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Daniel Haßkerl

Economic Performance Optimization by Direct Optimizing Control Applied to Reactive Distillation Processes

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Chemieingenieurwesen

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“*Tu’n Sie, was getan werden muss!*”

„*Do whatever is necessary!*“

Prof. Engell, project meeting, August 2013

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The citation above matches perfectly with my personal point of view. The path I have chosen is definitively not the easiest one nor is it the one I have expected when I was working on the farm of my dad. With the support of the aforementioned persons, I was able to finish high school and my diploma thesis, despite the fact that it was demanding, financially exhausting and sometimes demotivating. As the last step of my educational path, I herewith submit my PhD thesis. All along that path every piece was new to me, inspiring but challenging, interesting, but correlated to large efforts. For me, it is personally important to accept challenges and to solve them to a reasonable extend, which means *'till the end'*. A proof of concept to my opinion is that all individual parts are fully understood AND the concept is working in reality. It is worthless if you can show/ produce something that is theoretically of interest, but with no practical benefit as it does not apply to real-life systems. "Do whatever is necessary!" therefore contains three stages for dealing with any challenge, not only in terms of projects or scientific work: In the first step, the goal to be reached must be defined. Secondly, the milestones should be placed which have to be fulfilled while avoiding unnecessary pieces of work. And lastly, someone has to catch up and to realize the milestones. All in all, these stages are individually already quite demanding, but this statement gave me a lot of confidence, because I interpreted in these words, that it is believed that I can tackle all of the stated items in order to reach the specified goal. So I did and I can only hope that in the end, I could demonstrate, that choosing me for this undertaking was a correct choice.

Abstract

By the use of economic performance optimization, the profitability of any chemical process can be enhanced while meeting the process, environmental and ecological constraints at the same time. Two prominent methods are established techniques to achieve economic goals for chemical processes by means of advanced process control (APC), the well-known real-time optimization (RTO) and direct optimizing control (also called one-layer approach or dynamic RTO/ D-RTO). To assure a good controller performance, both approaches rely on accurate models by which the process is described mathematically. D-RTO schemes, which combine nonlinear model predictive control (NMPC) with an economic objective, have received increasing attention from the control community and from the industry over the past years. Compared to the widely-applied RTO approach, D-RTO schemes offer the advantage that the processes are dynamically steered towards the most profitable region. Despite the intense research effort dedicated to study and develop efficient computational methods to assist the economics optimizing control approaches, their application to lab-scale, pilot-scale or even production-scale chemical processes is rarely (if at all) reported. There exist numerous scientific and implementation challenges among which two major obstacles stand out: if high-fidelity models are utilized for control purpose, the size of the resulting optimization problem that has to be solved in a moving-horizon fashion usually leads to considerable computation times, and even when an accurate model is available, modelling uncertainties can be present in complex chemical processes leading to performance deterioration of the controlled systems. Novel methods in dynamic optimal control make it possible to overcome the issues caused by the problem size and to deal with modeling uncertainties in a less conservative way. To tackle the issue of response times, efficient optimization techniques are used which can handle optimization problems with thousands of optimization variables while using the automatic differentiation functionality for efficient computations of first and second-order derivative information. Automatic differentiation can also speed up algorithms for state estimation which are required to return process information to the controller. To overcome the issue related to modeling uncertainty, a control strategy based on the multi-stage NMPC approach (so-called robust approach in contrast to the nominal approach which neglects modelling uncertainties) can be employed.

In this thesis, it will be demonstrated that nominal and robust optimizing control schemes are mature methods and are only one step away from the application to pilot-scale or larger chemical processes. To highlight the important features of an application of economics optimizing control to a large-scale and complex chemical process, reactive distillation processes are studied. Reactive distillation is the most well-known example of an intensified chemical processing unit with numerous challenges in process operations. Two case studies representing two different types of reactions are investigated in computer simulations out of which one case study is investigated in an experimental work. The case study studied in practice is the homogeneously-catalyzed two-step transesterification reaction of dimethyl carbonate with ethanol to produce the intermediate product ethyl methyl carbonate (EMC) and the final product diethyl carbonate (DEC). Not only the production of each valuable product according to a certain specification is demonstrated, but also the transient product changeover that is realized by means of optimizing control is investigated. The performance of the controller and its effect on the overall process performance is discussed with respect to important process-related performance indicators. The details of the software realization that implements the economics optimizing control approach in real-time are described and limitations of the approach, open issues and possible future directions are pointed out.

Zusammenfassung

Durch den Einsatz von ökonomischer Optimierung als Teil gehobener Prozessführungsstrategien kann die Rentabilität chemischer Prozesse unter Einhaltung kritischer Prozessparameter und Umweltauflagen maßgeblich erhöht werden. Die beiden bekanntesten Verfahren um chemische Prozesse unter ökonomischen Gesichtspunkten zu optimieren sind die stationäre und die dynamische Echtzeitoptimierung. Um eine möglichst hohe Regelgüte und somit einen gesteigerten Profit zu erzielen, wird in beiden Verfahren ein hochgenaues Prozessmodell benötigt. Während die stationäre Echtzeitoptimierung bereits eine Standardmethode mit vielen industriellen Anwendungen ist, erhält die dynamische Echtzeitoptimierung in den letzten Jahren vermehrt Aufmerksamkeit. Bei der dynamischen Echtzeitoptimierung wird im Gegensatz zur klassischen Echtzeitoptimierung kein stationäres Optimierungsproblem gelöst, dessen Lösung von einer unterlagerten Regelung nachgefahren werden. Die Anlagenökonomie wird stattdessen direkt in die dynamische nichtlineare modell-prädiktiven Regelung (NMPC) in Form einer Zielfunktion integriert. Obwohl diese Integration viele Vorteile bietet, gibt es zahlreiche Herausforderungen, die einer Anwendung im Wege stehen, von denen zwei Herausforderungen besonders herausstechen. Wenn ein hochgenaues Prozessmodell zur dynamischen Optimierung verwendet wird, führen die Anzahl der Variablen und die resultierende Größe des Optimierungsproblems unweigerlich zu hohen Rechenzeiten bei der Lösung des gestellten Problems. Zudem muss selbst bei der Nutzung eines hochgenauen Prozessmodells davon ausgegangen werden, dass nicht alle physikalischen Vorgänge, die bei einem komplexen chemischen Prozess auftreten, genau erfasst sind. Somit liegen Modellungenauigkeiten vor, die zu einer Verschlechterung der Regelgüte des modell-prädiktiven Reglers führen können. Die hohen Rechenzeiten können mit Hilfe von modernsten Optimierungsalgorithmen und der automatischen Differentiation maßgeblich verkürzt werden. Automatische Differentiation kann zudem bei der Zustandsschätzung, die für die Rückführung von Prozessinformationen unerlässlich ist, Einsatz finden. Die mehrstufige nichtlineare modell-prädiktive Regelung ist ein neues Konzept um Modellunsicherheiten zu betrachten und –durch die spezielle Formulierung des Optimierungsproblems – eine bessere, da robustere Regelung des Gesamtsystems zu gewährleisten.

In der vorliegenden Arbeit wird gezeigt, dass die dynamische Echtzeitoptimierung sowohl unter Berücksichtigung von Modellungenauigkeiten als ohne deren Betrachtung für den Einsatz an Pilot- oder Produktionsanlagen reif ist. Um einige Faktoren, die bei der Realisierung berücksichtigt werden müssen, herauszustellen, wird das Verfahren der dynamisch-ökonomischen Echtzeitoptimierung anhand der Reaktivrektifikation evaluiert. In Simulationsstudien werden zwei verschiedene Reaktivrektifikationsprozesse, die stellvertretend für unterschiedliche Reaktionssysteme stehen und mit Hilfe von Gleichgewichtsmodellen mathematisch beschrieben werden, dynamisch optimiert. Für die Anwendung von dynamischer Echtzeitoptimierung an einer Pilotanlage im Technikumsmaßstab wird die zweistufige homogenkatalysierte Umesterung von Ethanol mit Dimethylkarbonat betrachtet. In diesem Prozess kann sowohl das Zwischenprodukt Ethylmethylkarbonat als auch das Endprodukt Diethylkarbonat in einer einzelnen Rektifikationskolonne hergestellt werden. Es werden die ökonomische Produktion beider Produkte sowie der dynamische Produktionswechsel betrachtet. Die Details der Software, die benötigt wird, um die dynamische Echtzeitoptimierung zu realisieren, werden beschrieben und noch bestehende Grenzen und Herausforderungen werden erläutert.

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