Comparison of systemic, compartmental and CFD modelling approaches: Application to the simulation of a biological reactor of wastewater treatment

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ABSTRACT

Nowadays there exist two main approaches to simulate the hydrodynamics of chemical reactors: the systemic method, based on the description of a given reactor as a limited number of elementary reactors, and the more theoretical CFD approach, based on the resolution of the Navier–Stokes equations in a large number of computing cells. This work describes another recent modelling approach based on the description of the reactor as a network of both structural and functional compartments. The complete methodology to build such a model, using CFD simulations, tracer experiments, mass transfer and chemical processes, is described. The simulation results with such a model are then compared to those obtained with the systemic and CFD models in the case of a biological gas–liquid reactor for wastewater treatment, involving oxygen transfer and complex biological kinetics. This work shows that the compartmental model gives results very similar to those of a full CFD simulation but with lower calculation time (10 times in most cases) with the advantage of remaining almost as simple to manipulate as the systemic approach.

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1. Introduction

The modelling of complex reactors combining hydrodynamics, transfer and kinetics aspects, which are often coupled, is one of the major challenges in chemical engineering. The first step often consists in modelling the hydrodynamics and then to take into account transfer processes and chemical kinetics. Two most different methods have been used for several years to model the hydrodynamics of reactors. The first one often called "systemic modelling" has been developed by Levenspiel. It consists in describing the flow behaviour using a combination of properly interconnected elementary reactors (plug flow, perfect mixing reactor, dead volume, etc.). These models emphasize the functional aspects of the reactor and do not detail the localisation of those phenomena. The initial structure is often derived from tracer experiments interpretation from which a network of elementary reactors is deduced; then, transfer and kinetics processes can be introduced. It is a global approach that has been extensively used in the past to simulate chemical reactors. It gives quite rapidly and with moderate efforts a first approximation of the reactor behaviour. These models have a good robustness in the range of experimental and size conditions for which they have been developed. However, they remain unsatisfactory when numerous local

phenomena are involved and they have only limited predictability for extrapolation. For the last fifteen years, computational fluid dynamics (CFD) with chemical reaction has been more and more used to simulate the behaviour of chemical reactors. This is a structural approach which discretises the reactor using a computational grid. However, despite numerous developments and improvements, this approach still remains difficult to handle for reactors involving complex and coupled local hydrodynamics, heat and mass transfer and chemical reactions because of the high computational requirements.

Nowadays, another third approach, namely the compartmental model, is emerging (Rigopoulos and Jones 2003; Debangshu et al., 2006). It relies upon the description of the reactor by a structural and functional network of compartments derived from CFD investigations. Because, they studied a relatively homogeneous bubble column, Rigopoulos and Jones emphasized the importance of the connectivity between the network compartments more than the shape and the number of compartments. The reactor was divided into a limited number of main zones subdivided into several compartments based on their different behaviours or/and composition. Three heuristic rules were used in order to build this network: flow must not change direction along the boundaries; residence time must be constant for all the particles crossing a zone and each homogeneous concentration volume corresponds to a given compartment. Flowrates between the compartments were computed from CFD velocity fields, the mixing due to turbulence was modelled as an exchange flux. These turbulent flowrates were calculated in such a

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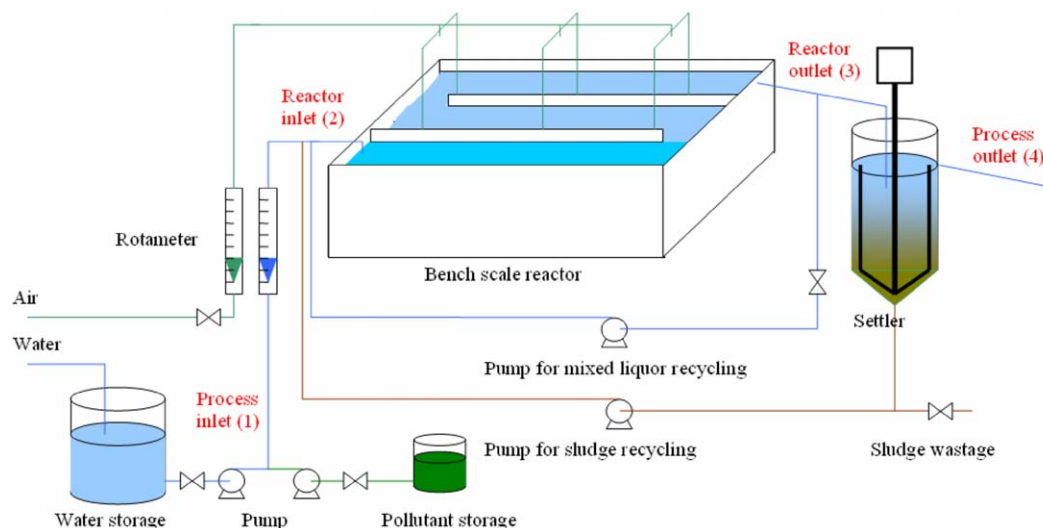
Fig. 1. Scheme of the experimental set-up.

way that the simulated numerical residence time distribution (RTD) matches the experimental one.

Debangshu et al. (2006) determined the volume and shape of compartments using the kinetics characteristic time: the time necessary for a fluid particle to cross a compartment must be less or equal than the characteristic time of the reaction. This condition, applied in three dimensions, gives the shape of each compartment. The compartment crossing times and the flowrates between each compartment are determined using the CFD velocity fields. Turbulence mixing is modelled as mass transport terms between each compartment. This methodology is difficult to carry out when kinetics is complex because it leads to characteristic times of different magnitudes which can be difficult to determine. Moreover, when the characteristic time of the reactions is small, this method generates a large number of compartments.

Networks of elementary reactors are more and more used to model wastewater treatment reactors based on process knowledge (Alex et al., 1999) or global information derived from CFD simulations (Alex et al., 2002). But the building of such models is not derived straightforwardly from the local information calculated from CFD simulations.

The present contribution details a methodology to produce compartment models and compares the three above-mentioned modelling methods (systemic, CFD and compartmental) for a biological reactor for wastewater treatment. This reactor is a gas–liquid reactor where hydrodynamics and mass transfer phenomena are coupled to complex biological reactions. Therefore this type of reactor allows testing the robustness of the three approaches.

2. Pilot reactor

The studied reactor is a pilot gas/liquid reactor with a very long length compared to its height and width (channel reactor). In this type of reactor, water flows mainly along the length and gas is injected at the bottom. Because the biological kinetics involved are well represented by Monod equations with apparent reaction orders greater than zero, the pollution removal efficiency depends on the hydrodynamics (Levin and Gealt 1993).

The total length of this bench scale reactor is 3.6 m with a rectangular section of width and height, respectively, equal to 0.18 and 0.2 m (Fig. 1). One side of the walls is fitted with stainless-steel tubes where 1 mm holes have been drilled every centimetre for air

sparging. The mixed liquor is partially recycled at the inlet. A settler of 0.88 m^3 is used to clarify the mixed liquor and to produce sludge which is also partially recycled at the reactor inlet. The mixed liquor and sludge recycling rates are, respectively, 4 and 1. These choices have been made to have a standard reactor behaviour and to ensure the presence of a significant amount of biomass in the reactor.

3. Kinetics model

The biological kinetics model chosen for this study is the ASM1 model (Henze et al., 2001). This model considers 12 different components and eight kinetic processes (ρ_i, $i = 1–8$). The biomass is composed of heterotrophic, autotrophic and inert biomass. Heterotrophic biomass grows with the consumption of soluble biodegradable pollution and oxygen (aerobic process) or nitrate (anoxic process). Autotrophic biomass grows with the consumption of ammonium and oxygen and produces nitrate. Both heterotrophic biomass and autotrophic biomass decay into inert biomass, particulate biodegradable pollution and particulate nitrogen pollution. Both particulate biodegradable pollution and particulate organic nitrogen are hydrolysed with the presence of heterotrophic biomass into, respectively, soluble biodegradable pollution and soluble organic nitrogen. Finally soluble organic nitrogen is transformed into ammonium by the action of heterotrophic biomass. The different components are briefly described in Table 1. The standard advised set of values is used for all stoichiometric and kinetics coefficients (Copp, 2001).

4. Hydrodynamics and mass transfer modelling

4.1. Systemic approach

The liquid hydrodynamics in this reactor is well modelled either by the plug flow reactor with axial dispersion model or by the equivalent perfect mixing reactors in series model (Le Moullec et al., 2008a). The number of perfect mixing reactors (or equivalently, the axial dispersion coefficient) depends on the gas flowrate and on the reactor geometry. It has been shown that a series of perfectly mixed reactors with backmixing presents the advantage to take into account the variation of the number of perfect mixing reactors with the flowrate by adjusting the backmixing rate (Potier et al., 2005). Eq. (1) gives the backmixing rate α needed to simulate a series of J_{app} perfectly mixed reactor without backmixing from J reactors

Table 1
Brief description of the components and structure of the ASMI model.

Notation	Description	Process(es) in which every component is involved
S_I	Soluble inert pollution	None
S_S	Soluble biodegradable pollution	Aerobic and anoxic growth (ρ_1 and ρ_2), hydrolysis (ρ_7)
X_I	Particulate inert pollution	None
X_S	Particulate biodegradable pollution	Decay (ρ_4 and ρ_5), hydrolysis (ρ_7)
$X_{B,H}$	Heterotrophic biomass	Aerobic and anoxic growth (ρ_1 and ρ_2), decay (ρ_4)
$X_{B,A}$	Autotrophic biomass	Aerobic growth (ρ_3), decay (ρ_5)
X_P	Inert biomass	Decay (ρ_4 and ρ_5)
S_O	Dissolved oxygen	Aerobic growth of $X_{B,H}$ and $X_{B,A}$ (ρ_1 and ρ_3)1
S_{NO}	Nitrate and nitrite	Anoxic growth of $X_{B,H}$ and aerobic growth of $X_{B,A}$ (ρ_2, ρ_3)
S_{NH}	Ammonium	Aerobic growth (ρ_3), ammonification (ρ_6)
S_{ND}	Soluble organic nitrogen	Ammonification (ρ_6), hydrolysis (ρ_8)
X_{ND}	Particulate organic nitrogen	Decay (ρ_4 and ρ_5), hydrolysis (ρ_8)

with a backmixing rate α:

$$J_{app} = \frac{J}{1 + 2\alpha - \dfrac{2\alpha(1+\alpha)}{J} + \dfrac{2\alpha^{1+J}(1+\alpha)^{1-J}}{J}} \qquad (1)$$

In practice, the coefficient J_{app} has been determined experimentally using experimental residence time distribution curves (RTD). Preliminary calculations have been performed to verify that the same results are achieved with a classical series of J_{app} reactors and with a series of J reactors with a backmixing rate α calculated according to Eq. (1).

The oxygen transfer is modelled with a volumetric gas–liquid mass transfer coefficient ($k_L a$) which has been determined experimentally using the following method (Le Bonté et al., 2005): a defined quantity of biomass is taken from the steady-state reactor and then introduced into a watertight perfectly mixed respirometer equipped with an oxygen probe. The evolution of the oxygen concentration in this respirometer allows the determination of the oxygen uptake rate which is equal to the oxygen transfer due to gas bubbling in the reactor.

4.2. CFD approach

The CFD study has been carried out with the FLUENT package. A drag coefficient suitable for bubbles, bubble induced turbulence source terms and a degassing boundary condition have been implemented by user-defined functions. The simulated liquid phase velocity fields and turbulence characteristics have been compared to laser Doppler velocimetry measurements and the gas fraction field has been compared to optical probe measurements, with a satisfying agreement (Le Moullec et al., 2008b).

The oxygen transfer is calculated using the Higbie's film penetration theory (Cockx et al., 2001; Fayolle et al., 2007) as follows:

$$k_L a = 2\sqrt{\frac{D_O |\mathbf{u}_g - \mathbf{u}_l|}{\pi d_g}} \frac{6\alpha_g}{d_g} \qquad (2)$$

where D_O is the molecular diffusivity of oxygen (1.97×10^{-9} m^2/s at 20 °C), d_g the bubble diameter, α_g the gas fraction and $\mathbf{u}_g$ and $\mathbf{u}_l$ are, respectively, the gas and liquid phase velocities. Each of the 12 components concentration involved in the kinetics process is simulated by a transport equation coupled with a source term for the biological reaction. This hydrodynamics/kinetics coupling is satisfactory because the smallest kinetics timescale is much larger than the hydrodynamics timescales.

4.3. Compartmental modelling approach

The compartmental modelling describes the reactor as a network of functional compartments spatially localized. It is based on the determination of volumes in which physico-chemical properties are homogeneous with a given tolerance. In our case, we based the choice of the pertinent properties, and the determination of the compartments, on both process knowledge and CFD results.

For the channel reactor, the flow is invariant along the length. Therefore, the reactor was split into slices of equal sizes along its length. Each slice is divided into different compartments. The number, the shape and the connectivity of these compartments are determined using a detailed analysis of three key parameters:

- The gas fraction, since the mass transfer between phases has a preponderant role, and the gas fraction is highly inhomogeneous across a slice of the reactor.
- The liquid velocity field in order to compute flowrates.
- Liquid turbulence characteristics (k and ε) because a previous study (Le Moullec et al., 2008b) has shown that the dispersion coefficient along the reactor is mainly dependent on them.

In practice, image analysis allows quantifying the homogeneity of physical variables and has been used to identify these compartments. The number of compartments is increasing with the decrease of the tolerance. In order to simplify the structure of the network, the very small compartments can be included straightforwardly into adjacent larger ones. By construction, the gradients of these variables along boundaries between compartments are very low.

This methodology led to the following structure for each slice (Fig. 2):

Zone 1: a large recirculation zone, containing only the liquid phase, with high velocity magnitude and high turbulent kinetics energy.

Zone 2: the centre of zone 1 which is, also, a liquid phase zone, but with low velocity magnitude and low turbulent kinetics energy.

Zone 3: the aeration zone, which is a gas–liquid zone, with high velocity magnitude and high turbulence.

Zone 4: two dead corners at the opposite side of the sparger device, with low velocity magnitude and low turbulent kinetics energy.

The flowrates between two adjacent compartments due to convective transport are computed from CFD simulations. Turbulent dispersion between two adjacent compartments is more difficult to quantify: we made an analogy similar to the one used in the systemic approach, i.e. the equivalence between the plug flow with axial dispersion model and the perfect mixing cells in series with backmixing model. With this analogy, since the compartments are considered by pairs, the apparent number of compartments is deduced from
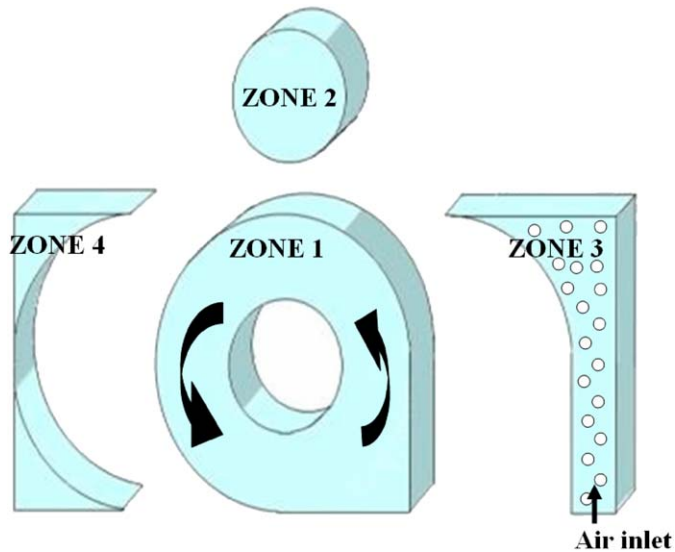
Fig. 2. Representation of the four compartments of a reactor slice.

Fig. 3. Structure of the compartment model.

Eq. (1) and is calculated as follows:

$$x = \frac{2(1 + \alpha_{i,j})}{1 + 2\alpha_{i,j}} \tag{3}$$

where $\alpha_{i,j}$ is the turbulent backflow rate between compartments i and j.

Moreover, the Peclet number which characterises the turbulent dispersion can be approximated by $2(x-1)$ (this is a strong approximation since x is lower than 10). This leads to

$$2(x - 1) = Pe = \frac{u_{t,i,j}\Delta L_{i,j}}{D_t} = \frac{u_{t,i,j}\Delta L_{i,j} Sc_t \varepsilon}{C_\mu k^2} = \frac{\alpha_{i,j} Q_{i,j}\Delta L_{i,j} Sc_t \varepsilon}{S_{i,j} C_\mu k^2} \tag{4}$$

where Pe is the Peclet number, D_t is turbulent dispersion coefficient, $u_{t,i,j}$ represents an equivalent fluid velocity between compartments i and j due to turbulence, $\Delta L_{i,j}$ is the distance between the centres of compartments i and j, Sc_t the Schmidt turbulent number ($= 0.7$), C_μ a constant of the $k-\varepsilon$ turbulence model ($= 0.09$), ε the turbulent dissipation rate, k the turbulent kinetic energy, $S_{i,j}$ the surface between compartments i and j, $Q_{i,j}$ the convective flowrate between compartments i and j and $\alpha_{i,j}$ the fraction of this flowrate due to turbulent mixing.

Finally, $\alpha_{i,j}$ can be deduced from Eqs. (3) and (4) using the following expression:

$$\alpha_{i,j} = \frac{\sqrt{A^2 + 8A}}{4A} - \frac{1}{4} \quad \text{where} \quad A = \frac{Q_{i,j}\Delta L_{i,j} Sc_t \varepsilon}{2S_{i,j} C_\mu k^2} \tag{5}$$

From these equations, we can find two extreme theoretical cases. Without turbulent mixing two adjacent compartments represent a series of two perfectly mixed reactors, and the flowrate is only the convective one derived from the CFD velocity field. For a very high turbulent mixing, the turbulent backflow rate is preponderant and the two adjacent compartments can be assimilated to one perfectly mixed reactor.

Once the structure of the slices has been determined, the number of slices is calculated by fitting the simulated RTD to the experimental one. CFD RTD results can also be used. An iterative procedure has been carried out: a number of slices is assumed, this allows to calculate the convective flowrates and turbulent backmixing rates between compartments. The process is repeated until the calculated RTD matches the experimental one.
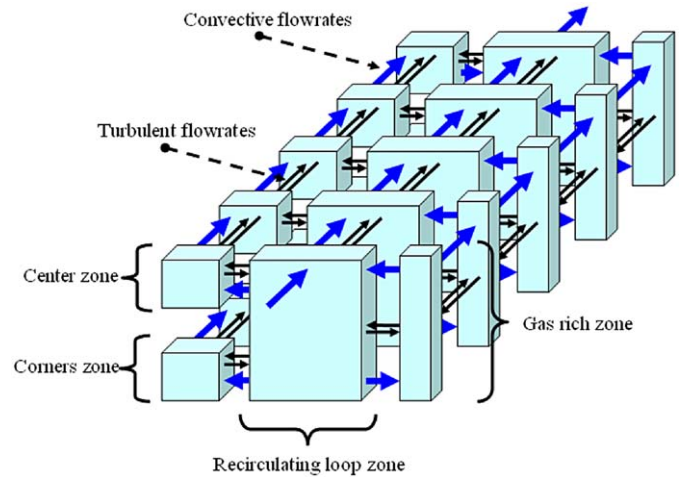
The final structure of the compartment model is presented in Fig. 3 (with a reduced slice number).

5. Comparison of the three modelling approaches

5.1. Modelling of the settler

The purpose of this work is to compare the three different modelling methods. In our case, the behaviour of the reactor is strongly linked to the behaviour of the settler. Therefore the modelling of the settler can impact the results for the reactor. In order to avoid any interference between these two parts of the process, the separation efficiency of the settler is considered identical for each model. Experiments allow an estimation of settler efficiency in steady-state which is close to 100% with a relative error of 1%. The efficiency of our experimental settler calculated using the IWA model (Copp, 2001) is 99.6% which corresponds to our experimental results within the experimental uncertainty range. Therefore the quality of separation of particulate compounds has been considered constant and equal to 99.6%.

5.2. Simulation results

In the present paper, the three modelling approaches have been compared in a theoretical case, without reference to experiments. These comparisons have been performed for theoretical conditions defined as follows: 2.5 h of retention time, with a gas flowrate of 35 L/min and the average standard effluent composition recommended by the ASM1 benchmark (Copp, 2001) (Si: 30 mg/L, Ss: 69.5 mg/L, Xi: 51.2 mg/L, Xs: 202.3 mg/L, Xbh: 28.2 mg/L, Snh: 31.6 mg/L, Snd: 6.9 mg/L and Xnd: 10.6 mg/L; all other concentrations have been taken equal to 0). The general tendencies of the three models can thus be compared in a situation with high concentration gradients along the reactor length: this allows focusing on the models comparison in a more discriminating case than realistic experimental conditions. The CFD results have been compared to experimental data in another paper (Le Moullec et al., 2009) where it has been shown that the agreement between experimental and simulated concentration profiles along the reactor is really acceptable for oxygen, nitrate and COD concentrations but CFD was not able to represent the profile of ammonium concentration: the differences between CFD simulations and experimental data were mainly due to the kinetics model and to the difficulty of estimate the sludge characteristics.
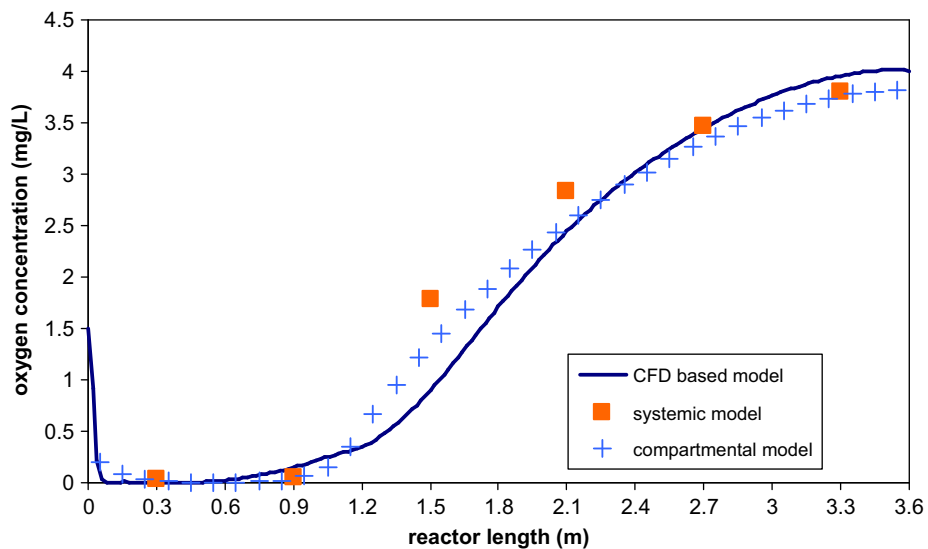
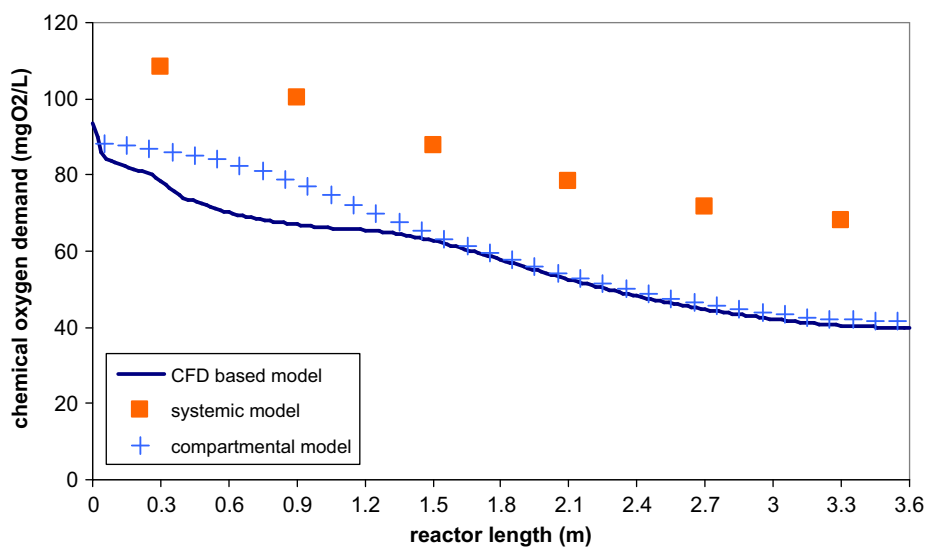**Fig. 4.** Comparison of the three models for the dissolved oxygen concentration.

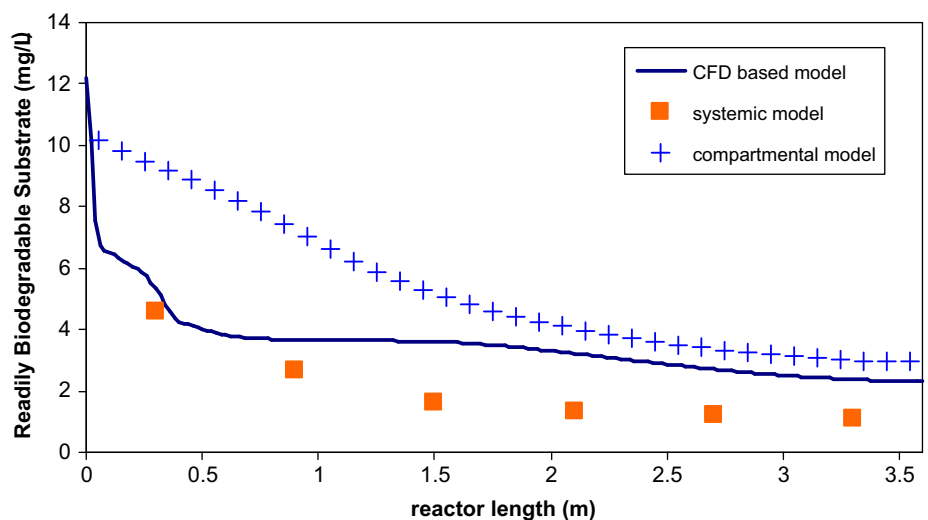**Fig. 5.** Comparison of the three models for the chemical oxygen demand.

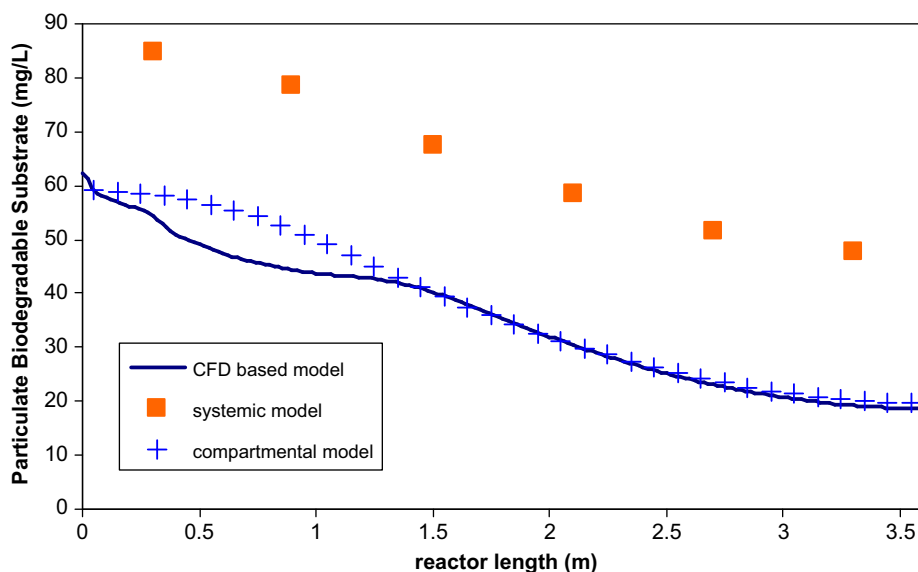**Fig. 6.** Comparison of the three models for the soluble biodegradable substrate.

Fig. 7. Comparison of the three models for the particulate biodegradable substrate.
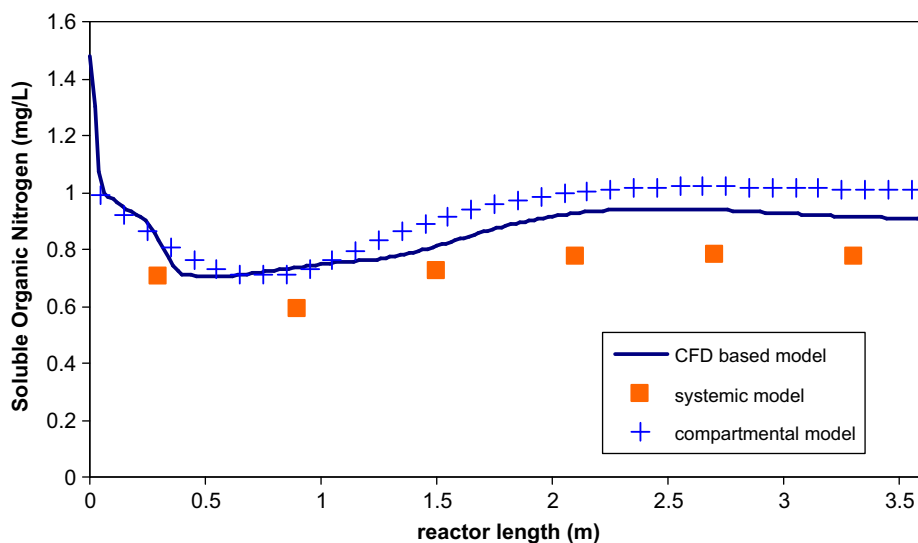

Fig. 8. Comparison of the three models for the soluble organic nitrogen.

In the present case, all three models follow the same main trends, especially with the soluble compounds: dissolved oxygen, soluble biodegradable substrate and soluble organic nitrogen (Figs. 4, 6 and 8). In the case of the slowly biodegradable compounds (particulate biodegradable substrate and particulate organic nitrogen), the systemic model presents a significant difference with the CFD based model (Figs. 7 and 9). This may be due to the calculated hydrolysis process which is affected by the inhomogeneity of the particulate compounds concentration on a section of the reactor. This inhomogeneity is accounted for in the CFD and compartmental models but not in the systemic approach. The fact that Figs. 6 and 8 present a smaller concentration for the systemic model than for the CFD model shows that the hydrolysis reaction must be slower than in the other two models. It can be highlighted that the compartmental model gives results very similar to those of CFD. The discrepancy observed in Fig. 6 between the CFD and compartment modelling is probably due to the incomplete mixing accounted for in the CFD results due to the more realistic admission of effluent (in the compartmental model, the effluent mixing takes place in the first slice). In fact, the degradation of soluble substrates kinetics is very fast and the concentrations of the reactants are locally higher in the CFD simulation than in the compartment model, which leads to a rapid decrease of S_S. On the contrary, in the compartment model, the reactant concentration is lower because diluted in the first slices and the decrease is more progressive along the slices. The differences between CFD and compartment simulations are still present but much lower in Figs. 7 and 9 because the involved kinetics are very slow. The DCO, defined as the sums of S_i, S_S, S_{nd}, X_S, X_i and X_{nd} presents the same behaviour as particulate compounds (Fig. 5).

6. Discussion

Complete comparison between these three complex approaches is not straightforward. It should take into account complexity, quantity and quality of the obtained information, level of detail required, possible experimental validations, calculation time, etc. In order to
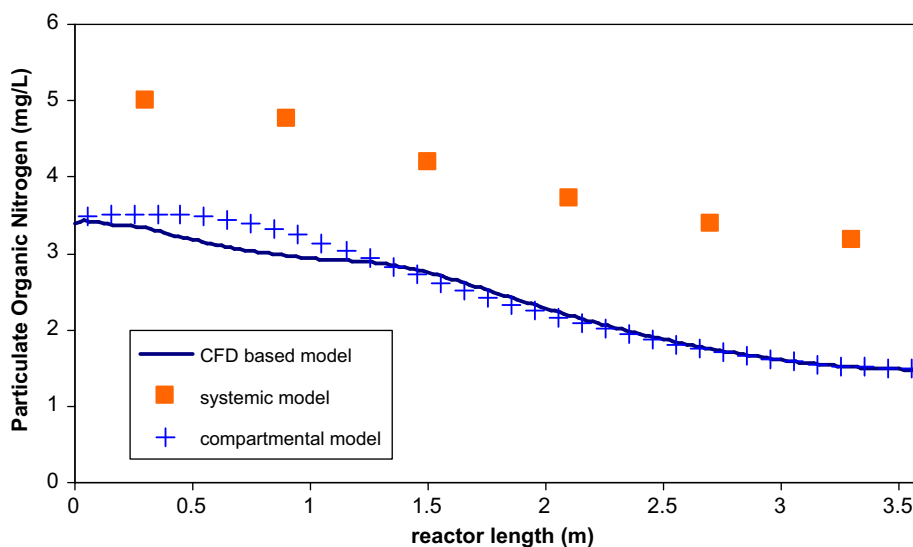
Fig. 9. Comparison of the three models for the particulate organic nitrogen.

compare the different approaches, a series of criteria, divided into four main groups, has been taken into account:

1. Preparation time which accounts for the work needed to obtain the usable model, such as:
   - Programming: the efforts needed to produce a simulation program or to learn how to use such a program (Fluent for example).
   - Process knowledge: this represent the level of knowledge required to develop the model.
   - Experimental study: this represents the amount of experiments needed to evaluate the model parameters (kinetics parameters for example).
2. Scientific value of the model:
   - Predictability: Is this model usable in a large operating zone?
   - Simplicity: Is this model easy to understand and manipulate?
   - Scientific accuracy: Is this model based on scientific theory or empirical observation? Are numerous concessions necessary in order to make this model computable?
3. Computing time: The calculation time needed to obtain results.
4. Comparison with experiments:
   - Precision: The accuracy compared to experimental values.
   - Robustness: Is the model very sensitive to parameters? Could it easily lead to discrepancies?
   - Pertinence: Gives access to the same kind of information as experience, with an equivalent precision.

The interest of the systemic approach relies in its simplicity and easy experimental access, but its main drawback is its lack of predictability: for example, the k_La and the axial dispersion coefficient values have to be measured experimentally for each gas flowrate. The program is quite simple, coded in FORTRAN, and uses the DDASSL subroutine for the numerical integration. The calculation is instantaneous for a steady state simulation and takes a few minutes for a hundred days of transient simulation. The model parameters can be easily fitted to the experimental measurements and therefore a very good precision can be achieved with this model, when calibrated; it is therefore particularly adapted to industrial applications (process control, debottlenecking, etc.).

CFD is predictable, as far as the employed models have been validated at a given scale but, with complex kinetics and physical

phenomena as those encountered in biological water treatment, it remains a time-consuming approach, especially because of the different time scales involved in the ASM1 model. This approach also requires fine models and detailed knowledge of physical parameters. For instance, in our work, oxygen transfer and bubble size have not been sufficiently studied and the k_La value estimated with Eq. (2) is 30% larger than the measured one (Le Moullec et al., 2009), therefore a value based on experimentation has been used. A complete hydrodynamics steady-state simulation takes 3 h, the RTD validation takes another 3 h and the steady-state complete kinetics calculation takes approximately four days (Intel Xeon, 3.5 GHz bi-processor, 4 Go RAM). CFD simulations give lots of information, but a great amount of this information is not used, and therefore the calculation time is not completely effective. Finally, CFD models are very complex with numerous parameters and choices. This can lead to high discrepancy with reality if not enough precaution is taken as experimental validation for example.

The compartmental model is programmed in the same way as the systemic approach but its hydrodynamics parameters are taken from a steady-state CFD hydrodynamics calculation. Compared to the CFD model, only pertinent values are calculated and it gives the same useful results as the CFD based model. Moreover, this model describes the main behaviour of the reactor in a more intuitive way than the CFD.

Table 2 summarizes the differences between the three models with respect to the criteria previously discussed, except the experimental comparison criterion.

7. Conclusion and perspectives

In this paper the whole development of a compartment model has been established. It consists in a structural and functional model based on CFD hydrodynamics calculation. This development has been applied to a channel reactor used in wastewater treatment. This reactor is a gas–liquid reactor with oxygen transfer and complex kinetics. It is therefore particularly suited to compare a compartmental model to a systemic model and a CFD model.

This work has shown that CFD remains a useful tool for the hydrodynamics design of a new wastewater treatment reactor, but seems rather limited by its calculation time when kinetics models are coupled to the hydrodynamics solution. Systemic modelling allows a

Table 2
Summary of the models comparison.

	Systemic model	Compartmental model	CFD based model
Preparation	Good process knowledge. Only a few experiments is needed. Fast programming	Combine systemic and CFD based models needs but without the experimental part	Very complex programming but limited process knowledge or experiments needed
Scientific approach	Simple, based on empirical observations and not predictable	Quite simple, based on CFD hydrodynamics calculations and a few empirical observations. Possibly predictable	Very complex, based only on transport equations and possibly predictable
Run time			
Steady-state	Less than 1 s	Less than 1 min	4 days
Transient simulation of a 100 day run	A few minutes	Approximately 1 h	Not realized

fast simulation of the kinetics behaviour of the reactor and therefore is adapted to applications such as process optimization and control.

It has also been shown that the same useful information and the same predictability as CFD can be obtained with the compartmental model. This modelling method consists in a CFD study limited to the hydrodynamics, followed by the development of a simplified model used to solve the kinetics model. When limited to hydrodynamics, the CFD calculation time is ten times shorter as for a complete CFD study including kinetics and mass transfer. Then the calculation of the compartmental model is instantaneous compared to a CFD one. Experiments have been carried out in the bench scale reactor and the model predictability will be evaluated in a future paper. It can be noticed that the methodology developed in this work is applicable only if the kinetics does not influence the hydrodynamics, this condition is almost always verified in liquid phase reactors. Moreover the compartmental methodology will be tested on other reactors.

Notation

C_μ	constant of the $k-\varepsilon$ turbulence model
d_g	bubble diameter, m
D	dispersion coefficient, m^2/s
D_O	molecular diffusivity of oxygen in water at $20\,°C$, m^2/s
J	number of perfectly mixed reactor (PMR) in a series of PMR
k	turbulent kinetics energy, m^2/s^2
k_{La}	volumetric mass transfer coefficient, s^{-1}
L	length, m
Pe	peclet number, dimensionless
Q	flowrate, m^3/s
S	surface, m^2
Sc	schmidt number, dimensionless
$\mathbf{u}_g, \mathbf{u}_l$	respectively gas phase velocity and liquid phase velocity vectors, m/s

Greek letters

α	backmixing rate in a series of PMR with backmixing, adimensional
α_g	gas fraction, adimensional
ε	turbulent dissipation rate, m^2/s^3

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