

Modeling and Control of Emulsion Polymerization Processes with Evaporative Cooling

Zur Erlangung des akademischen Grades eines

Dr.-Ing.

vom Fachbereich Bio- und Chemieingenieurwesen
der Universität Dortmund
genehmigte Dissertation

von

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aus

Kanpur (India)

Tag der mündlichen Prüfung: 16. Mai 2007

1. Gutachter: Prof. Dr. S. Engell

2. Gutachter: Prof. Dr. G. Sadowski

Dortmund 2007

Schriftenreihe des Lehrstuhls für Anlagensteuerungstechnik
der Universität Dortmund (Prof.-Dr. Sebastian Engell)

Band 3/2008

Sachin Arora

**Modeling and Control of Emulsion Polymerization
Processes with Evaporative Cooling**

D 290 (Diss. Universität Dortmund)

Shaker Verlag
Aachen 2008

Bibliographic information published by the Deutsche Nationalbibliothek

The Deutsche Nationalbibliothek lists this publication in the Deutsche Nationalbibliografie; detailed bibliographic data are available in the Internet at <http://dnb.d-nb.de>.

Zugl.: Dortmund, Univ., Diss., 2007

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Printed in Germany.

ISBN 978-3-8322-7219-7

ISSN 0948-7018

Shaker Verlag GmbH • P.O. BOX 101818 • D-52018 Aachen

Phone: 0049/2407/9596-0 • Telefax: 0049/2407/9596-9

Internet: www.shaker.de • e-mail: info@shaker.de

Acknowledgements

First of all, I would like to express my sincere gratitude to Prof. Sebastian Engell, who offered me the opportunity of experiencing graduate research under him. I heartily acknowledge his able guidance and constant motivation throughout the scope of this project. I am thankful to him for giving me a lot of freedom to explore new ideas and further on, for showing me light whenever I got lost. The enthusiasm he brought into every aspect of the work was truly inspiring. I would also like to thank Prof. G. Sadowski, Prof. A. Górac and Prof. D. W. Agar for being members of my PhD examination committee.

I am highly grateful to the former senior researcher Dr. Ralf Gesthuisen for being my mentor during the early phase of my project. His suggestions and intelligent directions from time to time were of great help to me. I also thank Dr. Stefan Krämer for taking the initiative of inviting me to Dortmund and for encouraging me during the course of my study.

When I came to Germany, I had hardly imagined that I would meet a person as lively and helpful as Wolfgang Mauntz. His cheerful and friendly attitude on one hand made my work enjoyable, and on the other hand quickly filled the vacuum of a close friend in a foreign land. I gratefully acknowledge his constructive feedbacks and suggestions. I am also thankful to Dirk Nitsche for his numerous helps. I fondly remember the outdoor trips that I have enjoyed going out together with him. I value the friendship and guidance of Dr. Mehdi Rajabi who shared the same office with me. I wholeheartedly thank Sven Lohmann and Christian Sonntag for the cheerful atmosphere they created in our partly separated offices. I convey very special thanks to our technician Ralf Kneirim and student coworker Viswanath Chintala for helping me in the laboratory experiments. I also wish to thank the rest of the colleagues at AST, who apart from being very good friends, also made AST a very special and interesting place to work at.

I am thankful to the secretaries, Gisela Hensche and Dorothea Weber for their kind support and cooperation. I thank the 'Graduate School of Production Engineering and Logistics' coordinator, Meni Syrou and the secretary Gundula Pläp for their organizational helps. The financial support from the Graduate School is gratefully acknowledged. The social activities and excursions organized by AST and by the Graduate School have left many beautiful memories of my days in Dortmund.

I would like to thank all my colleagues from the RSO team at BASF, who helped me adjust comfortably in the new environment. I acknowledge my group leader Dr. Joachim Birk, for being very kind and supportive. I specially thank Dr. Bernd Mahn, Dr. Jens Neumann, Dr. Veit Hagenmeyer, Dr. Tobias Kleinert, Markus Schladt, Marcus Nohr and Olaf Kahrs for their warm and friendly nature.

I would not have been able to accomplish this work without the moral support and love of a lot of people. I wish to acknowledge here a few of them, from a very long list. The residents of the D-New wing of Nilgiri House at IIT Delhi, who were once an integral part of my life, but are now spread all over the world, still have the effect of making my day by their irregular emails and sudden calls. I feel fortunate to have such wonderful friends in my life. I wish to express my profound gratitude to my high school teacher Ms. C. Sinha for playing a motivating role in my life. I acknowledge the friendship and support of my school friends Satya Jyoti, Vishal Jain and Vikas Jain for over two decades.

I would like to thank my whole family for their support, encouragement and love over the years, especially Babli maama jee and the Singhal family, who stood by me in trying moments of my life. Finally, I would like to conclude by rendering my deepest thanks and paying homage to my parents for their unconditional love and for enduring innumerable hardships while encouraging me for continuing my educational pursuits.

Sachin Arora

Abstract

Emulsion polymerization is an important industrial process, which is used for producing a wide range of polymeric materials. From an industrial perspective, one of the major objectives is that of fast and safe operation with consistent polymer product quality. The polymerization usually proceeds as a double bond addition reaction initiated via a free-radical mechanism. The polymerization reaction kinetics is normally quite fast and is extremely exothermic. The latter restricts the speed of the process to the maximum cooling capacity available. The aim of this dissertation is to explore the possibility of extending the bottleneck of limited cooling capacity of jacketed reactors by the use of evaporative cooling.

The mentioned goal is pursued in a stepwise manner, starting from the development of a mathematical model that extends the physical and chemical phenomena involved in a conventional emulsion polymerization process by the vaporization phenomenon. The multi-component gas-liquid mass transfer is described by the Maxwell-Stefan diffusion equations. First principle models are used that help to understand the underlying mechanisms and also for providing a solid basis for the development of model based optimization and control techniques.

The developed model is then validated by several experimental data sets from the literature as well as from own experiments. To gain further insight into the role of the parameters involved in the gas-liquid mass transfer, a local sensitivity analysis is performed.

Based on the extended model, a novel process operation strategy is developed. Controlled vaporization is done by which additional heat is removed from the reaction system running in a time optimal manner. This enables to extend the restrictions imposed by the heat removal capacity of the cooling jacket considerably.

In order to maximize the productivity with the minimum usage of nitrogen, an online optimizing control problem is then formulated in the model predictive control framework. Due to the online optimization of performance criteria, the scheme has a distinct advantage of adapting according to the changing conditions without depending on fixed setpoints.

Applicability and robustness of the control schemes are demonstrated by simulation studies on homopolymerization of vinyl acetate in an industrial sized reactor. The results show that a significant amount of heat can be removed by evaporative cooling thus leading to a higher productivity. Although, this dissertation is focussed on emulsion polymerization processes, it also serves as a guide to general polymerization modeling principles and devising control strategies for complex processes, which require stringent control and optimized production processes.

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