Thesis for the Degree of Master of Engineering

Phenol fate simulation for wastewater treatment plant by using ASM3+ model

by

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ASM3+ model을 이용한 하수처리장 페놀 거동 시뮬레이션

Advisor: Prof. Byung Hun Lee

by

Dan Wang

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Phenol fate simulation for wastewater treatment plant by using ASM3 model

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Abstract

The growing population, urbanization and modernization has led to the release of toxic organic compounds into the environment, Phenol is one of the most common organic water pollutants, which is regarded as a priority pollutant by USEPA is a widespread pollutant found in many industrial effluents. To protect human health and ecosystems, the research of phenol-laden waste waters is of great importance. Literatures on biodegradation kinetics of phenol as individual pollutant is though plenty, study of phenol treatment in the wastewater treatment plant by using the ASM3 modeling in Korea has never been reported.

Activated sludge model 3(Computer Program for the Identication and Simulation of Aquatic Systems)developed in 1999. As the biological reaction can be changed arbitrarily based on the user in Aquasim, simulating the new concept modeling is possibility. We add the phenol treatment process in ASM3 matrix. Using the average phenol concentration of all the wastewater treatment plants in Busan, we estimate parameters through the surface response methodology. The simulation of phenol in AQUASIM is operated

successfully. The ASM3 model with the process of phenol treatment for the imitation of wastewater treatment is possibility.

The proposed method will be useful to designers and operators of wastewater treatment plants, who need reliable kinetic parameters to predict the fate of toxic contaminants in wastewater treatment plants.

Ⅰ. Introduction

Phenol which is regarded as a priority pollutant by USEPA is a widespread pollutant found in many industrial effluents. It is used in variety of industries, such as in production of steel, resins, ceramics, fungicides and herbicides. (Edalatmanesh *et al.*, 2008; Tsai and Juang, 2006; Juang and Tsai, 2006; Rodriguez *et al.*, 2006). Phenol is released into the environment mainly through industrial wastewater discharges (Huang *et al.*, 2007).

Phenol is one of the most common organic water pollutants, because it is toxic even at low concentrations, and also its presence in natural waters can lead further to the formation of substituted compounds during disinfection and oxidation processes(Busca *et al.*, 2008). Currently, phenol is produced at a rate of about 6million ton/yr worldwide, with a significantly increasing trend(W. Jordan *et al.*, 2002).

Phenol in the environment may present many adverse health and environmental effects; for example, phenol can alter aquatic ecosystems and damage valuable resources (Babich and Davis, 1981; Busca *et al.*, 2008). To protect human health and ecosystems, the research of phenol-laden waste waters is of great importance.

Phenol is also relevant in the field of environmental research, because it has been chosen frequently as a model pollutant and many data are available on its removal and destruction in particular with respect to wastewater treatments (Busca *et al.*, 2008).

However, to the best of our knowledge, Literatures on biodegradation kinetics of phenol as a individual pollutant is though plenty, The study of phenol treatment in the wastewater treatment plant by using the ASM3 modeling in Korea has never been reported.

The objective of this paper is to calibrate known treatment plant configurations, using existing data, to derive the appropriate modeling parameters for phenol treatment process in the wastewater treatment plant. In this calibration effort, the aim was to match known effluent and musk concentration to predicted values, based on existing influent concentrations and variables of treatment plant design and operation.

The proposed method will be useful for designers and operators of wastewater treatment plants, who need reliable kinetic parameters to predict the fate of toxic contaminants in wastewater treatment plants in Korea. In obtaining a better understanding of the processes that are taking place in wastewater system, engineers will be able to more accurately predict the degradation of toxic contaminants in wastewater treatment plant by using ASM3 modeling.

Ⅱ. Background

2.1 Toxic compounds in wastewater

The growing population, urbanization and modernization has led to the release of toxic organic compounds into the environment, including the endocrine disrupting compounds (EDCs). Interest in EDCs has risen over the last few years as new, highly sensitive analytical technologies have been developed to be capable of detecting these compounds at extremely low levels (nano and pico−levels) in the environment. These compounds are called "endocrine disruptors" as exposure to them results in disruption of normal endocrine function with possible adverse health impacts.

Most of the organic compounds in domestic wastewater and some in industrial wastewater are of natural origin and can be degraded by common bacteria in aerobic or anaerobic processes. However, currently there are over 70,000 synthetic organic chemicals, termed *xenobiotic compounds,* in general use (Schwarzenbach *et al.*, 1993).

Unfortunately, some of these organic compounds pose unique problems in wastewater treatment, due to their resistance to biodegradation and human health. Organic compounds that are difficult to treat in conventional biological treatment processes are termed *refractory.* In addition, there are naturally occurring substances, such as those found in petroleum products that are of similar concern.

Examples of petroleum compound sand synthetic organic compounds found in different types of wastewater are reported in Table 2.1.

Table 2.1 Examples of toxic and recalcitrant organic compounds found in wastewater[a]

Type of waste	Types of organic compounds
Petroleum	Alkanes,alkenes,polyaromatic hydrocarbons,monocyclic aromatics−benzene,toluene,ethylbenzene,xylenes, naphthenes
Nonhalogenated solvents	Alcohols,ketones,esters,ethers,aromatic and aliphatic hydrocarbons,glycols,amines
Halogenated solvents	Chlorinated methanes−methylene chloride, chloroform, carbon tetrachloride; chlorinated ethenes−tetrachloroethene,trichloroethene;chlorinated ethanes−trichloroethane;chlorinated benzenes
Pesticides, including insecticides,herbicides,fungicides	Organochloride compounds, organophosphate compounds, carbamate esters, phenyl ethers, creosotes, chlorinated phenols
Munitions and explosives	Nitroaromatics,trinitrotoluene,nitramines,nitrate esters
Industrial intermediates	Phthalate esters, benzene, phenol, chlorobrnzenes, chlorophenols, xylenes
Transformer and hydraulic fluids	PCBs
Production products	Dioxin,furans

Watts(1997).

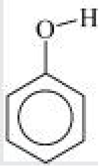
2.2 Phenol properties and pollution sources

2.2.1. Phenol chemical and physical properties

Some chemical and physical properties of phenol (also called phenic acid or carbolic acid) are reported in Table 2.2. Phenol was first isolated from coal tar in 1834 by the German chemist Runge. It is an aromatic compound.

At ambient temperature and pressure it is a hygroscopic crystalline solid. When pure, solid phenol is white but is mostly colored due to the presence of impurities. Phenol is very soluble in ethyl alcohol, in ether and in several polar solvents, as well as in hydrocarbons such as benzene. In water it has a limited solubility and behaves as a weak acid. As a liquid phenol attacks rubber, coatings, and some forms of plastic. Hot liquid phenol attacks aluminum, magnesium, lead, and zinc metals. It is characterized by a typical pungent sweet, medicinal, or tar-like odour (J. E. Amore and E. Hautala, 1983). It is a combustible compound.

Table 2.2 Chemical and physical properties of phenol(Kirk−Othmer, 1999;W. Jordan *et al.*, 2002)

Formula	C_6H_5OH 
Molecular weight (g/mol)	94.11
Tmelt (°C)	40.9
Teb (°C)	181.75
Water solubility (r.t.)	$9.3g_{phenol}/100ml_{H2O}$
pKa	9.89
Flammability limits in air (vol%)	1.7(lower) 8.6(higher)
Flash point (°C)	79 (closed cup)
Autoignition temperature (°C)	715

2.2.2. Phenol industrial syntheses and sources

Industrial processes generate a variety of molecules that may pollute air and waters due to negative impacts for ecosystems and humans (toxicity, carcinogenic and mutagenic properties). Phenol is one of the most common organic water pollutants, because it is toxic even at low concentrations, and also its presence in natural waters can lead further to the formation of substituted compounds during disinfection and oxidation processes.

Phenol is an aromatic compound that is used as raw material for the production of a variety of resins, including phenolic, epoxy, polycarbonate, and polyamide, for various applications (Kirk-Othmer, 1978).

In addition, phenol and its derivatives are commonly found in effluents from (i) industries manufacturing synthetic chemicals, pesticides, paper and (ii) coal conversion, oil-refining process, etc. The concentration of phenols in these effluent ranges from10 to 17,500 mgl^{-1}(Veeresh *et al.*, 2005).

Currently, phenol is produced at a rate of about 6million ton/yr worldwide, with a significantly increasing trend(W. Jordan *et al.*, 2002). The so called Hock processes, i.e., the three-step cumene synthesis and oxidation processes (such as the Sunoco-UOP, the KBR and the GE-Lummus processes), consisting in the simultaneous syntheses of phenol and acetone from benzene, propylene and oxygen, produces about 95% of the phenol used in the world.

These processes(R. J. Schmidt, 2005) involve: (i)alkylation of benzene with propene to form cumene, catalyzed by phosphoric acid, aluminum chloride or, recently, by beta or MCM22 zeolite(G. Busca, 2007);(ii) oxidation of cumene to cumene hydroper oxide (CHP) with air proceeding via a free−radical mechanism that is essentially auto−catalyzed by CHP; (iii) cleavage of cumene hydroperoxide to phenol and acetone, catalyzed by sulphuric acid.

Several alternative industrial syntheses of phenol exist(W. Jordan *et al.*, 2002;H.G. Franck and J. W. Stadelhofer, 1989; H. A. Wittcoff and B. G. Reuben, 1996;K. Weissermel and H.−J. Arpe, 1997),i.e., through chlorobenzene (reactionwith caustic soda at 350°C) or by sodic benzensolfonate alkaline fusion or by oxidation of toluene via benzoic acid.

Phenol is also present in benzole and coal tar produced during coal coking. It may be separated from these by−products by extraction with caustic solutions as sodium phenate. It is shipped in the molten state at elevated temperatures or in the solid or crystalline form; it is also available as an aqueous solution.

Phenol and many substituted phenols are natural components of many substances (e.g., tea, wine and smoked foods), and phenol is also emitted from the combustion of fossil fuels and tobacco. It is also present in animal wastes and decomposing organic material and may be formed in air as a product of benzene photo oxidation. Bacteria in the environment quickly break down phenol, and so levels in air (1-2 days),water (9 days) and soil (2-5 days) are generally quite low.

2.2.3. Phenol industrial applications

As a pure substance, phenol is used as a disinfectant, for the preparation of some cream and shaving soap for its germicidal and local anesthetic properties, in veterinary medicine as an internal antiseptic and gastric anesthetic, as a peptizing agent in glue, as an extracting solvent in refinery and lubricant production, as a blocking agent for blocked isocyanate monomers, as a reagent in chemical analysis and as a primary petrochemical intermediate.

Its largest use (35%) is to produce phenolic resins like phenol-formaldehyde resins (Bakelite) which are low-cost thermosetting resins applied as plywood adhesive, construction, automotive and appliance industries. By reaction with acetone it may also be converted into bisphenol A, a monomer for epoxy-resins (28%).

It is also used to produce cyclohexanone and cyclohexanone-cyclohexanol mixtures by selective catalytic hydrogenation. Cyclohexanone is later converted into its oxime and further to ε-caprolactame, the monomer for nylon 6 (16% of phenol applications).

The mixture cyclohexanone-cyclohexanol is oxidized by nitric acid to adipic acid, one of the monomers for the production of nylon-6,6. Phenol is also used to produce polyphenoxy and polysulphone polymers, corrosion-resistant polyesterand polyester polyols.

Phenol may be converted into xylenols, alkylphenols, chlorophenols, aniline, and other secondary intermediates in the production of surfactants, fertilizers, explosives, paints and paint removers, textiles, rubber and plastic plasticizers and antioxidants, and curing agents and so on. Phenol is also a building block for the synthesis of pharmaceuticals, such as, e.g., aspirin.

2.2.4. Phenol and health

The sterilizing activity of phenol was discovered by the English surgeon Joseph Lister in 1865. The germicidal activity of phenol appears associated to its protein denaturing ability. It has lipofile properties, so it binds itself to the batteric proteine by hydrogen bonds.

On the other hand, phenol has relevant health effects for humans(Priority Substances List Assessment Report, 1999). The manufacture and transportation of phenol as well as its many uses may lead to worker exposures to this substance, through inhalation, ingestion, eye or skin contact, and absorption through the skin. Phenol is rapidly absorbed through the skin and can cause skin and eye burns upon contact. Comas, convulsions, cyanosis and death can result from overexposure to it. Internally, phenol affects the liver, kidneys, lungs, and vascular system. The ingestion of 1 g of phenol is deadly for man.

The Nazi used phenol toxicity for refining extermination techniques, making phenol injections for killing the prisoners. Death was coming up in a few seconds and the method was considered to efficacious and economic(R. J. Lifton, 1986). No evidence exists to indicate that phenol has any carcinogenic potential.

2.3. Biological removal of toxic and recalcitrant organic compounds

Biodegradation of phenol in wastewater is generally more cost-effective than the physicochemical treatment processes(Loh *et al.*, 2000). The process has been carried out for many years either aerobically or an aerobically. The potential mechanisms of degradation of phenols during activated sludge treatment include volatilization, biological metabolism, adsorption onto biomass and chemical reaction; in an efficient biological detoxification system (Rayback, 1992; Knowles and Bunch, 1986; Aronstein *et al.*, 1994).

Though the degradation pathways of such compounds have been studied in detail(Shingler *et al.*, 1992; Paller *et al.*, 1995) and the removal of these compounds by effective treatment of distillery waste by physicochemical means has been reported earlier(Lilov *et al.*, 2000; Hong *et al.*, 2000; Blonskaja *et al.*, 2003; Mendonca *et al.*, 2004), bioremediation techniques using particular microorganisms or microbial consortia may be more effective and cost-beneficial than physico-chemical methods (Wolmarans and de Villiers, 2002;Nandy *et al.*, 2002).

2.3.1 Biological treatment methods

Importance of Specific Microorganisms

The ability to degrade toxic and recalcitrant compounds will depend primarily on the presence of appropriate microorganism(s) and acclimation time. In some cases, special seed sources are needed to induce and sustain the enzymes and bacteria required for degradation. Acclimation times can vary from hours to weeks depending on the microorganism population and organic compound.

Biodegradation Pathways

The three principal types of degradation pathways that have been observed are (1)the compound serves as a growth substrate; (2)the organic compound provides an electron acceptor; and (3) the organic compound is degraded is not part of the microorganism's metabolism. Degradation of the compound is brought about by a nonspecific enzyme and provides no benefit to the cell growth. Complete biodegradation of toxic and recalcitrant organic compounds to harmless end products such as CO_2 and H_2O or methane may not always occur, and instead biotransformation to a different organic compound is possible. Care must be taken to determine if the organic compound produced is innocuous, or just as harmful as or more harmful than the initial compound.

Anaerobic Degradation

Many toxic and recalcitrant organic compounds are degraded under anaerobic conditions, with the compound serving as a growth substrate with fermentation and ultimate methane production. Typical examples include nonhalogenated aromatic and aliphatic compounds such as phenol, toluene, alcohols, and ketones. However, most chlorinated organic compounds are not attacked easily under anaerobic conditions and do not serve as growth substrates. Fortuitously, many of these compounds also serve as electron acceptors in anaerobic oxidation reduction reactions.(McCarty, 1999).

Aerobic Biodegradation

With proper environmental conditions, seed source, and acclimation time, a wide range of toxic and recalcitrant organic compounds have been found to serve as growth substrates for heterotrophic bacteria. Such compounds include phenol, benzene, toluene, polyaromatic hydrocarbons, pesticides, gasoline, alcohols, ketones, methylene chloride, vinyl chloride, munitions compounds, and chlorinated phenols. However, many chlorinated organic compounds cannot be attacked readily by aerobic heterotrophic bacteria and thus do not serve as growth substrates.

While a large amount of the chlorinated organic compounds that may be present in municipal and industrial biological wastewater treatment processes are more likely lost from the process by volatilization during aeration, because of their high volatility and the minimal potential for cometabolic bacteria to be present. Fortunately, a number of chlorinated organic compounds are degradable by cometabolic degradation. It should be noted that organic compounds that are saturated fully with chlorine are degraded only by anaerobic dechlorination (Stensel and Bielefeldt, 1997).

Abiotic Losses

Due to concerns about environmental and health effects of toxic and recalcitrant compounds, it is important to understand their fate and transport in biological treatment processes. For many toxic and recalcitrant organic compounds entering biological wastewater treatment processes, nonbiological or abiotic losses may be more significant than biodegradation. Abiotic losses include adsorption of the compound to the mixed liquor solids in the reactor with subsequent transport out of the system by the waste sludge and volatilization with release of the compound to the surrounding atmosphere.

Losses Due to Adsorption

For certain compounds, removal by partitioning (i.e., adsorbing) onto the biomass can be more significant than biodegradation or volatilization. To describe solids partitioning, the Freundlich Isotherm model is modified to a general linear equilibrium relationship (n=1) for adsorption to solids at relatively low liquid organic concentrations:

$$q = K_p S \qquad (2-1)$$

where,

q = g organic adsorbed/g adsorbent

K_p = partition coefficient, L/g

S = concentration of organic compound in liquid, g/m3

Absorption of organic compounds in biological treatment processes has been observed to be relatively fast (Melcer *et al.*, 1994), so that Eq.(2−1) can be used to describe the distribution of the compound between the solid biomass and liquid phases as a function of the partition coefficient K_p for the compound. The value for K_p depends on the hydrophobic nature of the compound and the adsorption characteristics of the solids. Solids with high carbon content and greater surface area result in higher values. The following equation by Dobbs *et al.* (1989) can be used to obtain an estimate of the partition coefficient for wastewater treatment process solids as a function of the compound octanol−water partition coefficient K_{ow}:

$$\log K_p = 0.58 \log K_{ow} + 1.42 \qquad (2-2)$$

where,

K_p = partition coefficient, L/kg
K_{ow} = otanol/water partition coefficient (dimensionless)

Greater amounts of more hydrophobic compounds will be found in the octanol layer. and these compounds will have greater K_p values in solids/water mixtures. Ranges of K_p values for various types of compounds are shown in Table 2.3.

Table 2.3 Comparison of selected estimated partition coefficients(K_p) values for different types of organic compounds.

Organic compound	Kp, L/g
Benzene	0.23
Dinitrotoluene	0.29
Trichloroethene	0.33
Dieldrin	1.48
Phenanthrene	5.33
Pentachlorophenol	10.96
PCB	43.87
Benzopyrene	45.15

[a] Adapted from LaGrega, 2001

Using the equilibrium partition coefficient, the amount of organic compound removed by sludge wasting can be estimated from the ratio of the mass of organic compound adsorbed to the mass of solids wasted per day:

$$q = \frac{r_{ad}}{r_{X,w}} \qquad (2-3)$$

where,

q = g organic compound adsorbed/g solids

r_{ad} = rate of organic compound absorbed daily, g/d

$r_{X,w}$ = rate of solids wasted daily, g/d

By substituting Eq.(2-1) for q and solving for r_{ad} ,the amount of compound lost daily due to adsorption is

$$r_{ad} = -r_{X,w} K_p S \qquad (2-4)$$

At steady state, the amount of solids wasted daily is related to the averrage SRT value for the activated−sludge system :

$$r_{X,w} = \frac{X_T V}{\mathrm{SRT}} \qquad (2-5)$$

Substituting Eq. (2−5) into Eq. (2−4) yields the following expression for mass loss due to adsorption:

$$r_{ad} = \frac{X_T V K_p S}{\mathrm{SRT}} \qquad (2-6)$$

Losses Due to Volatilization

The removal of volatile organic compounds due to aeration (volatilization) is reviewed briefly here.

$$r_{sv} = -K_L a_s (S) \qquad (2-7)$$

where,

r_{sv} = loss due to volatilization, mg/L·d

$K_L a_s$ = $K_L a$ of organic compound, d−1

S = concentration of organic compound in liquid, mg/L

2.3.2 Separation of phenol from water solutions

Phenol-containing wastewater may not be conducted into open water without treatment because of the toxicity of phenol. It also contributes to off-flavours in drinking and food processing waters. Due to the toxic nature of some of these compounds the Environmental Protection Agency has set a water purification standard of less than 1 part per billion (ppb) of phenol in surface waters.

A comparison of the experimental condition for most of these techniques is given, with some comments, in Table 2.4. Actually, several phenol derivatives are also possible water contaminants. The data concerning phenol abatement could be also taken as references for the treatment of waters polluted by phenol derivatives.

Table 2.4 Summary of experimental conditions for technology for the treatment of phenol-water mixtures(G. Busca, *et al.*, 2008).

Technique	Temperature range(°C)	Pressure	Reactor	Additional chemicals	Ref
Distillation	95-180	~1 atm	Distillation column	No	(M. B. King 1969)(QVF Engineer)
Liquid-liquid extraction	I 20-50; II 60-180 (regeneratin)	~1 atm	I washing column; II distillation column	DIPE or MIBK (recycled)	H. G. Franck*et al.*, (1989); C. J. King *et al.*, (1982);QVF Engineering Gmbh
Adsorption (AC)	20-50	~1 atm	I washing column; II distillation column	AC	L. R. Radovic *et al.*, (2000); Z. Hubicki *et al.*, (2005)
Pervaporatin	20-50	~1 atm/1 -20 Torr	Membrane module	Membrane	J. E. Amore *et al.*,(1983);R.J. Schmidt(2005)
Membrane extraction (ex.MTBE)	20-50	~1 atm	Membrane module	Membrane Solvent	J. E. Amore *et al.*,(1983);R.J. Schmidt(2005)

2.4 Activated sludge modeling

2.4.1 Modeling biotic and abiotic losses

A number of models have been developed and evaluated that account for the fate of recalcitrant organic compounds in biological treatment processes (Melcer *et al.*, 1995; Melcer *et al.*, 1994; Monteith *et al.*, 1995; Parker *et al.*, 1993; Grady *et al.*, 1997; and Lee *et al.*, 1998). In general, the models contain basic mechanisms and mass balances that account for the mass rate of the organic compound entering the treatment process, and leaving in the liquid effluent, by biodegradation, by volatilization, and by adsorption on waste solids.

In the following discussion, all of these mechanisms as discussed above are combined into a general model to describe the fate of specific compounds in a biological treatment process. The following steady−state mass balance (i.e., accumulation = 0) across a complete−mix activated−sludge process can be prepared to predict the fate of an organic compound subject to biotic and abiotic processes.

$$0 = \text{organic constituent in influent} - \text{loss of organic constituent due to biodegradation} - \text{loss of organic constituent due to sorption} - \text{loss of organic constituent due to volatilization} - \text{loss of organic constituent in effluent}$$

$$QS_0 = r_{su} + r_{ad} + r_{sv} + QS \quad (2-8)$$

where,

QS_0 = mass of compound in wastewater influent, g/d

r_{su} = biodegradation rate, g/d

r_{ad} = solids adsorption rate, g/d

r_{sv} = volatilization rate, g/d

QS = mass of compound in wastewater effluent, g/d

Substituting the appropriate reaction terms for each component of the mass balance yields the following expression:

$$QS_0 = \left(\frac{1}{Y}\right)\frac{\mu_m S}{(K_s + S)}(X_s)(V) + \frac{X_T V K_p S}{\mathrm{SRT}} + K_L a_s S V + QS \quad (2-9)$$

The fate of the compound in the influent wastewater as a function of the solids concentration, liquid concentration, τ, SRT, and rate terms is obtained by dividing Eq.(2-9) by Q:

$$S_0 = \left(\frac{1}{Y}\right)\frac{\mu_m S}{(K_s + S)}(X_s)\tau + K_p S X_T\left(\frac{\tau}{\mathrm{SRT}}\right) + K_L a_s S(\tau) + S \quad (2-10)$$

Note in Eqs. (2-9) and (2-10), X_s is the biomass concentration capable of degrading the specific organic compound, and X_T is the total MLVSS concentration that includes all the biomass grown on various substrates plus the nonbiodegradable VSS. The value of X_s can be calculated as a function of the amount of substrate that is biodegraded and kinetic coefficients, and the system τ, and SRT. The following expression is used to calculate X_s at steady state for a complete−mixed reactor with consideration for losses of the substrate by volatilization and adsorption:

$$X_s = \frac{Y[(S_0 - S) - K_p S X_T(\tau/\mathrm{SRT}) - K_L a_s S(\tau)]}{k_d(\tau) + (\tau/\mathrm{SRT})} \qquad (2-11)$$

For most cases where biodegradation is occurring and the loss is not overwhelming due to volatilization and/or solids adsorption, the liquid constituent concentration, for a complete−mix reactor at steady state is given by

$$S = \frac{K_s[1 + (k_d)\mathrm{SRT}]}{\mathrm{SRT}(\mu_m - k_d) - 1} \qquad (2-12)$$

For the other exceptional cases, Eq.(2−10) and (2−11) can be solved simultaneously.

The approach outlined above can be used to estimate the fate of an organic compound in a complete−mix activated−sludge reactor assuming steady−state conditions, a constant input of the organic constituent, and a fully acclimated culture.

2.4.2 ASM3 model

2.4.2.1. Explanation of rate expressions

Hydrolysis($\rho 1$)

This process makes available all slowly biodegradable substrates X_S contained in the influent to an activated sludge system. Hydrolysis is assumed to be active independently of the electron donor. This process is different from the hydrolysis process in ASM1; it is of less dominating importance for the rates of oxygen consumption and denitrification.

$$\rho 1 = k_H \cdot ((X_s / X_H) / (K_x + ((X_s / X_H))) \cdot X_H$$

Aerobic storage of X_{STO}($\rho 2$)

This process describes the storage of readily biodegradable substrate S_S in the form of cell internal storage products X_{STO}. This process requires energy, which is obtained from aerobic respiration. It is assumed that all substrates first become stored material and later are assimilated to biomass. This is definitely not observed in reality, however at this moment no reliable model is available which can predict the substrate flux into storage, assimilation and dissimilation respectively. Therefore the Task Group suggests for the time being this simplest assumption. However using a low yield coefficient for storage (Y_{STO}) and a higher one for subsequent growth (Y_H) allows to approximate the consequences of direct growth rather than storage followed by growth.

$$\rho 2 = k_{STO} \cdot (S_o / (K_{O.H} + S_o))\cdot(S_s / (K_s + S_s))\cdot X_H$$

Anoxic storage of X_{STO}(ρ3)

This process is identical to aerobic storage, but denitrification rather than aerobic respiration provides the energy required. Only a fraction of the heterotrophic organisms X_H in activated sludge is capable of denitrification. ASM3 considers this by reducing the anoxic heterotrophic storage rate as compared to the aerobic rate.

$$\rho 3 = k_{STO} \cdot \eta_{NO} \cdot (K_{O.H} / (K_{O.H} + S_{O.H})\cdot(S_s /(K_s + S_s))\cdot(S_{NO} /(K_{NO}+ S_{NO}))\cdot X_H$$

Aerobic growth (ρ4)

The substrate for the growth of heterotroohic organisms is assumed to consist entirely of stored organics X_{STO}. This assumption simplifies ASM3 considerably.

$$\rho 4 = u_H \cdot (S_o / (K_{O.H} + S_o)) \cdot (S_{NH} / (K_{NH} + S_{NH}) \cdot (S_{PO4} / K_{PO4.H} + S_{PO4})) \cdot (S_{ALK} / (K_{ALK} + S_{ALK}))\cdot ((X_{STO} / X_H) / (K_{STO} +(X_{STO} / X_H))) \cdot X_H$$

Anoxic growth(ρ5)

This process is similar to aerobic growth but respiration is based on denitrification. Olny a frantion of the heterotrophic organisms X_H in activated sludge is capable of denitrification. ASM3 considers this by reducing the anoxic heterotrophic storage rate as compared to the aerobic rate.

$$\rho 5 = u_H \cdot \eta_{NO} \cdot (K_{O.H} / (K_{O.H} + S_{O.H}) \cdot (S_{NO} / (K_{NO} + S_{NO})) \cdot (S_{NH} / (K_{NH} + S_{NH}) \cdot (S_{PO4} / (K_P + S_{PO4})) \cdot (S_{ALK} / (K_{ALK} + S_{ALK})) \cdot ((X_{STO} / X_H) / (K_{STO} + (X_{STO} / X_H))) \cdot X_H$$

Aerobic endogenous respiration(ρ6)

This process describes all forms of biomass loss and energy requirements not associated with growth by considering related respiration under aerobic conditions: decay, endogenous respiration, lysis, predation, motility, death, and so on. The model of this process is significantly different from the decay process introduced in ASM1.

$$\rho 6 = b_H \cdot (S_O / (K_{O.H} + S_O)) \cdot X_H$$

Anoxic endogenous respiration(ρ7)

This process is similar to aerobic endogenous respiration but typically slower. Especially prorozoa are considerably less active under denitrifying than under aerobic conditions.

$$\rho 7 = b_H \cdot \eta_{NO.end} \cdot (K_{O.H} / (K_{O.H} + S_{O.H}) \cdot (S_{NO} / (K_{NO} + S_{NO})) \cdot X_H$$

Aerobic respiration of X_{STO}(ρ8)

This process is analogous to endogenous respiration. It assures that storage products, X_{STO}, decay together with biomass.

$$\rho 8 = b_{STO} \cdot (S_o / (K_{O.H} + S_o)) \cdot X_{STO}$$

Anoxic respiration of X_{STO}(ρ9)

This process is analogous to the aerobic process but under denitrifying conditions.

$$\rho 9 = b_{STO} \cdot \eta_{NO.end} \cdot (K_{O.H} / (K_{O.H} + S_{O.H}) \cdot (S_{NO} / (K_{NO} + S_{NO})) \cdot X_{STO}$$

Growth(ρ10)

$$\rho 10 = u_A \cdot (S_o / (K_{O.A} + S_o)) \cdot (S_{NH} / (K_{NH} + S_{NH}) \cdot (S_{PO4} / K_{PO4.H} + S_{PO4})) \cdot (S_{ALK} / (K_{ALK} + S_{ALK})) \cdot X_H$$

Aerobic endogenous respiration(ρ11)

$$\rho 11 = b_A \cdot (S_o / (K_{O.A} + S_o)) \cdot X_A$$

Anoxic endogenous respiration(ρ12)

$$\rho 12 = b_A \cdot \eta_{NO.end.A} \cdot (K_{O.A} / (K_{O.A} + S_O) \cdot (S_{NO} / (K_{NO.A} + S_{NO})) \cdot X_{STO}$$

Storage of X_{PHA}(ρ13)

$$\rho13 = q_{PHA} \cdot (Ss / (K_{S.PAO} + Ss)) \cdot (S_{ALK} / (K_{ALK.PAO} + S_{ALK})) \cdot ((X_{PP} / X_{PAO}) / (K_{PP.PAO} + (X_{PP} / X_{PAO}))) \cdot X_{PAO}$$

Aerobic storage of X_{PP}(ρ14)

$$\rho14 = q_{PP} \cdot (So / (K_{O.PAO} + So)) \cdot (S_{PO4} / K_{PO4.PP} + S_{PO4})) \cdot (S_{ALK} / (K_{ALK.PAO} + S_{ALK})) \cdot ((X_{PHA} / X_{PAO}) / (K_{PHA} + (X_{PHA} / X_{PAO}))) \cdot (((K_{MAX.PAO} - (X_{PP} / X_{PAO})) / (K_{IPP.PAO} + K_{MAX.PAO} - (X_{PP} / X_{PAO}))) \cdot X_{PAO}$$

Anoxic storage of X_{PP}(ρ15)

$$\rho15 = q_{PP} \cdot \eta_{NO.PAO} \cdot (K_{O.PAO} / (K_{O.PAO} + So)) \cdot (S_{NO} / (K_{NO.PAO} + S_{NO})) \cdot (S_{PO4} / K_{PO4.PAO} + S_{PO4})) \cdot (S_{ALK} / (K_{ALK.PAO} + S_{ALK})) \cdot ((X_{PHA} / X_{PAO}) / (K_{PHA} + (X_{PHA} / X_{PAO}))) \cdot (((K_{MAX.PAO} - (X_{PP} / X_{PAO})) / (K_{IPP.PAO} + K_{MAX.PAO} - (X_{PP} / X_{PAO}))) \cdot X_{PAO}$$

Aerobic growth(ρ16)

$$\rho16 = u_{PAO} \cdot (So / (K_{O.PAO} + So)) \cdot (S_{NH} / (K_{NH.PAO} + S_{NH}) \cdot (S_{PO4} / K_{PO4.PP} + S_{PO4})) \cdot (S_{ALK} / (K_{ALK.PAO} + S_{ALK})) \cdot ((X_{PHA} / X_{PAO}) / (K_{PHA} + (X_{PHA} / X_{PAO}))) \cdot X_{PAO}$$

Anoxic growth(ρ17)

$$\rho 17 = u_{PAO} \cdot \eta_{NO.PAO} \cdot (K_{O.PAO}/(K_{O.PAO}+So)) \cdot (S_{NO} / (K_{NO.PAO} + S_{NO})) \cdot (S_{NH} / (K_{NH.PAO} + S_{NH}) \cdot (S_{PO4} / K_{PO4.PAO} + S_{PO4})) \cdot (S_{ALK} / (K_{ALK.PAO} + S_{ALK})) \cdot ((X_{PHA} / X_{PAO}) / (K_{PHA} + (X_{PHA} / X_{PAO}))) \cdot X_{PAO}$$

Aerobic endogenous respiration(ρ18)

$$\rho 18 = b_{PAO} \cdot (So / (K_{O.PAO} + So)) \cdot X_{PAO}$$

Anoxic endogenous respiration(ρ19)

$$\rho 19 = b_{PAO} \cdot \eta_{NO.end.PAO} \cdot (K_{O.PAO}/(K_{O.PAO}+So) \cdot (S_{NO} / (K_{NO.PAO} + S_{NO})) \cdot X_{PAO}$$

Aerobic lysis of X_{PP}(ρ20)

$$\rho 20 = b_{PP} \cdot (So / (K_{O.PAO} + So)) \cdot X_{PP}$$

Anoxic lysis of X_{PP}(ρ21)

$$\rho 21 = b_{PP} \cdot \eta_{NO.lys.PP} \cdot (K_{O.PAO} / (K_{O.PAO} + So)) \cdot (S_{NO} / (K_{NO.PAO} + S_{NO})) \cdot X_{PP}$$

Aerobic respiration of X_{PHA}(ρ22)

$$\rho 22 = b_{PHA} \cdot (So / (K_{O.PAO} + So)) \cdot X_{PHA}$$

Anoxic respiration of X_{PHA}(ρ23)

$$\rho 23 = b_{PHA} \cdot \eta_{NO.resp.PHA} \cdot (K_{O.PAO} / (K_{O.PAO} + S_o)) \cdot (S_{NO} / (K_{NO.PAO} + S_{NO})) \cdot X_{PHA}$$

Phenol adsorption(ρ24)

$$\rho 24 = K_p \cdot S_{phenol} \cdot X_H$$

Phenol volatilisation(ρ25)

$$\rho 25 = K_{LV} \cdot S_{phenol}$$

Phenol growth(ρ26)

$$\rho 26 = \mu_{phenol} \cdot (S_{phenol}/(K_{phenol}+S_{phenol})) \cdot (S_O/(K_{O.H}+S_O)) \cdot (S_{NH}/(K_{NH}+S_{NH}) \cdot X_H$$

2.5 Response surface methodology

Response surface methodology (RSM) is the regression method exploring the relationships between several explanatory variables and one or more response variables. The method was introduced by Box and Wilson (1951). RSM is widely used in various fields, e.g. preparation of chitosan from beet molasses (E.I. Ferreira, *et al.*, 2005), synthesis of N−carboxybutylchitosan (K. Ravikumar, *et al.*, 2005), dye removal by absorbent (Y. Goksungur, 2004) and radiolytic degradation of poly−vinyl alcohol(S.J. Zhang, 2005).

Response Surface Methodology (RSM) is a collection of statistical and mathematical methods that are useful for developing, improving and optimizing a process. The main advantage of RSM is the reduced number of experimental trials required to assess multiple parameters and their interactions(S. Sharma, *et al.*, 2009;M.J. Chen, *et al.*, 2005;F. Karacan, et al., 2007). This methodology can be usefully applied in the development of suitable water treatment technology as it considers the effects of operational parameters on the removal process(S. Sharma, *et al.*, 2009;R. H. Myers, *et al.*, 2002;K. Ravikumar, *et al.*, 2005).

The design procedure for RSM is as follows (V. Gunaraj and N. Murugan, 1999):

(i) Performing a series of experiments for adequate and reliable measurement of the response of interest.

(ii) Developing a mathematical model of the second−order response surface with the best fit.

(iii) Determining the optimal set of experimental parameters that produce a maximum or minimum value of response.

(iv) Representing the direct and interactive effects of process parameters through two and three-dimensional (3-D) plots.

If all variables are assumed to be measurable, the response surface can be expressed as follows:

$$y = f(x1, x2, x3, \cdots, xk)$$

where y is the answer of the system, and xi the variables of action called factors.

The goal is to optimize the response variable (y). An important assumption is that the independent variables are continuous and controllable by experiments with negligible errors. The task then is to find a suitable approximation for the true functional relationship between independent variables and the response surface (V. Gunaraj and N. Murugan, 1999).

Process engineers need to determine the values of the design parameters at which the response reaches its optimum. The optimum could be either a maximum or a minimum of a function of the design parameters. One of the methodologies for obtaining the optimum results is response surface methodology. It is essential that an experimental design methodology be economical for extracting the maximum amount of complex information, a significant reduction in experimental time, saving both material and personnel cost(M. Kincl, *et al.*, 2005).

RSM is a statistical method based on the multivariate non−linear model that has been widely used for optimization of the process variables of adsorption(Z. R. Holan and B. Volesky, 1994;M. M. D. Zulkali, *et al.*, 2006;J. Goel, *et al.*, 2006). Further, RSM consists of designing experiments to provide adequate and reliable measurements of the response, developing a mathematical model having the best fit to the data obtained from the experimental design, and determining the optimal value of the independent variables that produces a maximum or minimum response (D. C. Montgomery, 2001;G. M. Clarke and R. E. Kempson, 1997; J. A. Cornell, 1990;G. Box and N. Draper, 1987).

It is also useful in studying the interactions of the various parameters affecting the process. RSM examines the responses of several factors by varying them simultaneously with limited number of experiments. It is worthy to quote that the response surface methodology does not elucidate the mechanism of the processes studied but only ascertains the effects of factors upon response and the interactions between the factors. Nevertheless, the RSM is a powerful tool for statistical modelling and optimization of the separation processes using lesser number of experimental runs planned according to experimental design (C. Cojocaru and G. Zakrzewska−Trznadel, 2007).

Ⅲ. Experiment methods

In this study, for simulating the fate of phenol in the wastewater treatment plant, ASM3 modeling are used, by the actual average data of all the wastewater treatment plants in Busan and use of the program of response surface methodology, we estimate the efficiency of the modeling.

3.1 The selection of simulator

AQUASIM

In this study, the simulator which we used is the AQUASIM(Computer Program for the Identification and Simulation of Aquatic Systems) (Gujer *et al.*, 1999) developed in 1999. As the biological reaction can be changed arbitrarily based on the user in Aquasim, simulating the new concept modeling is possibility. Table 3.1 is a summary of the simulation characteristic of wastewater treatment plant.

Table 3.1 Simulator types(Jaesin Han, 2010)

Class	Program	Advantage	Disadvantage
Text base	Aquasim ASIM Simnon	1.Suitable for researcher 2.Good composed attitude 3.Generally cheap 4.Quick computing speed	1.Difficult for beginner 2.Generally difficult sediment modeling
Graphic base	GPS-X WEST Simba Bio-win	1.Suitable for beginner and operator in site 2.Easy to use	1.Little composed attitude 2.Generally expensive
General purpose	MATLAB ACSL C+ Fortran	1.Suitable for researcher 2.Great composed attitude 3.Convenient for expert	Difficult for inexperienced person

3.2 Phenol concentration of wastewater treatment plants

The data of phenol from all the wastewater treatment plants in Busan is used for the modeling. The modeling researched in my study is applied for all the wastewater treatment plant in Busan.

Table 3.2 Phenol concentration of all the wastewater treatment plants in Busan in 2010.

WWTP	Phenol (mg/L)	
	Influent	Effluent
Suyoung	0.67	0.54
	0.66	0.52
	0.81	0.21
	0.75	0.21
Gangbyun	0.8	0.51
Nambu	0.6	0.49
	0.75	0.31
Haewoondai	0.77	0.37
	0.91	0.43
	1.91	1.61
Noksan	1.05	0.24
Seobu	0.89	0.39
	0.95	0.36
Jungang	0.5	0.22
	0.55	0.15
Gijang	0.48	0.27
	0.49	0.23
Junkwan	1.5	0.8
	1.2	0.5

3.3 Sensitivity analysis and estimation of parameters

We will add the phenol removal process in ASM3 modeling. Carrying out the sensitivity analysis by Aquasim. We establish and approve the parameters through the actual average effluent concentration of phenol and using the program of response surface methodology.

Ⅳ. Results and discussion

4.1 The data of phenol from lewater all the wastewater treatment plants in Busan

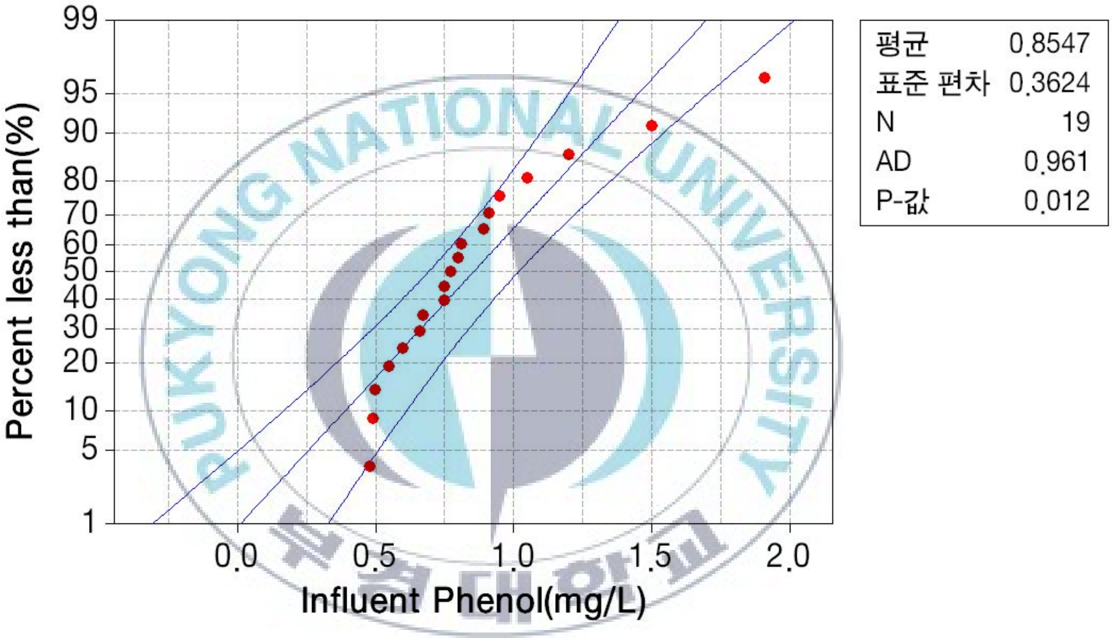


Fig.4.1 Influent concentration percent of phenol in all the wastewater treatment plants in Busan.

The actual data of influent concentration of phenol from all the wastewater treatment plants in Busan is showed in Fig.4.1.

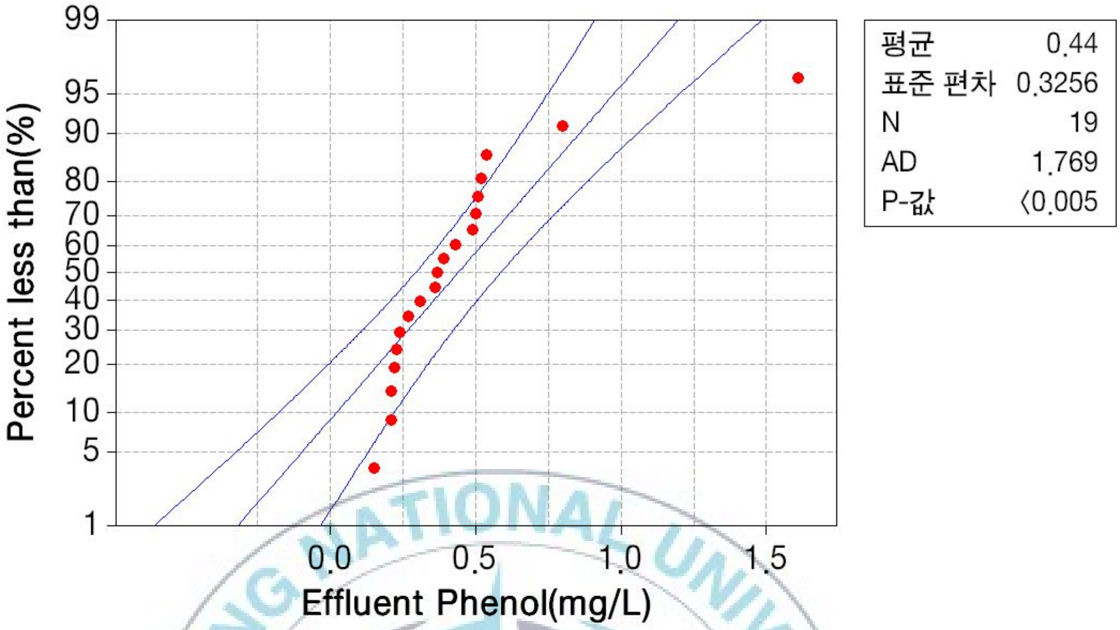


Fig.4.2 Effluent concentration percent of phenol in all the wastewater treatment plants in Busan.

The actual data of effluent concentration of phenol from all the wastewater treatment plants in Busan is showed in Fig.4.2.

4.2 The development of the treatment of phenol added in ASM3 modeling

ASM3 includes only the microbiological transformation processes. Chemical precipitation processes are not included, but may easily be added based on the information provided for ASM2 (Henze *et al.*, 1995). Though ASM3 trace the removal of organic matter and nitrogen for a basis, the process of toxic organic compounds's removal can be added possibly when the basic rescue is not changed by the form of a module.

4.2.1 The assortment of matters

The modeling include 19 kinds of matters. There are dissolved maters S(Soluble) and particle matters X(Particulate) generally. The total matters described in the following Table 4.1 .

Table 4.1 Description of state variables

State Variable Descriotion	State Symbol	Units
Soluble component		
Dossolved Oxygen	S_o	kg O_2/m^3
Readily biodegradable organic substrate	S_s	kg COD/m^3
Phenol	S_{Phenol}	kmol P/m^3
Inert soluble organic material	S_I	kg COD/m^3
Ammonium	S_{NH4}	g N/m^3
Nitrate and nitrite nitrogen	S_{NO}	kmol N/m^3
Dinitrogen(N_2)	S_{N2}	kmol N/m^3
Alkalinity	S_{ALK}	kmol HCO_3^-/m^3
Particulate component		
Inert particulate organic material	X_I	kg COD/m^3
Slowly biodegradable substrate	X_S	kg COD/m^3
Heterotrophic organisms	X_H	kg COD/m^3
Internal storage product of heterotrophic organisms	X_{STO}	kg COD/m^3
Phosphorus Accumulating Organisms	X_{PAO}	kg COD/m^3
Polyphophate	X_{PP}	kg COD/m^3
Cell−internal storage product of X_{PAO}	X_{PHA}	kg COD/m^3
Nitrifying organisms	X_A	kg COD/m^3
Total Suspended Solid	X_{TSS}	kg TSS/m3

4.2.2 The addition of ASM3 matrix with phenol treatment process

It is the responsibility of the user of ASM3 to determine the concentrations of relevant compounds in the wastewater, as well as the stoichiometric and kinetic parameters, which apply to the specific case to be dealt with. Absolute values of these parameters are not part of ASM3. They are necessary, however, if ASM3 is to be applied to any specific case.

In Table 4.2−4.3 a set of typical model parameters are provided for convenience. They are merely presented here as a reference for testing computer code and as a first estimate for the design of possible experiments that may be used to identify these parameters more accurately.

Table 4.2 Stoichiometric matrix of ASM3+phenol

	i Variable	1	2	3	4	5	6	7	8
j	Precess ↓	S_O	S_S	S_{phenol}	S_I	S_{NH4}	S_{NOX}	S_{N2}	S_P
Hydrolysis									
1	hydrolysis		$1-f_{SI}$		f_{SI}	$i_{N,XS}-i_{N,SS}(1-f_{SI})-i_{N,SI}\cdot f_{SI}$			$i_{P.XS}-i_{P.SS}$
Heterotrophic organisms, X_H									
2	Aerobic storage of X_{STO}	$-(1-Y_{STO})-(2.383-YHP)/YHP$	-1	-1/YHP		$i_{N,SS}$			$i_{P,SS}$
3	Anoxic storage of X_{STO}		-1	-1/YHP		$i_{N,SS}$	$-(1-Y_{STO,N})/2.86$	$(1-Y_{STO,N})/2.86$	$i_{P,SS}$
4	Aerobic growth	$1-(1/Y_H)$				$-i_{N,BM}$			$-i_{P,BM}$
5	Anoxic growth					$-i_{N,BM}$	$(1-(1/Y_{STO,N}))/2.86$	$-(1-(1/Y_{STO,N}))/2.86$	$-i_{P,BM}$
6	Aerobic endogenous respiration	$-(1-f_{XI})$				$i_{N,BM}-f_{XI}\cdot i_{N,XI}$			$i_{P,BM}-f_{XI}\cdot i_{P,XI}$
7	Anoxic endogenous respiration					$i_{N,BM}-f_{XI}\cdot i_{N,XI}$	$-(1-f_{XI})/2.86$	$(1-f_{XI})/2.86$	$i_{P,BM}-f_{XI}\cdot i_{P,XI}$
8	Aerobic respiration of X_{STO}	-1							
9	Anoxic respiration of X_{STO}						-1/2.86	1/2.86	
Autotrophic organisms, X_A									
10	Growth	$1-(4.57/Y_A)$				$-(1/Y-i_{N,BM})$	$1/Y_A$		$-i_{P.BM}$
11	Aerobic endogenous respiration	$-(1-f_{XI})$				$i_{N,BM}-f_{XI}\cdot i_{N,XI}$			$i_{P,BM}-f_{XI}\cdot i_{P,XI}$
12	Anoxic endogenous respiration					$i_{N.BM}-f_{XI}\cdot i_{N.XI}$	$-(1-f_{XI})/2.86$	$(1-f_{XI})/2.86$	$i_{P,BM}-f_{XI}\cdot i_{P,XI}$
Phosphorus accumulation organisms, X_{PAO}									
13	Storage of X_{PHA}		-1			$i_{N,SS}$			$Y_{PO4}+i_{P.SS}$
14	Aerobic storage of X_{PP}	$-Y_{PHA}$							-1
15	Anoxic storage of X_{PP}						$-Y_{PHA}/2.86$	$Y_{PHA}/2.86$	-1
16	Aerobic growth	$1-(1/Y_{PAO,O2})$			$-i_{N,BM}$				$-i_{P.BM}$
17	Anoxic growth					$-i_{N,BM}$	$(1-(1/Y_{PAO,NO}))/2.86$	$-(1-(1/Y_{PAO,NO}))/2.86$	$-i_{P.BM}$
18	Aerobic endogenous respiration	$-(1-f_{XI})$				$i_{N,BM}-f_{XI}\cdot i_{N,XI}$			$i_{P,BM}-f_{XI}\cdot i_{P,XI}$
19	Anoxic endogenous respiration					$i_{N,BM}-f_{XI}\cdot i_{N,XI}$	$-(1-f_{XI})/2.86$	$(1-f_{XI})/2.86$	$i_{P,BM}-f_{XI}\cdot i_{P,XI}$
20	Aerobic lysis of X_{PP}								1
21	Anoxic lysis of X_{PP}								1
22	Aerobic respiration of X_{PHA}	-1							
23	Anoxic respiration of X_{PHA}						-1/2.86	1/2.86	
24	Phenol adsorption			-1					
25	Phenol volatilisation			-1					
26	Phenol growth			$-(1-Y_{HP})/(2.383-Y_{HP})$					

Table 4.2 Stoichiometric matrix of ASM3+phenol (continued)

	i Variable	9	10	11	12	13	14	15	16	17	18
j	Precess ↓	S_{ALK}	X_I	X_S	X_H	X_{STO}	X_{PAO}	X_{PP}	X_{PHA}	X_A	X_{TSS}
Hydrolysis											
1	hydrolysis	$\nu_{1,ALK}$		-1							$\nu_{1,TSS}$
Heterotrophic organisms, X_H											
2	Aerobic storage of X_{STO}	$\nu_{2,ALK}$				$Y_{STO.O2}$					$\nu_{2,TSS}$
3	Anoxic storage of X_{STO}	$\nu_{3,ALK}$				$Y_{STO.O2}$					$\nu_{3,TSS}$
4	Aerobic growth	$\nu_{4,ALK}$			1	$-(1/Y_{H.O2})$					$\nu_{4,TSS}$
5	Anoxic growth	$\nu_{5,ALK}$			1	$-(1/Y_{H.NO})$					$\nu_{5,TSS}$
6	Aerobic endogenous respiration	$\nu_{6,ALK}$	f_{XI}		-1						$\nu_{6,TSS}$
7	Anoxic endogenous respiration	$\nu_{7,ALK}$	f_{XI}		-1						$\nu_{7,TSS}$
8	Aerobic respiration of X_{STO}	$\nu_{8,ALK}$				-1					$\nu_{8,TSS}$
9	Anoxic respiration of X_{STO}	$\nu_{9,ALK}$				-1					$\nu_{9,TSS}$
Autotrophic organisms, X_A											
10	Growth	$\nu_{10,ALK}$								1	$\nu_{10,TSS}$
11	Aerobic endogenous respiration	$\nu_{11,ALK}$	f_{XI}							-1	$\nu_{11,TSS}$
12	Anoxic endogenous respiration	$\nu_{12,ALK}$	f_{XI}							-1	$\nu_{12,TSS}$
Phosphorus accumulation organisms, X_{PAO}											
13	Storage of X_{PHA}	$\nu_{13,ALK}$						$-Y_{PO4}$	1		$\nu_{13,TSS}$
14	Aerobic storage of X_{PP}	$\nu_{14,ALK}$						1	$-Y_{PHA}$		$\nu_{14,TSS}$
15	Anoxic storage of X_{PP}	$\nu_{15,ALK}$						1	$-Y_{PHA}$		$\nu_{15,TSS}$
16	Aerobic growth	$\nu_{16,ALK}$					1		$-(1/Y_{PAO.O2})$		$\nu_{16,TSS}$
17	Anoxic growth	$\nu_{17,ALK}$					1		$-(1/Y_{PAO.NO})$		$\nu_{17,TSS}$
18	Aerobic endogenous respiration	$\nu_{18,ALK}$	f_{XI}				-1				$\nu_{18,TSS}$
19	Anoxic endogenous respiration	$\nu_{19,ALK}$	f_{XI}				-1				$\nu_{19,TSS}$
20	Aerobic lysis of X_{PP}	$\nu_{20,ALK}$						-1			$\nu_{20,TSS}$
21	Anoxic lysis of X_{PP}	$\nu_{21,ALK}$						-1			$\nu_{21,TSS}$
22	Aerobic respiration of X_{PHA}	$\nu_{22,ALK}$							-1		$\nu_{22,TSS}$
23	Anoxic respiration of X_{PHA}	$\nu_{23,ALK}$							-1		$\nu_{23,TSS}$
24	Phenol adsorption										
25	Phenol volatilisation										
26	Phenol growth				1						

Table 4.3 Activated sludge model NO. 3 (ASM3) Process

j	Process ↓	Process Rate, ρ_j [$ML^{-3}T^{-1}$]
Hydrolysis		
1	hydrolysis	$k_H\cdot((X_S/X_H)/(K_X+(X_S/X_H)))\cdot X_H$
Heterotrophic organisms, X_H		
2	Aerobic storage of X_{STO}	$k_{STO}\cdot(S_O/(K_{O.H}+S_O))\cdot(S_S/(K_S+S_S))\cdot X_H$
3	Anoxic storage of X_{STO}	$k_{STO}\cdot\eta_{NO}\cdot(K_{O.H}/(K_{O.H}+S_{O.H})\cdot(S_S/(K_S+S_S))\cdot(S_{NO}/(K_{NO}+S_{NO}))\cdot X_H$
4	Aerobic growth	$\mu_H\cdot(S_O/(K_{O.H}+S_O))\cdot(S_{NH}/(K_{NH}+S_{NH})\cdot(S_{PO4}/(K_{PO4.H}+S_{PO4}))\cdot(S_{ALK}/(K_{ALK}+S_{ALK}))\cdot((X_{STO}/X_H)/(K_{STO}+(X_{STO}/X_H)))\cdot X_H$
5	Anoxic growth	$\mu_H\cdot\eta_{NO}\cdot(K_{O.H}/(K_{O.H}+S_{O.H}))\cdot(S_{NO}/(K_{NO}+S_{NO}))\cdot(S_{NH}/(K_{NH}+S_{NH})\cdot(S_{PO4}/(K_P+S_{PO4}))\cdot(S_{ALK}/(K_{ALK}+S_{ALK}))\cdot((X_{STO}/X_H)/(K_{STO}+(X_{STO}/X_H)))\cdot X_H$
6	Aerobic endogenous respiration	$b_H\cdot(S_O/(K_{O.H}+S_O))\cdot X_H$
7	Anoxic endogenous respiration	$b_H\cdot\eta_{NO.end}\cdot(K_{O.H}/(K_{O.H}+S_{O.H})\cdot(S_{NO}/(K_{NO}+S_{NO}))\cdot X_H$
8	Aerobic respiration of X_{STO}	$b_{STO}\cdot(S_O/(K_{O.H}+S_O))\cdot X_{STO}$
9	Anoxic respiration of X_{STO}	$b_{STO}\cdot\eta_{NO.end}\cdot(K_{O.H}/(K_{O.H}+S_{O.H})\cdot(S_{NO}/(K_{NO}+S_{NO}))\cdot X_{STO}$
Autotrophic organisms, X_A		
10	Growth	$\mu_A\cdot(S_O/(K_{O.A}+S_O))\cdot(S_{NH}/(K_{NH}+S_{NH}))\cdot(S_{PO4}/(K_P+S_{PO4}))\cdot(S_{ALK}/(K_{ALK\,A}+S_{ALK}))\cdot X_H$
11	Aerobic endogenous respiration	$b_A\cdot(S_O/(K_{O.A}+S_O))\cdot X_A$
12	Anoxic endogenous respiration	$b_A\cdot\eta_{NO.end.A}\cdot(K_{O.A}/(K_{O.A}+S_O)\cdot(S_{NO}/(K_{NO.A}+S_{NO}))\cdot X_{STO}$
Phosphorus accumulation organisms, X_{FAO}		
13	Storage of X_{PHA}	$q_{PHA}\cdot(S_S/(K_{S.PAO}+S_S))\cdot(S_{ALK}/(K_{ALK.PAO}+S_{ALK}))\cdot((X_{PP}/X_{FAO})/(K_{PP.FAO}+(X_{PP}/X_{FAO})))\cdot X_{FAO}$
14	Aerobic storage of X_{PP}	$q_{PP}\cdot(S_O/(K_{O.PAO}+S_O))\cdot(S_{PO4}/(K_{PO4.PP}+S_{PO4}))\cdot(S_{ALK}/(K_{ALK.PAO}+S_{ALK}))\cdot((X_{PHA}/X_{FAO})/(K_{PHA}+(X_{PHA}/X_{FAO})))\cdot(((K_{MAX.PAO}-(X_{PP}/X_{PAO}))/(K_{IPP.PAO}+K_{MAX.PAO}-(X_{PP}/X_{FAO})))\cdot X_{FAO}$
15	Anoxic storage of X_{PP}	$q_{PP}\cdot\eta_{NO.FAO}\cdot(K_{O.PAO}/(K_{O.PAO}+S_O))\cdot(S_{NO}/K_{NO.PAO}+S_{NO}))\cdot(S_{PO4}/(K_{PO4.PP}+S_{PO4}))\cdot(S_{ALK}/(K_{ALK.PAO}+S_{ALK}))\cdot((X_{PHA}/X_{FAO})/(K_{PHA}+(X_{PHA}/X_{PAO})))\cdot(((K_{MAX.PAO}-(X_{PP}/X_{FAO}))/(K_{IPP.PAO}+K_{MAX.FAO}-(X_{PP}/X_{PAO})))\cdot X_{PAO}$
16	Aerobic growth	$\mu_{FAO}\cdot(S_O/(K_{O.FAO}+S_O))\cdot(S_{NH}/(K_{NH.FAO}+S_{NH}))\cdot(S_{PO4}/(K_{PO4.PAO}+S_{PO4}))\cdot(S_{ALK}/(K_{ALK.PAO}+S_{ALK}))\cdot((X_{PHA}/X_{PAO})/(K_{PHA}+(X_{PHA}/X_{PAO})))\cdot X_{PAO}$
17	Anoxic growth	$\mu_{FAO}\cdot\eta_{NO.PAO}\cdot(K_{O.PAO}/(K_{O.FAO}+S_O))\cdot(S_{NO}/(K_{NO.FAO}+S_{NO}))\cdot(S_{NH}/(K_{NH.PAO}+S_{NH}))\cdot(S_{PO4}/(K_{PO4.PAO}+S_{PO4}))\cdot(S_{ALK}/(K_{ALK.FAO}+S_{ALK}))\cdot((X_{PHA}/X_{FAO})/(K_{PHA}+(X_{PHA}/X_{PAO})))\cdot X_{PAO}$
18	Aerobic endogenous respiration	$b_{FAO}\cdot(S_O/(K_{O.PAO}+S_O))\cdot X_{FAO}$
19	Anoxic endogenous respiration	$b_{FAO}\cdot\eta_{NO.end.PAO}\cdot(K_{O.PAO}/(K_{O.FAO}+S_O)\cdot(S_{NO}/(K_{NO.PAO}+S_{NO}))\cdot X_{FAO}$
20	Aerobic lysis of X_{PP}	$b_{PP}\cdot(S_O/(K_{O.PAO}+S_O))\cdot X_{PP}$
21	Anoxic lysis of X_{PP}	$b_{PP}\cdot\eta_{NO.lys.PP}\cdot(K_{O.PAO}/(K_{O.PAO}+S_O)\cdot(S_{NO}/(K_{NO.PAO}+S_{NO}))\cdot X_{PP}$
22	Aerobic respiration of X_{PHA}	$b_{PHA}\cdot(S_O/(K_{O.PAO}+S_O))\cdot X_{PHA}$
23	Anoxic respiration of X_{PHA}	$b_{PHA}\cdot\eta_{NO.resp.PHA}\cdot(K_{O.PAO}/(K_{O.FAO}+S_O)\cdot(S_{NO}/(K_{NO.PAO}+S_{NO}))\cdot X_{PHA}$
24	Phenol adsorption	$K_p\cdot S_{phenol}\cdot X_H$
25	Phenol volatilisation	$K_{LV}\cdot S_{phenol}$
26	Phenol growth	$\mu_{phenol}\cdot(S_{phenol}/(K_{phenol}+S_{phenol}))\cdot(S_O/(K_{O.H}+S_O))\cdot(S_{NH}/(K_{NH}+S_{NH})\cdot X_H$

4.2.3 Mathematical Formulation

Mathematical formulation of all the state variables are discussed below. Biological processes affect almost all variables except the inert component which are only affected by physical processes like sedimentation, mixing and resuspension.

1. Oxygen (So)

Dissolved oxygen plays a fundamental role in natural wastewater treatment systems.The concentration of dissolved oxygen in the pond is determined by the joint action of the following main mechanisms.

1. Consumption of oxygen by the aerobic bacteria (autotrophic and heterotrophic)
2. Generation of oxygen by algal photosynthesis
3. Oxygen reaeration through the air-water interface

$$dSo/dt = (-(1-Y_{STO}) - (2.383-Y_{HP}) / Y_{HP}) * \rho 2 + (1-(1/Y_H)) * \rho 4 + (-(1-f_{XI})) * \rho 6 + (-1) * \rho 8 + (1-(4.57/YA)) * \rho 10 + (-(1-f_{XI})) * \rho 11 + (-Y_{PHA}) * \rho 14 + (1-(1/Y_{PAO.O2})) * \rho 16 + (-(1-f_{XI})) * \rho 18 + (-1) * \rho 22$$

2. Inert soluble (S_I)

Inert soluble materials flow unchanged through the waste stabilization pond.

$$dS_I/dt = f_{SI} * \rho 1 + (-i_{N.BM}) * \rho 16$$

3.Readily biodegradable component (S_S)

Readily biodegradable components are composed of simple (low molecular) compounds. They are consumed by hetrotrohic and autotrophic bacteria and produced during hydrolysis of slowly biodegradable particulate.

$$dSs/dt=(1-f_{SI}) * \rho1 + (-1) *\rho2+ (-1) * \rho3+(-1)* \rho13$$

4. Slowly biodegradable particulate COD (X_S)

These are composed of high molecular compounds. They are produced during decay of biomasses in waste stabilization ponds. The hydrolysis process convert them to readily biodegradable materials.

$$dXs/dt = (-1) * \rho1$$

5. Particulate inert organic matter (X_I)

$$dX_I/dt = f_{XI} * \rho6 +f_{XI} * \rho7 + f_{XI} * \rho11+f_{XI} *\rho12+ f_{XI} *\rho18+f_{XI} *\rho19$$

6. Nitrate (S_{NO})

The concentration of nitrate is increased by aerobic growth of autotrophs (nitrification) and decreased by anoxic growth of hetrotrophs (denitrification). Algal growth also decreases the concentration of nitrate. Algae prefer to take up ammonium instead of nitrate (M. A. Senzia, *et al.*, 2002). Therfore, when ammonium concentration is high, nitrate uptake is low due to switching function added to the growth equation.

$$dS_{NOX}/dt = (-(1-Y_{STO.N})/2.86) * \rho 3 + ((1-(1/Y_{STO.N}))/2.86) * \rho 5 + (-(1-f_{XI})/2.86) * \rho 7 + (-1/2.86) * \rho 9 + (1/Y_A) * \rho 10 + (-(1-f_{XI}) / 2.86) * \rho 12 + (-Y_{PHA} / 2.86) * \rho 15 + ((1-(1/Y_{PAO.NO}))/2.86) * \rho 17 + (-(1-f_{XI})/2.86) * \rho 19 + (-1/2.86) * \rho 23$$

7. Phosphorus-accumulating organisms(X_{PAO})

These organisms are assumed to be representative for all types of polyphosphate-accumulating organisms. They are all assumed to grow aerobically and some of them anoxically. The concentration of X_{PAO} does not include the cell-internal storage products X_{PP} and X_{PHA}, but only the "true" biomass.

$$dX_{PAO}/dt = \rho 16 + \rho 17 + (-1) * \rho 18 + (-1) * \rho 19$$

8. Cell−internal storage product of phosphorus−accumulating organisms(X_{PHA})

It primarily includes poly−hydroxy−alkanoates (PHA) and glycogen. Although it occurs only in association with X_{PAO}, it is not included in the mass of X_{PAO}. X_{PHA} cannot be compared directly with analytically measured PHA concentrations; it is a functional component required for modeling but cannot be directly identified in chemical terms. However, it is recovered in COD analysis, where it must satisfy ThOD conservation. For stoichiometric considerations, X_{PHA} is assumed to have the chemical composition of poly−hydroxy−butyrate $(C_4H_6O_2)n$.

$dX_{PHA}/dt = \rho 13 + (-Y_{PHA}) * \rho 14 + (-Y_{PHA}) * \rho 15 + (-(1/Y_{PAO.O2})) * \rho 16 + (-(1/Y_{PAO.NO})) * \rho 17 + (-1) * \rho 22 + (-1) * \rho 23$

9. Polyphosphate (X_{PP})

This is a cell−internal inorganic storage product of PAO. It is assumed to be associated only with X_{PAO} but is not included in the latter's mass. It forms part of the particulate phosphorus and may be analytically observed. For stoichiometric considerations, poly−phosphate is assumed to have the composition of $(K_{0.34}Mg_{0.33}PO_3)n$. Since the Bio−P module does not account for K^+ and Mg^{2+}, an electric charge of −1/31 must be included to compensate for this term.

$dX_{PP}/dt = (-Y_{PO4}) * \rho 13 + \rho 14 + \rho 15 + (-1) * \rho 20 + (-1) * \rho 21$

10. Phenol

$dS_{phenol}/dt = (-1/YHP) * \rho 2 + (-1/YHP) * \rho 3 + (-1) * \rho 24 + (-1) * \rho 25 + (-(1-Y_{HP})/(2.383-Y_{HP})) * \rho 26$

11. Ammonium (S_{NH4})

For the balance of the ionic charges, S_{NH4} is assumed to be all NH_4^+.Because ASM3 assumes that organic compounds contain a fixed fraction of organic nitrogen, the influent $S_{NH4,0}$ cannot be observed directly but should be computed from wastewater composition ; Kjeldahl nitrogen − organic nitrogen. In the activated sludge reactors and in the effluent S_{NH4} is equivalent to observed concentrations. With the redox reference level chosen, S_{NH4} does not have a ThOD.

$dS_{NH4}/dt = (i_{N.XS}-i_{N.SS}(1-f_{SI})- i_{N.SI} \cdot f_{SI}) * \rho 1 + i_{N.SS} * \rho 2 + i_{N.SS} * \rho 3 + (-i_{N.BM}) * \rho 4 + (-i_{N.BM}) * \rho 5 + (i_{N.BM} - f_{XI} \cdot i_{N.XI}) * \rho 6 + (i_{N.BM}-f_{XI} \cdot i_{N.XI}) * \rho 7 + (-(1/Y-i_{N.BM})) * \rho 10 + (i_{N.BM}-f_{XI} \cdot i_{N.XI}) * \rho 11 + (i_{N.BM}-f_{XI} \cdot i_{N.XI}) * \rho 12 + i_{N.SS} * \rho 13 + (-i_{N.BM}) * \rho 17 + (i_{N.BM}-f_{XI} \cdot i_{N.XI}) * \rho 18 + (i_{N.BM}-f_{XI} \cdot i_{N.XI}) * \rho 19$

12. Dinitrogen (S_{N2})

S_{N2} is assumed to be the only product of denitrification. S_{N2} may be subject to gas exchange, parallel with oxygen, S_{O2}. It can then be used to predict problems due to supersaturation with N_2 in secondary clarifiers. Alternatively the N_2 contained in the influent and gas exchange can be neglected. S_{N2} may then be used to calculate the amount of nitrogen lost due to denitrification. S_{N2} has a negative ThOD.

$dS_{N2}/dt = ((1-Y_{STO.N})/2.86) * \rho 3 + (-(1-(1/Y_{STO.N}))/2.86) * \rho 5+((1-f_{XI})/2.86) * \rho 7+ (1/2.86) * \rho 9 + ((1-f_{XI}) / 2.86) * \rho 12 +(Y_{PHA} / 2.86) * \rho 15+ (-(1-(1/Y_{PAO.NO}))/2.86) * \rho 17 +((1-f_{XI})/2.86) * \rho 19 + (1/2.86) * \rho 23$

13. Alkalinity of the wastewater (S_{ALK})

Alkalinity is used to approximate the conservation of ionic charge in biological reactions. Alkalinity is introduced in order to obtain an early indication of possible low pH conditions, which might inhibit some bilogical processes. For all stoichiometric computations, S_{ALK} is assumed to be bicarbonate, HCO_3, only.

$dS_{ALK}/dt = \nu_{1.ALK} * \rho 1 + \nu_{2.ALK} * \rho 2+ \nu_{3.ALK} * \rho 3+ \nu_{4.ALK} * \rho 4 + \nu_{5.ALK} * \rho 5 + \nu_{6.ALK} * \rho 6+ \nu_{7.ALK} * \rho 7+\nu_{8.ALK} * \rho 8 +\nu_{9.ALK} * \rho 9 + \nu_{10.ALK} * \rho 10 + \nu_{11.ALK} * \rho 11+ \nu_{12.ALK} * \rho 12 +\nu_{13.ALK} * \rho 13 +\nu_{14.ALK} * \rho 14 +\nu_{15.ALK} * \rho 15+ \nu_{16.ALK} * \rho 16 \ \nu_{17.ALK} * \rho 17 + \nu_{18.ALK} * \rho 18+ \nu_{19.ALK} * \rho 19+ \nu_{20.ALK} * \rho 20 + \nu_{21.ALK} * \rho 21+ \nu_{22.ALK} * \rho 22+ \nu_{23.ALK} * \rho 23$

14. Heterotrophic organisms (X_H)

These organisms are assumed to be the "allrounder" heterotrophic organisms, they can grow aerobically and many of them also anoxically. These organisms are responsible for hydrolysis of particulate substrates X_S and can metabolize all degradable organic substrates, They can form organic storage products in the form of poly−hydroxy−alkanoates or glycogen. X_H are assumed to have no anaerobic activity except cell external hydrolysis, which is the only anaerobic process in ASM3.

$$dX_H/dt = \rho 4 + \rho 5 + (-1) * \rho 6 + (-1) * \rho 7 + 1 * \rho 26$$

15. A cell internal storage product of heterotrophic organisms (X_{STO})

It includes poly−hydroxy−alkanoates(PHA), glycogen, etc. It occurs only associated with X_H; it is, however, not included in the mass of X_H. X_{STO} cannot be directly compared with analytically measured PHA or glycogen concentrations; X_{STO} is only a functional compound required for modelling but not directly identifiable chemically. X_{STO} may, however, be recovered in COD analysis and must satisfy ThOD conservation. For stoichiometric considerations, X_{STO} is assumed to have the chemical composition of poly−hydroxy− butyrate$(C_4H_6O_2)_n$.

$$dX_{STO}/dt = Y_{STO.O2} * \rho 2 + Y_{STO.O2} * \rho 3 + (-(1/Y_{H.O2})) * \rho 4 + (-(1/Y_{H.NO})) * \rho 5 + (-1) * \rho 8 + (-1) * \rho 9$$

16. Nitrifying organisms (X_A)

Nitrifying organisms are responsible for nitrification; they are obligate aerobic, chemo−litho−autotrophic. It is assumed that nitrifiers oxidize ammonium, S_{NH4}, directly to nitrate, S_{NOX}. Nitrite as an intermediate compound of nitrification is not considered in ASM3.

$$dX_A/dt = \rho 10 + (-1) * \rho 11 + (-1) * \rho 12$$

17. Total suspended solids (X_{TSS})

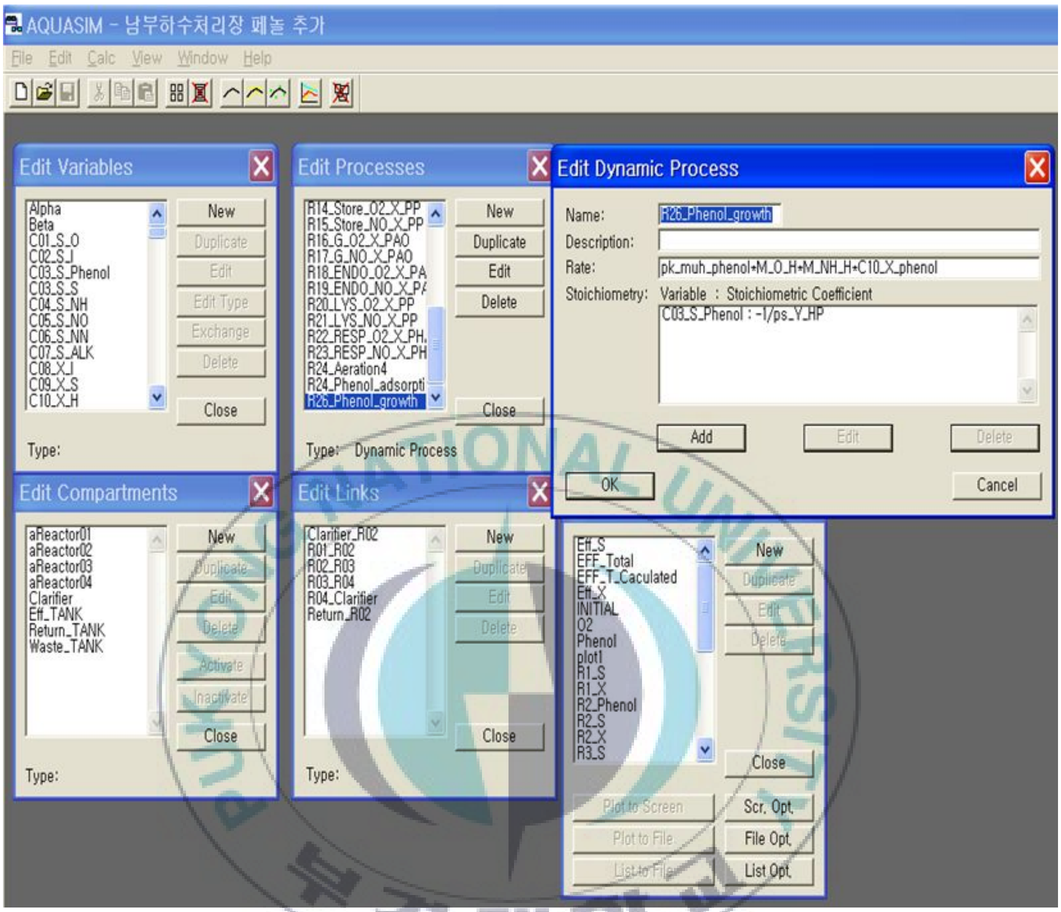
Suspended solids are introduced into the bio−kinetic models in order to compute their concentration via stoichiometric. Treatment plant operators typically follow SS in day to day analysis. In the influent, SS include an inorganic fraction of SS and the "soluble' fraction of XS.0, which passes membrane filters.

$$dX_{TSS}/dt = \nu_{1.TSS} * \rho1 + \nu_{2.TSS} *\rho2+ \nu_{3.TSS} * \rho3+ \nu_{4.TSS} * \rho4 + \nu_{5.TSS} * \rho5 + \nu_{6.TSS} * \rho6 + \nu_{7.TSS} * \rho7 +\nu_{8.TSS} * \rho8 +\nu_{9.TSS} * \rho9+ \nu_{10.TSS} * \rho10+ \nu_{11.TSS} * \rho11+ \nu_{12.TSS} * \rho12+\nu\nu_{13.TSS} * \rho13 +\nu_{14.TSS} * \rho14 +\nu_{15.TSS} * \rho15+ \nu_{16.TSS} * \rho16 + \nu_{17.TSS} * \rho17+ \nu_{18.TSS} * \rho18 + \nu_{19.TSS} * \rho19+ \nu_{20.TSS} * \rho20 + \nu_{21.TSS} * \rho21 + \nu_{22.TSS} * \rho22+ \nu_{23.TSS} *\rho23$$

18. Soluble orthophosphate(S_P)

$$dS_P/dt = (i_{P.XS.} \cdot i_{P.SS}) * \rho1+(i_{P.SS}) * \rho2 + (i_{P.SS}) * \rho3 + (-i_{P.BM}) * \rho4+(-i_{P.BM}) * \rho5 + (i_{P.BM} - f_{XI} \cdot i_{P.XI}) *\rho6+(i_{P.BM} - f_{XI} \cdot i_{P.XI}) *\rho7+ (-i_{P.BM}) * \rho10 +(i_{P.BM} - f_{XI} \cdot i_{P.XI}) * \rho11+ (i_{P.BM}-f_{XI} \cdot i_{P.XI}) * \rho12+ (Y_{PO4}+ i_{P.SS}) * \rho13 +(-1)* \rho14+ (-1) * \rho15+ (-i_{P.BM}) * \rho16 +(-i_{P.BM}) * \rho17 +(i_{P.BM} - f_{XI} \cdot i_{P.XI}) *\rho18 + (i_{P.BM} - f_{XI} \cdot i_{P.XI}) * \rho19+ \rho20 + \rho21$$

4.3 Sensitivity analysis and parameters estimation



Name: R26_Phenol_growth
Description:
Rate: pk_muh_phenol*M_O_H*M_NH_H*C10_X_phenol
Stoichiometry: Variable : Stoichiometric Coefficient
C03_S_Phenol : -1/ps_Y_HP

Fig.4.3 The process of ASM3 and the addition of phenol in AQUASIM

The average concentration of phenol from all the wastewater treatment plants in Busan in 2010 is used for parameter estimation by Aquasim. The results of sensitivity analysis is shown as follow.

Table4.4 The results of sensitivity analysis

	Parameter:	r(av(SensAR^2)) [gCOD/m^3]	Comparing the relatives
1	K_P	0.08169	1
2	μ_{phenol}	0.001995	0.0244
3	K_{LV}	0.000199	0.0024

The result of sensitivity analysis values of Kp and μ_{phenol} are larger than the K_{LV}. The comparing the relatives values of K_P, μ_{phenol} and K_{LV} are 1, 0.0244 and 0.0024, respectively.

Table 4.5 The connection of μ value , Kp and absolute value of phenol

μphenol(/day)	Kp(L/g)	Eff. Phenol(mg/l)	Abs(Error)
0.0018	0.007172	0.5611	0.1211
0.0018	0.012828	0.3995	0.0405
0.0025	0.012	0.3893	0.0507
0.0018	0.01	0.4614	0.0214
0.0018	0.01	0.4614	0.0214
0.0018	0.01	0.4614	0.0214
0.0018	0.01	0.4614	0.0214
0.00279	0.01	0.418	0.022
0.0018	0.01	0.4614	0.0214
0.0025	0.008	0.4883	0.0483
0.0011	0.012	0.4407	0.0007
0.0011	0.008	0.5637	0.1237
0.00081	0.01	0.5048	0.0648

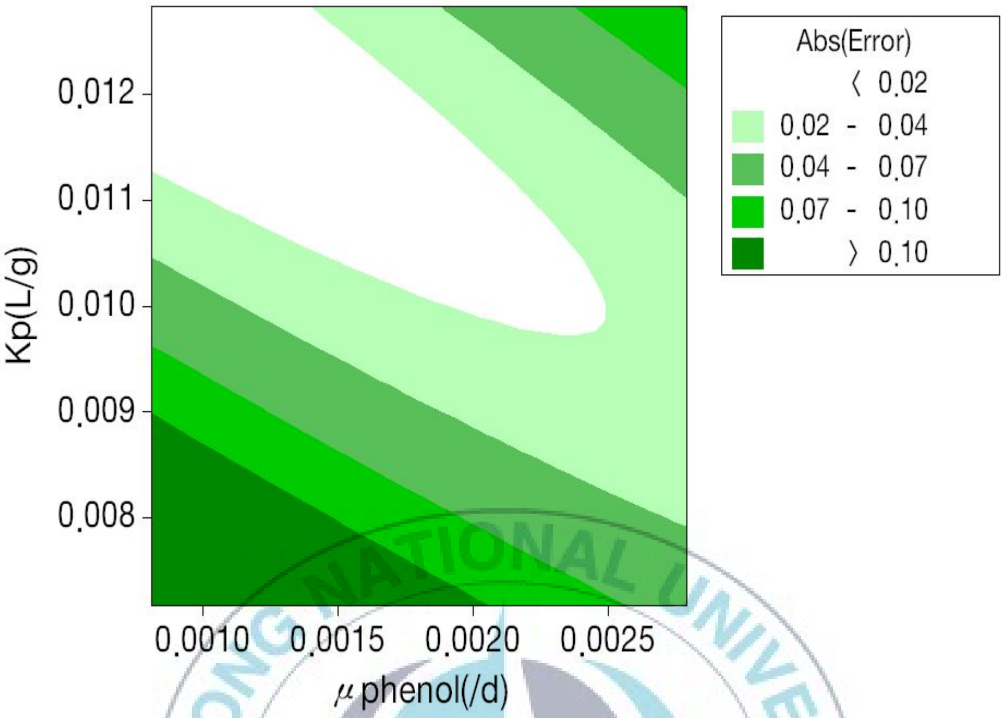


Fig.4.4 The connection of μ value and Kp of phenol

From the Fig.4.4, we can know that the best result is shown in the blank area.

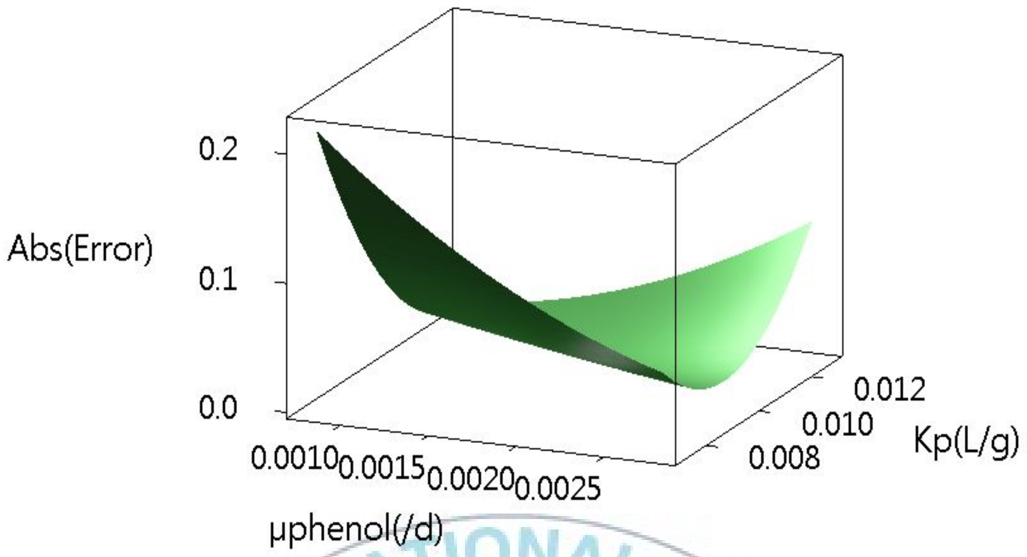


Fig.4.5 The connection of μ value , Kp and absolute value of phenol

From Fig.4.5 we can know when the Kp value at 0.010L/g, the value of μphenol is the more larger, the best absolute value is shown.

We can check the compared result of phenol addition in AQUASIM after the eatimation .

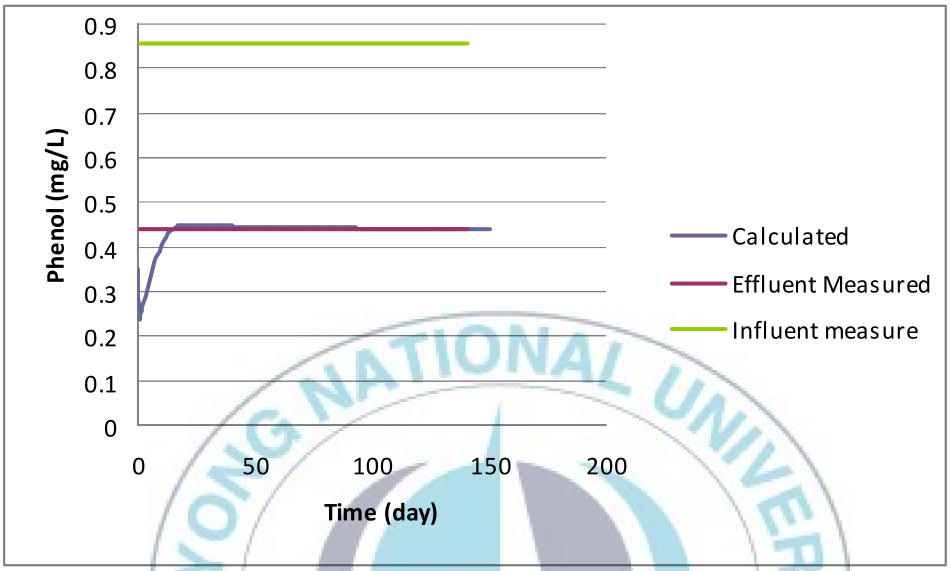


Fig.4.6 The comparison of calculated results with the actual influent and effluent results of phenol

We can get a intuitive result that the calculated result and the actual result are very similar in Fig.4.6.

Ⅴ. conclusion

The results of the addition of ASM3 model with phenol treatment process in wastewater treatment plant in Busan is as follow shown.

1. The addition of activated sludge modeling ASM3 with phenol treatment process is possibility.

2. The model of activated sludge ASM3 with phenol addition can estimate phenol effluent concentration of wastewater treatment plants in Busan,

3. Sensitivity analysis for phenol is carried out about biodegradation, adsorption and volatilization according to the removal mechanism. Compared to biodegradation and adsorption, volatilization has small affect to the concentration of effluent.

4. The result of parameter estimation about biodegradation and adsorption for phenol according to the removal mechanism show that the value of μ_{phenol} is 0.0011/d, K_p is 0.012 (L/g).

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감사의 글

한국에 대학원 생활은 눈문을 마치면서 끝이 되네. 2년 동안 학교를 다니면서 감사해야 하는 분들이 참 많습니다. 정말 많은 분들의 도움을 받아온 것 같습니다.

먼저 저에게 많은 가르침을 주시는 저희 지도교수님 이병헌교수님께 감사하다는 말씀을 드립니다. 제가 교환학생으로 여기에 왔을 때 많이 긴장한 저에게 먼저 따뜻하게 웃으면서 말씀을 준 적이 있습니다. 교수님이 아마 기억하지 않지만 그때 교수님의 모습이 저한테 깊은 인상을 주었습니다. 그리고 제가 대학원생 되고 싶어서 저를 받아주시는 것도 항상 감사하게 새각합니다. 2년동안 부적한 저에게 많이 챙겨주셔서 감사합니다. 참 좋은 교수님이세요, 교수님의 은혜는 평생 잊지 않겠습니다. 그리고 바로 옆방에서 항상 관심을 가져주신 강임석 교수님, 논문심사 할 때 지도 해 주신 여석준 교수님, 자주 뵙지는 못하는 김일규 교수님, 또 김상단 교수님, 이태윤 교수님께도 감사드립니다.

밥을 많이 사 주신 은주 선배님, 저를 많이 관심을 주신 대수 선배님, 수업을 도와 주신 빈정인 선배님께 진신으로 감사합니다. 창욱선배~ 말을 잘 안 들은 저를 항상 봐 주셔서 수고했어요. 많이 도움을 줘서 감사해요, 상엽선배~우리가 미운정만 있다는 거 들렸어요. 우리가 나쁜 일이 있었지만 지금 좋은 정이 이겼어요. 제가 선배한테 속상하게 만들어서 죄종해요. 처음부터 끝까지 잘 챙겨 줘서 감사해요. 제가 좋은 기억을 가지고 따날께요~그리고 재신언니~저한테 많이 신경 써 줘서 감사해요. 은미언니, 인정언니~ 많이 잘해 줘서 감사해요. 예쁘고 착한 수진이 잘 지내~마지막 학기에 만난 병기씨~ 석사과정 잘 하세요~많이 도와 줘서 감사해요. 승진

이 나한테 한국말 발음을 가르쳐 줘서 감사했어요. 근영씨는 실험실을 위해 많은 일을 해서 고생했다. 마지막 P군~~나한테 네 웃음 기억할 께 ~ 너한테 직접 이별 인사 하려고 했는데 이제 못 보겠네, 보고 싶을 께~해복하세요.

한국에 있을 때 저와 같이 신간을 보태 오는 친구들!!내 roommate 가완여 네가 있어서 나 외롭하지 않는다. 마문가~항상 옆에 있게 줘서 고마워~왕미~미미~나 좋아해서 고마워~ 마레시아에 있는 Jennis~너랑 같이 보내는 시간이 즐거웠어요~나는 너 찾아갈 수도 있어~빨리 좋은 남자랑 결혼 해~행복하세요! 원원아~~우리 이제 친하지만 너는 참 좋은 친구 생각한다. 너의 들이 있어서 나는 힘든 시간 이겨 왔어, 너무 고마워, 우리 중국에서 만나자, 결혼식에서 ㅋㅋㅋ

그리고 나 2년을 기다려 준 중국에 있는 친구들, 양양, 큰 언니,둘째 언니, 가가, 나 이제 졸업한다, 우리 인생 남은 시간에 같이 있어 하자.항상 걱정, 관심을 해 줘서 고마워 ,너들이 나한테 너무 소중하게 생각한다. 우리 이제 해복하게 살자, 영원히!!!

절대 잊어서는 안 될 저에겐 너무 소중하고 사랑하는 우리 가족들. 하늘에 게시는 외 할머니~덕분에 나 이제 졸업했다, 옆에 있으면 얼마나 좋겠어요, 보고 싶어요! 대학원까지 공부하게 해주신 우리 아빠, 엄마. 항상 감사히 생각하고 있어요. 이제는 열심히 사회생활하면서 아빠랑 엄마한테 더 잘하는 딸이 될께요. 또 다른 가족들도 관심 해 줘서 감사합니다.

절 생각해주시고 챙겨주신 모든 분들에게 이 논문을 바치며, 항상 감사하는 마음 잊지 않고 열심히 하겠습니다. 감사합니다.