CFD-aided modelling for hydrodynamic analysis of biological reactor

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Abstract: The performance testing of treatment plants is of great concern in the field of environmental engineering, especially regarding the management of wastewater plants devoted to treatment and reuse. The efficiency of the treatment process is strictly related to both biological kinetics and hydrodynamics, influencing each other. In fact, the actual hydrodynamic behaviour of a biological reactor can deviate significantly from the design hypotheses, leading to hydraulic defects such as formation of dead volume and bypass. These problems exert a strong influence on the biological process and therefore affect the treatment efficiency of the plant. The Residence Time Distribution (RTD) analysis is commonly adopted for quantifying the type and amount of the functioning deficiencies affecting the process. However, to address the corrective intervention, these deficiencies should be localized by integrating RTD method with Computational Fluid Dynamics (CFD). This paper shows the early studies of a wider research project aiming at developing a standardized method combining RTD and CFD techniques for mitigating or eliminating functioning defects in biological reactors. An application of CFD-aided modelling for assessing hydrodynamic behaviour of an activated sludge (AS) pilot plant is illustrated. The obtained results are compared with experimental results from RTD analysis, showing how the CFD model can help supporting design of new facilities and the optimization or retrofitting of existing facilities for wastewater treatment.

Key words: finite volume modelling, RTD analysis, biological reactor, pilot plant, experimental verification, hydrodynamic analysis, functioning defects, dead volume

1. INTRODUCTION

Biological processes represent the central step in the urban wastewater treatment, as well as in the treatment process of several industrial wastewater. Their management has been significantly improved in the last century on the basis of both scientific and technical experiences thus meeting the specific requirements imposed by discharge permits (Hreiz et al., 2015).

Anyway the cost-effective management of these plants to match high treatment efficiency with suitable quality standard of the effluent is still an open challenge (Karpinska and Bridgeman, 2016).

As well known, the treatment efficiency is equally determined by biological kinetics and the hydrodynamic behaviour; thus similar treatment efficiencies can be obtained with reactors of quite different volume depending on their hydrodynamics and possible related defects (most frequently, bypass and dead volume).

The experimental verification of the hydrodynamic behaviour of a reaction tank can be carried out through the retention time distribution (RTD) analysis (Nauman, 2007); it derives from the well-established knowledge in the field of chemical engineering (Levenspiel, 1998) that has been successfully applied to pilot plants for biological nutrient removal with the aim of evaluating volume utilization through the identification of both short circuiting and dead volumes (Newell et al., 1998).

The experimental stimulus-response test can be carried out by injecting a tracer at the reactor's inflow and measuring over time its concentration at the outflow. The obtained experimental RTD curve can be interpolated through tank-in-series analytical models that mimic the reactor's hydrodynamic response by accounting for possible bypass and dead volume.

This diagnostic phase of the RTD analysis provides "global" information about the presence of possible hydrodynamic defects and their extent. In order to address proper remedial interventions, a
corrective phase is necessary in which the "local" flow conditions should be evaluated; such a goal can be achieved, for example, with the adoption of computational fluid dynamics (CFD) techniques (Le Moullec et al., 2010).

The numerical modelling allows evaluating, at each elementary volume inside the reactor, the local mean residence time of the occupying fluid particle, that is the average time to reach that volume since this particle entered the inlet's reactor. This calculation is of major concern in order to characterize the process (Baléo et al., 2000) and to detect possible hydrodynamic defects.

This work presents the early results of a wider study that integrates the RTD analysis with finite volume modelling applied to the AS reactor in a pilot plant for wastewater treatment with the aim of assessing and localize possible hydrodynamic defects. It is assumed that the pilot plant operates with a steady state flowrate.

In the following sections, the basic features of the numerical model of the reactor are illustrated. Subsequently, the relevant results are commented, concerning the spatial distribution of the mean residence time that helps to localize the hydrodynamic defects in the worse functioning condition. The numerical results are compared with the experimental results from the RTD analysis carried out in the pilot plant to assess the reliability of the finite volume modelling.

2. NUMERICAL MODELLING

The stationary hydrodynamic analysis of the biological reactor has been carried out with a finite volume commercial software (CD-adapco, STAR-CCM+).

To reduce computational effort, the symmetry of the tank has been taken into account; the simulated half geometry of the reactor is shown in Fig. 1. An upstream compartment is devoted to nitrogen removal, while the downstream compartment combines substrate oxidation and nitrification.

Since the study is focused on the hydrodynamics, the pilot plant operates with clear water; furthermore, all the diffusers at the bottom of the reactor are turned off because the organic matter is absent. These conditions allow simplifying the numerical model by carrying out single-phase stationary analysis of a Newtonian-fluid.

The inflow and outflow rate are equal to about $Q = 0.02$ L/s, while the total volume of the half reactor is roughly $V = 0.22$ m$^3$. Therefore, the average hydraulic retention time of the reactor is approximately $\bar{t} = V/Q = 3$ h.
The steady turbulent incompressible isothermal flow is obtained through numerical solution of RANS model that, in general, assumes the following form:

\[ \nabla \cdot \mathbf{v} = 0 \]

\[ \frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} = -\frac{1}{\rho} \nabla p + (\nu + \nu_t) \nabla^2 \mathbf{v} + \mathbf{g} \quad (1) \]

The symbols in Eq. (1) are: \( \mathbf{v} \) ensemble average velocity vector, \( \rho = 1000 \text{ kg/m}^3 \) fluid density, \( p \) pressure, \( \nu = 1.0-6 \text{ m}^2/\text{s} \) kinematic viscosity, \( \nu_t \) eddy viscosity, \( \mathbf{g} \) gravity acceleration.

The Eq. (1) is coupled with standard \( k-\varepsilon \) model to obtain closure of the mathematical problem.

The following balance differential equations of the specific turbulent kinetic energy \( k \) (TKE) and its specific dissipation rate \( \varepsilon \) are considered:

\[ \frac{\partial k}{\partial t} + v_j \frac{\partial k}{\partial x_j} = \frac{\partial}{\partial x_j} \left[ \left( \frac{\nu_T}{\sigma_k} + \nu \right) \frac{\partial k}{\partial x_j} \right] + \nu_T \left( \frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right) \frac{\partial v_j}{\partial x_i} - \varepsilon \quad (2) \]

\[ \frac{\partial \varepsilon}{\partial t} + v_j \frac{\partial \varepsilon}{\partial x_j} = \frac{\partial}{\partial x_j} \left[ \left( \frac{\nu_T}{\sigma_\varepsilon} + \nu \right) \frac{\partial \varepsilon}{\partial x_j} \right] + C_{1\varepsilon} \frac{\varepsilon}{k} v_i \left( \frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right) - C_{2\varepsilon} \frac{\varepsilon^2}{k} \]

The symbol \( v_i \) denotes the Cartesian components of the average velocity \( \mathbf{v} \) in the coordinate system \( x_i \) \( (i = 1, 2, 3) \); summation convention is assumed for repeated indices. The symbols \( C_{1\varepsilon} = 1.44, C_{2\varepsilon} = 1.9, \sigma = 1.3, \sigma_k = 1.0 \) in the transport Eq. (2) are empirical coefficients; the turbulent coefficient \( v_T \) is related to the empirical coefficient \( C_\mu = 0.09 \) by the following relation:

\[ v_T = C_\mu \frac{k^2}{\varepsilon} \quad (3) \]

Once the stationary flow field has been calculated through the solution of the balance Eq. (1) coupled with the turbulence quantity transport Eq. (2), the local mean residence time \( T_{res} \) of a fluid particle at any elementary volume within the reactor is evaluated by solving a transport equation for the passive scalar field \( \Theta \):

\[ \frac{\partial \Theta}{\partial t} + \mathbf{v} \cdot \nabla \Theta = \left( \frac{\mu}{\sigma} + \frac{\mu_T}{\sigma_T} \right) \nabla^2 \Theta \quad (4) \]

In Eq. (4) \( \sigma \) and \( \sigma_T \) are, respectively, the laminar and turbulent Schmidt numbers.

The three dimensional computational domain has been discretized by means of polyhedral meshes resulting in a total number of about 316000 elementary volumes.

The constant flow rate \( Q \) has been assigned at the inflow boundary, while constant pressure of 0.0 Pa is assumed at the outflow section (Fig. 1). The obtained solution is identical to the one that would be obtained by mirroring the mesh about the symmetry plane outside the computational domain. All the solid surfaces delimiting the tank are treated as impermeable wall boundaries.

### 3. RESULTS, DISCUSSION AND CONCLUSIONS

Two functioning conditions of interest have been investigated: \( a) \) only upstream impeller turned on, and \( b) \) upstream and downstream impellers turned off (no-mixing).

In both cases the numerical results confirm the experimental results obtained from RTD analysis of the pilot plant through pulse injection of non-reactive tracer at the inflow.
No bypass occurs in both operating conditions $a$) and $b$); this is due to the peculiar geometry of the reactor that avoids hydraulic short-circuiting. Therefore the inflowing fluid crosses the whole reactor's volume before reaching the outflow section (see also Fig. 3).

Concerning the operating condition $b$) with absence of mechanical mixing, the numerical model confirms the results of the RTD analysis that has detected an overall dead volume of about 5%.

This is visible in Fig. 2 where is plotted the cumulative distribution of the residence time as percentage of the reactor's volume (blue curve). The $y$-parallel dashed black line is traced at $T_{res} = 30$ h, that is ten times the average hydraulic retention time $\tilde{t}$, which can be assumed as a limit of the retention time to detect a dead volume (Collivignarelli et al., 1995).

The ordinate of the intersection point between the black line and blue curve is equal to about 0.95 meaning that approximately 5% of the total reactor's volume is characterized by a residence time that exceed 30 hours.

![Figure 2. Cumulative distribution of the residence time (no-mixing).](image1)

From Fig. 3 it can be seen that the major part of the detected dead volume is located in the upper left-hand portion of the downstream compartment: in this zone the calculated local mean residence time exceeds the above mentioned limit of 30 hours.

![Figure 3. Dead volume distribution with both impellers turned off (no-mixing).](image2)
The pale-blue area between the two green streamlines shows, in a qualitative manner, the average hydrodynamic path of the fluid inside the reactor and points out those zones outside the path where recirculating flow occurs. Among these zones, those ones located at the bottom left-hand corner of the upstream compartment and at the bottom right-hand corner of the downstream compartment are almost negligible.

In conclusion, CFD modelling proved to be effective for quantifying and localizing dead volume in the investigated reactor. This is also confirmed by the comparison with the RTD experimental analysis of the pilot plant.

Further studies will be carried out to evaluate the effects of possible remedial measures for reducing the amount of dead volume, such as changing the position of the outflow section or modifying the tank geometry near the outflow.

This numerical tool seems therefore reliable to support the design of new facilities and optimization or retrofitting of existing plants by helping to address proper corrective interventions for mitigating hydrodynamic defects.

REFERENCES