Optimal Process Operation by Using Economics Optimizing Nonlinear Model Predictive Control

Zur Erlangung des akademischen Grades eines

Dr.-Ing.

der Fakultät Bio- und Chemieingenieurwesen
an der Technischen Universität Dortmund
vorgelegte Dissertation

von

Elrashid Abdelrahman Noureldin Idris, M.Sc.

aus

Omdurman, Khartoum, Sudan

Tag der mündlichen Prüfung: 15. November 2013

1. Gutachter: Prof. Dr.-Ing. Sebastian Engell, Dortmund
2. Gutachter: Prof. Dr.-Ing. Günter Wozny, Berlin

Dortmund, 2013

Schriftenreihe des Lehrstuhls für
Systemdynamik und Prozessführung
herausgegeben von Prof. Dr.-Ing. Sebastian Engell

Band 1/2014

Elrashid Abdelrahman Noureldin Idris

Optimal Process Operation by Using Economics Optimizing Nonlinear Model Predictive Control

D 290 (Diss. Technische Universität Dortmund)

Shaker Verlag
Aachen 2014

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, Technische Univ., Diss., 2013

Printed in Germany.

ISBN 978-3-8440-2668-9
ISSN 1867-9498

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

It would have been beyond the bounds of possibility to realize this dissertation without the encouragement and assistance of helpful people in my surroundings. Only representatives of whom could be named in what follows.

I truthfully express my thorough gratitude and respect to my supervisor, *Prof. Dr.-Ing. Sebastian Engell*, the head of the Chair of Process Dynamics and Operations (DYN) and the dean of the Faculty of Biochemical and Chemical Engineering, Technische Universität Dortmund. His widespread expertise, his outstanding way of thinking and his constructive criticism have been of great value to me. The realization of the present doctoral thesis was a direct consequence of his encouraging personal guidance.

My sincere respect and thanks are due to the official referees *Prof.Dr.-Ing. Günter Wozny*, *Prof.Dr.-Ing. Andrzej Górak*, *Prof.Dr.-Ing. David W. Agar* and *Prof.Dr.-Ing. Rolf Wichmann* for their detailed review, constructive criticism, excellent advices and the nice environment during my PhD defense.

I thankfully acknowledge the financial support of the International University of Africa (IUA). I especially and warmly thank the former head of the department of Applied Chemistry, *Dr. Shiekh Idris Ahmed Elshiekh*, the former faculty dean of Pure and Applied Science *Prof. Ali Ahmed Mahmoud* and the former deputy vice-chancellor for scientific affairs *Prof. Mohammed Ali Hussien*.

In the course of this research study I have cooperated with elite of colleagues for whom I have great regards and respect, and I would like to offer my hottest appreciation to all those who have provided helping hands and supporting ideas during my research studies in the Department of Biochemical and Chemical Engineering in Dortmund.

I am most grateful to the PhD candidate *Mr. Gaurang Shah* and to *Dr. Alaeldin Bouaswaig* for their valuable academic supports. I pass my gratitude to all other friends and colleagues in the chair for the fruitful discussions and for the cordial environment. I would like to primarily mention *Mr. Ali Houssieni* and *Dr. Le Chi Pham*. I am deeply indebted to *Mr. Malte Behrens* and to *Mr. Johannes Beyer* who greatly and tirelessly helped me with German translations and administrative tasks. Special thanks go to *Dr. Subanatarajan Subbiah*, *Mr. Christian Sonntag* and *Dr. Wolfgang Mauntz* for helping me during my first arrival to Dortmund. I'm much obliged to *Dr. Tobias Keller* from the FVT Group for his significant assistance.

I gratefully acknowledge the funding received during the research leading to the results presented in this thesis from the European Union Seventh Frame-work Programe FP7 / 2007 - 2013 under grant agreement number FP7 - ICT - 2009 - 4248940 (EMBOCON).

I delightfully thank my close friends and colleagues in Sudan, Germany and elsewhere for their help and support throughout, some of whom have already been mentioned. I am deeply grateful to the PhD candidate *Mahmoud Mohammed Ali* for his great assistance and support.

Last, but by no means least, I offer my warmest and affectionate thankfulness to my great family in Sudan especially my mother *Muna Yousif Mohamed Ali* and my father *Abdelrahman Noureldin Idris*. Both have sacrificed a lot during my long-term studies. Without their stimulation and patience it wouldn't have been manageable to reach such a step. Exceptional regards and blessings are due to my sister *Hipa* and to my brothers *Noureldin* and *Moumin*.

Dedication

This dissertation is dedicated

to the memory of my beloved father

Abdelrahman Noureldin Idris (1940-2010)

You are exceptionally appreciated for inculcating in me the valuable meanings of fortitude and determination and for your purposeful commitment to my academic progress!

May God rest your soul.

&

to my mother

Muna Yousif Mohammed Ali

Your graces and sacrifices are myriad and beyond being lumped in words!

May your life be satiated with vivacity, robust health and merriments in a lap of luxury,

&

may God lengthen your life.

Abstract

Process profitability is a decisive criterion for successful long-term operation of industrial processes. Economics-driven optimization based on rigorous first-principles models has been progressively integrated into the operation of chemical processes in order to improve the competitiveness of these processing units. Decisions on the most profitable conditions are usually made based on infrequent optimizations of stationary rigorous first-principles models (real-time optimization, RTO). However, the neglect of the dynamic process behaviour in these models can lead to feasibility issues and performance degradation. The inclusion of rigorous dynamic models in the decision-making policies makes it possible to overcome these difficulties and therefore higher process efficiency and profitability can simultaneously be achieved. This can be realized by using different strategies of economics-based nonlinear model predictive control (NMPC).

Nonlinear model predictive control is perhaps the most advanced feedback control technique that introduced a significant impact on the industrial chemical processes. Its abilities to handle multivariable control systems, to incorporate constraints into the control problem formulation and to enable the integration of economics optimizing criteria into the feedback control design are the most outstanding advantages among many others.

An economics optimizing NMPC controllers to optimize and control the operations of a non-minimum phase continuous stirred tank reactor (CSTR) and the operations of a complex dynamics pilot-scale continuous catalytic distillation (CCD) process are investigated in this thesis. This direct economic optimization scheme is compared with a compromise scheme, the economics-oriented tracking controller. Besides the inherent nonlinearity of these processes, non-minimum phase behaviour, input multiplicity and local minima are among the complex phenomena encountered in both case studies. Different control structures are used to explore the potential benefits of the dynamic online economics-based nonlinear control strategies. Online state and disturbance estimation is an integral part of the investigated NMPC control schemes particularly in the presence of disturbances and plant-model mismatch. Two conceptually different state and disturbance estimation techniques are used in this thesis namely the extended Kalman filter (EKF) and the nonlinear gain-scheduling observer, which is a modified version of the extended Luenberger observer (ELO).

In this thesis, global as well as local optimization algorithms are used. The global optimization algorithm is used primarily to locate the optimal region (i.e. good initial guess) to a local optimization algorithm and to avoid those potentially optimal parts of the space from being overlooked. The local optimization algorithm finds the best point in that optimal region.

The outcome of this work indicates that by using direct economics optimizing NMPC the plant economics can be handled better while guaranteeing the product specifications. The economics of the process can be enhanced when more degree of freedom are manipulated at the price of more complex optimization problems. The concept of the economics optimizing NMPC can straightforwardly be applied to similar chemical processes and the findings and conclusions deduced from this work are important for analogous chemical processes.

Zusammenfassung

Die Prozess-Rentabilität ist ein entscheidendes Kriterium für einen erfolgreichen langfristigen Betrieb industrieller Prozesse. Ökonomische Optimierungen basierend auf rigorosen Modellen wurden schrittweise in den Betrieb von chemischen Prozessen integriert, um die Wettbewerbsfähigkeit zu verbessern. Die Entscheidungen für die profitabelsten Bedingungen basieren in der Regel auf der Grundlage unregelmäßiger Optimierungen von stationären rigorosen Modellen (*real-time optimization, RTO*). Allerdings kann die Vernachlässigung des dynamischen Prozessverhaltens in diesen Modellen zu Unzulässigkeit und Suboptimalität führen. Die Einbeziehung dynamischer rigoroser Modelle in die Entscheidungsfindung macht es möglich, diese Schwierigkeiten zu überwinden und damit eine höhere Prozesseffizienz und damit höhere Rentabilität zu erreichen. Dies kann durch verschiedene Strategien der ökonomie-basierten nichtlinearen Modellprädiktiven Regelung (*NMPC*) realisiert werden.

Die nichtlineare modellbasierte prädiktive Regelung ist unter den Vertretern der gehobenen Regelungstechnik der mit der größten Bedeutung für industrielle chemische Prozesse. Ihre Fähigkeit zur Mehrgrößenreglung, die Modellgleichungen als Nebenbedingungen in das Optimierungsproblem zu integrieren und die Einbeziehung der allgemeinen wirtschaftlichen Optimierungskriterien in das Regeldesign zu ermöglichen sind die wichtigsten Vorteile.

In dieser Arbeit wird ein ökonomie-orientierter optimierender NMPC- Regler zur Optimierung und Steuerung eines kontinuierlichen Rührkessels (*CSTR*) mit Nicht-minimalphasen-Charakteristik und zum Betrieb eines kontinuierlichen katalytischen Destillations-(*CCD*)-Verfahrens mit einer komplexen Dynamik mittels Simulation im Pilotmaßstab untersucht. Dieses direkt ökonomisch optimierende Sche-ma wird mit einer ökonomie-orientierten Folgeregelung verglichen. Neben der inhärenten Nichtlinearität dieser Prozesse tragen die Nichtminimalphasen-Charakteristik, die Multiplizität von Eingangsgrößen und lokale Minima zur Komplexität dieser beiden Fallstudien bei. Verschiedene Kontrollstrukturen werden verwendet, um die potenziellen Vorteile von dynamischen online-ökonomie-basierten nichtlinearen Regelstrategien zu identifizieren. Eine online Zustands- und Störungsabschätzung ist ein wesentlicher Bestandteil der untersuchten NMPC Regelschemata, besonders in Gegenwart von Störungen und Modellfehlern. Zwei konzeptionell unterschiedliche Zustands- und Störungsschätzer wurden in dieser Arbeit verwendet, und zwar der erweiterte Kalman-Filter (*Extended Kalman Filter, EKF*) und ein nichtlinearer gain scheduled-Beobachter (*Gain-scheduled Observer*), eine modifizierte Version des erweiterten Luenberger Beobachters (*Extended Luenberger Obsever, ELO*).

In dieser Arbeit werden sowohl globale als auch lokale Optimierungsalgorithmen eingesetzt. Der globale Optimierungsalgorithmus wird verwendet, um den optimalen Bereich (d.h. gute Anfangsbedingungen) für einen lokalen Optimierungsalgorithmus zu finden und zu vermeiden, potenzielle optimale Bereiche des Suchraumes zu übersehen. Der lokale Optimierungsalgorithmus optimiert innerhalb dieser optimalen Regionen.

Das Ergebnis dieser Arbeit zeigt, dass durch die Verwendung direkt ökonomie-optimierender NMPC-Regler das ökonomische Potential der Beispielprozesse unter Einhaltung der Produktspezifikationen besser ausgenutzt werden kann Die Wirtschaftlichkeit der Verfahren kann verbessert werden, wenn mehr (auch dynamische) Freiheitsgrade in der Optimierung erlaubt sind, zu dem Preis erhöhter Komplexität der Optimierungsprobleme. Das Konzept der hier verwendeten ökonomie-optimierenden NMPC-Regler kann auf andere chemische Prozesse übertragen werden und auch die Ergebnisse und Schlussfolgerungen aus den hier dargestellten Fallstudien sind relevant für analoge chemische Prozesse.

Contents