Computer Aided Process Engineering Forum 7-8 February 2008, Thessaloniki, Greece

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Model-based Investigation of the Microbial Production of Polyhydroxyalcanoates (PHAs)

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Polyhydroxyalkanoates (PHAs) are microbial thermoplastics produced in a variety of microorganisms as intracellular carbon and energy storage compounds. These compounds exhibit significant advantages over conventional polymeric materials as they are non-toxic, they come from renewable sources and they are 100% biodegradable. Polyhydroxybutyrate (PHB) constitutes the most important and widely studied representative of the PHAs. It is a biopolymer with mechanical properties similar to conventional commercial polymers like polypropylene or polyethylene. Therefore, PHB or its blends can potentially replace synthetic polymers in a variety of different applications. Despite the promise of these new materials, their introduction to the worldwide market is inhibited by a series of economic and engineering considerations. Commercially available biopolymers are at present, significantly more expensive than their synthetic alternatives. Therefore, there is an emerging need to reduce the overall cost of PHB production by designing novel processes and separation procedures in order to maximize its yield and productivity.

An attractive candidate microorganism for the production of PHB is the bacterium *Alcaligenes latus*. This specific bacterium exhibits certain advantages, as it utilizes a cheap substrate (i.e. sucrose) and accumulates PHB even during its growth phase with increased efficiency and selectivity. PHB is accumulated in the cytoplasm of *A. latus* as a membrane enclosed granule at a percentage up to 80-90% of the dry cell mass. The production rate/yield of PHB has been found to increase by imposing limitations on the nitrogen concentration in the presence of excess carbon source during non-growth conditions. Furthermore, yield and productivity of the PHB can be enhanced by eliminating the possible inhibition effect of the substrates on the specific growth rate of the microorganism.

In the present study a mathematical model was developed for the prediction of the dynamic evolution of the active biomass, substrates (i.e. carbon and nitrogen) and product (i.e. PHB) concentrations. In order to describe the specific growth rate of the micro-organism, different expressions available in literature were considered. Product formation was assumed to comprise growth and non-growth associated terms. Sucrose consumption was presumably due to the growth of catalytically active (residual) biomass, product formation and maintenance of the microorganism whereas nitrogen was consumed exclusively for the growth of the biomass.

Initially, the parameters of the model were adjusted using experimental data from batch and fed batch reactors. Subsequently, the effect of carbon and nitrogen levels on biomass growth and PHB accumulation in *A. latus* on a batch reactor was examined. The model was used to determine the optimal initial nitrogen-to-sucrose ratio and the composition of the culture medium, which correspond to the maximum PHB productivity. Finally, the model was applied for the simulation of an ideal fed-batch reactor system. Different feeding policies of the two substrates were examines in order to establish an optimal design strategy for the production of PHB.

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CAPE FORUM 2008 7-8 February 2008 CERTH Convention Hall Thessaloniki, Greece



Thursday February 7th, 2008

08:30-09:15		Registration
09:15-09:40		Opening - Welcome
		Oral presentations S1 – Chairs: N. Vaklieva and S. Bezergianni
09:40-10:20	OP1.0	Capturing Dynamics in Supply Chain Integrated Management L. Puigjaner
10.20 10.40	OD1 1	Universitat Politecnica de Catalunya, Spain
10:20-10:40	OP1.1	Sc-MOPP – Platform for Planning and Scheduling Multi-site Manufacturing Systems B. Ivanov , J. M. Lainez, N. Vaklieva-Bancheva, K, Minchev, E. Shopova, L. Puigjaner, and A. Espuna Bulgarian Academy of Sciences, Bulgaria
10:40-11:00	OP1.2	A Toolbox for Early Market Introduction of New Energy Technologies I. Bulatov and J. Koppejan The University of Manchester, U.K.
11:00-11:10		Coffee Break
11:10-11:30	OP1.3	Modelling the Intra-Particle Transport Phenomena and Chemical Reactions of Olive Kernel Fast Pyrolysis T. Damartzis and A. Zabaniotou Aristotle University, Greece
11:30-11:50	OP1.4	<i>Improving the Maximum Conversion of Ethanol Esterification</i> M. Emtir , I. M. Mujtaba, and E. A. Edreder Libyan Institute of Petroleum Libya
11:50-12:10	OP1.5	Biorefinery: Analysis of Process Design Alternatives N. Al Haque and R. Gani Technical University of Denmark
12:10-12:30	OP1.6	Modeling and Simulation of Crystallization Processes for the Purification of Phosphorous Acid U. Brinkmann and E. Kenig Universitaet Dortmund Germany
12:30-14:00		Lunch
		Oral presentations S2 – Chairs: C. Botar and C. Chatzidoukas
14:00-14:40	OP2.0	<u>Process Performance Monitoring – Towards Model Based Approaches</u> J. Morris Newcastle University, U.K.
14:40-15:00	OP2.1	A Systematic Approach to Optimization-Based Control of Wastewater Treatment <u>Plants</u> J. Busch and W. Marquardt RWTH Aachen, Germany
15:00-15:20	OP2.2	Multivariable Fuzzy-Neural Model of Polymer Process V. Chitanov and M. Petrov Technical University of Sofia Bulgaria
15:20-15:40	OP2.3	Model Predictive Control of a Cyclic Propylene Steaming Pilot Plant I. Anastasiou, C. Ziogou, K. Kostaras, S. A. Papadopoulou, S. Voutetakis , and P. Seferlis CPERI/CERTH, Greece
15:40-16:00	OP2.4	An Adaptive Backstepping Technique for the Control of a Neutralization Process E. H. El Mazoudi and B. Messnaoui Ecole Mohammadia d'Ingénieurs, Morocco

16:00-16:20	OP2.5	Life Cycle Assessment Coupled with Process Simulation Under Uncertainty for <u>Reduced Environmental Impact: Application to Phosphoric Acid Production</u> A. D. Bojarski , G. Guillin-Gosalbez, and L. Jimenez Universitat Politocnica do Catalumya, Spain
16:20-16:30		Coffee Break
20:30-24:00		Poster presentations SP – Chairs: P. Seferlis, S. Voutetakis
	PP01	Model-Based Investigation of the Microbial Production of Polyhydroxyalcanoates (Phas) G. Penloglou, A. I. Roussos, C. Chatzidoukas , and C. Kiparissides Aristotle University and CPERI/CERTH. Greece
	PP02	Analysis and a Metabolic Interpretation of the Ph Evolution During Grape Must Alcoholic Fermentation H. Akin, I. Touche, C. Brandam, P. Strehaiano, and X. M. Meyer ENSIACET. France
	PP03	Energy Saving Potential of Phosphoric Acid Production by Wet Process L. L. Tovazhnyansky, P. Kapustenko, L. M. Ulyev, and S. A. Boldyryev SODBUL Ukraine
	PP04	Dynamic Simulation and Control Studies of the Main Fractionation Column of a Heat Integrated Fluid Catalytic Cracking Plant E. Jara-Morante, R. Roman, and P. S. Agachi
	PP05	 Babes-Bolyai University, Romania <u>Study of a Complex Petrochemical Process Based on Dynamical Mathematical</u> <u>Modeling Analysis</u> R. Roman, Z. K. Nagy, M. V. Cristea, E. Jara Morante, and S. P. Agachi
	PP06	Babes-Bolyai University, Romania <u>Application of Principal Component Analysis on a Hydrotreating Process</u> S. Bezergianni and A. Kalogianni CDEDI/CEDITH. Converse
	PP07	 CPERI/CERTH, Greece <u>The Simulation of Closed-loop Barometric Condenser System in Wet Phosphoric</u> <u>Acid Production Process</u> P. Kapustenko, G. Khavin and A. Perevertaylenko SODBUL Ukraine
	PP08	A Non-Linear MPC Strategy for Feed Conversion Targeting in a FCC Pilot Plant I. Anastasiou, S. A. Papadopoulou, S. S. Voutetakis, and P. Seferlis CPERI/CERTH Greece
	PP09	The Impact of Product Lifecycle on Capacity Planning Best Policies of the Reverse Supply Chain with Remanufacturing E. Athanasiou Aristotle University
	PP10	Generic Modelling, Design and Optimization of Industrial Phosphoric Acid Production Processes A. I. Papadopoulos and P. Seferlis CPEDUCEDTH_Graces
	PP11	 Operating Policy and Simulation Studies of a Stand-Alone Power System Using <u>Renewable Energy Sources and Hydrogen Storage</u> D. Ipsakis, S. Voutetakis, P. Seferlis, F. Stergiopoulos, S. Papadopoulou, and C. Elmasides CDEDUCEDTIL C.
	PP12	OIL Production Optimization in Petroleum Reservoir F. Razavi and F. Jalali Farahani University of Tehran, Iran Conference Dinner



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