

Predication of Fhhh potential in PTA wastewater treatment

CHENG Shu-pei*, SHI Lei, ZHANG Xu-xiang, YAN Jun, DING Zhong-hai, HAO Chun-bo

(The National Key Laboratory of Pollution Control and Resource Reuse, Department of Environmental Sciences, Nanjing University, Nanjing 210093, China. E-mail: chengsp@nju.edu.cn)

Abstract: Ebis is the intelligent environmental biotechnological informatics software developed for judging the effectiveness of the microorganism strain in the industrial wastewater treatment system(IWTS) at the optimal status. The parameter, as the objective function for the judgment, is the minimum reactor volume(V_{min}) calculated by Ebis for microorganism required in wastewater treatment. The rationality and the universality of Ebis were demonstrated in the domestic sewage treatment system(DSTS) with the data published in USA and China at first, then Fhhh strain's potential for treating the purified terephthalic acid(PTA) was proved. It suggests that Ebis would be useful and universal for predicating the technique effectiveness in both DSTS and IWTS.

Keywords: software; strain; potential; predication; purified terephthalic acid wastewater

Introduction

With the development of the informatics sciences and computer techniques, the environmental informatics software has made great achievements for evaluating the feasibility of the urban water cycle and the land resource management, for optimizing the wastewater treatment process and for designing the wastewater treatment plant(Mitchell, 2001; Zhang, 2000; Argent, 2001; Petrides, 2001; Yan, 2000).

Although the experts and officials had judged the technical schemes before IWTS set, some IWTS including the PTA IWTS were still invalid for removing pollutants or thoroughly did not run. The benzyl compounds in PTA wastewater could be transformed the toxic substances and induce cancer(Kluwe, 1982). It is necessary to predicate the effectiveness of the strain potential and to optimize treatment process before build and run a PTA IWTS.

One of the Ebis(environmental biotechnological informatics software) fundaments is a reformative TASP(the traditional activated sludge process)(Cheng, 2002). Most of the wastewater treatment software occurred base on TASP for DSTS(Ohtsuki, 1998; Gabaldon, 1998) in the last decade. And the technique of the TASP has been recognized more than one century. The range of the Ebis IWTS parameter values designed includes that of DSTS and is wider than that of the DSTS. The objective function V_{min} 's value was used to evaluate the Fhhh strain potential in PTA IWTS.

Fhhh is a genetically engineered microorganism strain(GEMs) constructed from the gene recombination of intracellular in the protoplast fusion of the three parental strains(Chen, 2002; Yan, 2001). Fhhh could integrate the high degradability of the first parental strain PC(*Phanerochaete chrysosporium*), the high flocculation of the second parental strain SC(*Saccharomyces cerevisiae*) and the high adaptability of the third parental strain YZ1(a native bacterium)(Zhong, 2000; Tao, 2001; Barr, 1994; Bogan, 1996; Lu, 1998). Fhhh is a safe GEMs to environment, because the protoplast fusion process does not create new gene.

In a wastewater biological treatment system, the degradation of

pollutants depends on the microorganism strain's character. PTA IWTS needs the specific functional strain and the optimized treatment process. After the rationality and universality of Ebis to DSTS demonstrated with the data from both USA(Corbitt, 1998) and China(Tang, 2000), the potential of Fhhh in the PTA IWTS was proved. The results suggested that Ebis has a useful universality for forecasting the effectiveness of the strain potential and optimizing the treatment process for both IWTS and DSTS.

1 Process of Ebis construction

Fig. 1 is the outline of the software and hardware in construction and operation of Ebis. The steps, form (1) to (6) on the left of Fig. 1, are the construction processes of Ebis. The processes of running and operating Ebis system are shown on the right of Fig. 1.

2 Mathematical models of Ebis

The mathematical models should be useful, reasonable, brief and effective for setting the Ebis. The mathematical models of Ebis consisted of 4 parts(Wanner, 1992; Cheng, 2000; Deng, 1996; Qi, 1988). They are: (1) the objective function mathematical model for obtaining V_{min} value and for evaluating the Fhhh potential in PTA IWTS; (2) the constraint mathematical models involving the objective function, the controllable parameters and the other processing parameters; (3) the degradation kinetics mathematical models for representing the specific characters of Fhhh in PTA IWTS; (4) the mathematical models for screening out the wrong value of the objective function and the other parameters in the end.

Ebis has 28 parameters selected from the above mathematical models. According to the function, resource, feature and occurring time of the parameters, they could be divided into 6 parts:

(1) The objective function parameter is V_{min} , the minimum reactor volume, needed for the microorganism strain in wastewater treatment. The value of V_{min} is the result of the Ebis optimal calculation and it was used to forecast the Fhhh strain potential in PTA IWTS in this research.

(2) The 3 native parameters are the raw wastewater flow(Q_0), the

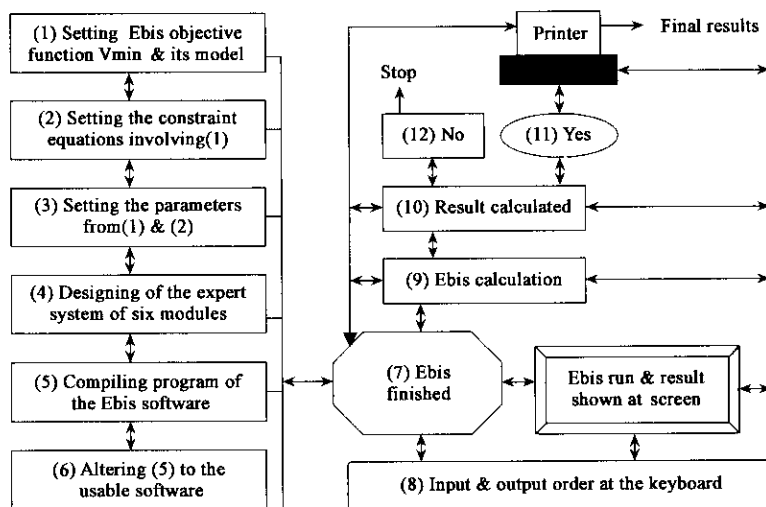


Fig.1 The construction, constitution, composition and operation systems of Ebis

organic pollutant concentration (S_o) and the biomass concentration (X_o). The values of Q_o , S_o and X_o show the quality and quantity of the raw wastewater. The 3 native parameter values were inputted in Ebis for the optimal calculation.

(3) The 6 kinetics parameters are the maximum specific degradation rate (q_{max}) and the organic substance concentration (K_{sq}) at $q_{max}/2$, the maximum specific growth rate (μ_{max}) and the organic substance concentration (K_{sp}) at $\mu_{max}/2$, the decay coefficient (K_d) and the theoretical yield coefficient (Y_T). The values of the six kinetics parameters from the test were inputted in the Ebis program for the optimal calculation. They present the features of Fhfh in the PTA IWTS.

(4) The 14 temporary parameters are the influent flow of the reactor (Q_i), the organic pollutant concentration (S_i) and the biomass concentration (X_i) of Q_i , the biomass concentration in the reactor (X), the organic pollutant concentration (S_e) in and out of the reactor, the wastewater discharge flow (Q_e) and the biomass concentration (X_e) of Q_e , the sludge discharge flow (Q_s) and the biomass (X_s) of Q_s , the specific degradation rate (q) and the specific growth rate (μ) in the

reactor, the hydraulic retention time (θ) and the sludge retention time (θ_c), the observation yield coefficient (Y_{obs}), the maximum biomass concentration (X_{max}) in reactor and the reactor volume (V). All the 14 temporary parameters are the treatment process parameters basing on TASP (Fig.2) and their values were variables in the optimal calculation process of Ebis.

(5) The 2 controllable parameters are the sludge recycle flow (Q_r) and the biomass concentration (X_r) of Q_r . The regulation of the values of X_r and Q_r was the key operation to improve the effectiveness for getting the function value of V_{min} . Q_r and X_r , they also belong to the treatment process parameters were variables in the Ebis optimal calculation.

(6) The 2 parameters should be controlled in the wastewater discharge are the effluent organic pollutant concentration (S_e) and the effluent biomass concentration (X_e). Referring the document of [GB8978-1996] published by the Chinese government, the values of S_e and X_e are inputted Ebis.

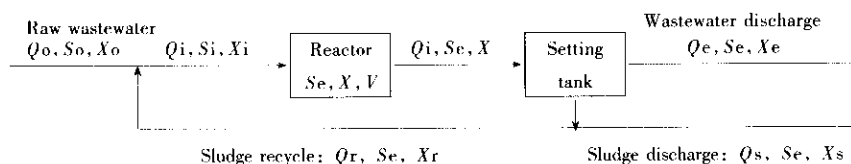


Fig.2 Flow sheet of TASP

The Ebis mathematical models based on TASP are shown in Fig.2. The TASP for DSTS has been recognized over one century practice. The wastewater treatment process of Ebis is a reformed TASP. The range of the IWTS parameter values designed is wider than the DSTS of TASP in Ebis. Because the IWTS wastewater quality is more complex than DSTS's, the various IWTS strain needed is different from DSTS.

3 Construction of Ebis software

Ebis has an expert system consisted of the six programming modules (Rodrigue-molina, 1998; Ci, 1997; Liu, 1997), which are: (1) the initialized module: defining all the variables and parameters, units and values, and fixing the properties of the object and form windows; (2) the input and output module: inputting the data including the normal

native values of the raw wastewater quality, the degradation kinetic parameter values, the control values for wastewater discharge; outputting the optimized results to the user, transferring the parameter value among the forms; (3) the calculation module: according to the logic arrangement of the mathematical model calculating and getting all the local optimized values; (4) the judgment module: filtrating all the parameter values and getting the final optimized results from all the local optimized values; (5) the conservation and printing module: saving the data to file and printing the results; (6) the switch module: linking and switching the forms.

The least system requirements of Ebis: Intel PII 300 processor, 64MB (megabyte) RAM (random access memory) and 10 M (megacycle) hard disk space; and the operation system: Windows98 or later editions.

Microsoft Visual Basic 6.0. Ebis program size 1.8 MB after transferred to the user's available software directly.

4 Judging Ebis universality to DSTS

Before Ebis used to evaluate the Fhhh potential in the PTA IWTS, the universality and reality of Ebis should be judged by the data published and recognized. The V_{min} values from Ebis calculation and the V values from normal calculation shown in Table 1 were obtained from the published and recognized data. The difference between the values of V_{min} and V is 0.80% with Corbitt *et al.* data(Corbitt, 1998) published in USA, and the difference between the values of V_{min} and V is 7.32% with Tang *et al.* data(Tang, 2000) published in China.

Table 1 The values of DSTS reactor volume from Ebis and traditional calculations

Style	V value from normal calculation		V_{min} value from Ebis calculation	
	Corbitt <i>et al.</i> , 1998	Tang <i>et al.</i> , 2000	Corbitt <i>et al.</i> , 1997	Tang <i>et al.</i> , 2000
Data from				
Q_o , m ³ /d	10000	10000	10000	10000
S_o , kg/m ³	12.03	6.78	12.03	6.78
X_o , kg/m ³	0	0	0	0
S_e , kg/m ³	4.16	0.68	4.16	0.68
X_e , kg/m ³	0.15 ≤ -	0.15 ≤ -	0.126	0.0082
Volume, m ³	2500	2500	2480	2317

(1) From the normal calculation, the values between the Corbitt *et al.* data(Corbitt, 1998) and the Tang *et al.* data(Tang, 2000) are shown in Table 1. The value of removed pollutant for Corbitt *et al.* data (Corbitt, 1998) is 7.87 kg/m³ (12.03 - 4.16). The value of removed pollutant for Tang *et al.* data(Tang, 2000) is 6.1 kg/m³ (6.78 - 0.68).

The difference of the values for removed pollutant between Corbitt *et al.* (1998) and Tang *et al.* is 1.77 kg/m³ (7.78 - 6.1) . It means that, the Corbitt *et al.* (1998) could remove 1.77 kg/m³ of the organic pollutant more than Tang *et al.* (2000) both in the 2500 m³ of DSTS reactor according to the normal calculation.

(2) From the calculation of Ebis, the values between the Corbitt *et al.* data(Corbitt, 1998) and the Tang *et al.* data(Tang, 2000) are also shown in Table 1. The ΔV_{min} value between Corbitt *et al.* (1998) and Tang *et al.* (2000) is 163 m³ (2480 - 2317).

It means that Corbitt *et al.* DSTS(1998) needs 163 m³ reactor volume more than that of Tang *et al.* (2000), and Corbitt *et al.* (1998) could remove 1.77 kg/m³ of the organic pollutant more than that of Tang *et al.* (2000) .

Anyway, the values of the differences between V_{min} and the normal V are very small for both with Corbitt *et al.* data(1998) and Tang *et al.* data(2000), and it demonstrates that Ebis might have the universality and the rationality to DSTS both in USA and China.

The value of V_{min} calculated from Ebis for the native strain is 2072 m³ in UASB (upflow anaerobic sludge blanket) for treating 10000 m³/d PTA wastewater with Cheng *et al.* data(Cheng, 1997) from China. And the value of V_{min} calculated from Ebis for the native strain is 2154 m³ in UASB for treating 10000 m³/d PTA wastewater with the Kleerebezem *et al.* data(Kleerebezem, 1997) from The Netherlands. The difference of the V_{min} values between Kleerebezem *et al.* (Kleerebezem, 1997) and

Cheng *et al.* (Cheng, 1997) is as low as 3.81% . It means that Ebis also has the universality and the rationality to PTA IWTS in both The Netherlands and China.

5 Fhhh potential in PTA IWTS

Fhhh potentials were evaluated with the marked parameter and the optimized function value V_{min} from the Ebis optimal calculation. And the Fhhh value of the Ebis V_{min} was compared with that of its parental strains shown in Table 2.

(1) The value of V_{min} calculated from Ebis for Fhhh is the lowest one among the three strains. It is 1329 m³ needed for treating 10000 m³ /d PTA wastewater.

(2) The value of V_{min} calculated from Ebis for the native parental strain YZ1 is the highest one. It is 8065 m³ needed in the same system as Fhhh. It is near to the actual data.

(3) The value of V_{min} calculated from Ebis for the fungous parental strain PC is the middle one, lower than that of YZ1 and higher than that of Fhhh.

(4) The another parental strain of the fungus SC could not grow in the PTA wastewater and have no data. But SC flocculation gene integrated in Fhhh could improve the sludge sedimentation of Fhhh.

Table 2 The results from the Ebis optimal calculation

Parameters	Parental strains			Parameters	GEMs		
	YZ1	PC	Fhhh		YZ1	PC	Fhhh
V_{min} , m ³	8065	4030	1329	K_d , d ⁻¹	0.0200	0.1900	0.0026
Q_o , m ³ /d	10000	10000	10000	Y_T , %	67.00	45.00	79.70
S_o , kg/m ³	4.66	4.66	4.66	q , d ⁻¹	0.0035	0.0914	0.0441
X_o , kg/m ³	0	0	0	μ , d ⁻¹	0.0027	0.0599	0.0305
q_{max} , d ⁻¹	0.018	4.00	5.424	Q_r , m ³ /d	10000	2530	9850
K_{sq} , kg/m ³	1.92	1.71	6.55	X_r , kg/m ³	2.46	11.45	3.41
μ_{max} , d ⁻¹	0.012	2.200	1.608	S_e , kg/m ³	0.47	0.04	0.05
K_{sft} , kg/m ³	1.64	1.43	2.58	X_e , kg/m ³	0.0002	0.0452	0.0035

It is clear that the Fhhh Ebis V_{min} value was lower than those of its parental strains and the native strains in UASB reported by Cheng *et al.* (Cheng, 1997) from China and by Kleerebezem *et al.* (Kleerebezem, 1997) from The Netherlands. And it might illustrate that Fhhh had the potential in PTA IWTS better than its parental strains and the native strains in UASB.

6 Principle for predication

The principles for the environmental biotechnological informatics software(Ebis) to predicate the Fhhh potential in PTA wastewater treatment are shown in the followed processes of operation.

Inputting all the values of the four kinds of parameters into Ebis, the four kinds of parameters are the kinetic parameters from the measurements, the wastewater discharge standard parameters ruled by the government, the native parameters of the raw wastewater tested and the experience parameters of the treatment process published.

According to the reasonable mathematical models for the wastewater treatment process and the restricted levers of the parameters set before, computer of Ebis begins to calculate with all the values of the parameters input into.

The large amount data obtained from the initial results of Ebis calculation will be screened to meet the requirements for restricted

factors. The screening processes include the data range selected, utilizable data selected, the substance balance selected and the optimal data selected. The optimal data is the final useful data in this research.

7 Summaries

Ebis is an intelligent system for predicating the strain potential in IWTS and base on the informatics sciences, the computer techniques, the experts' experiences, and TASP DSTS.

Ebis mathematical models consist of the function equation, the constraint equations, the kinetics models and the identification models. All the parameters are from the models.

Ebis software is an expert system consist of the 6 modules, which are the functions of the information input, result output, filter data, terminal judgment, operation linkage and switch.

Ebis has the universality and rationality to TASP DSTS through the optimal calculation with the data published in both USA and China.

Ebis has the universality and rationality to PTA IWTS through the optimal calculation with the data published in both The Netherlands and China.

Fhhh has the potential for PTA IWTS better than its parental strains and the native strains in UASB judged through the Ebis optimal calculation.

Acknowledgements: The authors appreciate Prof. Wang for PC strain and NJYZ for the PTA wastewater and YZ1 strain.

References:

- Argent R M, Houghton B, 2001. Land and water resources model integration software engineering and beyond[J]. *Advances in Environmental Research*, 5: 351—359.
- Barr D P, Aust S D, 1994. Mechanisms of white rot fungi used to degrade pollutants[J]. *Environ Sci Tech*, 28: 78—89.
- Bogan B W, Schonenike B, Lamar R T *et al.*, 1996. MnP mRNA and enzyme activity levels during bioremediation of PAH-contaminated soil with *Phanerochaete chrysosporium*[J]. *Appl Environ Microbiol*, 7(62): 2381—2386.
- Chen X, Chen W Q, Tao J *et al.*, 2002. Transcription of *mnp* gene in inter-kingdom fusant Fhhh for degradation of PTA wastewater[J]. *J Nanjing University*, 39(4): 544—549.
- Cheng S P, Pei D P, You L *et al.*, 2000. Optimal parameters for *P. chrysosporium* degradation of PTA wastewater[J]. *Toxico Environ Chem*, 76: 229—238.
- Cheng S S, Ho C Y, Wu J H, 1997. Pilot study of UASB process treating PTA manufacturing wastewater[J]. *Wat Sci Tech*, 36(6—7): 78—79.
- Cheng S P, 2002. The intelligent environmental biotechnological informatics software for forecasting the technological effectiveness of wastewater treatment [Z]. Center for Protection of Publication Right of China, 200214966.
- Ci M J X, Fu D Y F, 1997. The optimal method[M]. Beijing: The World Publish Inc. 38—67.
- Corbitt R A, Crawford H B, Gleason D, 1998. Standard handbook of environmental engineering [M]. Second edition. New York: McGraw-Hill Company. 6—17.
- Deng L W, Cheng S P, 1996. Biodegradation kinetics of the soybean processing wastewater with the fusants between photosynthetic bacteria and yeast[J]. *J Shanghai Jiaotong University*, 30: 60—65.
- Gahaldon C, Ferrer J, Seco A *et al.*, 1998. A software for the integrated design of wastewater treatment plants[J]. *Environmental Modelling & Software*, 13: 31—44.
- Kleerebezem R, Mortier J, Huishoffpol L W *et al.*, 1997. Anaerobic pretreatment of petrochemical effluents: terephthalic acid wastewater[J]. *Wat Sci Technol*, 36(2—3): 237—248.
- Kluwe W M, 1982. Carcinogenicity testing of phthalate esters and related compounds by NTP[J]. *Environ Health Persp*, 45: 129—133.
- Liu L F, Zheng W Y, 1997. Model mathematics and model construction[M]. Beijing: Beijing Normal University Press. 27—87.
- Lu P, Cheng S P, 1998. The stability of FLO1 flocculation gene in the inter-kingdom fusant cell in the treatment of soybean wastewater[J]. *J Nanjing University*, 34(3): 18—27.
- Mitchell V G, Mein R G, McMahon T A, 2001. Modelling the urban water cycle [J]. *Environmental Modelling & Software*, 16: 615—629.
- Ohtsuki T, Kawazoe T, Masui T, 1998. Intelligent control system based on blackboard concept for wastewater treatment processes[J]. *Wat Sci Technol*, 37(12): 77—85.
- Petrides D Intelligen Inc, USA, 2001. Process modelling evaluates feasibility of water recycling[Z]. *Filtration + Separation*, 26—31.
- Qi Y B, Huang Y X, Liang M S, 1988. Principles and methods of genetic engineering[M]. Chengdu: Sichun University Press. 235—246.
- Rodriguez-molina J J, Garcia-Martinez R, 1998. Hydrotrack: a graphical software system for the simulation of pollutant discharges in water[J]. *Environmental Modelling & Software*, 13: 211—223.
- Tang S Y, Dai Y Z, 2000. Engineer manual for waste treatment[M]. Beijing: Chemical Industrial Press. 336—337.
- Tao J, Chen X, Chen W Q *et al.*, 2001. The characters and the optimal levels for GEMs Fhhh in the degradation of PTA wastewater [J]. *J Nanjing University*, 37(6): 701—705.
- Wanner O, Kappeler O, Gujer W, 1992. Calibration of an activated sludge model based on human expertise and on a mathematical optimization technique —a comparison[J]. *Wat Sci Tech*, 25(6): 141—148.
- Yan C H, Song D L, Zhang C G, 2000. Visual software for evaluating and managing ground water resource in the Yangzhou City[J]. *Journal of China Universities*, 6(4): 595—599.
- Yan J, Gu J D, Cheng S P, 2001. Regulation of MnP level of inter-kingdom fusant Fhhh with metal elements in degradation of organic pollutants[J]. *J Nanjing University*, 37(3): 342—347.
- Zhang G G, Deng W, Li Q S *et al.*, 2000. A water resource optimization management professional software (REMAX)[J]. *Engineering of Hydrology and Geology*, 5: 38—40.
- Zhong Z H, Lu P, Cheng S P, 2000. Characteristics of the specific strain in the degradation of the purified terephthalic acid wastewater [J]. *J Nanjing University*, 36(3): 312—317.

(Received for review September 16, 2002. Accepted November 25, 2002)