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Biological Nutrient Removal Model N° 2 (BNRM2): A general model for Wastewater Treatment Plants

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Abstract

This paper presents the plant-wide model Biological Nutrient Removal Model N° 2 (BNRM2). Since nitrite was not considered in the BNRM1, and this previous model also failed to accurately simulate the anaerobic digestion because precipitation processes were not considered, an extension of BNRM1 has been developed. This extension comprises all the components and processes required to simulate nitrogen removal via nitrite and the formation of the solids most likely to precipitate in anaerobic digesters. The solids considered in BNRM2 are: struvite, amorphous calcium phosphate, hydroxiapatite, newberite, vivianite, strengite, variscite, and calcium carbonate. With regard to nitrogen removal via nitrite, apart from nitrite oxidising bacteria two groups of ammonium oxidising organisms (AOO) have been considered since different sets of kinetic parameters have been reported for the AOO present in activated sludge systems and SHARON reactors. Due to the new processes considered, BNRM2 allows an accurate prediction of WWTPs performance in wider environmental and operating conditions.

Keywords

Activated sludge models; BNRM1; Nitrite; Plant-wide mathematical modelling; Precipitation

INTRODUCTION

Whole wastewater treatment plant modelling is one of the most important topics for the scientific community. This issue has been tackled by two philosophical approaches: using separated models (which were developed for the different process units) that are connected to simulate the whole plant, or using one unique and general model for the whole plant. In 2004, the CALAGUA research group published the Biological Nutrient Removal Model N° 1 (BNRM1, Seco *et al.*, 2004) including different physical, chemical and biological processes taking place in a WWTP. The physical processes included were: settling and clarification processes (flocculated settling, hindered settling and thickening), volatile fatty acids elutriation and gas-liquid transfer. The chemical interactions considered were acid-base processes, where equilibrium conditions are assumed. The biological processes included were: organic matter, nitrogen and phosphorus removal; acidogenesis, acetogenesis and methanogenesis. This model has been successfully applied for the design and optimization of numerous WWTPs (Ruano *et al.*, 2010). However, these applications showed that nitrogen removal via nitrite and chemical precipitation processes should be considered to properly simulate WWTPs.

Nitrogen removal via nitrite was initially applied in side stream processes (Hellings *et al.*, 1998). Savings in aeration costs of 25% are reached in comparison with conventional nitrification to nitrate. Moreover, subsequent denitrification consumes 40% less carbon source (Hellings *et al.*, 1998). Nitrogen removal via nitrite can be carried out in activated sludge reactors operated at short sludge retention time (SRT) and low dissolved oxygen (DO) concentrations. This process is particularly important in those WWTPs with low influent COD:N ratio. Biologically induced precipitation, which is frequently reported in the literature, causes important operational problems

in anaerobic digestion and downstream processes such as: pipe blockage and precipitates accumulation on the surfaces of different sludge management devices such as centrifuges and pumps (see Doyle and Parsons (2002) for a detailed review). Although struvite (magnesium ammonium phosphate) is the most important precipitate reported in WWTPs, Barat *et al.* (2009) detected an important precipitation of calcium phosphate jointly with struvite during anaerobic digestion. Furthermore, recent studies (Barat *et al.*, 2008) have observed that phosphorus precipitation during the biological phosphorus removal process could affect the metabolism of Polyphosphate Accumulating Organisms (PAOs). Due to the importance of precipitation and nitrogen removal processes to properly simulate WWTPs, an extension of BNRM1 has been developed. The new model (Biological Nutrient Removal Model No.2, BNRM2) that is presented in this paper includes the results of the work carried out by the CALAGUA research group on mathematical modelling (Barat *et al.*, 2011, Jiménez 2010). The new processes included in BNRM2 are the formation of 8 different precipitates and all the processes involved in the nitrogen removal via nitrite considering two groups of Ammonia Oxidising Organisms (AOO).

MODEL DESCRIPTION

The model considers the most important physical, chemical and biological processes taking place in a WWTP to maximize its potential applicability. The physical processes included are: settling and clarification processes (flocculated settling, hindered settling and thickening), volatile fatty acids (VFA) elutriation and gas-liquid transfer. The chemical interactions included comprise acid-base and ion-pairing processes, where equilibrium conditions are assumed, and precipitation processes. The biological processes included are: organic matter, nitrogen and phosphorus removal; acidogenesis, acetogenesis and methanogenesis. As a general model, BNRM2 considers the possible growth of all the bacterial groups included in the model in each operation unit. The environmental conditions (aerobic, anoxic or anaerobic) will determine which bacterial groups can proliferate. This “natural selection” observed in WWTPs is modelled by including switching functions for electron acceptors in the kinetic expressions.

The settling processes model (Ribes *et al.*, 2002) consists in a one-dimensional model based on both the solids flux concept and the conservation of mass. The settling velocity is obtained by using the model proposed by Takács *et al.* (1991) for the flocculated and hindered settling. The settling velocity in the lower layers is corrected by a compression function similar to the one proposed by Otterpohl and Freund (1992). This model is linked to the biological model in order to consider the biological processes taking place in primary and secondary settlers, and gravity thickeners.

Components in the model

The model considers 42 components split in 19 soluble and 23 suspended components that are defined below:

S_{Ac} [g COD m⁻³]: Acetate.

S_{CH4} [g COD m⁻³]: Dissolved methane.

S_F [g COD m⁻³]: Fermentable readily biodegradable substrate. It does not include VFA.

S_H [kmol H m⁻³]: Total proton concentration. This component includes free protons and those associated with acidic components.

S_{H2} [g COD m⁻³]: Dissolved hydrogen.

S_U [g COD m⁻³]: Inert soluble organic material.

$S_{Ig,C}$ [kmol C m⁻³]: Inorganic carbon. It consists of CO₂, HCO₃⁻ and CO₃²⁻. For all stoichiometric computations S_{IC} is assumed to be CO₂.

S_{N_2} [g N m⁻³]: Dinitrogen (N₂).
 S_{NH_x} [g N m⁻³]: Ammonium plus ammonia nitrogen.
 $*S_{NO_2}$ [g N m⁻³]: Total nitrite concentration. This component is the sum of nitrite and free nitrous acid concentrations.
 S_{NO_3} [g N m⁻³]: Nitrate.
 S_{O_2} [g O₂ m⁻³]: Dissolved oxygen.
 S_{PO_4} [g P m⁻³]: Orthophosphates.
 S_{VFA} [g COD m⁻³]: Fermentation products except acetate. It is assumed to be propionate.
 $*S_{Ca}$ [g Ca m⁻³]: Total soluble inorganic calcium concentration.
 $*S_{Mg}$ [g Mg m⁻³]: Total soluble inorganic magnesium concentration.
 $*S_{K}$ [g K m⁻³]: Total soluble inorganic potassium concentration.
 $*S_{Fe}$ [g Fe m⁻³]: Total soluble inorganic iron concentration.
 $*S_{Al}$ [g Al m⁻³]: Total soluble inorganic aluminium concentration.
 X_{PRO} [g COD m⁻³]: Acetogenic bacteria.
 X_{AO} [g COD m⁻³]: Acidogenic bacteria.
 X_{OHO} [g COD m⁻³]: Heterotrophic organisms. They may grow aerobically and anoxically.
 $*X_{AOO,r}$ [g COD m⁻³]: Ammonium oxidizing organisms (r-strategist). These organisms are responsible for ammonium oxidation to nitrite.
 $*X_{AOO,K}$ [g COD m⁻³]: Ammonium oxidizing organisms (K-strategist). These organisms are responsible for ammonium oxidation to nitrite.
 $*X_{NOO}$ [g COD m⁻³]: Nitrite oxidizing organisms. These organisms are responsible for nitrite oxidation to nitrate.
 X_U [g COD m⁻³]: Inert particulate organic material.
 X_{ACO} [g COD m⁻³]: Methanogenic acetoclastic organisms.
 X_{HMO} [g COD m⁻³]: Methanogenic hydrogenotrophic organisms.
 X_{PAO} [g COD m⁻³]: Polyphosphate Accumulating Organisms (PAOs).
 $X_{PAO,Stor}$ [g COD m⁻³]: Poly-hydroxy-alcanoates stored by X_{PAO} , but not included in the mass of X_{PAO} .
 $X_{PAO,PP}$ [g P m⁻³]: Poly-phosphates stored by X_{PAO} , but not included in the mass of X_{PAO} .
 X_{CB} [g COD m⁻³]: Slowly biodegradable substrates.
 X_{TSS} [g COD m⁻³]: Total suspended solids.
 X_{NVSS} [g COD m⁻³]: Influent non-volatile suspended solids.
 $*X_{ACP}$ [kmol ACP m⁻³]: Amorphous calcium phosphate (Ca₃(PO₄)₂·xH₂O).
 $*X_{HAP}$ [kmol HAP m⁻³]: Hidroxiapatite (Ca₅(PO₄)₃OH).
 $*X_{MAP}$ [kmol MAP m⁻³]: Struvite (MgNH₄PO₄·6H₂O).
 $*X_{New}$ [kmol New m⁻³]: Newberite (MgHPO₄·3H₂O).
 $*X_{Viv}$ [kmol Viv m⁻³]: Vivianite (Fe₃(PO₄)₂·8H₂O).
 $*X_{Str}$ [kmol Str m⁻³]: Strengite (FePO₄).
 $*X_{Var}$ [kmol Var m⁻³]: Variscite (AlPO₄).
 $*X_{Cal}$ [kmol Cal m⁻³]: Calcium carbonate (CaCO₃).
 $*$ New components included in BNRM2

All these components and the model notation are defined by following the nomenclature proposed by Corominas *et al.* (2010).

Since previous research (Claros *et al.*, 2010; Jiménez, 2010) has shown that model parameter values required to reproduce the AOO behaviour in SHARON and activated sludge reactors are significantly different, two AOO groups ($X_{AOO,r}$, $X_{AOO,K}$) are considered in BNRM2. This approach, which is similar to the one proposed by Wett *et al.* (2011), is also based on bacterial quantification

results using FISH technique. These results have proven that the conditions prevailing in the SHARON reactor (short SRT, high substrate concentrations) promote the development of r-strategist species (high growth rate and low substrate affinity), such as *Nitrosomonas europaea* and *Nitrosomonas eutropha*; while the conditions prevailing in activated sludge reactors (long SRT, low substrate concentrations) promote the development of K-strategist species (low growth rate and high substrate affinity), such as *Nitrosomonas oligotropha* (Manser *et al.*, 2005; Claros *et al.*, 2010).

The components S_{Mg} , S_{Ca} , S_K , S_{Fe} , S_{Al} represent the sum of the ion concentration (e.g. Ca^{2+}) and the ion present in other inorganic dissolved species (e.g. $CaOH^+$, $CaPO_4^-$, $CaHCO_3^+$). The solids most likely to precipitate (Maurer *et al.*, 1999; Musvoto *et al.*, 2000b) are various magnesium and calcium phosphates, calcium carbonate, iron phosphates and aluminium phosphate, which have been included as new components in the model.

Kinetic processes

The developed model considers a total of 60 kinetically governed processes (39 biological, 15 chemical and 6 physical processes) which are shown in Table 1. In appendix A the stoichiometric matrix of all these processes is shown.

Besides the continuity equations for the elements included in the BNRM1 (Chemical oxygen demand, inorganic carbon, proton, suspended solids, nitrogen and phosphorus) the following elements, which are involved in the precipitation processes, have been included in order to guarantee its continuity in the model: calcium, magnesium, aluminium, iron and potassium. Although potassium is not directly involved in the precipitation processes it has been included in BNRM2 due to its requirement to maintain the polyphosphate electroneutrality together with magnesium (Barat *et al.*, 2005). Appendix A (Table A2 and Table A4) shows the conversion factors to be applied in the continuity equations for all the elements considered in BNRM2. The content of Fe and Al in the organic compounds and biomass could be assumed to be negligible.

In BNRM2 the stoichiometry of both biological processes carried out by $X_{AOO,r}$ and $X_{AOO,k}$ is the same (see appendix A Table A1 and Table A3). However, this model considers two different groups of AOO because they present different maximum growth rates and substrate and dissolved oxygen affinities (Jiménez, 2010). As regards the stoichiometry for the denitrification processes, although nitrite can be detected as intermediate in denitrification process under specific conditions, this model considers that nitrate is directly converted to nitrogen gas as it is modelled by Hellinga *et al.* (1998) and Volcke (2006). This assumption was made according to our denitrification experiments carried out with urban wastewater where nitrite was not detected during nitrate removal.

In appendix B the kinetic expressions of all the processes considered in BNRM2 are listed. Two different pH inhibition functions are considered in BNRM2 (see Appendix B Table B1): a combination of Monod and non-competitive inhibition functions (I_{pH1} equation 1) and a sigmoidal function (I_{pH2} equation 2). This sigmoidal function is only used to model the growth of X_{NOO} because the I_{pH1} type function was not able to reproduce the sharp activity decrease observed at low pH values (Jiménez *et al.*, 2011).

$$I_{pH1} = \frac{\frac{S_{[H]}}{K_{S,H} + S_{[H]}} \cdot \frac{K_{I,H}}{K_{I,H} + S_{[H]}}}{\frac{S_{[H],Opt}}{K_{S,H} + S_{[H],Opt}} \cdot \frac{K_{I,H}}{K_{I,H} + S_{[H],Opt}}} \quad (1); \quad I_{pH2} = \frac{1}{1 + e^{[A_H(K_{S,pH} - pH)]}} \quad (2)$$

In these equations $S_{[H],Opt}$ represents the optimum proton concentration obtained as $\sqrt{K_{I,H} \cdot K_{S,H}}$, and A_H is a fitting parameter.

Table 1. Kinetic processes considered in BNRM2.

Biological processes	
<i>Heterotrophic Bacteria</i>	<i>Polyphosphate Accumulating Bacteria</i>
1. Aerobic hydrolysis	14. Storage of $X_{PAO,Stor}$ over S_{Ac}
2. Anoxic hydrolysis	15. Storage of $X_{PAO,Stor}$ over S_{VFA}
3. Anaerobic hydrolysis	16. Aerobic storage of $X_{PAO,PP}$
4. Aerobic growth of X_{OHO} over S_F	17. Anoxic storage of $X_{PAO,PP}$ over S_{NO3}
5. Aerobic growth of X_{OHO} over S_{Ac}	*18. Anoxic storage of $X_{PAO,PP}$ over S_{NO2}
6. Aerobic growth of X_{OHO} over S_{VFA}	19. Aerobic growth of X_{PAO}
7. Anoxic growth of X_{OHO} over S_F and S_{NO3}	20. Anoxic growth of X_{PAO} over S_{NO3}
8. Anoxic growth of X_{OHO} over S_{Ac} and S_{NO3}	*21. Anoxic growth of X_{PAO} over S_{NO2}
9. Anoxic growth of X_{OHO} over S_{VFA} and S_{NO3}	22. Lysis of X_{PAO}
*10. Anoxic growth of X_{OHO} over S_F and S_{NO2}	23. Lysis of $X_{PAO,PP}$
*11. Anoxic growth of X_{OHO} over S_{Ac} and S_{NO2}	24. Lysis of $X_{PAO,Stor}$
*12. Anoxic growth of X_{OHO} over S_{VFA} and S_{NO2}	
13. Lysis of X_{OHO}	
<i>Ammonium Oxidizing Bacteria-r</i>	<i>Ammonium Oxidizing Bacteria-K</i>
*25. Aerobic growth of $X_{AOO,r}$	*27. Aerobic growth of $X_{AOO,K}$
*26. Lysis of $X_{AOO,r}$	*28. Lysis of $X_{AOO,K}$
<i>Nitrite Oxidizing Bacteria</i>	<i>Acidogenic Bacteria</i>
*29. Aerobic growth of X_{NOO}	31. Anaerobic hydrolysis
*30. Lysis of X_{NOO}	32. Anaerobic growth of X_{AO}
	33. Lysis of X_{AO}
<i>Acetogenic Bacteria</i>	<i>Methanogenic Hydrogenotrophic Bacteria</i>
34. Anaerobic growth of X_{PRO}	36. Anaerobic growth of X_{HMO}
35. Lysis of X_{PRO}	37. Lysis of X_{HMO}
<i>Methanogenic Acetoclastic Bacteria</i>	
38. Anaerobic growth of X_{ACO}	
39. Lysis of X_{ACO}	
Physical processes	
40. Stripping of $S_{[CO2]}$	43. Stripping of S_{H2}
41. Stripping of S_{O2}	44. Stripping of S_{N2}
42. Stripping of S_{CH4}	45. Stripping of $S_{[NH3]}$
Precipitation processes	
*46. Precipitation of X_{ACP}	*47. Dissolution of X_{ACP}
*48. Precipitation of X_{Str}	*49. Dissolution of X_{Str}
*50. Precipitation of X_{MAP}	*51. Dissolution of X_{MAP}
*52. Precipitation of X_{New}	*53. Dissolution of X_{New}
*54. Precipitation of X_{Viv}	*55. Dissolution of X_{Viv}
*56. Precipitation of X_{Var}	*57. Dissolution of X_{Var}
*58. Precipitation of X_{Cal}	*59. Dissolution of X_{Cal}
*60. Precipitation of X_{HAP}	

BNRM2 considers different substrates to model the growth of both AOO groups (see Table B1 in Appendix B). The $X_{AOO,r}$ growth rate depends on free ammonia concentration (Claros *et al.*, 2010; van Hulle *et al.*, 2007) while the $X_{AOO,K}$ growth rate depends on total ammonia nitrogen concentration (Jiménez 2010 and Jiménez *et al.*, 2012).

With regard to the precipitation kinetics, the processes have been modelled as reversible processes, according to its oversaturated or undersaturated degree following the theory of Koutsoukos *et al.* (1980). However, X_{HAP} has been considered as a stable solid (only precipitation and not dissolution) according to the results obtained by different authors (Koutsoukos *et al.*, 1980; Maurer *et al.* 1999). Furthermore, the precipitation rates have been modelled as surface controlled processes (Maurer *et al.*, 1999; Musvoto *et al.*, 2000a).

A sign() function is included in the kinetic expressions related to the precipitation and dissolution processes (see Appendix B, Table B1). This sign() function is defined as the sign (+1, 0, -1) of the saturation index (SI) for each precipitate. For instance, when the solution is oversaturated, SI is positive (+1), the function $(1-\text{sign}(\text{SI}_X))/2$ that is included in the dissolution kinetic is zero and the dissolution process rate is zero. In this case, the function $(1+\text{sign}(\text{SI}_X))/2$ that is included in the precipitation kinetic is one and consequently the precipitation process takes place.

Equilibrium governed processes

As can be seen in the aforementioned equations the kinetic expressions of the processes considered make necessary the chemical equilibrium calculation in order to know the concentration of the inorganic soluble components under its different species (e.g. Ca^{2+} , PO_4^{3-} , NH_4^+ , NH_3 , H^+ , HNO_2) which are involved in the precipitation and some biological processes.

BNRM2 includes, as equilibrium governed processes, the acid-base, ion-pairing and redox reactions in which any of the components are involved. In order to solve the chemical equilibrium, it was distinguished between components and species. Chemically, the aqueous phase system is represented by a set of components and a set of species. A species is defined as every chemical entity to be considered. For the set of species selected, a set of components is chosen so that each species can be written as the product of a reaction involving only components, and no component can be written as the product of a reaction involving other components. With this chemical representation, two characteristic variables are defined: the species concentration, C_i (ML^{-3}), and the component concentration, T_j (ML^{-3}), being T_j the sum of concentration of all the species in which this component participates. The species that can be formed from the components are listed on the matrix of components-species shown in Appendix C, Table C1.

This equilibrium is described by a set of non-linear algebraic equations including one law of mass action (eq. 3) for each species formed in each equilibrium system and one mass balance (eq.4) for each component. The redox reactions are solved using the Nerst equation. The application of these equations is described in Appendix C.

$$\text{Law of mass action: } x_i = K_i \cdot \prod_{j=1}^{N_C} x_j^{a_{ij}} \quad i= 1, 2 \dots N_{sp} \text{ (number of species)} \quad (3)$$

$$\text{Mass balance: } T_j = \sum_{i=1}^{N_{sp}} a_{ij} \cdot C_i \quad j= 1, 2 \dots N_C \text{ (number of components)} \quad (4)$$

where x_i is the activity of the i^{th} species, x_j is the activity of the j^{th} component, a_{ij} is the stoichiometric coefficient of the j^{th} component in the i^{th} species (see Appendix C, Table C1), K_i is the stability constant of the i^{th} species corrected for temperature variations by the van't Hoff equation and C_i is the concentration of the i^{th} species. N_{sp} is the number of species considered (93 in this case) and N_C is the number of components (15 in this case). The activity and concentration of every component or species are related through the correspondent activity coefficient that depends on the ionic strength (Davis equation):

$$x_i = \gamma_i C_i \quad i=1, 2, \dots, N_{sp} \quad (5)$$

where γ_i is the activity coefficient for the i^{th} species. This chemical model is described in detail elsewhere (Serralta *et al.*, 2004; Barat *et al.*, 2011).

Instead of using the charge balance, the BNRM2 considers a mass-balance for proton component as proposed in the software MINTEQA2 (Allison *et al.*, 1991). Therefore, proton is included as a component in the model. Since the unit of this component is $\text{kmol H}^+ \cdot \text{m}^{-3}$, a continuity equation for H^+ is applied to calculate the variation of total proton concentration in biological processes. Conversion factors i_{H_i} are defined to apply the continuity equation (see Appendix A, Table A2 and Table A4).

It should be highlighted that the consideration of the acid-base and the ion-pairing interactions as equilibrium governed processes hugely simplifies the numerical solution and the model calibration due to the absence of kinetic parameters to solve the aqueous equilibrium.

Simulation procedure

The simulation procedure involves a sequential iteration among the differential equations obtained from the kinetic governed processes (biological and precipitation model) and the algebraic equations obtained from the equilibrium governed processes (chemical model). The total concentration of each component (e.g. S_{PO_4} and S_{NH_x}) needed for applying the chemical model, is provided by the solution of mass-balance equations. The concentrations of the species (e.g. $S_{[\text{PO}_4^{3-}]}$, $S_{[\text{HPO}_4^{2-}]}$, $S_{[\text{H}_2\text{PO}_4^{1-}]}$, $S_{[\text{H}_3\text{PO}_4]}$, $S_{[\text{FeHPO}_4]}$, $S_{[\text{FeH}_2\text{PO}_4^+]}$, $S_{[\text{FeHPO}_4^+]}$, $S_{[\text{FeH}_2\text{PO}_4^{2+}]}$, $S_{[\text{MgPO}_4^-]}$, $S_{[\text{MgHPO}_4]}$, $S_{[\text{MgH}_2\text{PO}_4^+]}$, $S_{[\text{CaPO}_4^-]}$, $S_{[\text{CaHPO}_4]}$, $S_{[\text{CaH}_2\text{PO}_4^+]}$, $S_{[\text{KHPO}_4^-]}$, $S_{[\text{Al}_2\text{PO}_4^{+3}]}$ and $S_{[\text{AlHPO}_4^+]}$ related to S_{PO_4} ; and $S_{[\text{NH}_4^+]}$, $S_{[\text{NH}_3]}$, $S_{[\text{CaNH}_3^{2+}]}$, $S_{[\text{Ca}(\text{NH}_3)_2^{2+}]}$ and $S_{[\text{FeNH}_3^{2+}]}$ related to S_{NH_x}) involved in the kinetic expressions are provided by the solution of the chemical equilibrium.

The use of MINTEQA2 (Allison *et al.*, 1991) is recommended in order to solve the chemical model due to the high number of species involved. The main advantages of using this software can be summarised as:

- The chemical algebraic equations are already implemented in the software.
- The equilibrium composition is thoroughly calculated: temperature variations of equilibrium constants are taken into account, activity coefficient of each species is calculated to apply the law of mass action.
- The model can be easily enlarged because the equations required to calculate the equilibrium composition considering new components are already implemented.
- MINTEQA2 calculates the redox reaction $\text{Fe}^{2+}/\text{Fe}^{3+}$ using the Nerst equation. In this respect, this software requires the redox potential value that should be defined in the simulation platform for each element of the WWTP.

The data required to predict the equilibrium composition consist of total dissolved concentrations for the components of interest. As in this case the equilibrium calculation is linked to dynamic biological processes, the total concentration of each component is provided by the solution of mass balance equations. MINTEQA2 original code has been slightly modified and compiled through the dynamic link library (DLL) techniques, allowing the FORTRAN module to be linked promptly to every program working with Windows system. In this respect, MINTEQA2 obtains the required

information from the software solving the mass balance differential equations and can be applied in an iterative calculation. A schematic diagram of the solution procedure is shown in Fig. 1.

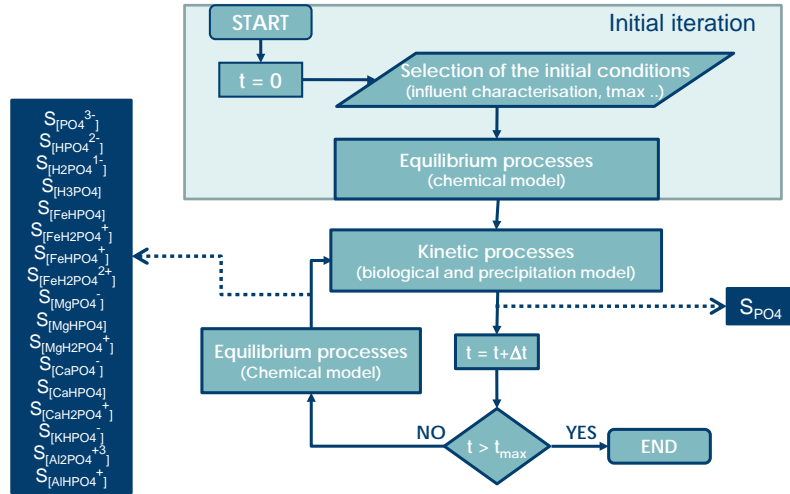


Figure 1. Schematic diagram of the proposed solution procedure to solve BNRM2.

MODEL VALIDATION

Different batch experiments were carried out in a laboratory scale SHARON reactor to determine the most important parameters related to $X_{AOO,r}$. Bacterial activity was measured as oxygen uptake rate (OUR) at different pH values (ranging from 6 to 9), substrate concentrations (from 45 to 10000 mg $\text{NH}_4\text{-N}\cdot\text{L}^{-1}$), dissolved oxygen concentrations (from 0.1 to 6 mg $\text{O}_2\cdot\text{L}^{-1}$) and nitrite concentrations (from 75 to 5000 mg $\text{NO}_2\text{-N}\cdot\text{L}^{-1}$). These experiments allowed to determine the following parameters related to $X_{AOO,r}$: $\mu_{AOO,r,Max}$, $K_{[\text{NH}_3],AOO,r}$, $K_{\text{O}_2,AOO,r}$, $K_{I,[\text{HNO}_2],AOO,r}$, $K_{I,pH,AOO,r}$, $K_{S,pH,AOO,r}$, and $Y_{AOO,r}$. The kinetic expression for the $X_{AOO,r}$ growth was defined on the basis of the experimental results obtained. These results showed that free ammonia should be considered as the substrate for these bacteria and that the reduction observed in the biomass activity at high ammonium concentration was due to salinity and not to free ammonia concentrations. Further details related to the results obtained and the calibration methodology can be found at Jiménez (2010) and Claros *et al.* (2010).

In addition, the most important parameters related to $X_{AOO,K}$ and X_{NOO} were determined in different laboratory batch experiments using biomass from a nutrient removal pilot plant. With regard to $X_{AOO,K}$ the following parameters were determined: $\mu_{AOO,K,Max}$, $K_{\text{NH}_x,AOO,K}$, $K_{\text{O}_2,AOO,K}$, $K_{I,[\text{HNO}_2],AOO,K}$, $K_{I,pH,AOO,K}$, $K_{S,pH,AOO,K}$, and $Y_{AOO,K}$. The experimental results obtained indicated that total ammonium concentration should be considered as the substrate for these bacteria. The different substrates for both AOO bacteria determined in the different experiments carried out, is one of the reasons to include two AOO groups in BNRM2. Concerning X_{NOO} the following parameters were determined: $\mu_{NOO,Max}$, $K_{\text{NO}_2,NOO}$, $K_{\text{O}_2,NOO}$, $K_{S,pH,NOO}$, and Y_{NOO} . The experimental results obtained indicated that total nitrite concentration should be considered as the substrate for these bacteria and that pH values up to 9.9 did not affect X_{NOO} growth rate. These experimental results contributed to define the kinetic expressions related to these bacteria. For further details about these experiments see Jiménez *et al.* (2011) and Jiménez *et al.* (2012).

With regard to the calibration and validation of the precipitation and dissolution processes considered in BNRM2, six batch experiments were carried out in a SBR operated for enhanced biological phosphorus removal (EBPR). Figure 2 shows the experimental and simulated values of acetic acid, phosphate, pH (see Figure 2a), calcium, potassium and magnesium profiles (see Figure 2b) during one of the experiments. The results obtained in all the experiments (as Figure 2 shows) indicated that the model predictions accurately reproduced the corresponding experimental data, not only for the components related to chemical processes (S_{Ca} and S_{PO_4} involved in calcium phosphate formation as X_{ACP} and X_{HAP}) but also those components related to biological processes (S_{PO_4} , S_{VFA} , S_K and S_{Mg} involved in EBPR). For further details see Barat *et al.* (2011).

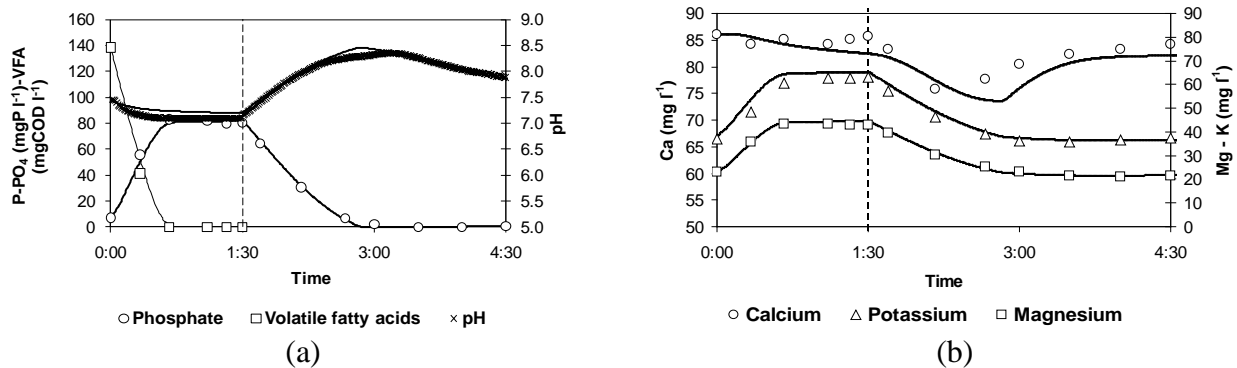


Figure 2. Experimental versus simulation results from an SBR operated for EBPR. Experimental data are plotted in dots and simulated data from BNRM2 are plotted in lines: (a) phosphate, volatile fatty acids and pH; (b) calcium, potassium and magnesium.

CONCLUSIONS

The BNRM2 has been presented in this paper as an extension of the general model BNRM1. This extension comprises the formation of 8 different precipitates and all the processes involved in the nitrogen removal via nitrite considering two groups of AOO ($X_{AOO,r}$, $X_{AOO,k}$). Thus, optimum operation conditions and plant configuration to improve nitrogen removal, to minimize the uncontrolled phosphorus precipitation and to maximize phosphorus recovery in the recycled streams can be established with BNRM2 as this model considers the nitrogen removal over nitrite and precipitation processes. Further research is being carried out in order to include other processes that take place in WWTPs which are not yet considered in this model, such as the ones related to sulphur containing species, i.e. the biological processes (by means of sulphate reducing bacteria) and the physico-chemical processes (e.g. sulphide oxidation and sulphate precipitation).

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