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# COMPUTATIONAL FLUID DYNAMICS IN WASTEWATER TREATMENT: REACTOR DESIGN AND INTENSIFICATION

Theses of the PhD dissertation

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# INTRODUCTION

Numerous wastewater treatment technologies have been established in order to reduce the pollution of the recipient. According to Kárpáti (2001), at first the wastewater treatment was a successful profession-oriented activity without any deep scientific background. Thanks to the development of the past two-three decades the scientific background have been strengthened remarkably, which allowed e.g. the efficient nutrient removal. Ideally, the new requirements for the treatment plants act as a drive of the further improvements and contribute the changing of the legislative background.

In order to observe the law, the current practice is usually based on empirical design using the average residence time, the surface load, the age of sludge, etc. The applied tank volumes are often overestimated and the hydraulic conditions are approximated with different reactor models (in good cases). The analysis of the flow pattern is not part of the planning. This approach usually leads to over-sizing of reactors, which is economically unsound. Recognizing this, more industrially developed countries are paying increased attention to the design and operation of their wastewater treatment plants (WTP) using mass transport-based models.

The current trends show the increase of the costs of energy (operation costs) and the threshold values for the effluent water quality get even stricter. The WTPs in the Central and Eastern European region hereafter have to face other problems (Somlyódy és Patziger, 2012) such as: (i) decreasing water consumption because of the infiltration in sewage system and the deficiency of rain water management resulting dilute or concentrated wastewater, (ii) under-loaded sedimentation tanks, which remove high amount of organic matter, causing inappropriate nitrification process, (iii) poor denitrification because of low C/N ratio, low age of sludge and bad design of anoxic reactor, (iv) poor phosphorous removal, because of the inappropriate coagulant dosing and deficiencies in mixing conditions, (v) under-loaded and poorly operated clarifiers, which have high influence on the effluent quality. Most of the problems occur due to the inadequate mass transport and fluid flow.

These problems called the attention to the fact that (i) the WTPs designed by traditional methods have extra capacity and (ii) it requires to improve the practice of planning taking into consideration the numerous specific problems. The latter one reflects the need of the correct description of reaction kinetics, optimization and intensification, which also requires fluid flow simulation. With CFD (Computational Fluid Dynamics) tools many above mentioned problems can be avoided. For example the inadequately operating volumes of the reactor characterized by high residence time and water age (these are the so-called dead-zones) can be eliminated, furthermore, the configuration of different reactors can be suggested. This novel approach in WTPs design could provide diversified applications. It means the utilization of the capacity, efficient intensification and reduction of the operational costs for the existing WTPs, smaller and more cost-effective reactors, and optimization of biodegradation process by taking into account the small scale flow phenomena for the new plants.

For large WTPs it may be particularly important to adapt the novel approaches in design, because the potential savings are higher than in small plants. The design process optimally has the following steps: (i) pre-experiment to determine the composition of the wastewater (ii) pilot experiments 1, (iii) planning 1, (iv) implementation partially, (v) full-scale and pilot measurements 2, (vi) planning including the investigation of the flow field 2 (vii) final implementation (here 1 and 2 refer to the order).

The Main Wastewater Treatment Plant of Vienna is an excellent example of the multi-step design process. Today, 680 000 $m^3$/day (dry weather flow) wastewater is treated (4 million of population equivalent) using nutrient removal. There are 15 clarifiers (designed with CFD tools), each has a diameter of 64 m, volume of 13500 $m^3$ (Kainz, 2008).

If we assume that the clarifiers are responsible for the 10-15 % of the investment costs and 20-30 % cost savings are achieved applying CFD, then 5-10 million euros are saved from the 220 million euros investment in such a way that the new clarifiers can be operated more effectively compared to the conventional construction. (Note that the conventionally designed Central Wastewater Treatment Plant of Budapest has an investment cost of 150 billion USD respectively.)

The frequently occurring opportunities for intensification are marked in Figure 1, which represents the overall wastewater treatment scheme.

1. Increasing the efficient volume of the reactors 2. Avoiding the washing out of suspended solids 3. Optimization of the inlet and outflow condition 4. Preventing the oxygen deficit or digestion 5. Achieving good simultaneous denitrification 6. Chemical phosphorous removal

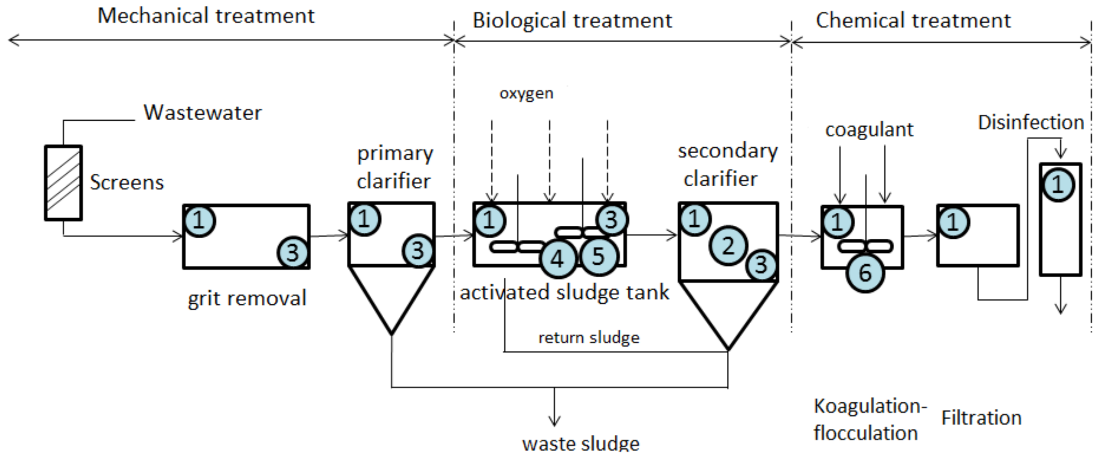


Figure 1: The overall scheme of the wastewater treatment

## AIMS OF THE RESEARCH

As it is mentioned in the introduction, the planning of modern WTPs or the intensification of technology requires the knowledge of the flow field. The efficiency of the reactors is determined by the hydraulic short-circuits, the volume of the dead-zones, the biochemical activity affected by the flow field and the opportunity for intensification of the processes, therefore these topics are investigated in my dissertation.

It is essential to **locate the dead-zones** within the reactors in order to be able to **terminate** them. The effects of temperature, discharge and density difference on dead-zones are investigated.

The effect of **mixing on coagulation-flocculation** technology of chemical phosphorous removal is analyzed by **coupling the hydrodynamics and mass transport model**.

Wastewater **sludge treatmen**t process was **upgraded** by introducing an **additional external force**. The aim was to establish a novel technology, which has an increased efficiency in settling-thickening of flock-size particles.

# SHORT SUMMARY OF RESEARCH RESULTS

## *Descriptive equations and solution*

The descriptive equations of hydrodynamics and mass transport were solved applying finite volume method, using different CFD software (Fluent 6.3, Ansys CFD, COMSOL). The results were verified by measurements and/or analytical approximations.

The local change of the concentration is determined by the convection, the diffusion and the reaction kinetics as follows:

$$\frac{\partial c}{\partial t} + \nabla(\underline{u} \cdot c) = \nabla D \nabla c + \lambda c, \text{ where}$$

c: concentration [g/m$^3$], $\underline{u}$: flow velocity [m/s], D: turbulent diffusion [m$^2$/s], λ: reaction kinetics [1/s].

Here, the molecular diffusion is replaced by turbulent diffusion, which is derived from the convection term and has higher order of magnitude. It can be calculated using turbulent viscosity ($\mu_t$), density of the fluid (ρ) and Schmidt number:

$$D = \frac{\mu_t}{\rho \cdot Sc}$$

The role of the different terms in the mass transport equation can be compared introducing dimensionless numbers; Peclet (Pe) number expresses the ratio of convection and diffusivity, Damköhler number (Da) is the ratio of reaction kinetics and convective transport. Both dimensionless numbers are derived from the numerical experiment of residence time distribution.

## *Hydrodynamic efficiency of reactors – detection of dead-zones*

Dead-zones in reactors or sedimentation tanks dissipate the energy of the flow, diminish the effective volumes and because of the high residence time these may cause poor effluent quality. Location of dead-zones can be estimated with CFD and then relying on the experience of the engineers, the poorly operating volumes can be reduced. The planning is based on the method of “empirical iteration”, namely, the solution alternatives greatly depend on the analyst’s skill and intuition.

In my dissertation I presented a novel method for detection of dead-zones and hydraulic short-cuts and I made recommendations to eliminate the problem. The procedure was tested for an activated sludge tank, Dorr sedimentation tank and swirl sedimentation trap using numerical tracer analysis (residence time distribution analysis, abbreviated as: RTD). A new quantity was introduced, the so-called “dead-zone ratio", with which the effect of various boundary and/or initial parameters (e.g. discharge, model geometry) on the hydrodynamic efficiency could be compared. The dead-zone ratio can be calculated as follows:

$$V_d / V = \max \left| F_{out} - \frac{1}{V} \sum_{i=1}^{N} F_i(t) \left| V_i \right| \right|$$, where

$V_d$: volume of the dead-zone, V: volume of the tank (i is the cell index), F(t): cumulative function of RTD curve (out: outflow section) N: number of the applied cells.

As a result of my calculation, I proved that the material properties of the sludge can be idealized, namely, the properties of the **applied fluid in the model can be approximated with the properties of the water.**

In the practice the permanent conditions are rare, therefore the investigation was completed with calculations of temperature, density, discharge differences between the reactor and inlet condition. For a 10 °C temperature difference between the inlet and inner fluid the average residence time was changed by nearly 10 %, but there was no significant effect on the dead-zones (the change in dead-zone ratio is smaller than 1 %). And nor the reduced or increased water discharge meant significant effect (dead-zone ratio decreases by 1-2 %). But it is remarkable that the dead-zone ratio reduced to one third if the outflow condition was modified.

*Improving the flocculation technology based on hydrodynamic calculations*

The orthokinetic flocculation depends on the fluid flow, which is generally taken to account by the so-called G-value, in other words, the average velocity gradient. Now, it is possible to determine not only an average value, but the distribution of G within the flocculator. In addition, the model requires the value of the residence time and the kinetic constant (Zhang és mtsai, 2004; van de Ven és Mason, 1977). **With the help of Da and Pe dimensionless numbers (Pe is calculated from RTD analysis) the conversion of orthokinetic flocculation described by Schmoluchovszky can be determined for different type of flocculators. The size of the flocks can be derived from the solution of the Schmoluchovszky equation and the separation of flocks can be calculated.**

Figure 2 shows a baffled flocculator, in which hydraulic short-circuits and large volume of dead-zones are presented. The theoretical residence time is 620 s, the water age at point 1 is 88 s, at point 2 it is 138 s, at point 3 it is 210 s, at point 4 it is 310 s, at point 5 it is around 8000 s and at the outflow section it is 380 s.

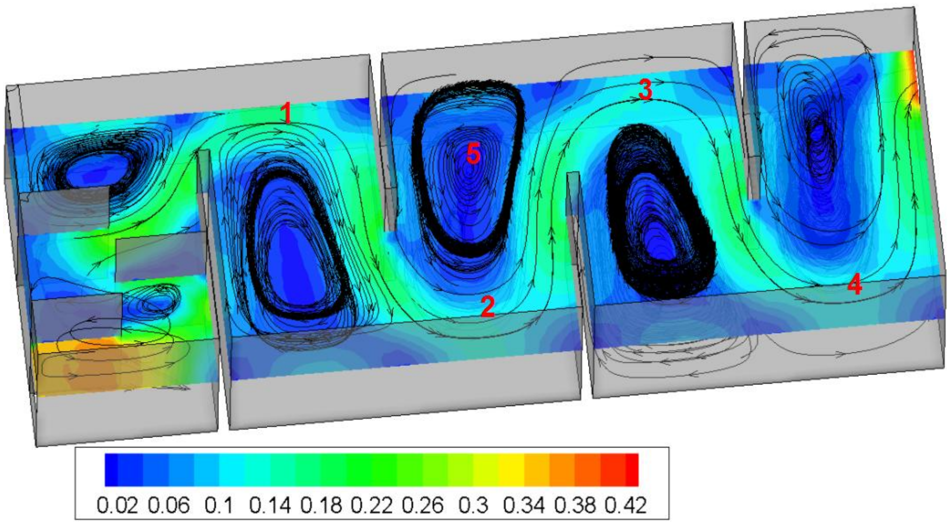


Figure 2: Contour of velocity magnitude [m/s], and some pathlines of water are highlighted. The numbers refer the points, where the water age is determined during the calculation

*Magnetic separation of floc-size particles*

Separation process is commonly used technique in wastewater treatment to retain the particulated matter. The efficiency of separation is mainly based on the density of particles (dry solid content) and the time required for the whole process. If an external field is introduced, which has an effect on the particles then the drive of the separation can be enhanced. The magnetic field is induced by permanent magnets and for the magnetization of the particles magnetic fluids (Fe(0)) or magnetite dispersion) were applied. The path of the particles during settling can be manipulated by the external field in order to achieve the maximum efficiency of separation.

We made the observations that the velocity of settling and thickening are increased so that 5-10 minutes were enough to achieve the same sludge blanket level with magnetic field as we achieve 30 minutes in the absence of the magnetic field. This has a consequence that the volume of reactors can be reduced, because then the detention time is enough at the same sludge load. The **achievable dry solid content nearly doubled using magnetic separation**, therefore the „traditional" thickening tanks may be eliminated from the technology.

Three main factors influence the separation; (i) sludge volume index, (ii) the amount of the magnetic fluid and (iii) magnetic field. Using two-factor analysis, the magnetic field proved to be the most sensitive parameter, but the magnetic fluid and magnet co-effect is also not negligible. The properties of the sludge have secondary importance on settling efficiency.

The aims of a numerical modeling were to investigate the magnetic separation, determine the main design parameters, reduce the measurements required and establish a novel model system for further applications.

The magnetostatic – CFD coupled model requires the summation of different forces acting on the particles. For this the strength of the magnetisability (in other word: susceptibility) and the magnetic field have to be known. The magnetic properties of the particles are calculated using Langevin function, where the slope of the linear part of the curve determines the magnetic susceptibility. This is the low-field limit of the function according to this formula (Rosenweig, 1997):

$$\chi_e = \frac{\pi}{18} \cdot \frac{\mu_0}{k \cdot T} \cdot \psi_v \cdot M_d^2 \cdot d^3 \text{, where}$$

$\chi_e$: susceptibility caused by external magnetic field [-], $\mu_0$: permeability of vacuum [H/m], k: Boltzmann constant [J/K], T: temperature [K], d: maximum diameter of magnetisable particles [m], $M_d$: dipole moment of the particle/magnetisation of the particle [A/m].

This susceptibility is modified by the so-called internal magnetisation, which is due to the fact that the magnetised particles also behave like small magnets and could modify the magnetic field. This effect is also built in the model.

The force acting on particles per unit volume can be determined by calculating the magnetic potential ($\underline{A}$) and the volume fraction of magnetic fluid, which is stirred to the sludge:

$$F_x = \frac{\chi}{\mu_0 \mu_r^2} \left( \frac{\partial A_z}{\partial x} \frac{\partial^2 A_z}{\partial x^2} + \frac{\partial A_z}{\partial y} \frac{\partial^2 A_z}{\partial x \partial y} \right) \cdot X_{ff}$$

$$F_y = \frac{\chi}{\mu_0 \mu_r^2} \left( \frac{\partial A_z}{\partial x} \frac{\partial^2 A_z}{\partial x \partial y} + \frac{\partial A_z}{\partial y} \frac{\partial^2 A_z}{\partial y^2} \right) \cdot X_{ff} \, .$$

Whereas the velocity field is given, the force balance for the particle (gravitational-, magnetic-, buoyancy- and drag force) is calculated and the flow of the particles can be determined. Equivalent diameter of the sludge particles is estimated (0.15-1.77 mm) by the literature (Hribersek et al, 2011), which is in a good agreement with the result of our laboratory measurement and estimated 0.23 mm for the average size of the flock-size particles. According to Hribersek et al (2011) the density of the sludge is 1070 kg/m$^3$, in which the solid core of the particles can be described with an average diameter of 2 μm and the density is in the range of 1400-1600 kg/m$^3$. On the basis of the experiments, in the free settling zone the settling velocity was in the range of 0,057 – 0,073 mm/s in the case of gravitational settling and this velocity range was 0.17- 0.24 mm/s using magnets. From this value the Reynolds number for settling is below than 0.4, therefore the settling is considered to be laminar.

The entire model concept schematic can be seen on the following Figure 3.

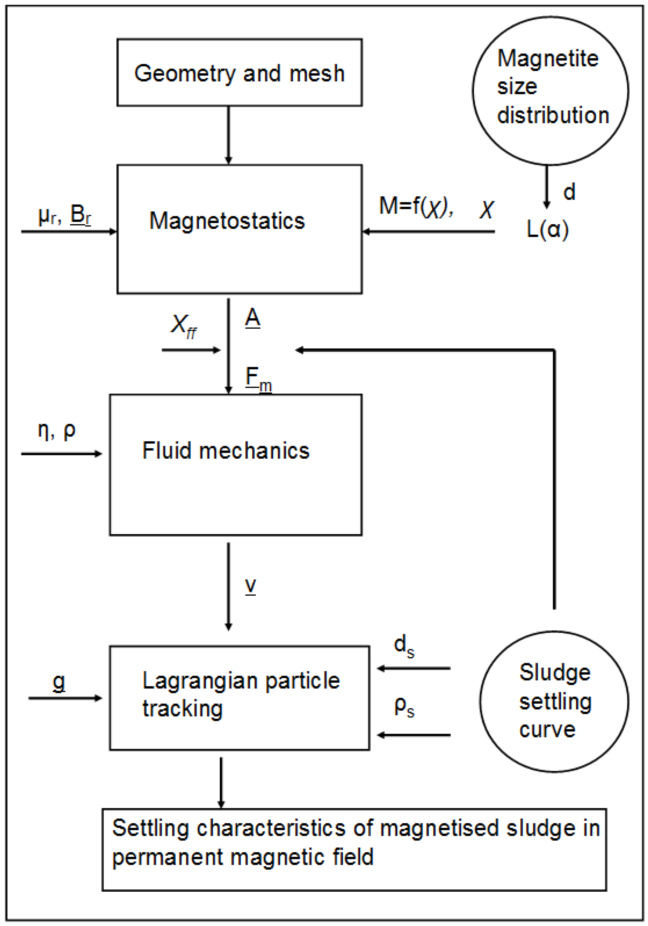


Figure 3: Magnetostatic – CFD coupled model. Symbols: d: diameter of the magnetasible particle, χ: magnetic susceptibility, $\underline{B}_r$: magnetic remanence, $\mu_r$: relative permeability, L: Langevin function, $\underline{M}$: magnetisation, $\underline{A}$: magnetic potential, $X_{ff}$: magnetic dispersion related to sludge volume, $\underline{F}_m$: magnetic force, v: velocity, g: gravitational acceleration, $d_s$: sludge particle diameter, $\rho_s$: density of sludge

As the model results revealed, the **character of the magnetic separation differs from the gravitational settling and thickening**. The former is characterized by high gradients of the external field force and the magnetic field properties have high importance on the separation efficiency. In the case of gravitational settling the properties of the flocks are relevant. This fact is also proved by laboratory measurements.

# THESES

## 1st Thesis

On the basis of the numerical residence time distribution (RTD) analysis it was demonstrated that the development of dead-zones in the tanks and reactors of wastewater treatment is determined by the geometrical conditions: the effect of temperature and discharge are secondary. A novel method was developed to determine the volume ratio of the dead-zones, which was derived from the RTD curve. It was verified that the properties of the applied fluid can be idealized, namely water can be used instead of wastewater. This method was applied and tested for various reactors such as stirred-, cascade-, plug flow reactor, activated sludge tank and sedimentation tank. [3,4,10]

## 2nd Thesis

It was shown that the Schmoluchovszky equation based particle collision probability, the Damköhler and Peclet number (calculated from RTD analysis) are necessary for the evaluation of the efficiency of the flocculators. With these parameters the grow of the flocks and the separation efficiency can be determined for different reactor construction. This method applies the residence time of the fluid and the velocity gradient. The latter can be estimated for all simulation points, therefore the effect of local small scale phenomena can be directly calculated. With the help of this method I suggested a modification on baffled reactors, with which the efficiency of flocculator could be improved. [1]

## 3rd Thesis

The settling and thickening characteristics of wastewater sludge can be improved by dosing magnetic fluid (zero valent nano iron or magnetite) and applying high-gradient magnetic field. It was demonstrated that the settling velocity and the achievable solid content increased by 2 - 3 times compared to “traditional” gravitational settling. However, the process requires only 50 – 150 g iron added per 1 $m^3$ sludge. The settling and thickening of sludge does not depend on the type of magnetic fluid (Fe(0) or magnetite), only the amount of dosed iron counts. [2,9,11]

## 4th Thesis

Magnetostatic – CFD coupled model was developed in order to analyze the settling of flock-size sludge particles. The model determines the settling trajectories of the particles based on the force balance, which is derived from the flow field modified by magnetic field. It was shown that the efficiency of the settling mainly depends on the magnetic behavior of the sludge. Despite the fact that the model is valid only for free settling zone, model alternatives can be compared. The results of the experiments and numerical simulations are in good agreement. [8,9]

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