Modeling, Validation and Time Optimal Control of Particle Size Distribution in Emulsion Polymerization

Zur Erlangung des akademischen Grades eines
Doktor-Ingenieurs
vom Fachbereich Bio- und Chemieingenieurwesen
der Universität Dortmund
genehmigte Dissertation

von
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aus
Yazd

Tag der mündlichen Prüfung: 8. Februar 2007

1. Gutachter: Prof. Dr.-Ing. S. Engell
2. Gutachter: Prof. Dr. techn. P. Walzel

Dortmund 2007

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

Band 1/2007

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Modeling, Validation and Time Optimal Control of Particle Size Distribution in Emulsion Polymerization

D 290 (Diss. Universität Dortmund)

Shaker Verlag
Aachen 2007

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 978-3-8322-6364-5
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

Acknowledgments

This thesis is the outcome of my research work as a Ph.D. student in the Department of Biochemical and Chemical Engineering at Universität Dortmund. The financial support of the Ministry of Science, Research and Technology of Iran is gratefully acknowledged.

Especially, I would like to express my profound gratitude to my supervisor Prof. Dr.-Ing. Sebastian Engell, as the center of my research circle, for giving me the opportunity to prepare my thesis at the Process Control Laboratory (AST), for his scientific supports and invaluable advices, for providing a chance to enhance my teaching skills and for many interesting discussions we had worthwhile for my future work. It was a great honor and recognition for me to have the opportunity to work in his group.

I would like to thank my former colleagues Dr.-Ing. Ralf Gesthuisen and Dr.-Ing. Stefan Krämer for their valuable discussions during the early stages of this project. Many thanks to Wolfgang Mauntz for his help all above for reading my articles and my thesis, for the careful preparation of the experimental setup in the laboratory and friendly relationships between our families. I am also thankful to my former co-worker Mr. Sachin Arora for having a cheerful and nice time in the same office.

Working with other members of the AST has been a lot of fun. It is the great team spirit that makes this group successful. I would like to thank our secretaries G. Hensche and D. Weber for their cooperation. I am very pleased to Dr. A. Shukla and Ms. M. Meuris for their collaboration in the preparation of PSD measurement facilities.

An dieser Stelle möchte ich all denen danken, die mir außerhalb der Universität, d.h. bei der Bewältigung der Alltagsprobleme in Deutschland behilflich waren und somit indirekt zu meinem Erfolg beigetragen haben. Besonders groß war die Unterstützung durch Herrn und Frau Althaus, die in wöchentlichen Sitzungen unsere deutschen Sprach- und Geschichtskenntnisse sowie unser Wissen über die europäische Kultur verbessert haben. Frau Althaus habe ich zu danken, dass Sie meiner Frau Fatemeh in der Zeit der Schwangerschaft und bei der Geburt unseres Kindes zur Seite stand und ihr die in einem fremden Land so wichtige psychische Unterstützung zukommen ließ.

Mein Dank gebührt auch unseren Nachbarn, den Familien Kroll, Milkert, Behrens und Roth, die uns herzlich in die Hausgemeinschaft aufgenommen, vorbildlich beraten und jederzeit unterstützt haben.
Zum Dank verpflichtet bin ich zudem meiner Familie, vor allem meiner Mutter und meinem Vater, die mir den Weg, den ich gegangen bin, ermöglicht haben.
Mein größter Dank gilt meiner lieben Frau Fatemeh und unserem über alles geliebten Sohn Parsa, die mit viel Geduld und Verständnis auf so manche gemeinsame Stunde verzichten mussten und mir dadurch die notwendige Rückendeckung zum erfolgreichen Abschluss dieser Arbeit gegeben haben.

Mehdi Rajabi-Hamane
Dortmund, October 2006

Abstract

The particle size distribution (PSD) is a key feature of a latex that strongly influences the viscosity and other attributes of the product which are critical in applications. The modeling of an emulsion polymerization process along with the PSD is very complex and still a challenging endeavor. The objective of this thesis is to establish a rigorous model for the simulation of the PSD and eventually use this model to perform optimal control of the PSD.

The established model consists of two major parts: a lumped and a distributed submodel. The lumped part is a kinetic submodel that describes the reaction kinetics, mass balances, the average number of radicals per particle and the thermodynamic relations between the concentrations of components in the different phases. This submodel provides the growth rate kernel which connects the two submodels. The distributed part makes use of a population balance equation (PBE) to compute the evolution of the PSD. The PBE is solved numerically using the method of orthogonal collocation on finite elements.

The validation of the model is investigated and demonstrated using simulation versus experimental data. The details about the experimental setup, the procedures and the required instruments are elucidated and discussed. A good agreement between the model and experimental data was observed albeit with some discrepancies between the experiments and distributed submodel.

In the optimization section, the computation of the monomer feed rate is performed in frame of a constrained optimization problem where the batch time is the performance index which is minimized and the difference between the specified and obtained particle size distributions (error) and the heat removal capacity of the reactor jacket enter as constrains. To solve the infinite dimensional optimization problem, the optimal control problem is transformed into a nonlinear programming problem using the control vector parametrization technique. The different aspects of the solution of the optimization problem are reported and discussed.

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