



# 计算机与应用化学

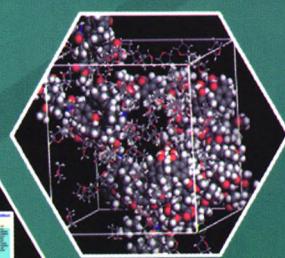
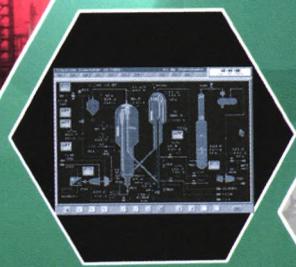
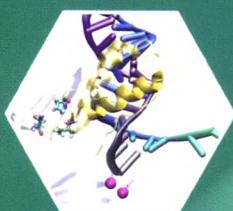
*Jisuanji Yu Yingyonghuaxue*

## COMPUTERS AND APPLIED CHEMISTRY

- Chinese Process Systems Engineering Society
- Computer Chemistry Committee,  
Chinese Chemical Society
- Committee for Information Technology Applications,  
Chemical Industry and Engineering Society of China

11  
2012

Vol.29 No.11  
第29卷 第11期



ISSN 1001-4160



9 771001 416114

中国系统工程学会过程系统工程专业委员会

中国化学会计算机化学专业委员会

中国化工学会信息技术应用专业委员会

会刊

# 计算机与应用化学

## JISUANJI YU YINGYONG HUAXUE

第 29 卷 第 11 期

2012 年 11 月

### 目 次

低碳经济下石化企业蒸汽动力系统运行优化研究	戴文智, 刘洋, 杨新乐	(1281)
定性趋势分析及其在化工过程中的应用	王兴, 李秀喜, 王慧	(1285)
燃气轮机—压缩机组仿真平台开发	徐宝昌, 宋永杰	(1289)
计算机模拟估算气体的扩散系数	晋宏营	(1294)
抑癌基因 p53 密码子偏好性分析及其突变致癌预测	谈承杰, 朱平	(1299)
从头算及变分过渡态理论研究尿素和甲醛的反应	马金广, 张纪明, 周建华	(1304)
基于模糊推理的本质 HSE 评价方法研究	焦巍, 肖源, 项曙光	(1307)
线型聚(N-杂环化)硅烷体系的电子结构与光谱性质的比较研究	王桂荣, 解菊, 董玉慧, 薛运生	(1313)
真空条件下肌酐的葫芦脲包合物的稳定性研究	张燕, 李代禧, 翟振, 刘宝林, 张冬兵, 刘立, 余华星	(1317)
硫酸烧渣煤基直接还原工艺的实验研究	郭振霆, 张宗旺, 魏连启, 仇小猛, 叶树峰	(1321)
一种基于虚拟现实技术的化工安全实时干预机理仿真平台	江志英, 朱群雄, 徐圆	(1326)
安全仪表系统的不同运行阶段实时可靠性分析	王丽君, 左信, 潘高峰	(1331)
基于二次型优化的单神经元 PID 控制器及其 pH 过程控制应用	于蒙, 邹志云, 赵丹丹, 刘兴红, 桂新军	(1335)
基于证据理论的共因失效因子不确定性分析	邓倩瑾, 左信, 岳元龙	(1339)
DMF 萃取精馏精制高纯度甲缩醛的模拟研究	张于弛	(1343)
基于 MATLAB 的双液系汽液平衡模型构建及其相图绘制	成忠, 张立庆	(1347)
苯管线泄漏扩散过程的模拟研究	张峰, 成云飞, 张军	(1351)
新戊二醇间歇精馏过程的模拟、优化与应用	田文广, 李雁, 陶红秀, 顾宇昕, 周年中, 解新安	(1355)
基于数据挖掘和因子试验设计的聚丙烯装置生产优化	张运陶, 徐前勇, 程正军, 李维存, 谢云颖, 郭正军	(1359)
酸性和碱性酶模式识别的研究	葛慧华, 张光亚	(1363)
广藿香酮电子结构及紫外光谱性质	王以武, 张海东, 蒋启华, 蒋君好, 邓萍	(1367)
化工销售物流损耗计算与优化研究	许高阳, 索寒生	(1371)
环体聚硅氧烷 $D_4^H$ 的密度泛函研究	陈婷, 杨祥, 刘斌, 周朝阳	(1375)
利用 GPU 技术使去噪方法并行化	林茂, 董玉敏, 蒋立, 许涛, 刘新军	(1379)
基于词汇链的多文档自动文摘研究	邓箴, 包宏	(1384)
MATLAB 在物理化学实验教学中的应用	杨涛	(1387)
多用途化学实验信息化教学平台建设	宋江闻, 赵会玲, 熊焰, 姚俊	(1391)
最大似然法在折光率-组成数据拟合中的应用	吴路平, 谭平华, 毛震波, 胡文励	(1395)
基于核最小二乘法的污水 BOD 软测量补偿方法研究	李瑞妮, 王小艺, 刘载文, 许继平, 魏伟, 董硕琦	(1399)
烟经济方法优化设计一个带有中间换热器的精馏塔	李岩梅, 胡仰栋	(1402)
环氧丙烷生产过程的模拟及扩产改造研究	夏力, 李尤, 项曙光	(1405)
《计算机与应用化学》征稿简则		(1366)
公告		(1408)

**CONTENTS**

Optimal operational planning for steam power system of petrochemical industry of low-carbon economy .....	Dai Wenzhi, Liu Yang and Yang Xinle	(1284)
Qualitative trend analysis and its application in chemical process .....	Wang Xing, Li Xiuxi and Wang Hui	(1288)
Development of gas turbine-compressor simulation platform .....	Xu Baochang and Song Yongjie	(1293)
Estimating diffusion coefficients of gases by use of computer simulation .....	Jin Hongying	(1298)
Analysis of codon bias of tumor suppressor gene p53 with forecast to gene mutation .....	Tan Chengjie and Zhu Ping	(1303)
<i>Ab initio</i> study on the reaction of urea and formaldehyde with variational transitional state theory .....	Ma Jinguang, Zhang Jiming and Zhou Jianhua	(1306)
The research of inherent hse evaluation method based on fuzzy inference .....	Jiao Wei, Xiao Yuan and Xiang Shuguang	(1312)
Comparative study on the structures and electronic spectra of chain (N-heterocyclic) oligosilane .....	Wang Guirong, Xie Ju , Dong Yuhui and Xue Yunsheng	(1316)
Investigation on the inclusion stability of creatinine-cucurbits[n](n=5, 6, 7) by molecular simulation .....	Zhang Yan, Li Daixi, Zhai Zhen, Liu Baolin, Zhang Dongbing, Liu Li and Yu Huaxing	(1320)
Experimental study on pyrite cinder of coal-based direct reduction process .....	Guo Zhenting, Zhang Zongwang, Wei Lianqi, Zhang Xiaomeng and Ye Shufeng	(1325)
A mechanism simulation platform of real-time intervention for chemical security based on virtual reality technology .....	Jiang Zhiying, Zhu Qunxiong and Xu Yuan	(1330)
Real-time reliability analysis for different operational phases of safety instrument system .....	Wang Lijun, Zuo Xin and Pan Gaofeng	(1334)
A single-neuron PID controller based on quadrics optimazation and its pH process control application .....	Yu Meng, Zou Zhiyun, Zhao Dandan, Liu Xinghong and Gui Xinjun	(1338)
Uncertainty analysis of common cause factor using the evidence theory .....	Deng Qianjin, Zuo Xin and Yue Yuanlong	(1342)
Simulation study of the methylal purification by extractive distillation with DMF .....	Zhang Yuchi	(1346)
Vapor-liquid equilibrium modeling and its phase diagram drawing for the ethanol-cyclohexane system based on MATLAB .....	Cheng Zhong and Zhang Liqing	(1350)
Simulation study on leakage and dispersion process of benzene from pipeline .....	Zhang Feng, Cheng Yunfei and Zhang Jun	(1354)
Simulation,optimization and application of batch distillation of neopentyl glycol .....	Tian Wenguang, Li Yan, Tao Hongxiu, Gu Yuxin, Zhou Nianzhong and Xie Xinan	(1358)
A polypropylene unit production optimization based on data mining and full factorial design .....	Zhang Yuntao, Xu Qianyong, Cheng Zhengjun, Li Weicun, Xie Yunying and Guo Zhengjun	(1362)
Classification of acidic and alkaline enzymes via pattern recognition methods .....	Ge Huihua and Zhang Guangya	(1366)
Theoretical study on the structure and UV spectra of pogostone .....	Wang Yiwu, Zhang Haidong, Jiang Qihua, Jiang Junhao and Deng Ping	(1370)
The study on chemical products sales logistics loss calculation and optimization .....	Xu Gaoyang and Suo Hansheng	(1374)
DFT study on 1,3,5,7-tetrahydrogen-1,3,5,7-tetramethylcyclotetrasiloxane .....	Chen Ting, Yang Xiang, Liu Bing and Zhou Zhaoxin	(1378)
Use of GPU technology parallelization denoising method .....	Lin Mao, Dong Yumin, Jiang Li, Xu Tao and Liu Xinjun	(1383)
Research of multi-document summarization based on lexical chains .....	Deng Zhen and Bao Hong	(1386)
Application of MATLAB in physical chemistry experimental teaching .....	Yang Tao	(1390)
Development of the information-based platform designed for multitask of teaching in chemistry experiment .....	Song Jiangchuang, Zhao Huiling, Xiong Yan and Yao Jun	(1394)
Application of maximum likelihood method in data fitting of refractivity and composition .....	Wu Luping, Tan Pinghua, Mao Zhenbo and Hu Wenli	(1398)
Research on the soft-sensing compensation method based on KPLS for BOD biosensors in sewage .....	Li Ruini, Wang Xiaoyi, Liu Zaiwen, Xu Jiping, Wei Wei and Dong Shuoqi	(1401)
Optimizing and designing an distillation column with side reboilers and condensers based on exergy-economics method .....	Li Yanmei and Hu Yangdong	(1404)
Simulation and production expansion for saponification process in propylene oxide plant .....	Xia Li, Li You and Xiang Shuguang	(1408)