right], \tag{5}$$

where:

Δx, Δt – space and time steps,
n – the time level ($n+1 = t_{n+1} = t_n + \Delta t$),
$F_{j+1/2}^n$, $F_{j-1/2}^n$ – approximations to the average flux of the c_i value along $x = x_{j+1/2}$ and $x = x_{j-1/2}$:

$$F_{j-1/2}^n \approx \frac{1}{\Delta t}\int_{t_n}^{t_{n+1}} f\left(c_i(x_{j-1/2},t)\right) dt, \tag{6}$$

$$F_{j+1/2}^n \approx \frac{1}{\Delta t}\int_{t_n}^{t_{n+1}} f\left(c_i(x_{j+1/2},t)\right) dt. \tag{7}$$

We can consider the flux to depend on derivatives of the solution as $\frac{\partial c_i}{\partial x}$:

$$f\left(\frac{\partial c_i}{\partial x}, x\right) = -\beta(x)\frac{\partial c_i}{\partial x}, \tag{8}$$

where β – a proportional coefficient.

Given two cell averages, C_{j-1} and C_j, the flux at the cell interface between them can be defined as

$$F_{j-1/2}^n \approx -\frac{1}{\Delta t}\int_{t_n}^{t_{n+1}} \left[\beta_{j-1/2}\left(\frac{\partial c_i}{\partial x}\right)_{j-1/2}\right] dt. \tag{9}$$

Equation (9) is a macroscopic version of the first Fick law and β (referred to as the proportional coefficient above), measuring the dispersity between neighboring cells.

There are numerous ways in which Equation (3) can be implemented for fluxes (6), (7) and (9) in numerical practice. Equation (2) can be solved using the splitting technique algorithm, a method assuming splitting the problem into two simple, autonomous tasks. In practice, it is often the simplest and most efficient to use different methods for the advection and dispersion parts [2].

In this paper, the two-step Lax-Wendroff method (LWM2), Figure 2, is used for the hyperbolic problem, *i.e.* advection Equation (4) and advection part of Equation (2). One approach is to first approximate c_i at the midpoint in time and evaluate the flux at this point. The LWM2 is of this form with fluxes:

$$F^n_{j-1/2} = f\left(C^{n+1/2}_{j-1/2}\right), \tag{10}$$

$$F^n_{j+1/2} = f\left(C^{n+1/2}_{j+1/2}\right), \tag{11}$$

where:

n – the time level ($n+1/2 = t_{n+1/2} = t_n + 0.5\Delta t$),

$C^{n+1/2}_{j-1/2}$, $C^{n+1/2}_{j+1/2}$ – the value of c_i at the midpoint of a time step,

$$C^{n+1/2}_{j-1/2} = \frac{1}{2}\left(C^n_{j-1} + C^n_j\right) - \frac{\Delta t}{2\Delta x}\left[F^n_j - F^n_{j-1}\right], \tag{12}$$

$$C^{n+1/2}_{j+1/2} = \frac{1}{2}\left(C^n_j + C^n_{j+1}\right) - \frac{\Delta t}{2\Delta x}\left[F^n_{j+1} - F^n_j\right], \tag{13}$$

and, finally, the main LWM2 formula is as follows:

$$C^{n+1}_j = C^n_j - \frac{\Delta t}{\Delta x}\left[F^{n+1/2}_{j+1/2} - F^{n+1/2}_{j-1/2}\right]. \tag{14}$$

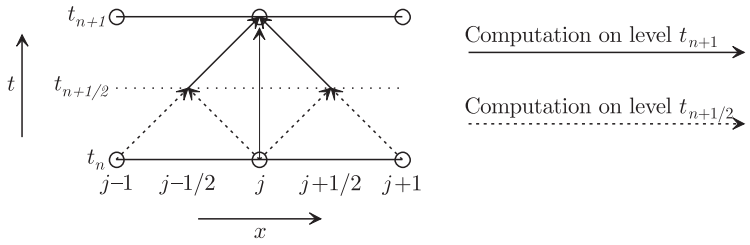

Figure 2. The two-step Lax-Wendroff method approach

This scheme enables achievement of second-order accuracy in approximation to integral (3) [2, 5]. Stability analysis leads to the Courant-Friedrichs-Lewy (CFL) necessary stability condition:

$$\nu \equiv \left|\frac{\bar{u}\Delta t}{\Delta x}\right| \leq 1, \tag{15}$$

where:

$\bar{u}$ – the average velocity,

ν – a ratio referred to as the Courant or CFL number.

As the second step of the splitting technique algorithm, the parabolic problem (dispersion equation) is solved using the implicit Crank-Nicholson Method (CNM). In this scheme, fluxes (9) will be as follows [5]:

$$F^n_{j-1/2} = -\frac{1}{2\Delta x}\left[\beta_{j-1/2}(C^n_j - C^n_{j-1}) + \beta_{j-1/2}(C^{n+1}_j - C^{n+1}_{j-1})\right], \tag{16}$$

$$F^n_{j+1/2} = -\frac{1}{2\Delta x}\left[\beta_{j+1/2}(C^n_{j+1} - C^n_j) + \beta_{j+1/2}(C^{n+1}_{j+1} - C^{n+1}_j)\right]. \tag{17}$$

Formulas (16) and (17) are natural approximations to the time-averaged flux (9) and make scheme second-order accurate and unconditionally stable [5].

4. Site measurements

Site measurements were carried out at the Gdansk Waste-Water Treatment Plant (WWTP). The bioreactors in the Gdansk WWTP work in the Modified University of Cape Town (MUCT) process configuration with an additional deoxic zone in the internal recirculation line from the aerobic zone to the anoxic zone (see Figure 3). The volume of a single bioreactor is 26 350 m^3, of which the aerobic zone occupies 11 700 m^3. During the measurements, the influent flow rate varied within the 1249–1580 m^3/h range, while the mixed liquor and returned activated sludge recirculations remained constant at 4694 m^3/h and 838 m^3/h, respectively. This data was used to determine the average velocity along the reactor chamber.

Tracer studies were carried out in the bioreactor aerobic zone at the Wschód WWTP using Rhodamine WT 20% (RWT) as a fluorescent tracer. The zone was designed as a plug flow reactor with the width of 8 m, height of 5.5 m and total length of 252 m. The dye samples were analyzed on-site with a Turner Designs Aquafluor handheld fluorometer. After background fluorescence analysis of mixed liquor samples, 1.0 dm^3 of the RWT was injected at the aeration zone's inlet. Mixed liquor samples ($V = 3$ cm^3) were taken for fluorescence measurements at three points located at the zone's inlet (sampling point SP_0, $x = 0$), in its middle (SP_1, $x = 130$ m) and at the outflow (SP_2, $x = 252$ m). Samples were withdrawn with frequencies of 5–20 min. The fluorometer was calibrated before each run of the fluorescence measurements.

During the tracer study, the dispersion coefficient, D_{TL}, was determined. The value of the dispersion coefficient was estimated using the statistical method of Fischer *et al.* [6] based on data series at two sampling points:

$$D_{TL} = \frac{\left(\frac{q}{A}\right)^2(\sigma_2^2 - \sigma_1^2)}{2\Delta T}, \tag{18}$$

where:

q – the flow rate (L^3T^{-1}),
A – cross-section area (L^2),
σ_i^2 – standard deviation of i series (T^2),
ΔT – time interval between series peaks (T^1).

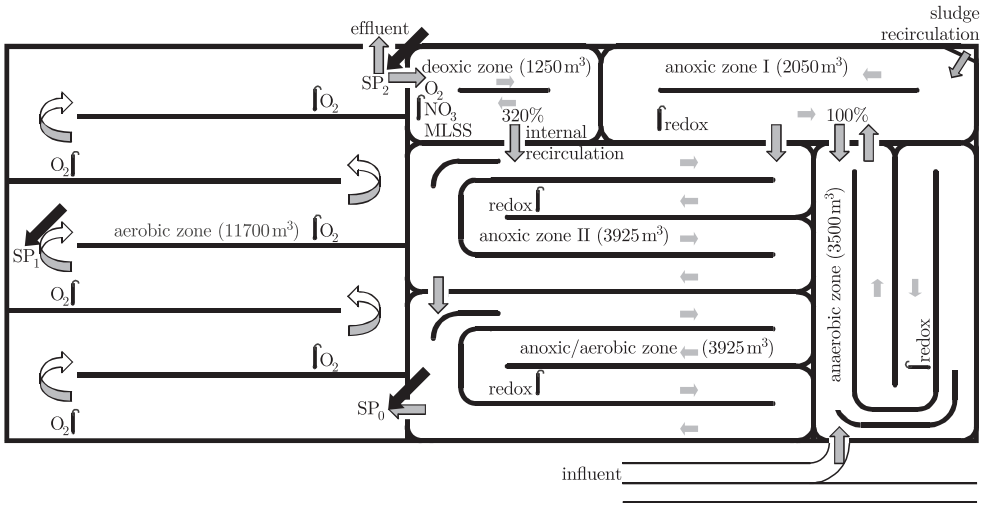

Figure 3. Layout of the aerated zone of the activated sludge bioreactor at the Wschód WWTP in Gdansk (black arrows indicate the sampling points, SP)

The standard deviation of i series is estimated from the following formula:

$$\sigma_i^2 = \frac{M_{2i}}{M_{0i}} - \mu_i^2 \quad (i = 1,2), \tag{19}$$

where μ_i – i series' mean value,

$$\mu_i = \frac{M_{1i}}{M_{0i}}, \tag{20}$$

where, in turn, M_{ji} – i series' moment distribution ($j = 0,\ 1,\ 2$):

$$M_{0i} = \int_{-\infty}^{\infty} c_i(x = \mathrm{SP}_i, t)dt, \tag{21}$$

$$M_{1i} = \int_{-\infty}^{\infty} t c_i(x = \mathrm{SP}_i, t)dt, \tag{22}$$

$$M_{2i} = \int_{-\infty}^{\infty} t^2 c_i(x = \mathrm{SP}_i, t)dt. \tag{23}$$

Using the tracer concentrations measured at the sampling points, marked as SP in Figure 3, values of the dispersion coefficient, D_{TL}, were calculated to be different in the different aerobic zones. Due to differences in mixing intensity between the aerobic zone's compartments, it was necessary to use different values of D_{TL} at the sampling points (compartments 1–3 and compartments 4–6):

- $D_{TL} = 0.47\,\mathrm{m}^2/\mathrm{s}$ in the first section (from $x = 0$ to $x = 130\,\mathrm{m}$) and
- $D_{TL} = 0.37\,\mathrm{m}^2/\mathrm{s}$ in the second section (from $x = 130\,\mathrm{m}$ to $x = 252\,\mathrm{m}$).

5. Numerical calculations and discussion of results

The mathematical model described by Equation (2) was used to simulate a tracer flow in the Gdansk WWTP's bioreactor. The flow parameters were steady and the advection part of Equation (2) assumed its standard hyperbolic form. In order to apply methods described in Section 3, the 1D domain x (the axis of symmetry of the

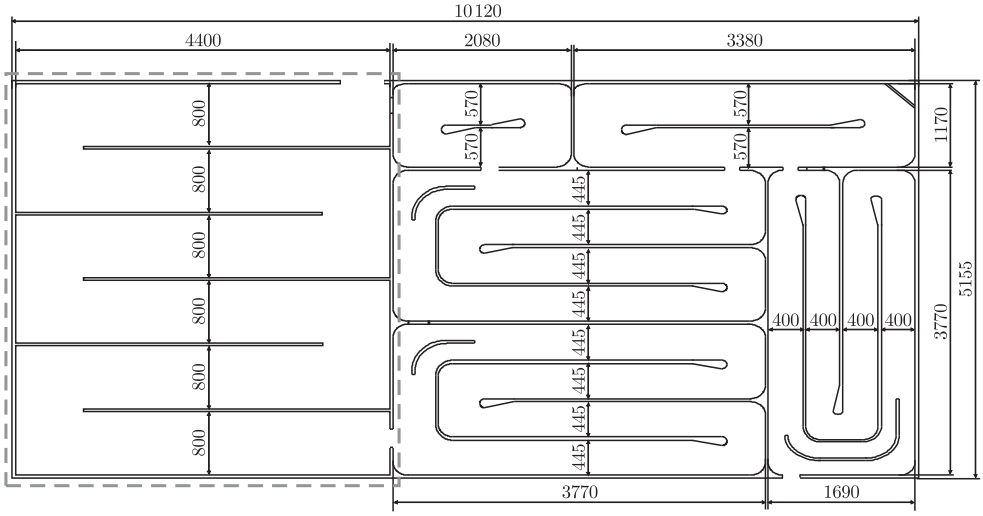

Figure 4. Dimensions of the activated sludge reactor located at the Wschód WWTP (in cm)

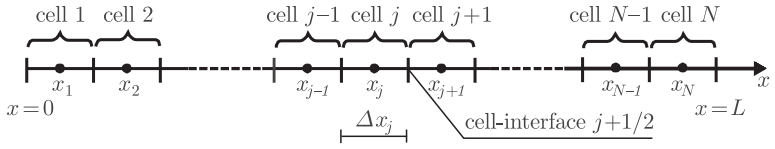

Figure 5. Discretization of the one-dimensional domain

bioreactor's compartments, see Figure 4) was discretized into a set of linear segments (cells). Each segment was defined by its edge points (cell interfaces, see Figure 5).

The domain's length ($L = 252\text{m}$) was divided into segments $\Delta x = 0.1\text{m}$. Equation (2) required initial and boundary conditions; the initial $c_i(x,t=0)=0$ condition and stability condition (15) were met during simulations and data from the SP_0 point was taken as the left boundary (Dirichlet-type) condition. The Neumann type of condition $\left(\frac{\partial c_i}{\partial x}=0\right)$ was used as the right boundary.

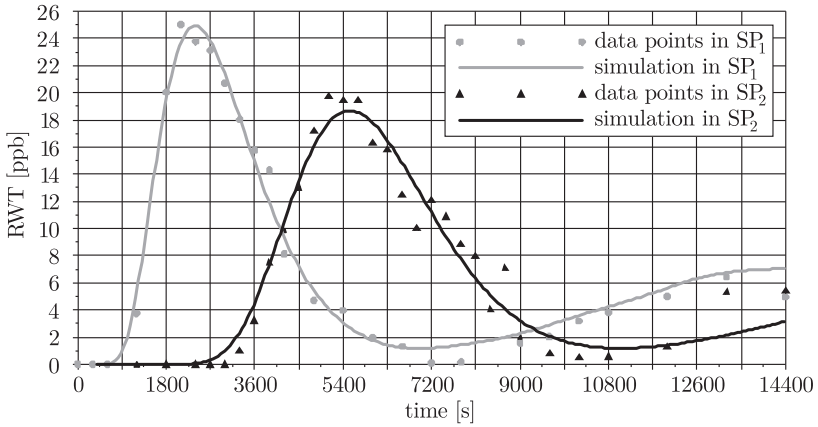

Figure 6. Measured vs. predicted concentrations of RWT in the aerobic zone of the activated sludge bioreactor during the tracer study at the Wschód WWTP

Figure 6 illustrates the simulation results obtained using 1D ADE without the source terms (Equation (2)). There is good correspondence between the numerical solution and the measurement data.

In the study next stage, the TIS model was used to numerically simulate tracer concentration profiles in the activated sludge system (Equation (4)). This model is the traditional approach, commonly used in designing biological reactors. The reactor's domain was partitioned into tanks: six tanks were applied in this approach, the number assumed on the basis of natural chamber construction. The results of those simulations, correlated with the ADE solution and the tracer concentrations at the sampling points, are shown in Figure 7. The hydraulic model (*tanks-in-series*) consisted of a series of six completely mixed reactors (without dispersion). In this case, the peak concentrations were predicted accurately but were shifted in time (10.5 and 22 min for SP_1 and SP_2, respectively).

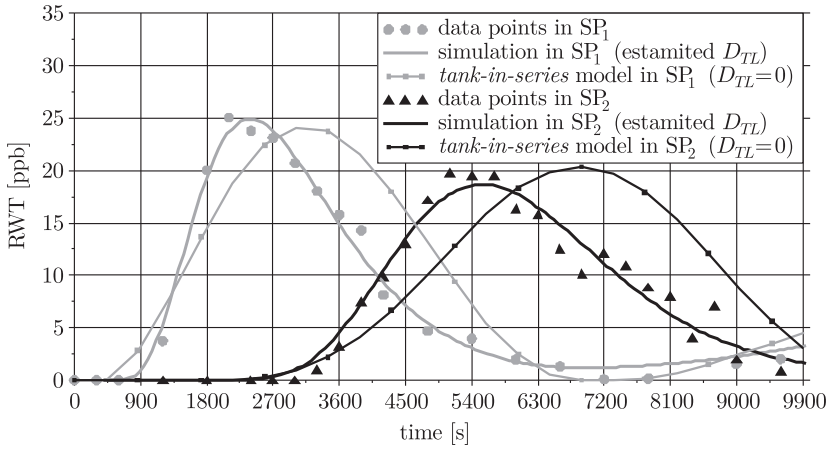

Figure 7. Concentrations of RWT in the aerobic zone of the activated sludge bioreactor during the tracer study at the Wschód WWTP: measured vs. predicted by two models

6. Summary and conclusions

The results of tracer studies carried out in the aerobic zone of the Wschód WWTP bioreactor enabled developing a complex Computational Fluid Dynamics (CFD) model (advection-dispersion) for predicting longitudinal profiles of non-reactive pollutant concentrations. The one-dimensional ADE without source terms was used, solved using FVM. The numerical solution of this model was split into two independent problems: the hyperbolic advection equation and the parabolic dispersion equation. The two-step Lax-Wendroff method was used for the hyperbolic problem, while the dispersion part was approximated using the implicit Crank-Nicholson scheme. The statistical method was used to estimate the values of the dispersion coefficient, D_{TL}, which were 0.47 and 0.37 m^2/s, respectively, in the bioreactor's two sections of different mixing intensities. The obtained numerical simulation results were compared with the traditional approach (the *tanks-in-series* model) and site data from the Gdansk WWTP bioreactors. The numerical simulations demonstrated meaningful

differences between the traditional and the presented methods of predicting non-active profile concentrations. The traditional *tanks-in-series* model was found to yield an inadequate description of dissolved matter's migration in reactors with intensive mixing. Better simulation results for such problems can be ensured using CFD equations.

The study of reactive substance in activated sludge bioreactors will be continued.

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