Third International Conference on CFD in the Minerals and Process Industries
CSIRO, Melbourne, Australia
10-12 December 2003

DEVELOPMENT OF SIMPLIFIED FLOW MODELS FROM CFD SIMULATIONS

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ABSTRACT

Reaction complexity in biological nitrogen removal (BNR) bioreactors has delayed the use of CFD simulations in this important field. The objective of this project has been to develop a method that can use the results of a CFD simulation of an activated sludge process to yield an equivalent model constituting a network of ideal reactors. The resultant simplified flow model will suitably account for the hydrodynamic behaviour of the process. This enables easy incorporation of complex physical phenomena such as activated sludge reaction kinetics, and can then be used for dynamic simulation of the whole plant and its incorporation into a control system, or the analysis of a badly performing process.

A general methodology has been developed to determine the optimal flow model. The flow-field generated using a Fluent CFD simulation was used to predict the movement of neutrally buoyant particles. The particle tracks provide a characteristic transfer matrix between the different sections of an organised set of zones. The transfer matrix is then used to lump the zones into a network of ideal reactors with exchange flows between each of the adjoining reactors. The method is presented as a case study of a bioreactor presently operating in Brisbane, Australia, using simplified reaction kinetics.

NOMENCLATURE

$F(t_S)$	transfer matrix defined for the time step t_S
$F_{IN}(t_S)$	inlet flow distribution vector
m_0	amount of conservative variable entering the system during a time step length
N	system dimension
R	reaction term vector
S	system state vector
t_1	beginning time of a time step
t_2	end of time step
t_m	mean residence time distribution
t_s	time step

INTRODUCTION

The biological reactions utilised to remove pollutants from wastewater occur primarily within so-called biocatalyst particles. The biocatalysts are suspended and subsequently transported, along with soluble reactants, through the reactor vessels. The transport of particles and reactants, and the resulting pollutants removal rate are governed by the hydrodynamics, which is determined by the reactor design.

Computational Fluid Dynamics enables one to predict accurately the hydrodynamics of Wastewater Treatment Plants (WWTP). Therefore, to model the whole process of Biological Nitrogen Removal (BNR) from wastewater, and determine correct pollutant removal rates, biological reaction kinetics have to be coupled to reactor hydrodynamics.

Considering current numerical methods available, the computational demands required to include sophisticated biological kinetics in 3D CFD models are not easily achievable. This means that different methods have to be used to model the whole process within reasonable computational demands. In this way, a simplified flow model can significantly reduce the amount of computational time for incorporation of complex phenomena, such as activated sludge reaction kinetics, compared to the direct implementation into a three-dimensional CFD code.

In the present work, a systematic method has been developed that can use the results of a CFD simulation of an activated sludge process to yield an equivalent model constituting a network of ideal reactors with a pattern of exchange flows between elements of the network, commonly called a compartmental system. The intrinsic assumption made is that the reaction process does not affect the flow.

This equivalent model is required to properly account for the hydrodynamic behaviour of the modelled reactor. This enables easy incorporation of various complex phenomena, and can then be used for dynamic simulation of the whole plant, incorporation into a control system, or the analysis of a badly performing process.

The accuracy of the method is attributed to the model's ability to reproduce the hydrodynamic performance of the reactor and removal rate performance for a kinetics model.

This type of methodology has been applied successfully in the combustion field to different scales of furnaces from pilot plants and industrial burners. It has been used to predict NOx emissions in combustion systems. Then, by changing key parameters of the model, it has been used to estimate the effect of some NOx reducing

techniques. It is beneficial for design and optimisation of industrial combustion systems (Falcitelli *et al.* 2002a),(Falcitelli *et al.* 2002c),(Benedetto *et al.* 2000). A similar application can be expected from such a methodology for wastewater treatment. Indeed, the implementation should be easier, as the coupling between reaction and flow is likely to be present in the combustion systems.

METHOD DESCRIPTION

The method presented below uses the results of a CFD simulation of an activated sludge process to yield an equivalent model constituting a network of ideal reactors. The method used is significantly different from what has been performed in previous work in this field, where the equivalent model is imposed onto the CFD simulation. Previous implementations have used the CFD data directly to compute flow rates between those zones (Falcitelli *et al.* 2002b).

Our method first divides the system into a relatively large number of geometrical cells, regardless of the CFD data. The WWTP is assumed to be an organised set of zones with connexions between elements, inlets and outlets. This organised set of zones has to be defined with a pattern of transfer rates between the cells.

The CFD simulation is used to track neutrally buoyant flow-following particles, to compute particle paths. Exchanges between different cells are generated from these trajectories. Indeed, these trajectories provide information on the channel mixing especially because they have a component which accounts for turbulent fluctuations. An important feature of our method is that transfer matrices are used to calculate exchange flows, rather than erroneously using the boundary transfer rates directly.

The cells are then lumped according to an algorithm using transfer matrices, until a required simplified system is reached. At any stage of the lumping algorithm, each set of zones defined with a transfer matrix can be turned into a network of reactors with a pattern of exchanges flows that can be used for various computations.

The different steps of the method we have developed are given below:

Steady State Solution

The first step to be completed is to solve the hydrodynamics of the reactor under investigation, so as to get velocity and turbulent diffusivity fields, which will govern particles trajectories.

System decomposition

The system is decomposed manually in small geometrical zones, which allows one to define the number of cells constituting the original set. This number has to be high enough so as original zones can be homogeneous enough. The upper bound of the number of zones chosen is based on the need to be able to get a statistically large enough number of cell transfer events measured.

Discrete Phase Modelling

Once the flow field of the activated sludge process is solved, it is used to track possible fluid paths within the system. The fluid packets tracked are neutrally buoyant, inert, flow-following particles. Trajectories will account for local turbulence within the system and will be subject to its stochasticity. To obtain statistically significant averages for the exchange coefficients, a large number of trajectories have to be computed.

The particle paths generated are indicators of the mixing occurring in the reactor and will provide characteristic transfer information between the different sections of the set of zones.

Transfer matrices generation.

The mixing behaviour of the system is accounted for through the definition of transfer matrices which represent interaction between internal zones, and also the initial fate of input and source of output flows. The matrix values are determined from the particle path outputs.

Definition

A transfer matrix is defined according to a time step t_S and will describe the system evolution during the time step length, in terms of exchanges between cells.

F (t_S) is an N-by-N matrix where N is the number of cells of the system, which will be called the system dimension. The element F_{ij} (t_S) of this transfer matrix is defined as the fraction of particles which are in cell i at time t and are in cell j at the time $t_2 = t_1 + t_s$.

Figure 1 represents the state of a 4x4 system at times t_1 and t_2:

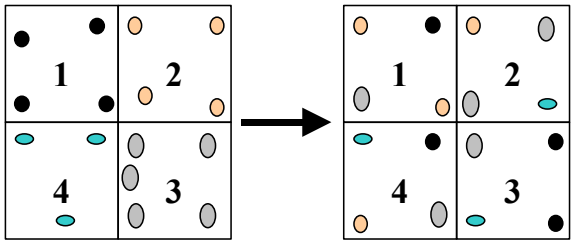

Figure 1: Evolution of a closed system during a time step length. The numbers refer to cell number.

The following transfer matrix describing the evolution between the two snapshots can be defined:

$$F(t_S) = \begin{bmatrix} 0.25 & 0 & 0.25 & 0.5 \\ 0.5 & 0.25 & 0 & 0.25 \\ 0.20 & 0.4 & 0.2 & 0.2 \\ 0 & 0.33 & 0.33 & 0.33 \end{bmatrix}$$

A transfer matrix expresses exchanges rates occurring between cells during a time step. Such matrices are generated looking along each particle path at particle positions for times t_1 and t_2, incrementing t_1 from the starting time to the final time.

Properties and Application of the transfer matrices

Properties of transfer matrices will be different when investigating closed or open systems. In general, the closed system properties are simpler.

When dealing with a closed system as the one represented above, $F(t_S)$ will have the property that the sum of the row elements is equal to 1, since none of the particles can leave the system. When the system is open, this property will not be satisfied, as particles can leave the system. Thus if the sum of a row is less than one, the difference expresses the fraction of particles that starts in a given cell and exits the system during t_S.

An open system requires as well the definition of inlet transfer vectors. These vectors are also defined according to a time step and describe the inlet flow contribution to the system evolution. When an amount of particles is released from the reactor inlet, $F_{IN}(t_S)$ is a vector of size N that represents the distribution of those particles in cells after the time step length. The sum of $F_{IN}(t_S)$ elements is equal to 1, unless some of the entering fluid exits before t_s

An important property of the transfer matrices is that the columns of $F_{ij}(t_s)$ need to sum to one (for a closed system). This is a statement that the fluid is incompressible and that a mass balance over each cell can be carried out. In general, given the stochastic simulation methods, this will *not* occur, as more particles will, due to random fluctuations, end up in some cells than others. (Figure 1 shows a simple example of this). It is necessary to apply a relaxation scheme to the initial transfer matrix to assure that this property is satisfied, as the iterative use of F to determine the fate of a tracer is dependent on the lack of arbitrary accumulation or loss.

Transfer matrices are used to simulate the mixing and hydrodynamic behaviour of a network of zones. Indeed, the fraction values have been calculated using the movement of particles elements, but they can be applied for every conservative variable.

If S_n is the vector defining the system state at the time t, so as S_n (i) represents the amount of a reacting component in cell i at time t, then the system state S_{n+1} after a time step length will be given by the following equation,

$$S_{n+1} = S_n * F(t_s) + F_{in}(t_s) * m_0 + R * S_n$$

In this equation, m_0 represents the total mass of the component entering the system during the time step length while R is the reaction rate. Thus, step-by-step computation can be performed on any system of cells.

Network generation from set of zones

A set of zones defined with transfer matrices can be turned into a network of ideal reactors. To generate a network, each zone is assumed to be a Completely Stirred Tank Reactor (CSTR), which is an ideal reactor assuming perfect. Flow rates between reactors are calculated by running a step-by-step computation on the full system of zones, applying an inlet pulse in concentration of a non-reacting tracer. The computation is run until the pulse is completely washed from the system. Exchange flows within the network are then computed by investigating exchanges of this variable between zones, which best-fit the observed concentrations in the zones.

Network simplification

The full zone network still represents considerable computational expense in its use for determination of reactor performance. The idea now is to use the full zone exchange information to generate a simplified network. Two general methods can be used, shown schematically in figure 2. These are simplification by the lumping of cells, and simplification by the reduction of the number of exchange flows. Only the first of these methods have been investigated in our study.

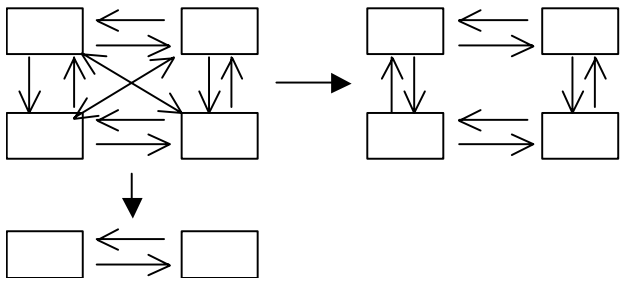

Figure 2: main ways of network simplification; (LHS): simplification by lumping cells; (RHS): simplification by reducing number of exchange flows

The system of zones originally defined is simplified by creating cell clusters. An algorithm has been created to perform the simplification, in which each step consists of lumping two connected cells into a single one. The whole simplification process is undertaken for a single value of t_s. The criterium chosen initially has been to identify the two adjoining cells which have the nearest concentration profile given an initial unit pulse input. This is not believed to be an optimal criterium, but appears reasonable. The method is iterative, with the new (N-1)

cell system used in the next simplification step, until, at the end, only one (stirred vessel) remains with N=1.

RESULTS

To demonstrate the method, the anoxic section of a bioreactor located at the Luggage Point Waste Water Treatment Facility, Brisbane, Australia, has been studied. In this part of the reactor, nitrate is biologically converted to nitrogen gas, through consumption of soluble carbon species. The configuration of the channel is shown in figure 3:

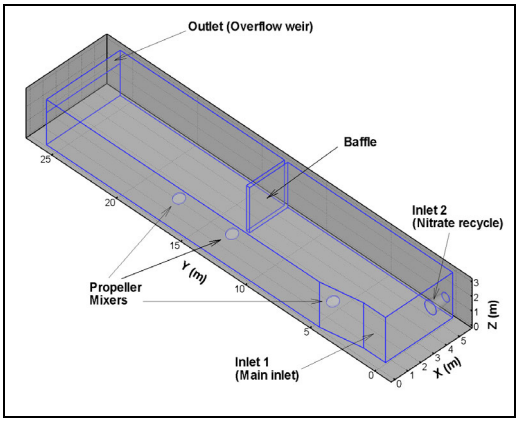

Figure 3: Anoxic channel configuration

This reactor is 25.7 m long, 5.7 m in width and 3.1 m deep. The channel is feed through two inlets, a main one for the wastewater stream and a smaller second one for nitrate recycling. The stream exits the reactor through a single outlet, constituted by an overflow weir. The flow rate through the bioreactor is 600 L/s and the volume is 447 m^3. Therefore, the mean residence time distribution of this system, t_m=745.3 s. It is mixed by three 1.5kW Flygtt propeller-like mixers, whose positions are shown in figure 3 (Brannock *et al.* 2002).

The CFD model of the system is composed of the hydrodynamic model along with the sludge and species. The sludge transport has a slip velocity in the vertical direction accounting for settling. The settling velocity of the sludge is a function of the local concentration. The mixers were modelled as sources of momentum in the axial direction only. In terms of boundary conditions measurements of the velocities and sludge concentration were made at the inlets and thus incorporated in a FLUENT CFD model. The free surface was modelled as a symmetry boundary.

Grid convergence was found at above 250,000 nodes. The simulation was solved transiently until the steady state is reached; this occurred at greater than 8 times the mean residence time. Further details of the simulation can be found in Brannock et al (2002). Figure 4 shows the flow simulated in the bioreactor.

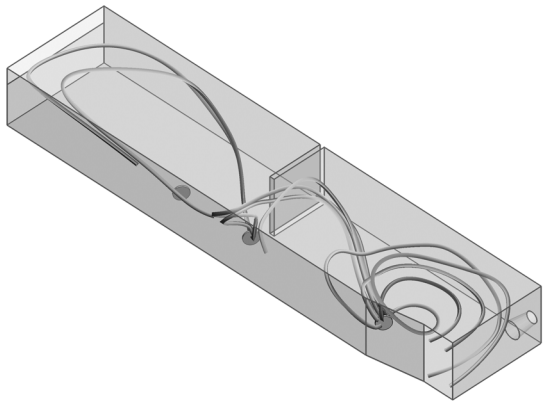

Figure 4: Flow-follower paths for four inlet particles (stochastic component removed)

Original set of zones

The choice has been made to work with an set of 512 zones, having 16 evenly spaced slices along the length, 8 along the width and 4 along the depth. To generate transfer matrices, 5270 trajectories have been computed.

From these trajectories, $F(t_s)$ can be calculated. The choice of the best value of t_s to use is crucial. If it is too small, then the inter-zone transport will be overestimated because mixing within each tank will not have time to take place, which is a key feature of the cells within the network. As t_s tends to zero the solution is the same as that calculated by measurement of the flux across cell boundaries, which is now clearly in error. If it is too large, then much of the interesting behaviour will not be noticed as either much of the fluid will have left the system and that inside the vessel will be well distributed. A value of t_s = 9 sec was found to be best for the generation of the transfer matrices. Figure 5 (in Appendix A) shows a comparison between the exit RTD predicted from the raw particle paths and that resulting from the network, using t_s = 9 sec.

Lumping influence

When decreasing the number of reactors constituting the network, a loss of accuracy in reproducing is expected. Figure 6 (in Appendix A) illustrates that simplifications modify slightly the exit RTD.

Looking at the influence of simplifications on the network RTD, it can be seen that a reduction in the number of cells tends to decrease residence time of fluid elements. Such a result was expected. When a concentration enters a CSTR, it is instantaneously evenly spread in the vessel, and there is no time lag before the first part exits it. Thus since when CSTRs are lumped the outlet becomes closer to the inlet, the influence on the performance is a global decrease of the initial exit time.

Kinetics implementation

The final step to be completed is the implementation of BNR kinetic models. Computations have been undertaken using numerical values from the European Co-operation in the field of Scientific and Technical Research (COST) simulation benchmark (COST 2002).

For this study the kinetics from the Activated Sludge Model Number 1. (ASM1) were simplified for CFD model to enable convergence (Henze 1987). The ASM1 has 13 components (state variables) and 8 processes. It has become a standard for mathematical modelling of biological wastewater treatment systems and is extensively used for design and operational applications (COST 2002). The main assumptions included no growth, decay or hydrolysis of biomass due to the low mean residence time and no autotrophic bacterial activity due to very low dissolved oxygen concentrations. This simplifies the full kinetics down to the following equations, which apply throughout the bioreactor:

$$S_{SS} = \underbrace{-\mu_H \frac{1}{Y_H}\left(\frac{X_{SS}}{K_{SS}+X_{SS}}\right)\left(\frac{X_{SN}}{K_{SN}+X_{SN}}\right)\eta_g X_{XH}}_{\substack{\text{Consumption of soluble substrate} \\ \text{due to heterotrophic biomass growth}}}$$

$$S_{SN} = \underbrace{-\mu_H \left(\frac{1-Y_H}{2.86 Y_H}\right)\left(\frac{X_{SS}}{K_{SS}+X_{SS}}\right)\left(\frac{X_{SN}}{K_{SN}+X_{SN}}\right)\eta_g X_{XH}}_{\substack{\text{Consumption of soluble nitrate} \\ \text{due to heterotrophic biomass growth}}}$$

S_{SS} and S_{SN} are the reactant source terms of soluble substrate and nitrate X_{SS} and X_{SN} are the concentrations of soluble substrate and nitrate; the others parameters are described by the COST simulation benchmark.

CFD simulations incorporating these kinetics have been completed and led to the following pollutant removal rates: 43.9% for S_{NO} and 95% for S_S. The kinetics have also been implemented into the networks, and the results in the table below show the removal rates for two simplified networks, the first containing 20 reactors and the second containing 100 reactors.

Table I: Pollutant removal rates for two simplified networks

	N=20	N=100
NO	44.14%	45.84%
Soluble Substrate	95.59%	97.91%

A good comparison is found between removal rates from CFD and network simulations. The proximity of results allows one to expect a good accuracy in results from implementation of complex phenomena.

CONCLUSIONS

A general methodology has been developed to generate an optimal flow model from 3D CFD simulations. The equivalent network of ideal reactors describes the reactor hydrodynamics. As expected, the accuracy of the simplification decreases with increasing simplifications. A balance has to be established between computational demand and result accuracy requirements. The incorporation of complex reaction phenomena is enabled and the whole process can be modelled rapidly in cases where reaction does not affect flow and diffusion behaviour.

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APPENDIX A: FIGURES

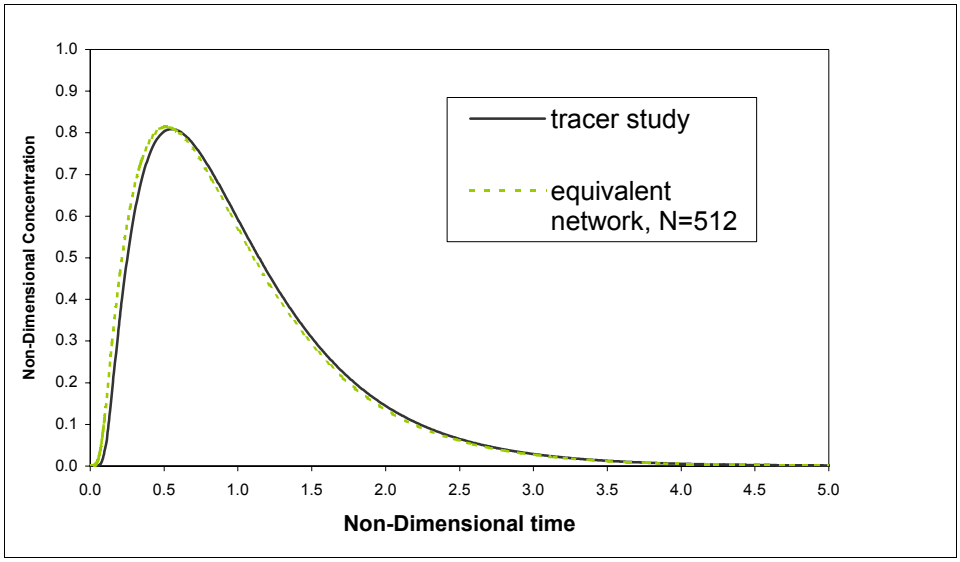

Figure 5: Comparison between the tracer study and the network generated from the first set of zones

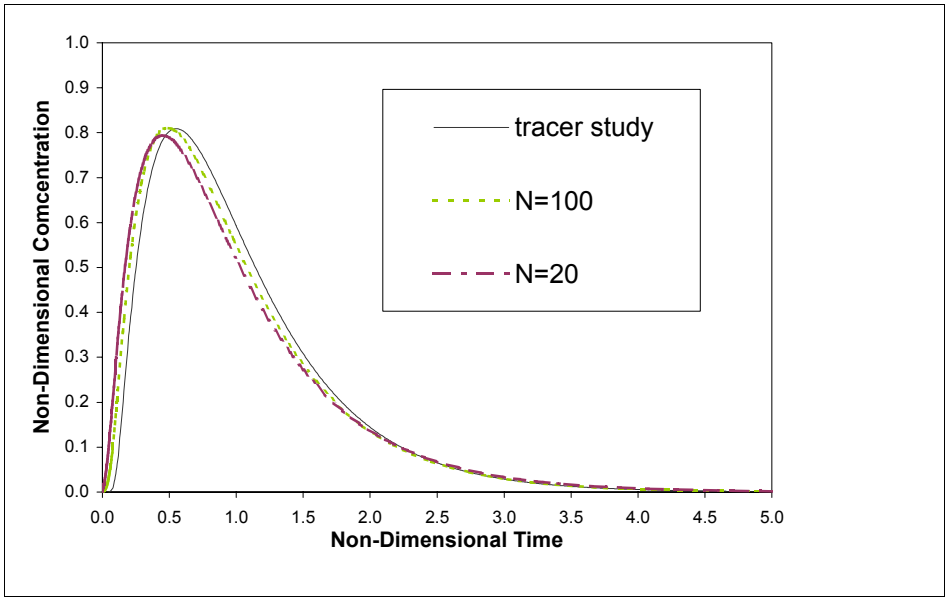

Figure 6: RTD comparison between tracer study and different lumping stages