The Application of ADM/ASM Interface in Sumo Wide Plant Model

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***Abstract*— Sumo is an innovative and most versatile wastewater simulation package on the market. The simulator is capable of modelling treatment plants of unlimited complexity, focusing largely on BOD, nitrogen and phosphorus removal; with digester, side streams, IFAS and MBBR, SBRs, trickling filters, primary and final settling, thickeners, centrifuges being process units typically found in Sumo which are used in municipal and industrial treatment plants. The model interface has numerous models including ASM (AM1, ASM2D, ASM2D_TUD, ASM3, and ASM3_BioP), Barker_Dold, and BUCTPHO plus. Sumo models can be run through several different interfaces. Though, ADM1 model is perhaps the most extensively applied for the simulation of anaerobic processes, it is not included in Sumo which incorporates a sludge model because of its complexity and ongoing modification. Simulation can still be achieved by simply interfacing ADM1 and ASM1 models by converting ADM1 state variables to ASM1 variables for use in Sumo.**

Keywords —ADM1, ASM1, Plant-wide modeling, Wastewater treatment

I. Introduction

Worldwide, mathematical modelling of wastewater treatment plants seems to answer the question as to how wastewater treatment plants (WWTPs) will perform under various operating conditions. One of the milestones in dynamic modelling of WWTPs was the study conducted by the University of Cape Town [1]. This dynamic model originated from the steady state model of Ekama and Marias [2]. In 1987, a task group was formed under the supervision of Prof. Henze and presented the first Activated Sludge Model, i.e. "ASM1 model", for combined biological carbon and nitrogen removal. This model was developed based on University of Cape Town's (UCT) model.

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The necessity to extend the model boundaries and to include other process units led to the development of the Anaerobic Digestion Model (ADM1) suggested in 2002 as a common platform to develop, design, and validate models of anaerobic digestion processes in WWTP [2]. Now, the ADM1 model has become one of the practical and dynamic tools for modelling anaerobic digestion systems [10], [3]. Though, ADM1 model is widely used for the simulation of anaerobic processes, it is not included in the Sumo; due to its complexity and ongoing modification. However, simulation can still be achieved by simply interfacing the ADM1 and the ASM1 models, thus, converting ADM1 state variables to ASM1 state variables for use in Sumo.

This paper aims to provide a review of how the ADM1/ASM1 interface can be applied in Sumo in order to simulate WWTPs performance.

II. ADM1 model description

The AMD1 model developed by the international water association (IWA) for mathematical modelling of anaerobic digestion processes is extensively detailed in the paper published by the IWA Task group [3]. The following is rather a brief summary of the model for discussion purposes.

ADM1 is an organized generic model that portrays the major process describing biochemical and physicochemical processes involved in the breaking down of complex organic matter into biogas and inert by-products [4]. ADM1 is a mathematical model grounded on COD as a common unit used in wastewater characterization representing performance the organic substrate concentration including removal [1].

The organic components considered by the model are the following: complex particulates, proteins, carbohydrates, sugars, lipids, amino acids (AA), long chain fatty acids (LCFA), volatile fatty acids and particulate matter including soluble inert substrates [5]. Fig. 1 illustrates the substrate and conversion processes pertaining to the presented model. Disintegration is the first biochemical conversion which involves the breakdown of complex particulate matters to monomers constituents of proteins, carbohydrates, lipids, particulate and soluble inert substrates. Hydrolysis of particulate monomers is the next conversion by which carbohydrates, proteins and lipids are converted into sugars, AA and LCFA by hydrolytic bacterial species. Once particulate monomers are hydrolyzed, then the fermentation of AA ensues to produce CO_2 and hydrogen (acidogenesis) [6]. Subsequently anaerobic oxidation of proprionic acid, valeric acid, butyric acid into CO_2 and

hydrogen including acetate (acetogenesis) ensues. The last step involves the production of biogas, which take place in two ways; either based on acetate or through the reduction of CO_2 by molecular hydrogen [1].

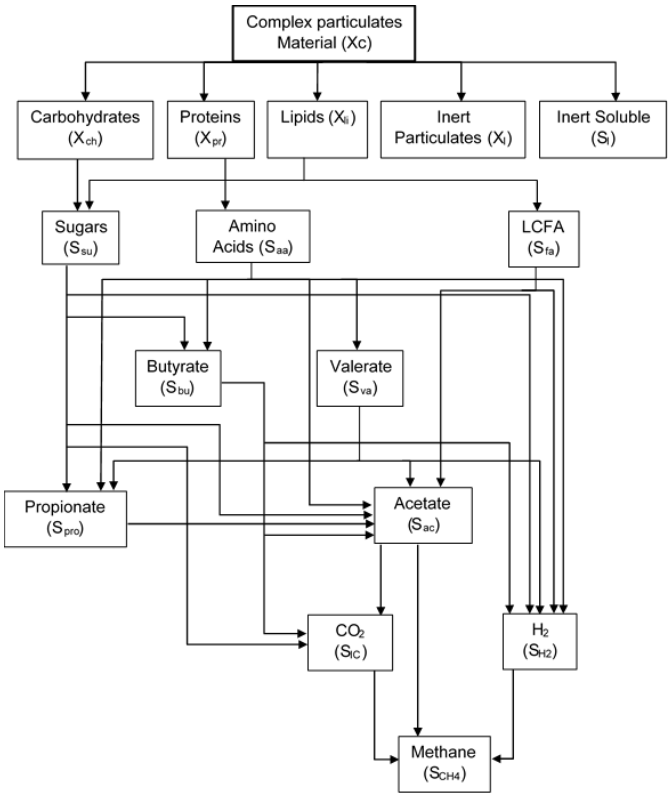

Fig.1 Biochemical conversion processes according to ADM 1 model

TABLE I: LIST OF THE DYNAMIC STATE VARIABLES IN ADM1 MODEL [7]

	Variables	Symbol	Units
Particulate	Composites	X_c	Kg COD m^{-3}
	Carbohydrates	X_{ch}	Kg COD m^{-3}
	Proteins	X_{pr}	Kg COD m^{-3}
	Lipids	X_{li}	Kg COD m^{-3}
	Particulate inerts	X_l	Kg COD m^{-3}
Soluble	Monosaccharides	S_{su}	Kg COD m^{-3}
	Amino acids	S_{aa}	Kg COD m^{-3}
	Long chain fatty acids	S_{fa}	Kg COD m^{-3}
	Valerate	S_{va}	Kg COD m^{-3}
	Propionate	S_{pro}	Kg COD m^{-3}
	Butyrate	S_{bu}	Kg COD m^{-3}
	Acetate	S_{ac}	Kg COD m^{-3}
	Soluble inerts	S_i	Kg COD m^{-3}
	Hydrogen gas	S_{h2}	Kg COD m^{-3}
	Methane gas	S_{ch4}	Kg COD m^{-3}
	Sugar degraders	X_{su}	Kg COD m^{-3}
	Amino acid degrader	X_{aa}	Kg COD m^{-3}
	LCFA degrader	X_{fa}	Kg COD m^{-3}
	Valerate and butyrate degraders	X_{c4}	Kg COD m^{-3}
	Propionate degraders	X_{pro}	Kg COD m^{-3}
	Acetate degraders	X_{ac}	Kg COD m^{-3}
	Hydrogen degraders	X_{h2}	Kg COD m^{-3}
	Inorganic nitrogen	S_{in}	Kmol N m^{-3}
	Inorganic carbon	S_{ic}	Kmol C m^{-3}
	Anions	S_{an}	Kmol m^{-3}
	Cations	S_{cat}	Kmol m^{-3}

A. Model Equation

The ADM1 model is an organized mathematical model comprising of 32 dynamic state variables to model change of different species for both in-/soluble and particulate components contained in the gaseous and liquid phases. Table I depicts the dynamic state variables contained in AMD1 model [7].

In the ADM1 model the total COD (COD_{total}) is a composite variable calculated through the addition of the organic state variables and the TKN (TKN_{total}) which is calculated as a sum of nitrogenous state variables plus the nitrogenous fraction of some organic state variables. Equation (1), (2), (3), (4) shows how total COD and TKN the calculated for the ADM1 model.

$$COD_{soluble} = S_i + S_{su} + S_{aa} + S_{fa} + S_{va} + S_{bu} + S_{pro} + S_{ac} + S_{h2} + S_{ch4} \quad (1)$$

$$COD_{particulate} = X_i + X_{su} + X_{aa} + X_{fa} + X_{c4} + X_{pro} + X_{ac} + X_{h2} + X_c + X_{ch} + X_{pr} + X_{li} \quad (2)$$

$$COD_{total} = COD_{soluble} + COD_{particulate} \quad (3)$$

B. Liquid phase equations

The mass balance equations utilized by the ADM1 model to describing the dynamic behavior of soluble and particulate substrate in the liquid phase are shown in Eq. (5), (6):

$$\frac{dS_{liq,i}}{dt} = \frac{Q}{V_{liq}}.(S_{in,i} - S_{liq,i}) + \sum_{j=1-19} \rho_j \nu_{i,j} \quad (5)$$

i=1…12; i=25-26

$$\frac{dX_{liq,i}}{dt} = \frac{Q}{Vliq}.(X_{in,i} - X_{liq,i}) + \sum_{j=1-19} \rho_j \nu_{i,j} \quad (6)$$

i=13,…,24

Where:

$S_{liq,i}$ is the concentration of each soluble state variable,

$X_{liq,i}$ is the concentration of each particulate and biomass state variable,

V_{liq} is the liquid reactor volume,

Q is the flow in and out of the reactor,

$S_{in,i}$ is the input concentration of soluble components,

$X_{in,i}$ is the concentration of particulate and biomass components,

$\sum_{j=1-19} \rho_j \nu_{i,j}$ The sum of the specific kinetic rates ρ_j for process j multiplied by the stoichiometric coefficients $V_{i,j.}$

C. Gas Phase Equations

The three main gaseous components modelled by the ADM1 model in the gas phase are biogas constituents. The rate transfer of these gasses can be attained by applying the two-film theory developed by Whitman [8]. Eq. (7) is an expression of the general dynamic gas concentration of each gas component "i".

$$\frac{dS_{gas,i}}{dt} = \frac{q_{gas}}{V_{gas}} S_{gas} + \frac{V_{liq}}{V_{gas}} \rho_{T,i} \quad (7)$$

Where:

q_{gas} is the gas flow,

V_{liq} is the liquid reactor volume (l),

V_{gas} is the gas volume (l);

S_{gas} is the gas phase concentration of gas component "i",

$\rho_{T,i}$ is the specific mass transfer rate of gas "i" expressed as in Eq. (8):

$$\rho_{T,i} = K_{La}.(K_H.P_{gas,i} - S_{liq,i}) \text{ i=Ch}_4, \text{ CO}_2 \text{ and H}_2 \quad (8)$$

Where:

K_{La} is the volumetric gas liquid mass transfer coefficient,

K_H ($M\ bar^{-1}$) is the Henry's law coefficient,

S_{liq} (M) is the liquid phase concentration of gas component "i",

P_{gas} is the gas phase pressure of each gas component "i" calculated from the ideal gas law as follows Eq. (9):

$$\begin{aligned} P_{gas,H_2} &= S_{gas,H_2}.\frac{R.T_{op}}{16} \\ P_{gas,CH_4} &= S_{gas,CH_4}.\frac{R.T_{op}}{64} \\ P_{gas,CO_2} &= S_{gas,CO_2}.R.T_{op} \end{aligned} \quad (9)$$

When assessing the dynamic gas phase concentration of all gas components and assuming that the total pressure of the gas phase above the liquid is equivalent to the difference between atmospheric and water vapor pressure at the specified reactor temperature and the rate at which the gas is produced can be estimated as in Eq. (10):

$$q_{gas} = \frac{R.T_{op}}{p_{atm} - p_{gas,H_2O}} V_{liq} \left(\frac{\rho_{T,H_2}}{16} + \frac{\rho_{T,CH_4}}{64} + \rho_{T,CO_2}\right) \quad (10)$$

D. SUMO Simulator

Sumo (Dynamita, France) is an innovative, open wastewater process modeling platform, having a multipurpose simulation platform developed for numerous environmental models, particularly municipal and industrial wastewater treatment plant modelling. A variety of plant designs can be simulated in Sumo. The models in the simulator are written in Excel based on an open source code language called SumoSlang (Sumo Simulation Language, copyright Dynamita), thus imparting ease in which both, steady-state and dynamic simulations can be performed.

Sumo can simulate steady-state, traditional bio-kinetic, mixed equilibrium-kinetic and direct algebraic models, depending on outcomes of the process being designed. The simulator comes with internally researched and developed wholes models including ASM models (AM1, ASM2D, ASM2D_TUD, ASM3_BioP, ASM3), Barker_Dold, and BUCTPHO plus. However, ADM1 model is not included in Sumo. A variety of model options can be selected:

- the calculation of the gas phase concentrations;
- the integration of the pH;
- the chemical precipitation of some components.

The limitation of the software is in its instability, especially when inputting complex process designs into the software.

III. Discussion

ADM1 has limitations associated with the application of plant-wide models. Another reported key limitation in the ADM1 model is the exclusion of bio-kinetics and physio-chemistry for sulfur and iron reduction, which interact with phosphorous via inhibit and precipitation mechanisms [9], [5]. This is very crucial, because the modeling of iron and sulphur improves the accuracy of pH variations attributed to precipitation.

A. ADM1 and ASM1Interface

Although the AMD1 model is not part of Sumo, simulation can still be achieved by simply converting the ADM1 state variable to ASM1 model parameters [7]. Future research will focus more on the conversion of ADM1 state variable to ASM1 state variable rather than ASM1 to ADM1, because converting ADM1 state variables to ASM1 is somewhat simpler [10]. Basically, the aim is to quantify and simulate maximum removal of S_i (soluble inert COD), X_s (slowly biodegradable substrate), S_s (readily biodegradable substrate), and X_i (particulate inert COD) in regard to the available COD X_{nd} (particulate organic nitrogen), S_{nh} (ammonia) and S_{nd} (soluble organic nitrogen) with respect to nitrogen. Fig. 2 and 3 represent of the COD and Total Kjeldahl Nitrogen (TKN) conversion, respectively.

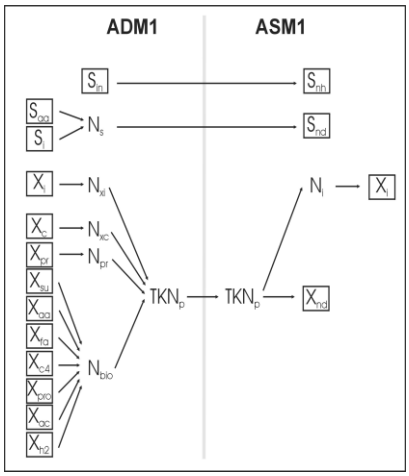

Fig.2 ADM1 to ASM1 state variable conversions for TKN.

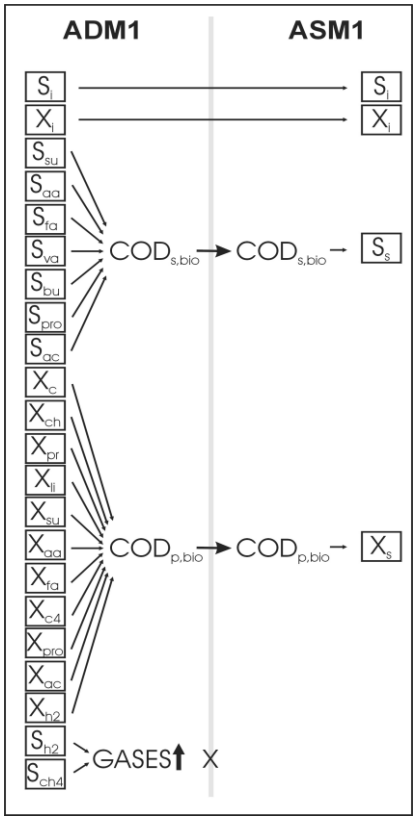

Fig.3 Schematic representation of COD conversion of ADM1 state variables to ASM1 state variables.

B. Dissolved COD

Maintenance of mass balance in any interface is very crucial. As shown in Fig. 2 and 3 the COD mass balance is maintained in the conversion to ASM1 with the exception of the dissolved gases (S_{h2} and S_{ch4}) [7]. As shown in Eq. (11) the difference between the influent COD and that used to generate biogas including that of dissolved gasses in the liquid represents the mass of COD conserved in the anaerobic system. This reduction in COD has no impact on the TKN since neither S_{h2} nor S_{ch4} has associate nitrogen components.

$$COD_{conserved} = COD_{t,anaerobic} - S_{h2} - S_{ch4} \quad (11)$$

C. COD Conversion

At this stage there is no conversion to be done. Si, $_{ASM1}$ is mapped as $S_{i,\ ADM1}$ and $X_{i,\ ASM1}$ as $X_{i,\ ADM1}$. The soluble biodegradable COD is summed and mapped to S_s (Eq. 12) and the particulate biodegradable COD is summed mapped to X_s (Eq. 13).

$$S_s = S_{su} + S_{aa} + S_{fa} + S_{va} + S_{bu} + S_{pro} + S_{ac} \quad (12)$$

$$X_s = X_c + X_{ch} + X_{pr} + X_{li} + X_{su} + X_{aa} + X_{fa} + X_{c4} + X_{pro} + X_{ac} + X_{h2} \quad (13)$$

D. TKN Conversions

The TKN conversion is relatively simple. Inorganic nitrogen is mapped directly to ammonia (S_{nh}) Eq. (14).

$$S_{nh} = S_{in} \quad (14)$$

VI. CONCLUSION

Mathematical modelling and use of software seems to be an answer to simulate and thus predict the behaviour of WWTPs under various operating conditions. The process engineering modelling software has become a widely accepted tool for the design, analysis, control, forecasting and optimization of WWTPs, thus helping to assure high effluent quality. Sumo is an innovative multipurpose simulation platform developed for common models, particularly for municipal and industrial wastewater treatment plant modelling. The AMD1 model regardless of its extensive use for the simulation of anaerobic processes, it is not part of Sumo. The use of an interface model, such as the one proposed here can allow others to transparently and consistently translate inputs to ASM1 and run the simulation in Sumo for better results.

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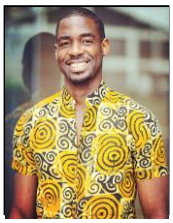

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