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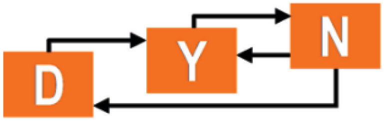
bci

The Dortmund Process Dynamics and Operations Group

Lehrstuhl für Systemdynamik und Prozessführung



Impressum

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This brochure informs about the members, the teaching and the research of the Process Dynamics and Operations Group in the Department of Biochemical and Chemical Engineering of TU Dortmund, in 2015, 25 years after my appointment as a professor in this department. When I got the information that I was offered the position of Professor of Process Control (Anlagensteuerungstechnik) in the middle of 1989, I was extremely happy, not only because the period of searching for a professorial position is a stressful one that also comes with disappointments, but mostly because I was really eager to start to work in a chemical engineering department, although my background was in electrical engineering and control theory. I wanted to work on challenges in control that are posed by nature itself, by chemistry, physics and biology.

In the BCI department at TU Dortmund I found an open space where I could spread out and follow a broad range of research interests, and good opportunities for collaboration. I learned a lot about chemical processes and their underlying principles, and by now, I almost feel like a chemical engineer.

The last 25 years were a great time for process control people, with the opportunities for the implementation of advanced control solutions continuously widening and a growing acknowledgement of the contribution of optimization and control to the success of the process industries by managers and other engineers. My position at the interface of the worlds of process engineering on the one hand and of control and ICT on the other hand side gave me a unique opportunity to transfer knowledge, to act as an integrator between these domains and to cooperate fruitfully with partners as well as with researchers coming from a wide range of backgrounds.

The breadth and the depth that the dyn group has reached in research and in teaching in 2015 is the result of the work of many generations of doctoral candidates and postdocs over the past 25 years, and of our secretaries and technicians. I am extremely grateful to all of them for their contributions and for the pleasure to work with them, and to see them grow and later make important contributions in industry and in other universities all over the world. I am very happy that with many former group members we are still in a fruitful exchange and collaboration, informally and in joint projects.

And there are enough challenges for the years to come!

Sebastian Engell

Back Row (l.t.r.):	Daniel Krahé, Reinaldo Hernandez, Lukas Hebing, Lukas Maxeiner, Alexandru Tătulea-Codrean
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Front Row (l.t.r.):	Sakthi Thangavel, Simon Wenzel, Gisela Hensche, Simone Herchenröder, Franziska Lanfer
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Research at dyn

The current research of the dyn group addresses five areas in process systems engineering:

- Process control methods and applications
- Plant management
- Logic control and scheduling
- Modeling, simulation and control of biosystems
- Process design and optimization.

One common feature of our approach in all these areas is the use of optimization methods. Optimization technology has developed tremendously during the last decades, and this has also changed the world of process control. Online computation of optimal control moves nowadays may still be challenging, but it is possible for most control tasks in the process industries. Drastic model simplifications in order to arrive at tractable optimization problems are no longer necessary, rigorous nonlinear models based on laws of physics and chemistry can be employed. The bottlenecks now are model development, model validation, and online model adaptation.

Another common thread is the insight that real-world control and optimization problems always are characterized by the presence of uncertainties. These can be model imperfections or unknown or unpredictable external influences. The presence of uncertainties and the need to react to them motivates continuous feedback control as well as logic control, and we take this fact into account also in scheduling and process design. In biological systems, the uncertainties are even larger than in other processing plants and a constitutive feature of the area.

Logic controllers and schedulers in the real world are acting in a feedback loop and react to disturbances and the arrival of new information, so they must be designed similar to model-predictive continuous controllers with an underlying basic regulatory control layer.

In process control, in scheduling, and in process design we have in recent years employed the same fundamental approach: *multi-stage (stochastic) optimization*. It builds on the fact that uncertainties materialize over time and that some decisions must be taken here and now (the next control move, the assignment of the next tasks, or the design of the plant equipment) while others can be taken in the future in order to react to the realization of the uncertain variables. The key idea is that the here-and-now decisions are computed anticipating the recourse options. This leads to the best possible use of the presently available information. In process control, we could show that model-predictive controllers that employ this idea give better performance than optimization for the nominal model or of the worst case. In scheduling, future uncertainties are anticipated and their effect is mitigated. In plant design, overdesign is avoided when the uncertain influences and parameters can be compensated by operational degrees of freedom.

In our research, we try to keep the right balance between addressing fundamental issues and dealing with specific processes and problems. A deep understanding of the real process that is controlled or optimized or of the real scheduling problem is needed to develop relevant solutions. On the other hand, our ambition is to develop generic methods that are applicable to a wide range of real-world problems.

For the future, besides further improving the available methods in control, management, and optimization and addressing even more demanding applications, the big challenge will be to bridge between the research areas listed above, i.e. to integrate from the basic control layer to plant management, to integrate logic control, continuous control and scheduling, and to take dynamics and control into account already in early stage process design.

Process control methods and applications

Feedback control is a basic principle that is employed in all natural and in human-made systems to ensure survival and safe and efficient operation. By using sensor information to adapt the degrees of freedom of the system, complex systems can be operated stably despite the influence of varying external factors and for varying and partly unknown internal dynamics. On the other hand, feedback control can lead to oscillations and instability, and the effect of the control law on the behavior of the controlled system is not straightforward which is why the design of feedback controllers has fascinated generations of control scientists since the 19th century.

Control for optimal plant performance

Starting from the design of feedback controllers for linear and nonlinear plants with the goal to achieve a good dynamic behavior of the controlled system, our focus of research has evolved to controller design for optimal plant performance. The key idea behind our work on process control is that the purpose of process control is to improve the operation of the plant, e.g. to consume less energy and raw materials, to avoid the production of off-spec material, to maximize the throughput, and to minimize the environmental impact. Controlling some variable to nicely track its set-point can contribute to this goal, but may have little effect and can even be counterproductive.

There are several ways of optimizing plant performance by feedback control: choosing a suitable control structure and suitable controlled and manipulated variables, tracking necessary conditions of optimality (as e.g. operating at the limits of the cooling power), stationary optimization of the set-points and implementation by tracking controllers, and direct optimizing control where the tracking criterion is replaced by an economic criterion, and adding the specifications of product purities and equipment limitations as constraints to the optimization problem. In recent years, we have worked on and applied all four approaches, with the main effort being devoted to direct optimizing control formulations and applications to chemical engineering problems.

Robust control and optimization

On the theoretical side, the main theme of our work is how to cope with the inaccuracies of the models that are used in model-based control. Three main lines of research are being currently pursued:

- Iterative optimization using gradient modifiers
- Multi-stage robust optimizing control
- Guaranteed parameter estimation and dual control.

On the applications side, we work on reactive distillation, chromatographic separations, polymerizations in semi-batch and continuously operated reactors, and on intensified processes.

Model-based optimizing control – from a vision to industrial reality - MOBOCON

MOBOCON is an ERC Advanced Investigator Grant Project that was awarded to Prof. Sebastian Engell of the dyn group (PI) and Prof. Hans-Georg Bock of IWR Heidelberg in 2012. The goal of this generously funded project is to overcome the obstacles for the industrial application of optimization-based control by developing methods for the enhanced robustness and failure resilience of model-based optimizing control solutions and for the reduction of the modeling effort, which is the major bottleneck in the development of optimizing controllers. Additionally, MOBOCON addresses the interaction with the plant operators, with the goal to achieve a symbiosis of optimization and human capabilities to detect and react to unforeseen situations. The group at IWR contributes advanced robust numerical solution algorithms for dynamic optimization problems as they arise in optimizing control. The results will be demonstrated for a challenging reactive distillation process in a pilot plant at the BCI department.

Publication

Engell, S.: Feedback Control for Optimal Process Operation. *J. of Process Control*, 17(3), 2007, 203–219.

Iterative online optimization via modifier adaptation

Iterative optimization is a strategy for improving the operation of cyclic or batch processes and for optimizing the operation of slow, essentially stationary processes (also called real-time optimization, RTO). Traditionally, real-time optimization is based upon rigorous nonlinear process models and adjusts the set-points of key process variables to optimize the economic performance while meeting constraints on product properties and operational limits. As for any model-based optimization scheme, a key issue is the accuracy of the model that is used in the optimization. Due to plant-model mismatch, the optimum of the real plant may differ considerably from the optimum that is computed for the model. Furthermore, the constraints may be violated by the theoretically optimal set-point.

Iterative optimization via modifier adaptation combines the use of models and of the data collected during the operation of the plant. The gradients of the cost function and the values and the gradients of the constraints are modified based on the information that was obtained at the previous set-points or from the previous batches. This correction ensures convergence to the true plant optimum and satisfaction of the constraints by the real process.

This technique has been demonstrated to be efficient for batch chromatography and other chromatographic processes (annular chromatography, MCSGP-process) in previous work of our group.

Currently, we are applying the iterative optimization with modifier adaptation to the online optimization of the operating conditions of the miniplants for the hydroformylation of n-Dodecene that are operated in the SFB Transregio InPROMPT at TU Berlin and TU Dortmund.

Publications

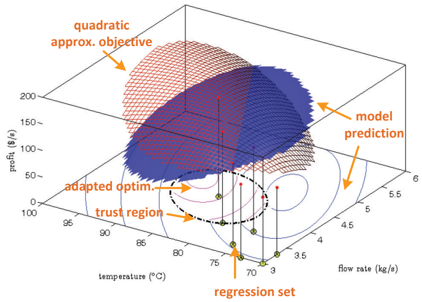
Gao, W., Engell, S.: Iterative set-point optimization of batch chromatography. *Comput. Chem. Eng., 29(6), 2005, 1401–1409.*

Behrens, M., Khobkhun, P., Potschka, A., Engell, S.: Optimizing set point control if the MCSGP process. In: Proc. of the *13th European Control Conference (ECC)*, Strasbourg, 2014, 1139–1144.

Iterative optimizing control by modifier adaptation with quadratic approximation

There is a fundamental problem with the use of the gradient modifiers in iterative optimization: the difficulty to correctly estimate the true plant gradients from the available measured data which has to be done by some sort of finite-difference approximation. We have therefore developed a new modifier adaptation scheme that uses ideas from derivative-free optimization (DFO).

The new scheme combines the quadratic approximation that is used in DFO with the modifier adaptation approach and integrates recent advances in both areas. Quadratic approximations of the cost function and of the constraints are constructed based on screened data, and the gradients with respect to the manipulated variables are computed from these approximated models. The next set-point move is then determined by modifier-adapted optimization in which the model is corrected by the empirical gradient information. Simulation studies have shown that the scheme leads to faster and more robust convergence to the true optimum and suppresses the oscillations around the optimum that are observed when using finite difference approximations. In future work, we will explore how to extend the scheme to updates during plant transients.



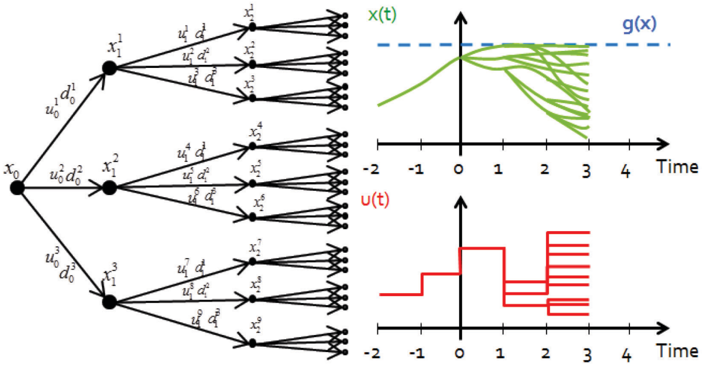
Publications

Gao, W., Wenzel, S., Engell, S.: Modifier Adaptation with Quadratic Approximation in Iterative Optimizing Control. In: *Proc. of the 14th European Control Conference (ECC)*, Linz, 2015, 2532–2537.

Gao, W., Wenzel, S., Engell, S.: Integration of Gradient Adaptation and Quadratic Approximation in Real-Time Optimization. In: *Proc. of the 34th Chinese Control Conference*, Hangzhou, 2015, 2780–2785.

Multi-stage nonlinear model-predictive control

Nonlinear Model-Predictive Control (NMPC) is a model-based strategy to achieve economic or tracking objectives for nonlinear systems while satisfying the process constraints. If the model does not describe the plant behavior accurately, there is the necessity of a robust control scheme which is not overly conservative. Multi-stage NMPC is a non-conservative real-time-implementable robust control scheme which guarantees constraint satisfaction for nonlinear systems under uncertainty. The evolution of the uncertainty is modeled as a scenario tree (see the figure.). The important aspect of the approach is



that it considers explicitly that new measurement information will be available at every stage of the prediction and that the decisions taken at every stage can be adjusted accordingly and thus can act as recourse to counteract the effects of the uncertainties. This improves the performance and reduces the conservativeness compared to traditional robust NMPC schemes.

When the state vector is not measured at each sampling interval but only noisy measurements of some outputs are available, additional uncertainty about the current state as well as inexact information about the future states must be taken into account. The presence of estimation error poses an interesting challenge of not only predicting the evolution of the plant under uncertainty but also the evolution of the plant under the control actions which result due to the presence of current and future estimation errors. With the assumption that the plant is observable and the innovations sequence is bounded, the samples of the innovations are modeled as new scenarios in the scenario tree in addition to the parametric uncertainties and the observer equations such as the EKF/UKF are used to predict the evolution of the future states/estimates. The proposed approach is shown to be robust to plant-model mismatch and to estimation errors.

If the values of a subset of the uncertain parameters can be estimated online using the state or parameter estimation techniques, the scenario tree can be adapted. Instead of having a global bound on the uncertain parameters, a less conservative local estimate of the bound of the (possibly time-varying) parameters can be obtained. The resulting innovations caused by the estimation errors in addition to the innovations generated by the possible parameter changes then have to be considered. The observer equations in the controller can be used to predict the future parameter estimates in addition to the states. Our approach considers the fact that not only the states but also the parameters are estimated at every sampling time and the future control inputs can act as a recourse for the effect of the changes in the parametric uncertainties along with the evolution of the plant at those times, resulting in further improvement in controller performance.

The dyn group has developed a modular and numerically efficient implementation of multistage NMPC in the framework of *DO-MPC*. It is an open source free software and can be downloaded from: https://github.com/do-mpc/do-mpc.

Publications

Lucia, S., Andersson, J., Brandt, H., Diehl, M., Engell, S.: Handling uncertainty in economic nonlinear model predictive control: a comparative case-study. *J. of Process Control*, 24(8), 2014, 1247–1259..

Subramanian, S., Lucia, S., Engell, S.: Economic multi-stage output nonlinear model predictive control. In: *Proc. of the 2014 IEEE Multi-Conference on Systems and Control*, 2014

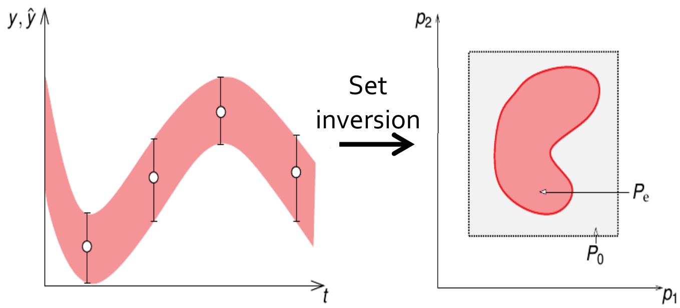
Lucia, S., Tatulea-Codrean, A., Schoppmeyer, C., Engell, S.: An Environment for the Efficient Testing and Implementation of Robust NMPC. In: *Proc. IEEE Multi-conference on Systems and Control*, Antibes, 2014

Subramanian, S., Lucia, S., Engell, S.: Adaptive Multi-stage Output Feedback NMPC using the Extended Kalman Filter for time varying uncertainties applied to a CSTR. *Proc. of the 5th IFAC Conference on Nonlinear Model Predictive Control, Sevilla, 2015*

Guaranteed parameter and state estimation

The quality of the results of model-based optimization strongly depends on the accuracy of the models that are employed. It is essential that the predictions of variables that are considered in the optimization problem, e.g. product quality parameters, are accurate. The quality of the models can be increased by online adaptation of crucial parameters by robust state and parameter estimation schemes.

In this respect, we pursue a guaranteed parameter estimation approach to obtain robust estimates of uncertain parameters while avoiding unreliable approximations that are associated with classical estimation approaches. The guaranteed estimation approach seeks to find the set of all possible parameter values such that the predicted outputs match the corresponding measurements within prescribed error bounds.



The solution of the guaranteed parameter and state estimation problems is found by the application of set inversion via interval analysis. We have developed a computationally efficient approach based on improved bounding techniques for parametric ordinary differential equations, and optimization-based domain and CPU-time reduction techniques.

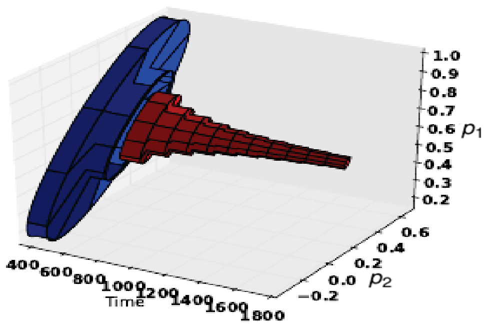
Publication

Paulen, R., Villanueva, M., Chachuat, B.: Guaranteed parameter estimation of non-linear dynamic systems using high-order bounding techniques with domain and CPU-time reduction strategies. *IMA J Math Control*, 2015.

Robust dual nonlinear model-predictive control

Dual control is a technique that seeks to solve the trade-off between probing control actions, which result in more precise estimation of unknown model parameters, and the optimal operation of a nonlinear dynamic system under parametric uncertainty.

We study robust approaches to dual control based on the multi-stage NMPC formulation that lead to a dual control formulation by taking explicitly into account the reduction of the uncertainty that future probing actions will provide over the prediction horizon. Using this formulation, our approach does not require any a priori heuristic decision on the relative importance of the probing actions with respect to the optimal performance of the controlled system, as proposed in some recent approaches, but takes this effect into account exactly.

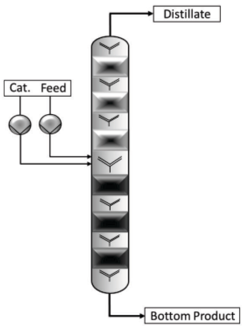


The novel dual robust NMPC formulation which is based on multi-stage NMPC reduces the conservatism of the robust control actions since it considers that future control inputs can be adapted to future observations and it predicts the future reduction of the uncertainty. The results show the advantage of using a dual robust NMPC over the classical adaptive control approaches, i.e. the sequential use of parameter estimation and optimization.

Publication

Thangavel, S., Lucia, S., Paulen, R., Engell, S.: Towards Dual Robust Nonlinear Model Predictive Control: A Multi-stage Approach. In: *Proc. American Control Conference*, Chicago, 2015, 428–433.

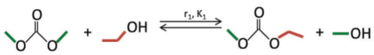
Model-based optimizing control of reactive distillation



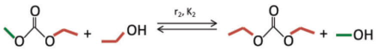
Reactive distillation (RD) combines chemical reaction and separation by distillation in one piece of equipment. It is the most often used integrated process because by applying reactive distillation, the number of pieces of equipment and the energy demand can be reduced significantly, in particular for equilibrium-constrained reactions. The dyn group has cooperated with the fluid separations group of Prof. A. Gorak (FVT) for many years in the dynamic mathematical modelling and optimal operation and control of reactive distillation processes.

In the context of the MOBOCON project, a very challenging reactive distillation process was chosen for the demonstration of online optimizing control at a pilot plant. The process, which has been developed by the FVT group, can be dynamically switched between two different target products. The reaction mechanism consists of two steps:

Trans-esterification of Dimethyl Carbonate with Ethanol:



Trans-esterification of Ethyl-Methyl Carbonate with Ethanol:



Both products are of interest industrially, but their individual production is difficult. By a proper choice of the operating conditions in a reactive distillation column, either product can be produced with a high selectivity in a single apparatus.

Dynamic mathematical modelling

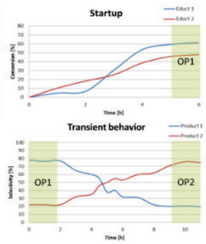
From several mathematical models of different complexity, an equilibrium-stage process model was chosen and implemented in MATLAB® and Python/CasADi for model-based control purposes. The resulting DAE model has 955 variables, among them 305 dynamic states.

Multi-rate state estimation

For model-based control, the internal states of the optimization model must be initialized using plant measurements. Possible estimators are particle filters or the DAE version of the EKF. A new formulation of the particle filter for DAE systems has been developed in which different sampling intervals of different measurements can be considered.

Model-based optimizing control

For nonlinear model-based control, the dyn group has developed a software-platform (called DO-MPC) that employs state-of-the-art methods for dynamic nonlinear optimization, such as automatic differentiation and multiple shooting, and supports robust multi-stage NMPC formulations.



The goal in MOBOCON is to apply direct optimizing control with an economic cost function to the real reactive distillation process in a 50 mm diameter pilot plant. Key challenges are the size and the nonlinearity of the process model and the inevitable plant-model mismatch as the complex physico-chemical phenomena are only approximately represented even by high-order models. The online optimizing controller should also handle the startup of the plant and the transition between the two modes of operation that lead to the two different target products.

Publications

Völker, M. C., Sonntag, C., Engell, S.: Control of integrated processes: A case study on reactive distillation in a medium-scale pilot plant. *Cont. Eng. Pract.*, 2007, 15(7), 863–881.

Idris, E.N.A.; Engell, S.: Economics-based NMPC strategies for the operation and control of a continuous catalytic distillation process. *J. of Proc. Control*, 2012, 22(10), 1832–1843.

Lucia, S., Tatulea-Codrean, A., Schoppmeyer, C., Engell, S.: An Environment for the Efficient Testing and Implementation of Robust NMPC. In: *Proc. IEEE Multi-conference on Systems and Control*, Antibes, 2014.

Model parameter estimation of the SMB process

Simulated Moving Bed (SMB) chromatography is a preparative chromatographic process which establishes a countercurrent movement of the solid bed by switching the feed and the product ports periodically in a ring of chromatographic columns. Compared to batch chromatography, the SMB process is more efficient in terms of solvent consumption and utilization of the adsorbent, but it is more difficult to design and to operate. Model-based online optimization techniques can improve the economic performance of the process. Due to the high sensitivity of the purities of the products to the adsorption behavior of the system, it is crucial to employ accurate models in the optimization.

The accuracy of the model parameters can be improved by optimal dynamic experiment design which is investigated in our research. By means of this technique, it has been possible to design start-up plant experiments which lead to a drastic reduction of the expected confidence intervals of the parameters of the isotherms of the individual columns, while respecting purity constraints for one of the product ports during the time horizon of the experiment. A critical aspect is the evaluation of the objective function of the experimental design problem, for which the adjoint-based derivative evaluation framework implemented in the optimal experiment design package VPLAN (IWR Heidelberg) is used together with an efficient implementation of the process model of the chromatographic plant.

We have also developed a technique for the estimation of individual column parameters based upon concentration measurements of the product ports when they are connected to the column under consideration.

In 2015, the dyn group will install a new SMB chromatography system which is capable of running the novel multi-column solvent gradient process (MCSGP), and we will study the online optimization of this mode of operation.

Publication

Lemoine-Nava, R., Engell, S.: Individual Column State and Parameter Estimation in the Simulated Moving Bed Process: An Optimization-based Method. In: Proc. of the 19th IFAC World Congress, Cape Town, 2014.

Interaction between operators and advanced control solutions

A challenge in advanced optimization-based control is the interaction with the operators. Professional plant operators have a good experience-based understanding of the behavior of the plant and can learn the effect of manual changes and disturbances whereas they cannot handle the interactions and constraints as well as the optimization-based solution. However, the operators are responsible for the monitoring of advanced controllers and have the authority to accept or to discard the proposed control moves and to switch the optimizing controller off if its behavior seems wrong to them.

Acceptance by the operators is therefore crucial to the long-term success of advanced control solutions; they must be viewed as a useful and reliable support in the daily work of the operators. Our goal is to provide information about the results of the optimization in order to convince and motivate the operators to rely on them. This requires that understandable explanations and reliable diagnosis of the results are provided in order to build trust.

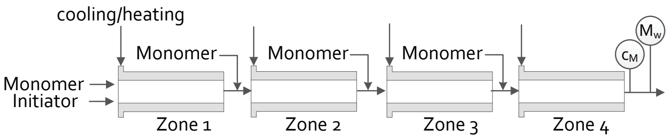
Moreover, the abilities of humans to detect and handle critical situations are important and will be needed for a long time to maintain an efficient operation of processing plants. Rather than asking the operators to make a yes/no decision on the acceptance of the proposed control moves, an improved performance could result from a two-way interaction between the model-based optimization and the operators so that their process experience can be used to influence the optimization, e.g. by anticipating changing conditions that are not known to the optimizer in advance.

Optimizing control of intensified processes

Intensified continuous processes have a large potential for the sustainable production of high-quality, high-value and customer-specific products at competitive prices in a sustainable fashion. To realize the potential of this technology, tightly controlled, fully automated and optimized production is a must. Starting with the F^3 project, the dyn group has investigated the optimizing control of intensified processes, in particular of tubular reactors.

Optimizing control and state estimation of a continuous polymerization reactor

The goal is to design and to implement optimizing control for a tubular polymerization reactor with side feeds of monomer and initiator to maximize the product throughput while meeting tight quality constraints. The molecular weight and the residual monomer of the produced polymer are considered as the quality indicators.



The tubular reactor system is described by a set of nonlinear PDEs and exhibits a very complex and dynamic behavior due to the superposition of the effects of the side feeds. Our approach combines state estimation by particle filtering and dynamic model-based optimization. A key challenge is the computation time due to the high order of the discretized process model. The weighted essentially non-oscillatory scheme (WENO) is used to simulate the system without the need for a very fine discretization grid.

Publications

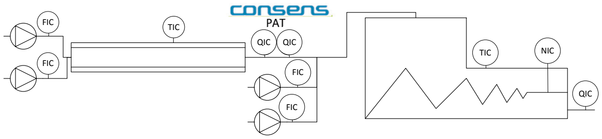
Bouaswaig, A.E., Engell, S.: WENO scheme with static grid adaptation for tracking steep moving fronts. *J. of Chem. Eng. Sci.*, 2009, 64(14), 3214–3226.

Hashemi, R., Engell, S.: Optimizing control and state estimation in a tubular polymerization reactor. In: *Proc. of the 19th IFAC World Congress*, Cape Town, 2014.

Integrated control and sensing for sustainable operation of flexible intensified processes

The goal of the HORIZON 2020 SPIRE project CONSENS is to advance the continuous production of high-value products in flexible intensified continuous plants by introducing novel online sensing equipment and closed-loop control of the key product parameters. CONSENS focuses on flexible continuous plants but the results will be transferable also to large-scale continuous processes. The research and development is driven by industrial case studies from three different areas, spanning the value chain of chemical production: complex organic synthesis, specialty polymers, and formulation of complex liquids. The project results will be validated in pilot plants, including production containers that have been developed in the F^3 Factory project.

In the dyn group, PAT-based control concepts for two CONSENS processes will be developed, an organic synthesis in a tubular reactor, and the production of high-viscosity polymers in two pieces of equipment, a tubular and a kneader reactor.



The challenge for both processes is to enhance the process performance applying the novel sensor data. In order to cope with the mismatch between plant models and reality, online model parameter estimation and iterative optimization using gradient modifiers will be applied. The model will be used for optimizing control. In addition, the dyn group will develop strategies for plant-wide control for modular continuous plants, integrating local control strategies into a plant-wide process control strategy.

Publication

Finkler, T., Kawohl, M., Piechottka, U., Engell, S.: Realization of online optimizing control in an industrial semi-batch polymerization. *J. of Proc. Control*, 2014, 24(2), 399–414

Plant management

Feedback control has traditionally been applied to the equipment and to the unit level while plant-wide and site-wide interactions have only been addressed on long time scales by stationary optimization. Disturbances, demand variations, and shutdowns are then handled by negotiations or phone calls. Increasingly, however, large plants and sites also are operated dynamically to exploit opportunities for cost saving or more sustainable operation. An example for this is a chemical plant or a steel plant with its own power plant for the generation of electricity and steam. Formerly, the operation of the power plant and the procurement of electricity from the grid followed the production plans that were optimized from the point of view of the production plants.

With the increased volatility of the markets for electricity and a multitude of possible contracts with utility providers, a more agile operation that reacts to the situation on the electricity supply side can save cost. In addition, the production can be made more sustainable by using electricity when there is a surplus of supply from renewables and reducing the demand in other periods.

When plants and sites are operated more dynamically, the different units have to be coordinated with respect to the use of internal resources for which no significant storages are available. In theory, with the available optimization technology, plant-wide optimization would be possible, however the lack of models in a uniform formulation, issues of missing information, and the autonomy of the different business units favor distributed solutions that build upon local optimization solutions. The EU-funded project DYMASOS addresses this challenge. In the future, we will extend this work in the context of the European ITN PRONTO in the direction of combined energy and production management.

Publication

Hadera, H., Harjunkoski, I., Sand, G., Grossmann, I., Engell, S.: Optimization of steel production scheduling with complex time-sensitive electricity cost. *Comput. Chem. Eng.*, 76, 2015, 117–136.

European roadmap on research and innovation in engineering and management of cyber-physical systems of systems (CPSoS)

Cyber-physical systems of systems (CPSoS) are large physical systems, such as railway systems, production sites, or the electric grid, that consist of many interacting physical elements and of distributed IT systems for monitoring, control, optimization, and interaction with human operators. These systems are of crucial importance for Europe as they represent some of the most important infrastructures and are the backbone of the European economy.

The dyn group is leading the EU-funded Support Action CPSoS. The goal of CPSoS is to develop a European research and innovation roadmap on cyber-physical systems of systems. CPSoS has collected inputs from a large number of experts, by discussions with the members of its three working groups on transportation and logistics, physically connected CPS, and tools and methods for engineering and management, and by many interviews with domain experts, in particular from industry. In its initial roadmap document, the CPSoS project has identified three key research and innovation challenges:

The first challenge, *distributed, reliable and efficient management of cyber-physical systems of systems*, results from the fact that control and management of CPSoS cannot be performed in a centralized or hierarchical top-down manner with one authority tightly controlling all subsystems. The second challenge addresses the *engineering support for the design-operation continuum of cyber-physical systems of systems.* The third challenge is the long-term goal to develop *cognitive cyber-physical systems of systems* in which big data and cognitive technologies support the users, system operators and managers in complexity management and systems operation.

Publication

Cyber-Physical Systems of Systems: Research and Innovation Priorities, Initial Roadmap Document, available at: http://www.cpsos.eu/roadmap/.

Dynamic management of physically coupled systems of systems (DYMASOS)

DYMASOS is a European project that is funded under the 7th Framework Programme in the area of Information and Communication Technology. It addresses the distributed management of systems of systems that are connected by flows of energy and material (cyber-physical systems of systems). Examples of such systems are chemical plants with many units that are coupled by flows of material and energy, e.g. via steam and gas networks and intermediates, or electric grids and electric vehicle charging systems. These systems are managed locally but should be operated such that the overall efficiency is as high as possible while the goals of the local systems (production plans of different business units or the interests of the users of electric cars to find their cars fully charged when they return to the charging stations) are achieved.

In DYMASOS, different techniques for control and optimization of such systems are investigated. The dyn group works on market-based algorithms for the coordination of large chemical plants. The idea of market-based algorithms is that the units are controlled by local optimization algorithms in which the resources, which are constrained and exchanged, are penalized with certain prices. By an iterative adaptation of the prices, which is driven by the imbalance of the networks, the local optimizers are steered towards the plant-wide optimum.

The benefits of this approach are that the scheme is more robust to missing local information or to the switching off of local optimizers than a centralized solution, and that the cost functions and the goals of the local systems do not have to be shared with others.

Publications

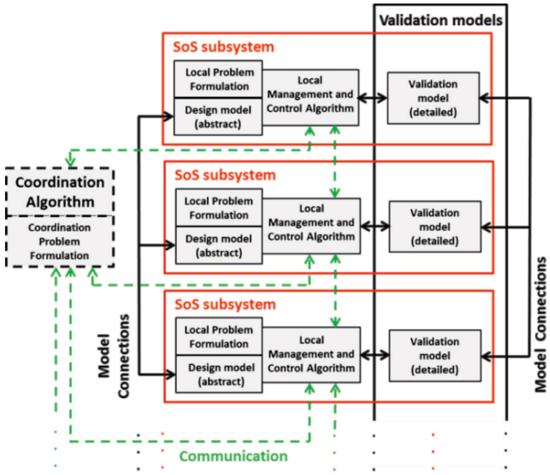
Paulen, R., Engell, S.: DYMASOS – Dynamic Management of Physically Coupled Systems of Systems. In: *ERCIM News 97*, April 2014, Special theme: Cyber-Physical Systems, 2014, 51–52.

Stojanovski, G., Maxeiner, L.S., Krämer, S., Engell, S.: Real-Time Shared Resource Allocation by Price Coordination in an Integrated Petrochemical Site. In: *Proc. European Control Conference*, Linz, Austria, 2015.

The DYMASOS simulation and validation framework

Before productive deployment, system of systems (SOS) management algorithms must be tested in simulations with faithful models of the controlled systems to validate the performance, correctness, and safety of the distributed management system. This task is facilitated by the DYMASOS simulation and validation framework that is tailored to large SOS with decentralized management.

The framework is based on the *Modelica* language for heterogeneous modelling and provides generic interfaces for the connection of models of the physical processes and implementations of distributed management algorithms. This plug-and-play approach eliminates the tedious task of manual model composition and interfacing, and simplifies the deployment of novel management algorithms to industrial automation systems.



Publications

Nazari, S., Sonntag, C., Stojanovski, G., Engell, S.: A Modelling, Simulation, and Validation Framework for the Distributed Management of Large-scale Processing Systems. In: *Proc. of 25th European Symposium on Computer Aided Process Engineering (ESCAPE)*, Copenhagen, 2015.

Kampert, D., Nazari, S, Sonntag, C., Epple, U., Engell, S.: A Framework for Simulation, Optimization and Information Management of Physically-Coupled Systems of Systems. In: *Proc. of 15th IFAC Symposium on Information Control Problems in Manufacturing (INCOM)*, Ottawa, 2015.

Real-time monitoring and optimization of resource efficiency

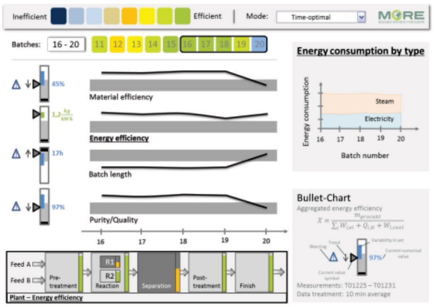
Operational decisions in the day-to-day business of production processes have a significant impact on the energy and material efficiency of the plants. Due to plant-wide interactions, the effect of the decisions is often not transparent to plant operators and managers. Currently, resource efficiency and sustainability indicators are only recorded on long time intervals, e.g. business years. The goal of the EU-funded project MORE—Real-time Monitoring and Optimization of Resource Efficiency in Integrated Processing Plants—is to introduce real-time resource efficiency indicators (REI) to monitor the energy and material efficiency of production plants in the process industries in (near) real-time and subsequently to use them in optimization and decision support for operating staff. Trade-offs between energy efficiency, material efficiency and economic success result in a multi-dimensional decision problem that must be efficiently visualized for easy perception by operators and managers.

Real-time resource efficiency indicators (RT-REI)

The MORE project has developed guidelines for the definition and computation of RT-REI. The REI are defined following a gate-to-gate approach based upon an integrated energy and material flow analysis within the boundaries of individual plants. The RT-REI are product- and resource-specific, i.e. different resources and products are taken into account separately, and independent from economic indicators and indicators of the environmental load are included. The indicators are normalized to theoretical or recorded optimal values to provide an efficient comparison of the actual state of the plant with the best possible operation. The indicators can be aggregated over a set of products. For individual process units, e.g. a distillation column, local indicators can be defined to support the operators. RT-REI have also been defined for batch plants and for mixed batch and continuous plants, taking into account the specific characteristics of such processes.

Visualization of resource efficiency indicators

Energy and resource efficiency has many aspects and is influenced by many operational decisions in a complex manner. The information provided by the RT-REI has to be presented to the operators in a transparent and intuitively understandable fashion. The dyn group therefore has developed a dashboard concept for multi-dimensional RT-REI that uses visualization elements that are best suited to highlight the intended relations and are easily comprehensible. To go beyond the possibilities of classical two- or three-dimensional representations, additional attributes as e.g. color, orientation, size, and specialized visualization elements are combined to dashboard solutions that visualize the contributions to the overall resource efficiency and their evolution.



Model-based decision support

The first step towards model-based decision support for the plant operators and managers is a tool for simulation-based what-if analysis that visualizes the effect of possible operation strategies. Beyond this, optimization techniques are used to determine optimal operation strategies with respect to resource efficiency under the current external factors imposed on the system. The approach was applied to an evaporator network of the Austrian viscose producer Lenzing AG. Based on the current fouling state of the evaporators, the optimal combination and loads of the evaporators are determined. Similar tools for other plants are currently under development.

Publication

Kalliski, M., Krahé, D., Beisheim, B., Krämer, S., Engell, S.: Resource efficiency indicators for real-time monitoring and optimization of integrated chemical production plants. In: *Proc. 25th European Symposium on Computer Aided Process Engineering (ESCAPE)*, Copenhagen, 2015.

Logic control and production scheduling

Since its beginnings, the dyn group has not only addressed the traditional field of continuous control but also the practically very relevant field of systems with discrete elements, i.e. logic control, hybrid systems, and production planning and scheduling.

Logic control code, including exception handling, switching between sensors and controllers etc., and sequence control represents the dominant part of the control software and exhibits a large complexity that makes it very difficult to verify its correctness, especially when the logic controllers are interacting with physical systems with continuous dynamics.

Despite significant research efforts, also by our group, a breakthrough in the systematic development and verification of logic controllers has not yet been achieved. Our most recent work concerned the systematic and intuitive specification of logic controllers and automatic generation of SFC code from the specification. For this, the DC/FT tool has been developed and is available for test users. In the European project MULTIFORM, we have worked on model transformations and tool chains to support the design of automated systems which forms the basis of the development of the DYMASOS simulation and validation framework.

In scheduling, our focus since long is on dealing with uncertainties in an anticipatory manner by employing the two-stage stochastic programming approach, and in a reactive manner by fast re-scheduling in the framework of rolling horizon scheduling based upon timed-automata models. The recent work in this area connects scheduling and logic control design to react to unexpected events in a flexible and efficient manner.

Publications

Hüfner, M., Fischer, S., Sonntag, C., Engell, S.: Integrated Model-based Support for Design of Complex Controlled Systems. *Computer Aided Chemical Engineering.* 31, 2012, 1672–1676.

Fischer, S., Teixeira, H., Engell, S.: Systematic Specification of a Logic Controller for a Delayed Coking Drum. *Computer Aided Chemical Engineering.* 31, 2012, 355–359.

Heuristic methods for solving two-stage stochastic chemical batch scheduling problems

Scheduling problems in which some information about the future evolution is uncertain at the time of the first decisions, but where more information arrives over time, can be modeled adequately by two-stage stochastic mixed-integer programs. Here the uncertainty is modeled by a discrete set of scenarios. The first-stage decisions have to be the same for all scenarios while the second-stage decisions can be adapted to the future evolution. The presence of these recourse decisions is taken into account when the first-stage decisions are optimized.

With an increasing number of scenarios, the resulting optimization problems become computationally very hard to solve in a monolithic fashion. In our previous work, we employed a stage decomposition approach where the first-stage decisions are optimized by an evolutionary algorithm and the scenario problems are solved by MILP methods.

In the context of the Research Training Group (DFG Graduiertenkolleg) "Discrete optimization of technical systems under uncertainty", the dyn group is investigating whether the ideas behind Ordinal Optimization: *'Order is easier than Value'* and *'Nothing but the best is very costly'* can be used to improve the computation times further. The key idea is to replace the exact MILP solution of the scenario problems by fast non-exact solutions and to perform a ranking (with small errors) of different promising first stage solutions. According to the theory of Ordinal Optimization, with a high probability one of the best solutions of this ranking is among the best solutions for the original optimization problem, hence good solutions can be found in relatively short computation times.

Publications

Sand, G.; Engell, S.: Modeling and solving real-time scheduling problems by stochastic integer programming. *Comput. Chem. Eng.*, 28(6-7), 2004, 1087–1103.

Tometzki, T.; Engell, S.: Systematic Initialization Techniques for Hybrid Evolutionary Algorithms for Solving Two-Stage Stochastic Mixed-Integer Programs. *IEEE Trans. Evol. Comput.*, 15(2), 2011, 196–214.

Timed automata-based scheduling

In all cases where resources (reactors, machines, robots, pallet movers) are used for different tasks or jobs that arrive in an irregular fashion, proper planning and scheduling is needed in order to achieve an efficient processing of the jobs, good resource utilization and customer satisfaction. In practice, schedules are often created manually or by applying simple heuristics which results in fast but suboptimal solutions. On the other hand, extensive scientific work has been done on formulating and solving scheduling problems by mathematical programming, but this is not yet widely applied. One of the reasons for this is that modelling is not intuitive and that realistic problems can only be solved by tailored algorithms.

In the last decade, we have explored an alternative approach: the modeling and solution of scheduling problems using timed automata. Timed-automata models are graphical and modular and the problem-specific parameters can be changed easily. Optimal schedules can be computed by the so-called reachability analysis for timed automata which computes the shortest path from an initial state to the final state where all jobs are finished by graph-search. The dyn group has developed the tool TAOpt that provides an intuitive modeling interface and advanced algorithms for graph search that solve medium-sized scheduling problems very efficiently. An advantage of the timed automata approach is that good solutions are provided very fast. Thus it is well suited for reactive scheduling problems where short response times are needed. For larger problems, time-scale decomposition by means of a rolling horizon approach can be applied.

Publications

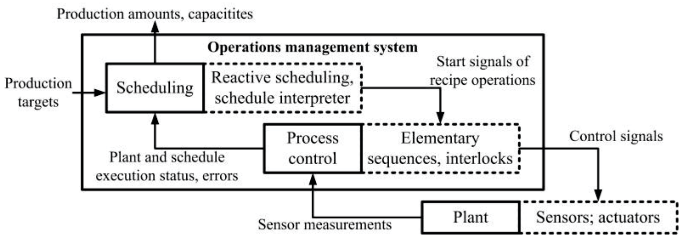
Subbiah, S., Schoppmeyer, C., Engell, S.: An intuitive and efficient approach to process scheduling with sequence-dependent changeovers using timed automata models. *Ind. Eng. Chem. Res.*, 50(9), 2011, 5131–5152.

Schoppmeyer, C., Subbiah, S., De La Fuente Valdès, J. M., Engell, S.: Dynamic Scheduling of Shuttle Robots in the Warehouse of a Polymer Plant Based on Dynamically Configured Timed Automata Models. *Ind. Eng. Chem. Res.*, 53(44), 2014, 17135–17154.

Integrating reactive scheduling with recipe control

The increasing demand for customized products with short life-cycles and the pressure to produce cheaper, faster, and more flexibly call for an efficient scheduling and a robust operation of multiproduct batch plants. Usually, the planning of the production is done for the next months, and a detailed scheduling is performed for each day. Currently, the scheduling and recipe control layers are not integrated so that disturbances and more severe errors that cannot be compensated by the recipe control layer and thus require quick rescheduling (e.g. machine breakdowns) cannot be handled efficiently.

To overcome this problem, the dyn group is working on operations management systems that integrate scheduling and recipe control by embedding timed automata-based schedule optimization into recipe-driven production based on sequential control logic combined with interlocks. The two levels are integrated by a feedback structure in which the scheduling level passes start signals to the corresponding elementary sequences of the recipe control level which in turn reports end and error signals to the scheduling level.



Experiments on a lab scale multiproduct pipeless batch plant have shown that this integrated system is able to respond quickly and robustly to uncertain events that occur during production.

Publication

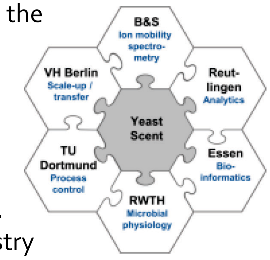
Schoppmeyer, C.; Fischer, S.; Steimel, J.; Wang, N.; Engell, S.: Embedding of Timed Automata-based Schedule Optimization into Recipe Driven Production. In Proc. 24th European Symposium on Computer Aided Process Engineering (ESCAPE), 2014, 415-420.

Modeling, simulation and control of biosystems

Biological production processes are far less well understood than chemical ones, and therefore the need for model-based control and optimization is even greater in this domain. However, the complexity of the biological processes makes modeling very challenging, and models of adequate complexity must be formulated that on the one hand represent the biological knowledge as much as possible but on the other hand do not have too many uncertain parameters.

Modeling and control of yeast fermentations

Saccharomyces cerevisiae, also known as budding yeast, is widely used in the food and beverage industry, in particular for baking, winemaking, and brewing. The early work of the dyn group focused on modeling of yeast cell cultures with respect to the cell cycle and on developing strategies to synchronize the budding of the cells. Currently, we investigate the transition of yeast cells to ethanol production and how to avoid this transition while achieving maximal growth rates. This phenomenon is called the Crabtree effect after its discoverer. The work is part of the BMBF project *„YeastScent"* in which ion mobility spectrometry (IMS) is used for the measurement of volatile metabolites in the off-gas of yeast fermentations and for the control of the feeding strategy. Our group develops a suitable mathematical model to predict the switching to ethanol production. The model is based on the biochemistry of the cell and extended by kinetics expressions.



Publications

Wegerhoff, S., Neymann, T.C., Engell, S.: Synchronization of a budding yeast cell culture by manipulating inner cell cycle concentrations. In: *Proc. of the 2012 IEEE Decision and Control Conference (CDC)*, Maui, USA, 2012.

Wegerhoff, S., Engell, S.: Simulation of the aerobic growth of Saccharomyces cerevisiae during fed batch fermentation by dynamic flux balance analysis. In: *Proc. of the 2015 Foundation of System Biology in Engineering (FOSBE)*, Boston, USA, 2015.

Dynamic models of biosystems based upon elementary modes

Mathematical models can support the development and the operation of bioprocesses significantly, by their use in model-based design of experiments to find optimal operating conditions, in optimizing batch trajectories, and in monitoring and control strategies. Recent advances in process-analytical technology provide access to a large amount of offline and online data of fermentation processes, but utilization of this data requires mathematical process models which characterize the important dependencies with a limited model complexity but sufficient accuracy.

In a project with Bayer Technology Services, we are developing a systematic modeling procedure so that dynamic process models can be generated within a short period of time. The procedure uses both knowledge-based and data-based modeling techniques and can be applied to batch- and fed batch processes. Elementary Modes are used as representative macro reactions for the cell metabolism. A newly developed data reconciliation procedure is used to test the importance of Elementary Modes. This method is further used in a multi-objective optimization for the selection of an ideal set of macro reactions. The influences of the process conditions are analyzed statistically and integrated in the kinetic expressions for the reaction rates. This approach utilizes the available biochemical knowledge and thus goes beyond the usual approach based only upon formal kinetics that depend on external concentrations and still leads to fast model development. The generated process models represent the process well within the design space and can be applied for online applications as e.g. state estimation and nonlinear model-predictive control (NMPC) at the real process.

Publication

Hebing, L., Neymann, T.C., Engell, S.: An Efficient Modelling Procedure for the Generation of Bioprocess Models with adaptable Complexity. In: *Proc. of the 2015 Foundation of System Biology in Engineering (FOSBE)*, Boston, USA, 2015.

Process design and optimization

Process design and optimization has been part of the dyn research portfolio for many years, starting from projects on the optimization of reactive distillation columns. Initially, rigorous mixed-integer nonlinear programming methods were applied, and robust model formulations were developed that ensured convergence for arbitrary initial values. Later, our focus shifted to memetic algorithms and to the support of process design in the early phase of process development.

Memetic algorithms for flowsheet optimization

In the work on the optimization of reactive distillation columns, it turned out that such optimization problems exhibit a significant number of different local optima. The combination of meta-heuristics (evolution strategies) and gradient-based local search algorithms in memetic algorithms was developed as a promising approach to the robust and efficient computation of many of these local optima. The evolution strategy performs a global search in the space of the discrete and continuous design decisions and a local rigorous optimization of the continuous design parameters improves the solution that is proposed by the evolutionary algorithm. The memetic algorithm has been applied successfully to the optimization of a process for the production of Methyl-tert-butyl-ether (MTBE) using a reactive distillation column with an optional external reactor.

Publications

Barkmann, S., Sand, G., Engell, S.: Modellierungsansätze für die Design-Optimierung von reaktiven Rektifkationskolonnen. *Chemie Ingenieur Technik*.80, 2008, 107–117.

Urselmann M., Barkmann S., Sand, G., Engell, S.: A memetic algorithm for global optimization in chemical process synthesis problems. *IEEE Trans. Evol. Comput*, 15, 2011, 659–683.

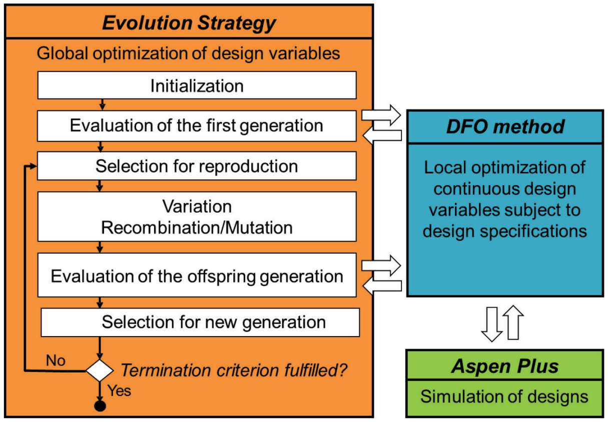
Urselmann, M., Barkmann, S., Sand, S., Engell, S.: Optimization-based design of reactive distillation columns using a memetic algorithm. *Comput. Chem. Eng.*, 35, 2011, 787–805.

Urselmann, M., Engell, S.: Design of memetic algorithms for the efficient optimization of chemical process synthesis problems with structural restrictions. Comput. Chem. Eng., 72, 2015, 87-108.

Design optimization by memetic algorithms coupled to *Aspen Plus*® process simulations

Design optimization by memetic algorithms is transferred to applications by the research project *„CHEMAX – Maximization of the energy efficiency of chemical processes*" funded by BMBF. Via ZEDO e. V., the dyn group collaborates in this project with divis intelligent solutions and SUPREN.

To improve the flexibility and the acceptance of the optimization software in industry, a memetic algorithm is coupled to the process simulator *Aspen Plus*® which provides large databases for physical properties and model libraries for many process units and facilitates setting up and simulating complex flowsheets. As *Aspen Plus*® does not provide information about derivatives, the gradient-based local optimization is replaced by a derivative-free method that is tailored to handle simulation failures and constraints. The robustness and the computation time needed for the optimization are improved by providing initial values for the simulation using data that was collected during the search.



Structure of the MA

Publication

Urselmann, M., Foussette, C., Janus, T., Tlatlik, S., Gottschalk, A., Emmerich, M., Bäck, T., Engell, S.: Derivative-Free Design Optimization of Chemical Processes by a Memetic Algorithm. *Proc. of the UK Workshop on Computational Intelligence*, Exeter, 2015.

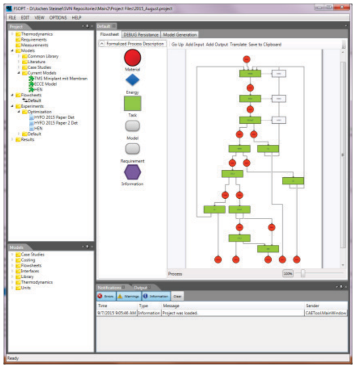
Model-based conceptual process design in the early phase of process development

Within the collaborative research center (SFB Transregio 63) *InPROMPT* funded by the German Research Foundation (DFG), the dyn group is developing methods and software for the optimization-based support of process design in the early phase of process development. The goal of the SFB Transregio InPROMPT is to develop novel liquid multiphase processes. Currently, the research focuses on the functionalization of long-chain olefins and esters.

The goal of the sub-project C1 "Model-based control of the development of novel chemical production processes" is to provide information about which process alternatives are most promising in the presence of significant uncertainties in the available models, and what experimental work should be performed to reduce the uncertainty in those parameters which are most important for the design decisions.

Two-stage stochastic programming formulation

In order to deal with the model uncertainty and to take the operational degrees of freedom of the plant into account, the process synthesis problem is decomposed into two stages: In the first stage, the design decisions are taken considering a set of discrete uncertainties. In the second stage, it is assumed that the values of the uncertain parameters are known and that the operational degrees of freedom can be adapted to the real situation.



The resulting large-scale optimization problem is decomposed by stages and solved using a hybrid algorithm that employs local gradient-based optimization algorithms for the evaluation of the mass and energy balances and of the operational degrees of freedom.

The flowsheet superstructure optimization tool FSOpt

During the course of the InPROMPT project a novel computer tool called FSOpt was developed with the goal to provide an integrated development environment for chemical process superstructures. FSOpt provides the user with capabilities for graphical and text-based modeling, as well as the automatic translation of the models into source code fit for execution and export into commercial optimization tools like GAMS® or MATLAB®.

Approximation of complex thermodynamic models in process synthesis

For process optimization, predictive thermodynamic models are indispensable. The more complex the phenomena are, e.g. if miscibility gaps exist, the more important are high-quality thermodynamic models. An example of this class of models is the Perturbed-Chain Associating Fluid Theory (PC-SAFT). But these models often use algorithmic procedures to solve large sets of coupled nonlinear equations, which are not compatible with equation-based optimization. If the model is reformulated in algebraic form and integrated into the flowsheet optimization, the computational effort increases significantly. In order to integrate advanced thermodynamic models into optimization-based flowsheet optimization, surrogate models can be used. As an example, one of the reactions considered in the InPROMPT project is the hydroformylation of 1-Dodecene in a thermomorphic multicomponent solvent system. The reaction medium is a 6-component-system and the solubility of CO and H_2 depends on pressure, temperature, and the composition of the liquid phase. Using a perceptron neural network fitted to solubility data calculated by the original PC-SAFT model, the mean relative deviations from the original model predictions are 0.05% for CO and 0.09% for H_2, while the computation time per phase equilibrium is reduced from 1.5 s to 0.005 s.

Publications

Steimel, J., Harrmann, M., Schembecker, G., Engell, S.: A framework for the modeling and optimization of process superstructures under uncertainty. *Chem. Eng. Sci.*, 115, 2014, 225–237.

Steimel, J., Engell, S.: Conceptual design and optimization of chemical processes under uncertainty by two-stage programming. *Comput. Chem. Eng.*, 81, 2015, 200–217.

Process control methods and applications:

- Thiago Finkler, 2015, Realization of Online Optimizing Control in Semi-Batch Polymerizations
- Malte Behrens, 2015, Iterative Optimierung kontinuierlicher chromatographischer Prozesse
- Sergio Lucia, 2015, Robust Multi-stage Nonlinear Model Predictive Control
- Ehsan Gholamzadeh-Nabati, 2014, Data-driven Adaptive Robust Control Based Upon Unfalsified Control
- Gaurang Shah, 2014, Bridging Model Predictive Control and Robust Linear Control Theory
- Elrashid Noureldin Idris, 2013, Optimal Process Operation by Using Economics Optimizing Nonlinear Model Predictive Control
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- Le Chi Pham, 2012, A Systematic Control Structure Selection for Economic Performance with Static and Dynamic Disturbances
- Ala Eldin Bouaswaig, 2011, Simulation, Control, and Inverse Problems in Particulate Processes
- Wolfgang Mauntz, 2010, A Contribution to Observation and Time-optimal Control of Emulsion Copolymerization Reactions

Plant management

- Hubert Hadera, 2014, Electricity Demand Side Management in Process Plants
- Chaujun Xu, 2013, Coordination and Decomposition of Large-Scale Planning and Scheduling Problems with Application to Steel Production

Process design and optimization

- Maren Urselmann, 2013, Designoptimierung chemischer Prozesse mit memetischen Algorithmen am Beispiel einer reaktiven Rektifikatinoskolonne mit optionalem Außenreaktor

Logic control and production scheduling

- Christian Schoppmeyer, 2015, Hierarchical Planning and Reactive Scheduling Using Timed-Automata Models
- Stephan Fischer, 2014, Entwurf und Verifikation von Ablaufsteuerungen
- Martin Hüfner, 2014, A Model-based Methodology for Tool Supported Design of Automated Systems
- Sabine Piana, 2012, Evolutionary Optimization of the Operation of Pipeless Plants with Variable Transfer Times
- Subanatarajan Subbiah, 2012, Modeling and Solution of Chemical Batch Scheduling Problems Using Timed Automata
- Sven Lohmann, 2011, Systematic Logic Controller Design as Sequential Function Chart Starting from Informal Requirements
- Thomas Tometzki, 2010, Hybrid Evolutionary Algorithms for the Efficient Solution of Planning Problems under Uncertainty
- Jian Cui, 2010, Medium-term Planning of a Multiproduct Batch Plant under Multi-period Multi-uncertainty by Means of Two-stage Stochastic Programming

All theses are published by the Shaker Verlag, Aachen, in the series “Schriftenreihe des Lehrstuhls für Systemdynamik und Prozessführung”.

Major collaborative projects

CONSENS: Integrated Control and Sensing for Sustainable Operation of Flexible Intensified Processes (2015-2017)
EC H2020 Research & Innovation Project, 15 partners, funding: 6.0 M€
Leader of work package *PAT-based Adaptive Control*

CPSoS: Towards a European Roadmap on Research and Innovation in Engineering and Management of Cyber-physical Systems of Systems (2013-2016)
EC FP7 Support Action, 4 partners, funding: 560 k€
Coordinator

DYMASOS: Dynamic Management of Physically Coupled Systems of Systems (2013-2016)
EC FP7 Collaborative Project, 12 partners, funding: 2.7 M€
Coordinator

MORE: Real-time Monitoring and Optimization of Resource Efficiency in Integrated Processing Plants (2013-2016)
EC FP7 Collaborative Project, 10 partners, funding: 2.8 M€
Scientific coordinator

MOBOCON: Model-based optimizing control - From a vision to industrial reality (2012-2017)
ERC Advanced Grant, 2 partners, funding: 3.5 M€
Coordinator

SFB/Transregio 63: Integrated Chemical Processes in Liquid Multiphase Systems - INPROMPT (2010-2017)
DFG-Transregio TU Berlin, OvGU Magdeburg, TU Dortmund, funding: 14,6 M€
Coordinator of *Project Area C: Systems Engineering*

DFG Project Cluster 635 (Paketantrag) Optimization-based Control of Uncertain Systems, RWTH Aachen, TU Dortmund, U Heidelberg, EPFL Lausanne, OvGU Magdeburg, U Stuttgart (2011-2015)
Coordinator

F^3 Factory: Creating the future of production (2011-2014)
EC FP7 Collaborative Project, 25 partners, funding: 30.0 M€
Leader of work package *Plant operation*

HYCON2: Highly complex and networked control systems (2010-2014)
EC FP7 Network of Excellence, 23 partners, funding: 3.9 M€
Leader of work package *System-wide coordination and control*

MULTIFORM: Integrated multi-formalism tool support for the design of networked embedded control systems (2008-2012)
EC FP7 Collaborative Project, 8 partners, funding: 2.8 M€
Coordinator

Awards

- Sebastian Engell, IFAC Fellow, 2006
- Sebastian Engell, Journal of Process Control Best Survey Paper Award 2005-2008 for the paper "Feedback control for optimal process operation", Journal of Process Control, 17, 203–219, 2007
- Sebastian Engell: Bayer Lecture, Carnegie-Mellon University, 2008
- Sebastian Engell: ERC Advanced Investigator Grant, 2012
- Sebastian Engell: 19^{th} Professor Roger W. R. Sargent Lecture, Imperial College London, 2012
- Abdelaziz Toumi, Dissertationspreis der TU Dortmund, 2005.
- Abdelaziz Toumi, NAMUR Award 2005 for the Dissertation "Optimaler Betrieb und Regelung von Simulated-Moving-Bed-Prozessen"
- Stefan Krämer, NAMUR Award 2006 for the Dissertation "Heat Balance Calorimetry and Multi-rate State Estimation Applied to Semi-Batch Emulsion Co-polymerization to Achieve Optimal Control"
- Anna Völker, NAMUR Award 2008 for the Master thesis "Optimization-based Safety Analysis of an Industrial-scale Evaporation System"
- Sebastian Panek, Olaf Stursberg and Sebastian Engell, Best Paper Award at Automatisierungstechnik 2008 for the paper "Produktionssteuerung auf der Grundlage von Echtzeitautomaten"
- Tomas Tometzki and Sebastian Engell: Best Paper Award IEEE Congress on Evolutionary Computation 2009 for the paper: "A Hybrid Multiple Populations Evolutionary Algorithm for Two-Stage Stochastic Mixed-Integer Disjunctive Programs"
- Ala Eldin Bouaswaig and Sebastian Engell, PSE Model-based Innovation Award 2010 for the paper "WENO scheme with static grid adaptation for tracking steep moving fronts", Chem. Eng. Sci., 64(14), 3214 – 3226, 2009
- Ala Eldin Bouaswaig, NAMUR Award 2012 for the Dissertation "Simulation, Control and Inverse Problems in Particulate Processes"
- Weihua Gao, Simon Wenzel and Sebastian Engell, Best Poster Award 34^{th} Chinese Control Conference (2015) for the paper "Integration of Gradient Adaption and Quadratic Approximation in Real-Time –Optimization"

With Industry:

With academia:

Education in Biochemical and Chemical Engineering at TU Dortmund

The BCI department of TU Dortmund educates chemical and biochemical engineers with a solid foundation in natural sciences, especially in chemistry, thermodynamics and in biochemistry and microbiology. Our graduates enjoy a very high reputation in the German chemical industry due to their broad knowledge and pragmatic approach. In the Bologna process, the study programs in Chemical Engineering and in Biochemical Engineering have been structured into a Bachelor phase (7 semesters) and a Master phase (3 semesters) which ends with 6 months thesis work. The yearly student intake in the past years has been between 240 and 300 on the bachelor level, from which about 60% finish with a Master degree. On the Master level, there is a significant additional intake from the German Fachhochschulen and from abroad. In terms of the number of students, the BCI department is by far the largest of its kind in Germany and one of the largest in Europe.

Specialization in Process Systems Engineering

Since more than 10 years, the BCI department offers an English Master program in Process Systems Engineering which has now become a specialization within the Master in Chemical Engineering. It is a 4 semester Master program that is entirely taught in English and offered on the international market. The focus is on modeling, simulation, dynamics, control, and optimization in the field of chemical engineering. Since the year 2008 more than 200 students from over 15 countries have taken part in the program and the vast majority of them finished the program successfully. Several of the graduates have taken up research positions for a doctoral degree, including some in our group, and many have found employment in the German industry.

Involvement of the dyn group

Within the Bachelor programs in Chemical and Biochemical Engineering, the responsibility of the dyn group is to teach computer programming, process dynamics and control, and process automation, complemented by student labs. Our core course is called Process Dynamics and Control. It starts from setting up dynamic first principles models, proceeds to the analysis of such models in the state space and state estimation and then moves on to an introduction to transfer function and classical control theory.

In the Master programs in Biochemical and Chemical Engineering, the students have to choose a number of core courses and elective courses. As a core course, we offer the course Process Performance Optimization; the electives cover a wide range from dynamic modeling and simulation over several courses in control to plant management and optimization (see the next pages). The students with specialization in PSE have to take Process Performance Optimization and the module Process Dynamics and Simulation from our group.

M.Sc. in Automation and Robotics at TU Dortmund

The M.Sc. program in Automation and Robotics is an international Master study program designed specifically to address the growing need of skilled engineers in the field of control and automation. After the first semester which consists of compulsory courses in mathematics, robotics, computer programming, computer systems, and control, the students can choose between three major fields of study, Robotics, Process Automation and Cognitive Systems. The program enrolls between 50 and 100 students per year and has a good success rate. Since the beginning of the A&R program, the dyn group has played a major role in it, teaching the compulsory course in control in the 1st semester and offering a large number of electives and a process control lab. In addition, the dyn group has supervised a large number of group projects.

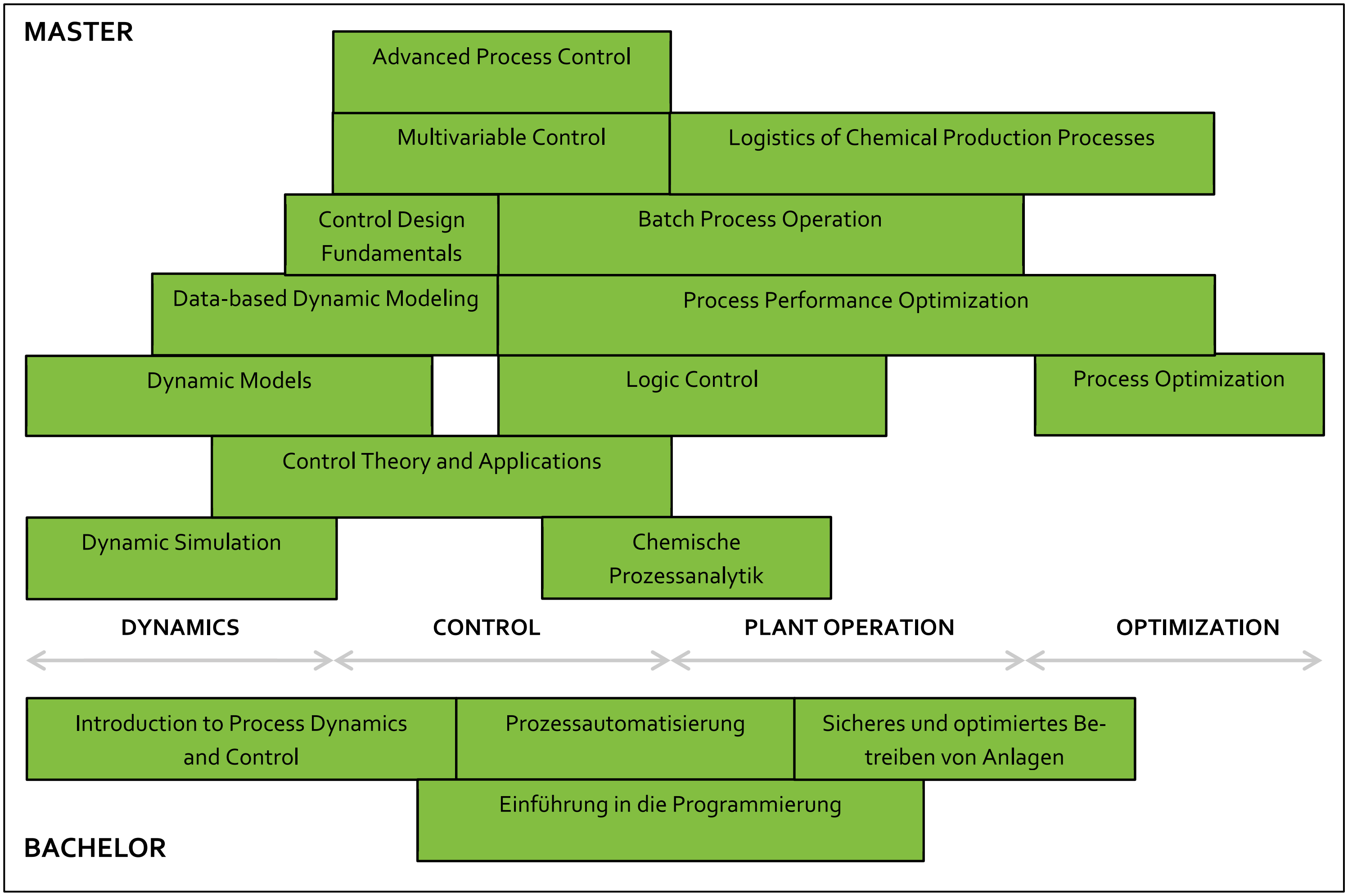
If the specialization in Process Automation is chosen, the course in Logic Control and the Process Control Lab are mandatory. In the past years, we have supervised a large number of Master thesis projects by A&R students, thereof many in collaboration with industry which helped us to progress in our research and also to gain new insights on challenges and approaches in industrial environments.

The graduates of the A&R program have good chances on the German and the international job markets, and quite a few have continued to work in research. So far, 11 graduates of the Automation and Robotics program have joined the dyn group as doctoral candidates and 4 have obtained a Dr.-Ing. degree.

dyn courses

In our lectures, we teach fundamentals and theory as well as how to apply the methods introduced in the lectures, which is why all the courses consist of a lecture and a tutorial. Some tutorials are taught as computer exercises in one of the PC pools of the BCI department.

We are very happy that we are supported by external lecturers with an industrial background. Our sincere thanks for this support go to Prof. Dr. Jörg Baumbach (B+S Analytik), Dr. Guido Dünnebier (Bayer Crop Science), Dr. Stefan Krämer (INEOS Köln) and Dr. Norbert Kuschnerus (formerly BTS and President of NAMUR).



Mandatory courses

- **Einführung in die Programmierung** *(Urselmann, Research assistants)*: Fundamentals of programming using MATLAB® to enable students to think in code and teach them how to use computer programs as tools to solve scientific problems B.Sc. BIW, CIW
- **Introduction to Process Dynamics and Control** *(Engell, Paulen)*: Basic understanding of modeling of dynamic systems, linear systems theory, Laplace transform, and its application for the design of single-loop controllers, B.Sc. BIW, CIW; M.Sc. PSE
- **Prozessautomatisierung** *(Engell)*: Introduction to sensor technology, logic control, process instrumentation, automation hierarchy, B.Sc. BIW, CIW
- **Process Performance Optimization** *(Engel, Paulen, Dr. Duennebier – Bayer Crop Science AG)* Basic and advanced process control, introduction to mathematical optimization, process monitoring and operator training simulators, M.Sc. PSE, BIW, CIW, A&R
- **Data-based Dynamic Modelling** *(Engell)*: Introduction to discrete time systems, linear model identification, neural network models, M.Sc. PSE, BIW, CIW, A&R
- **Dynamic Models** *(Engell)*: Derivation, solution, and analysis of continuous mathematical models in the form of ordinary and partial differential equations and differential algebraic systems and model order reduction techniques, M.Sc. PSE, BIW, CIW, A&R
- **Dynamic Simulation** *(Engell)*: Generation and solution of dynamic models using the equation based simulator gPROMS, M.Sc. PSE, BIW, CIW
- **Control Theory and Applications** *(Engell)*: Introduction to dynamic modeling, linear state space theory, Laplace transform, transfer functions, and frequency responses, single-loop controller design, M.Sc. A&R
- **Logic Control** *(Engell, Sonntag)*: Introduction to logic control languages for programmable logic controllers, automata models and their application, verification of control logic, M.Sc. A&R, BIW, CIW, PSE

Elective courses

- **Batch Process Operation** *(Dr. Krämer – INEOS Köln)*: Modeling, state estimation, data reconciliation, optimization, and scheduling of batch processes, M.Sc. BIW, CIW, PSE, A&R
- **Controller Design Fundamentals** *(Engell)*: Material from CTA for Chem.E. students: stability, frequency domain, SISO controllers and their tuning, M.Sc. BIW, CIW, PSE
- **Multivariable control** *(Engell)*: Single-input-single-output and multivariable controller design in the frequency domain, M.Sc. BIW, CIW, PSE, A&R
- **Advanced Process Control** *(Engell)*: Advanced linear state space theory, linear and nonlinear state estimation, gain scheduling control, linearizing control, model-predictive control, M.Sc. BIW, CIW, PSE, A&R
- **Sicheres und optimiertes Betreiben von Anlagen in der Chemie- und Pharmaindustrie** *(Dr. Kuschnerus – formerly Bayer Technology Services)*: Safe process operation, means to achieve production efficiency and flexibility in chemical and pharmaceutical production, .B.Sc. BIW, CIW; M.Sc. PSE
- **Logistics of Chemical Production Processes** *(Engell)*: Modeling and simulation of logistic systems, supply chains, production planning and scheduling, mixed-integer linear optimization M.Sc. BIW, CIW, PSE
- **Process Optimization** *(Paulen)*: Formulation and solution of mathematical optimization problems in chemical engineering and process control M.Sc. A&R
- **Chemische Prozessanalytik** *(Prof. Dr. Baumbach - Reutlingen University of Applied Science)*: Introduction to chemical analytics for chemical production processes, B.Sc. BIW, CIW; M.Sc. PSE

Courses in orange are mandatory for the study program
Courses in green are electives for the study program

Student labs

In all study programs, the practical application of the acquired knowledge and getting to know real process and control hardware is part of the education. The students have to show in experiments that they are able to transfer theory into practice. The dyn group offers several lab experiments on different levels. The complexity of the experiments varies according to the material taught in the corresponding courses, from simple liquid level control, which is solely installed for educational purposes, to advanced control, logic control design and schedule optimization of multi-product batch plants and pipeless plants. Some of the experiments are purely computer-based using the developments of the Learn2Control (L2C) project.

Even though the outcomes of the experiments are already known in theory, the practical application often provides an “aha experience“ to the students. E.g. the DYN 11 experiment concerns the creation of a schedule for a pipeless plant. While the scheduling tasks are not overly complicated, since it is easy to create a feasible schedule, due to the combinatorial explosion, it is a difficult task to create a good schedule. The comparison between the schedule produced by the students and the optimal schedule found using the timed automata based scheduling software motivates the investigation of advanced methods to solve scheduling and optimization problems.

Practical labs

- Liquid level control: Feedback control of a series of buffer tanks
- Computer aided design of the temperature control of a laboratory reactor: Model generation, validation and application for control
- Pressure control: System identification and controller design
- Control with a digital process control system: Sequential control logic design
- Flow measurement: Measurement errors
- Calorimetric measurement of the heat of reaction in a CSTR: Observer design
- Scheduling of a pipeless plant: Generation and application of production schedules

Computer labs

- Simulation of a tubular reactor: PDE modelling
- L2C - Heating system of a reactive rectification column: Rigorous process modelling
- L2C - Modeling and control of a CSTR
- L2C - Modeling and Analysis of a Reactor System: System analysis, linearization, linear control

Group projects

Higher education is not limited to acquiring domain specific technical knowledge, but also soft skills should be honed. This is one of the reasons why the curriculua of BCI, PSE, and A&R include a group project. The dyn group takes part in the organization and supervision of these projects, which involves to define suitable topics, to monitor and to guide the work of the students, and to discuss and to evaluate their intermediate and final reports as well as the presentations of their work.

The BCI and PSE students work on case studies provided by industry in groups of 8-10 students. The goal is to deliver the a basic engineering and a business assessment of a complete process, usually including the choice of the production route. The group composition is random and the results are finally presented in the department and at the partnering companies. Even though the students do not have access to the companies' resources and knowledge, the final design, which is mostly based on course material and scientific literature, often is of interest to companies due to the unbiased approach and open mindedness towards new technologies. The BCI students face this challenge at the end of the bachelor program where half of a semester in the curriculum is reserved for the group project. PSE students are expected to do the group project along with classes during a full semester.

The A&R group projects also span over a full semester but they are more flexible in scope and content. The goal is to produce "something that works", which can be software for control or design and analysis or systems that consist of hardware and software elements. The group size usually is 4-8.

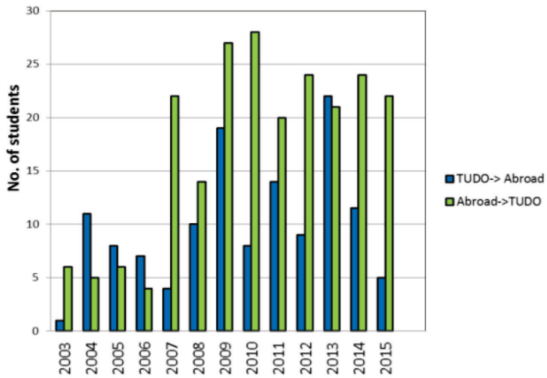
Besides having to apply the material from the courses and from the literature, the group project experience teaches the students to conduct project work under tight deadlines, to perform as a team, to manage a project and to interact with the supervisors. Also the supervisors learn a lot about how to guide students and to develop the team spirit.

International Summer Program

In 2003, the dyn group organized the International Summer Program (ISP) of TU Dortmund for the first time which in the following years has become a flagship project of TU Dortmund under the management of the International Office. The idea behind the ISP is to offer a low-threshold opportunity for students from top US and Asian universities to study in Germany. In turn, students from TU Dortmund can spend a semester at the partner universities with the fees being waived. The ISP takes place in the second half of the summer semester in Dortmund which is during the summer break for the foreign students who can acquire credits towards their degrees.

The ISP students have to take a compulsory German course as well as a course in German and European Culture and Politics, and they can choose from a broad range of courses in engineering, mathematics and business. All courses are taught in English. The students are provided with housing, insurance, semester ticket and offered a cultural program. Prof. Engell is one of the program directors, and several researchers of the dyn group each year are supporting the ISP students and involved in running the program.

The main partners in the ISP are University of Pennsylvania (USA), Hong Kong University of Science and Technology, Carnegie Mellon University (USA), Lehigh University (USA), Monterrey Institute of Technology and Higher Education (Mexico) and Universidad Federal do Rio Grande do Sul (Brazil). The graphics below shows the numbers of incoming and outgoing students in the framework of the ISP which is an important contribution to the internationalization of TUDO and to the creation of opportunities for engineering students to study abroad.



Process design and optimization


Dr. Maren Urselmann (9)
Research Associate


Tim Janus (15)
Research Assistant


Corina Nentwich (22)
Research Assistant

Head


Dr. Sebastian Engell (1)
Professor

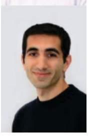
18
14
1,2,3,4,9,10,12,13,15,16,17,
19,20,22,23k,25,29,30

Process control


Clemens Lindscheid (19)
Research Assistant


Dr. Weihua Gao (6)
Research Associate


Thilo Goerke (10)
Research Assistant


Reza Hashemi (11)
Research Assistant


Elrashid Idris (7)
Research Associate


Roberto Lemoine (18)
Research Assistant


Daniel Haßkerl (12)
Research Assistant


Reinaldo Hernandez (14)
Research Assistant


Fabian Schweers (23)
Research Assistant


Sankaranarayanan Submaranian (26)
Research Assistant


Alexandru Tătulea-Codrean (27)
Research Assistant

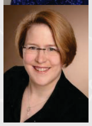

Sakthi Thangavel (28)
Research Assistant

Technician


Willi Hanika (4)

Secretaries

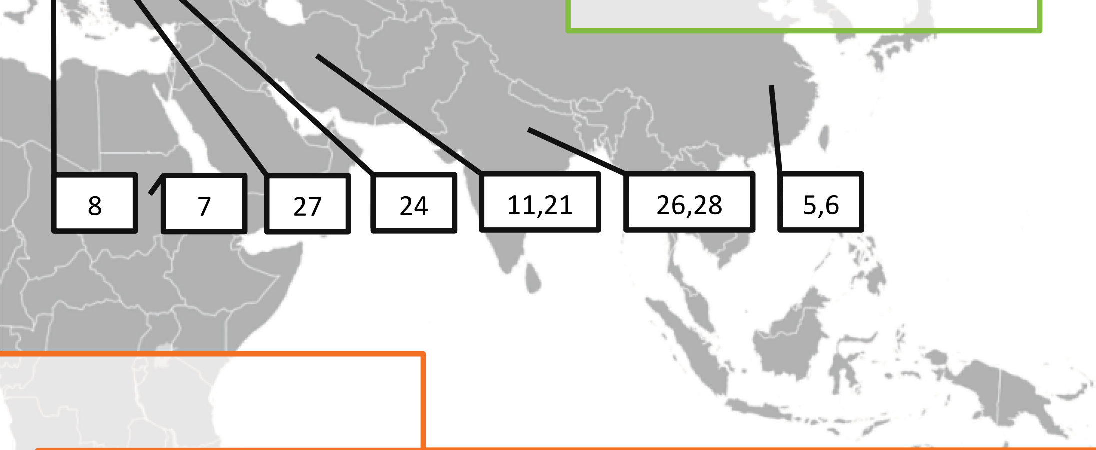

Giesela Hensche (2)


Simone Herchenröder (3)

Modelling, simulation, and control of biosystems


Lukas Hebing (13)
Research Assistant


Sven Wegerhoff (29)
Research Assistant



Logic control and scheduling


Thomas Siwczyk (24)
Research Assistant


Christian Sonntag (25)
Research Assistant

Plant management


Dr. Radoslav Paulen (8)
Research Associate


Dr. Jian Cui (5)
Research Associate


Daniel Krahé (17)
Research Assistant


Lukas Maxeiner (20)
Research Assistant


Shaghayegh Nazari (21)
Research Assistant


Marc Kalliski (16)
Research Assistant


Simon Wenzel (30)
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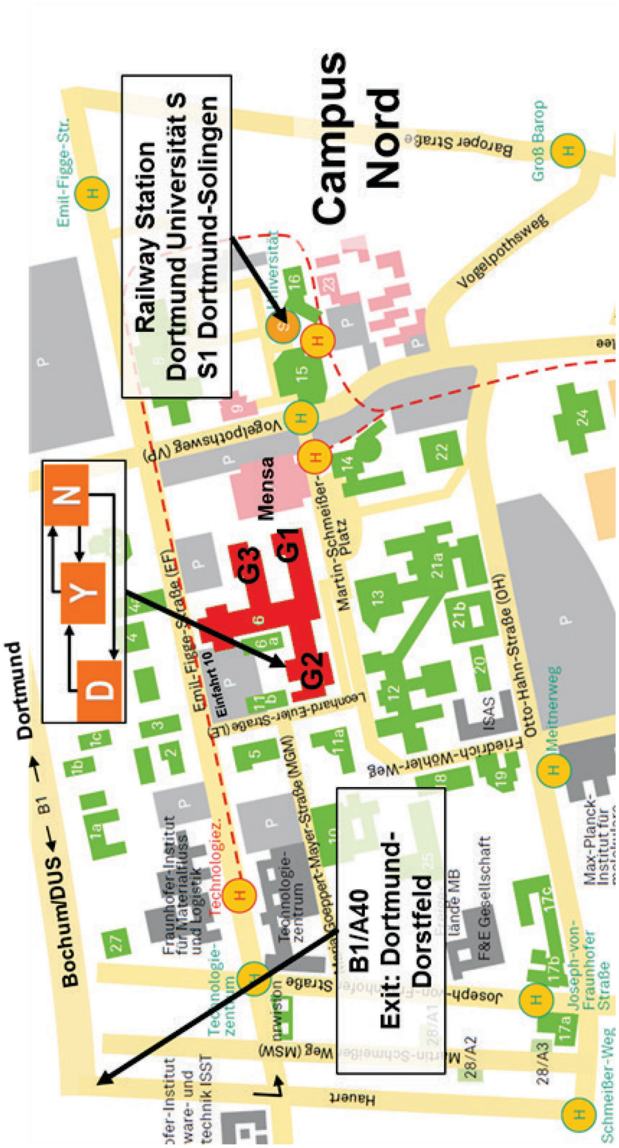

Directions

The TU Dortmund University is located on the west end of the City Dortmund. The Chair of Process Dynamics and Operations is located on the northern part of the University, Campus Nord, in the building BCI-G2. The secretariat is on the fifth floor in room 525.

By car:
TU Dortmund University can be reached by car via the A45 (Exit Dortmund-Eichlinghofen/Universität) or via the A40/B1/A44 (Exit Dortmund-Dorstfeld).

By train:
TU Dortmund University can be reached by local train S-train S1 (Dortmund-Solingen). Stop at S-Bahnhof Dortmund-Universität

By airplane:
Starting at Airport Dortmund (DTM): Bus 440 towards Dortmund Germania up to stop Dortmund-Eichlinghofen. Thence the H-train to Dortmund Universität S or Campus Nord. Starting with the car at Airport Dortmund, drive directly on the B1 in direction Dortmund and take the exit Dortmund-Dorstfeld.
Stating at Airport Düsseldorf (DUS): Take the Skytrain to Bahnhof Düsseldorf-Flughafen and change to the local S-train S1 in direction Dortmund till the stop S-Bahnhof Dortmund-Universität. As alternative take the regional trains RE1 or RE6 to Bochum central station or Dortmund central station and then change to the S-train S1.