technische universität
dortmund

Fakultät Bio- und Chemieingenieurwesen

TU Dortmund
Process Dynamics and Operations Group

Where is Dortmund?

- Dortmund is part of the Ruhr area (~ 4 million inhabitants)
  - Impressive industrial history - built upon coal and steel
  - Transformation and preservation of monuments of the past
  - It‘s not far to Paris, Amsterdam, Berlin…

Germany

Europe at night

Dortmund

Facts on TU Dortmund

- Dortmund is a part of the largest metropolitan area in Germany: The Ruhr
- Universität Dortmund was founded in 1968, as a step in the transition from a region of heavy industries to one of high-tec, services, and culture initially only science, engineering and business departments
- 1980 merger with a Teachers Education College (Pädagogische Hochschule Ruhr)
- 2008 renamed Technische Universität (Technical University)
- 22.000 students, 300 professors
- 16 departments, including all engineering disciplines
- Research university
- Before 2007 predominantly 4.5 year Diploma programs
- Since 2007 (forced) transition to a Bachelor/ Master system
  - 6-7 semesters for Bachelor, 3-4 for Master,
    5 years (10 semesters) overall

Department of Biochemical and Chemical Engineering

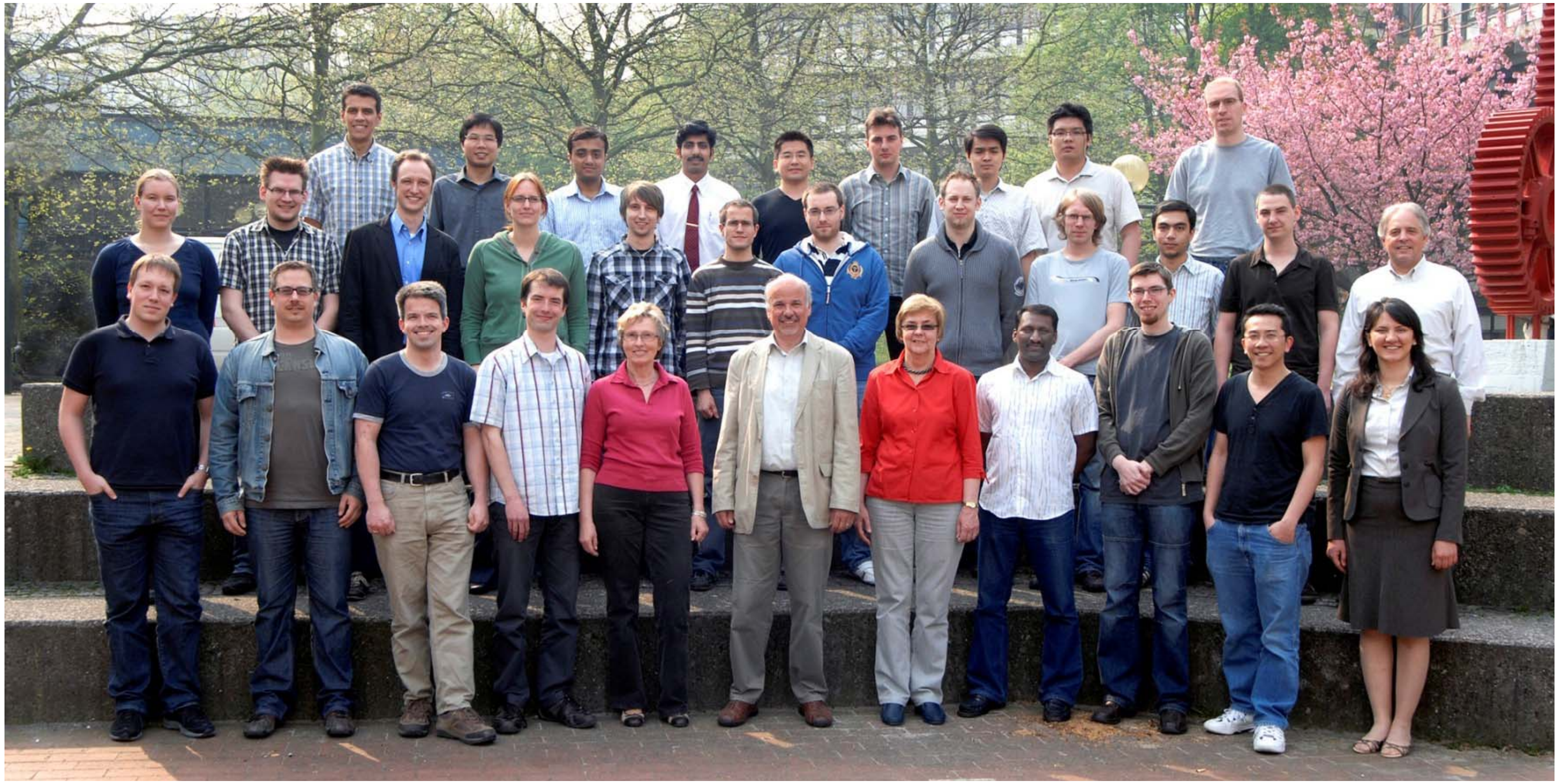
- The largest ChemE Department in Germany and among the largest in Europe
- Staff:
  - 14 Professors
  - ~ 120 doctoral students and post-docs, ~ 70 externally funded
  - ~ 20 doctoral students on scholarships
  - ~ 70 administrative and technical staff
- Programs:
  - Chemical Engineering – 140 beginners per year
    7 + 3 semesters Bachelor/Master programs
  - Biochemical Engineering – 90 beginners per year
    7 + 3 semesters Bachelor/Master programs
  - Master Program Process Systems Engineering
    - 4 semesters, 1 semester thesis work
    - Taught in English
  - Master Program Automation and Robotics/ Process Automation (interdepartmental)
- ~ 25 Dr.-Ing./ Dr. rer nat degrees granted per year

TU Dortmund
Biochemical and Chemical Engineering

Chemical Engineering Fundamentals	Industrial Chemistry	Plant Engineering	Materials Science	Biochemical Engineering
Thermodynamics *Gabriele Sadowski*	Chemical Process Development *Arno Behr*	Plant and Process Engineering *Gerhard Schembecker*	Biomaterials and Polymer Science *Jörg Tiller*	Biotechnology *Andreas Schmid*
Fluid Mechanics *Peter Ehrhard*	Reaction Engineering *David W. Agar*	Environmental Technology *Hans Fahlenkamp*		Technical Biochemistry *Oliver Kayser*
Fluid Separations *Andrzej Gorak*		Process Dynamics and Operations *Sebastian Engell*		Bioreaction Engineering *Rolf Wichmann*
Particle Technology Multiphase Processes *Peter Walzel*		BTS Professor of Equipment Design *Norbert Kockmann*		

- Process Intensification
- Sustainable Chemical & Biochemical Engineering
- Polymer Science and Polymer Production
- Model-based Design and Operation

The DYN Team



> 20 Dr.-Ing. candidates
3 technicians, 2 part-time secretaries
~ 15 student assistants

Process Dynamics and Operations

- Staff
  - Professor: Sebastian Engell
  - ~ 20 Dr.-Ing. candidates
  - 0 postdocs
  - 3 technicians, 2 part-time secretaries
- Teaching
  - B. Sc. Chemical Engineering / Biochemical Engineering
    - Process Dynamics and Control, Process Automation
    - Computer Programming, Control and Automation Lab
  - Master PSE / ChemE
    - Advanced Dynamics and Control, Batch Process Operations
    - PSE Lab
  - Master Automation and Robotics
    - Control Theory and Applications
    - Logic Control
    - Process Control Lab
    - Electives

A&R Class of 2010

DYN@TUDO: Areas of Research

Process Control Methods & Applications

Logic Controllers & Hybrid Systems

Modeling, optimization, and optimal operation of continuous and batch processes

Dortmund
Process Dynamics & Operations Group

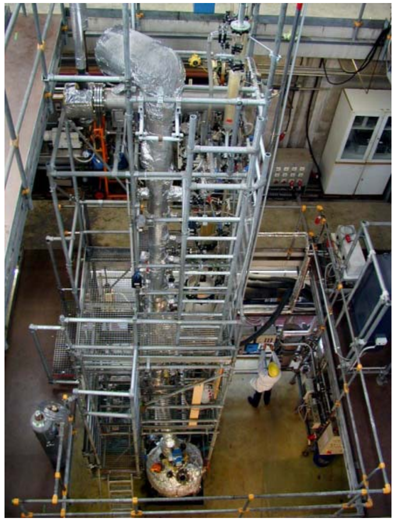
Control and operation of processes with discrete decisions

Process Design

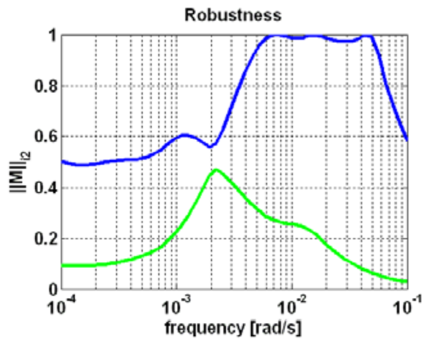
Scheduling of Batch Production

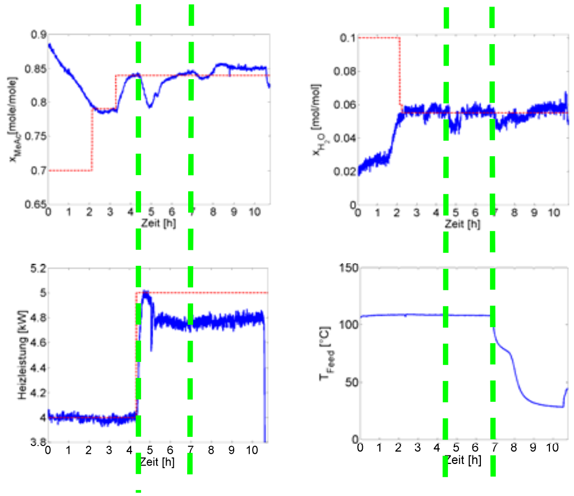
Process Control Methods

- General approach:
  Feedback control should lead to optimal operation of a production process
- Possible realizations:
  - Optimal control structure selection
  - Optimal controller tuning



Model error modeling

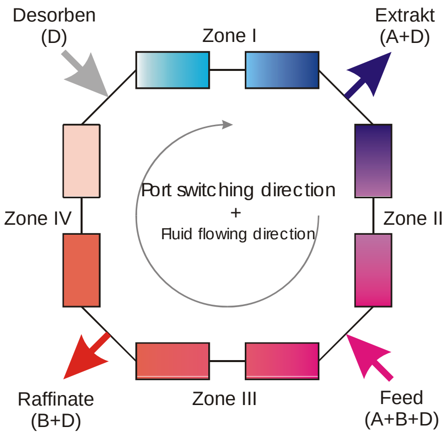


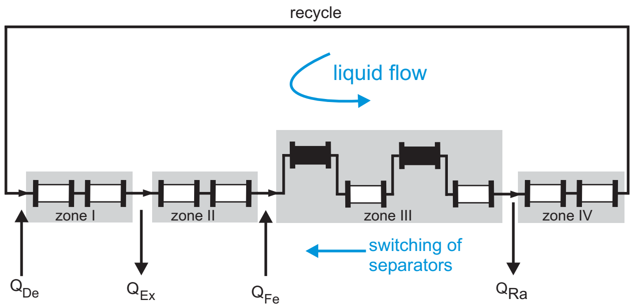


  - Implementation of optimal operation points by MPC (computed by RTO)
  - Online optimizing control

Online Optimizing Control

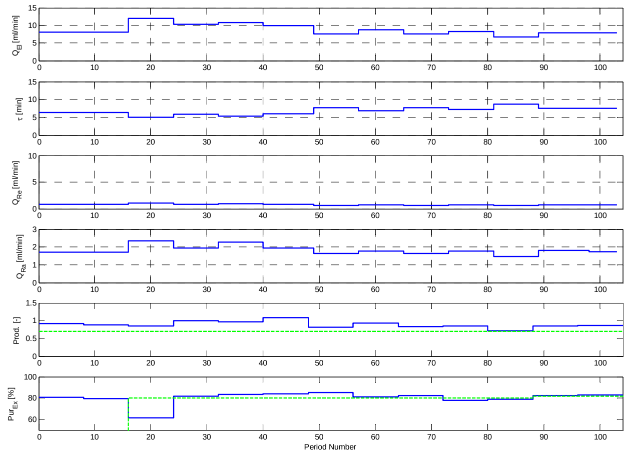
- Optimize the plant performance online over a certain prediction horizon
- Implement specifications (equipment limits, purities, yield, …) as constraints in the optimization problem – no set-point tracking
- Application: Control of (reactive) SMB processes





Novasep SMB plant, with reactors on top

Results at the real plant



Further research:
- Moving horizon state estimation
- Handling of model errors

Projects in Control Methods

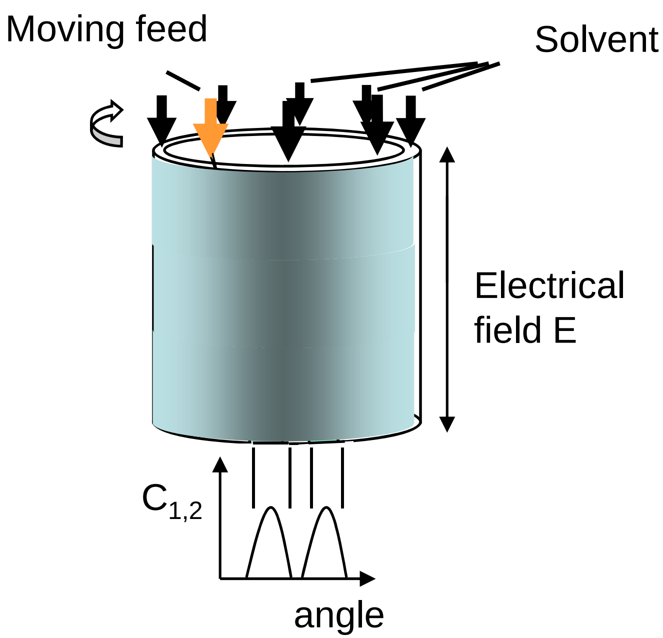
- Robust design of linear MPC controllers (Gaurang Shah)
- Selection of control structures based upon steady-state and dynamic performance (Le Chi Pham)
- Unfalsified control with controller adaptation (Ehsan Nabati)
- Robust NMPC by multi-stage optimization (Sergio Lucia, EU Project EMBOCON)
- Hierarchical control of coupled batch processes (Katja Pelz, EU NoE HYCON II)

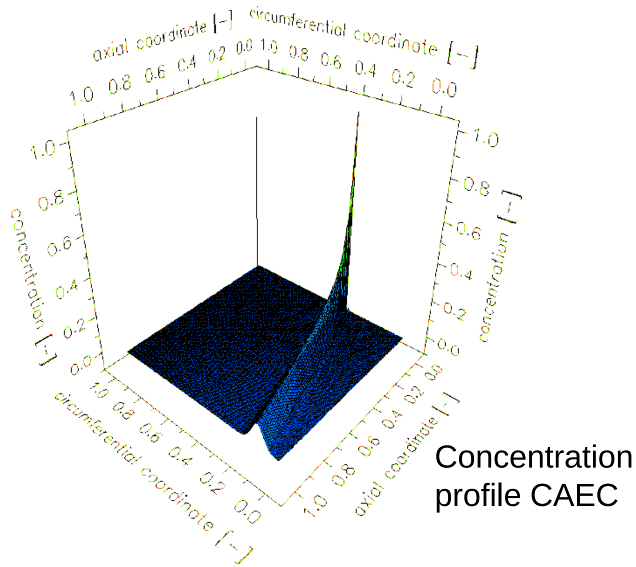
Applications Projects

- Dynamic modeling and control of electrochromatography (Yi Yu and Malte Behrens, EU project CAEC)
- Optimization and optimizing control of SMB processes (Malte Behrens and Roberto Lemoine, DFG)
- Modeling & control of the evolution of particle size distributions in emulsion polymerization (Ala Bouaswaig, Alireza Hosseini)
- Model-based control of complex emulsion polymerisation processes (Heiko Brandt, with BASF)
- NMPC of polymerization processes (Tiago Finkler, with Evonik)
- Continuous production of acrylic acid co-polymers (Daniel Kohlmann, EU project F3 with Rhodia and BASF)
- NMPC of reactive distillation (Elrashid Nour Eldin, funded by F3)

Continuous Annular Electrochromatography

- Combination of Annular Chromatography and Electrochromatography

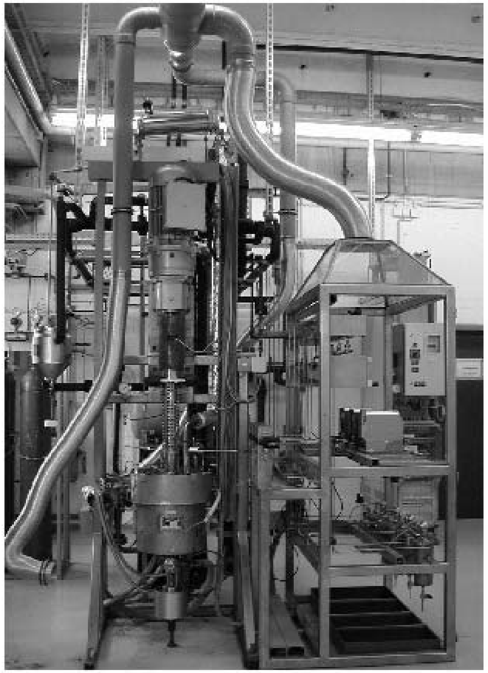




- A prototype is developed in the EU project CAEC
- Our contribution:
  - Dynamic modeling and simulation (2d pde)
  - Iterative optimizing control based upon gradient correction

Control of Polymerisation Processes

- Control of emulsion polymerization (with BASF)
  - First principles based predictive models
  - Batch trajectory optimization
  - State estimation
  - Batch time minimization by tracking the heat removal constraint
- Particle size distribution modeling and control
  - Development of numerical methods
  - Estimation of the growth kernel
  - Experiments in 1l scale
- Control of an industrial solution polymerization (with Evonik Industries and Leikon)



Pilot Plant
10l stainless steel reactor
DCS controlled

Process Systems Enterprise Limited
6th Floor East
26-28 Hammersmith Grove
London W6 7HA

t: +44 20 8563 0888 f: +44 20 8563 0999
w: www.psenterprise.com

12 October 2010

Ala Eldin Bouaswaig, Sebastian Engell
Process Dynamics and Operations Group
Technische Universitat Dortmund
44221 Dortmund
Germany

Dear Dr Bouaswaig & Prof. Engell,

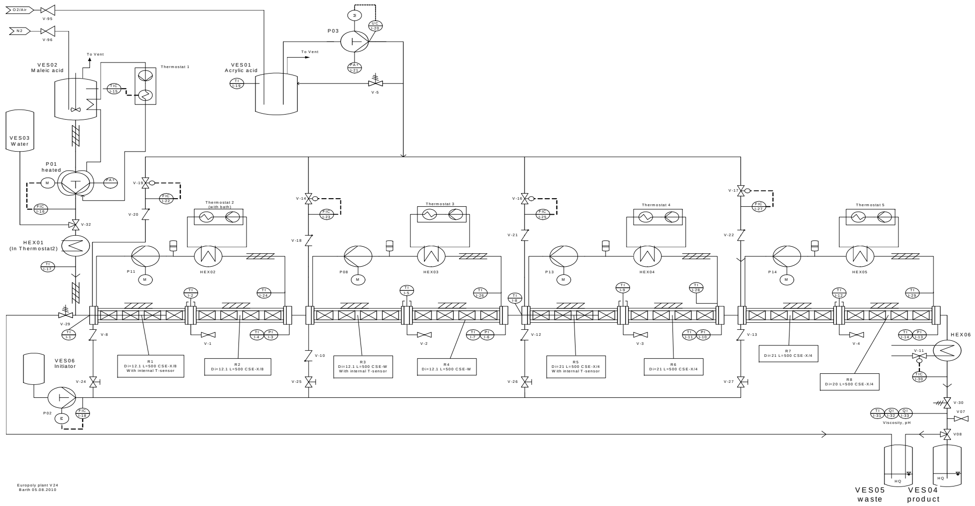
PSE Model-Based Innovation Prize winner

I am delighted to inform you that your paper "*WENO scheme with static grid adaptation for tracking steep moving fronts*" is the winner of the 2010 PSE Model-Based Innovation Prize.

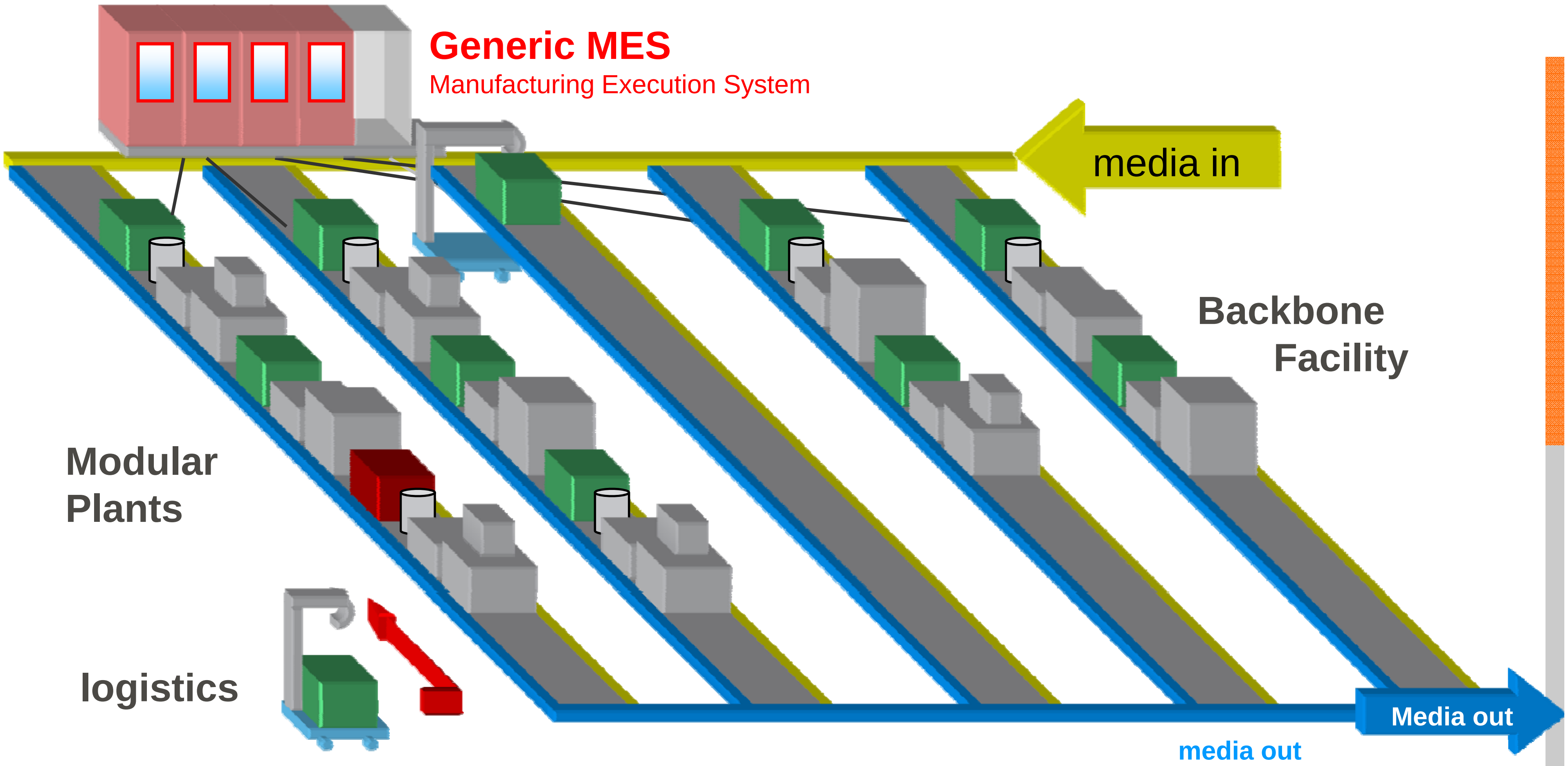
The judges were particularly impressed by the paper, summarising it as "*an excellent technical work proposing a new numerical method for the efficient solution of parabolic differential equations, with a very nice integration with gPROMS through a foreign object*".

Development and control of continuous polymerizations

- Co-polymerization of acrylic acid
- Cooperation with BASF, Rhodia in the EU Integrated Project F3



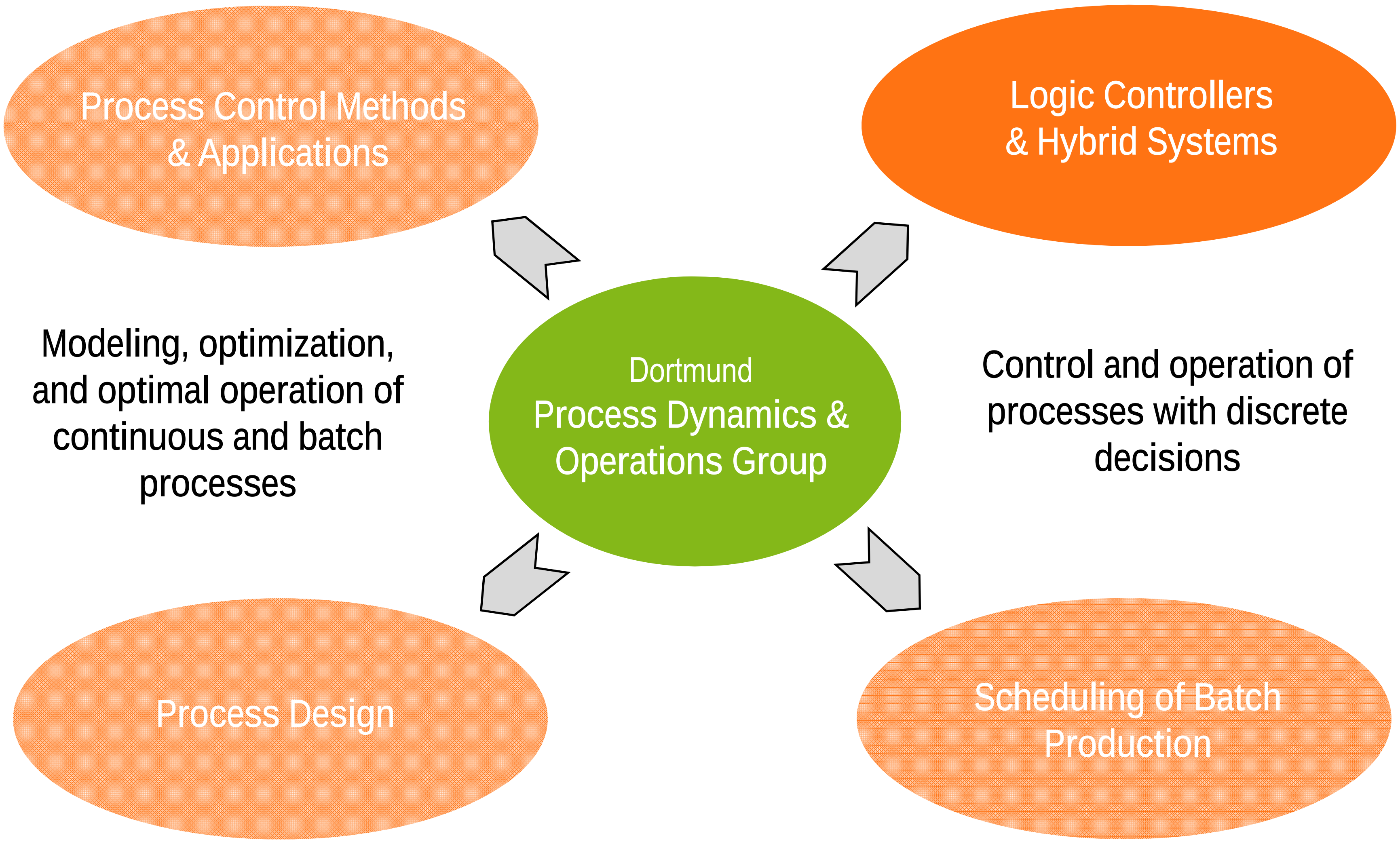
F3-Project (Bayer, BASF, Arkema, Rhodia, Astra Zeneca, Procter & Gamble + equipment manuf. + academia)



DYN: Lead of WP4 - Process operations

Controllability analysis and control design for prototypical applications

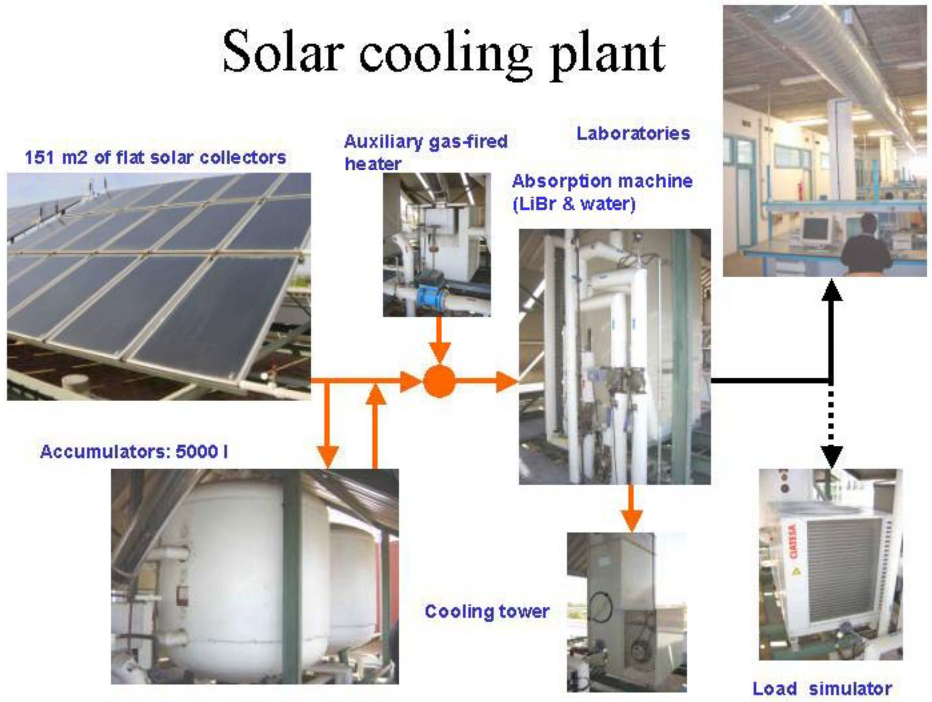
DYN@TUDO: Fields of Research

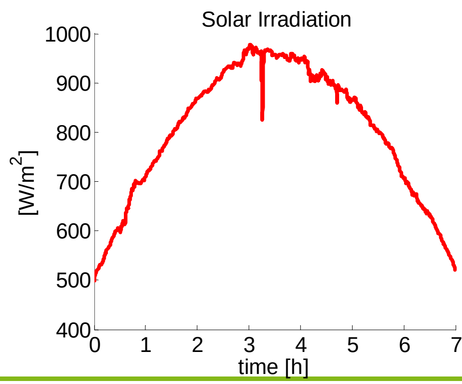


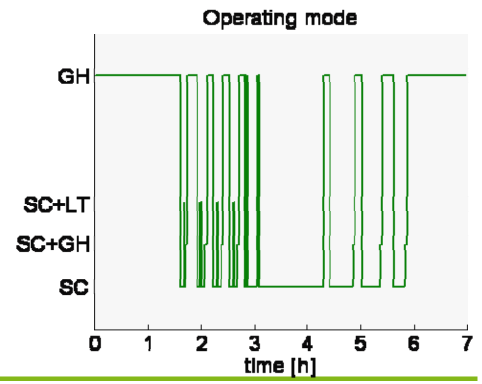
Example of Hybrid Control Design: Control of a Solar Cooling System

Competition organized by the
European Network of Excellence *HYCON*

- Plant located at the University of Seville
- Online computer control
- Remote monitoring and tuning via the internet
- Main problem: inaccurate model
- Winner: DYN@TUDO
- Optimizing switching strategy
- Controller provided good and robust performance in simulation and at the real plant







Design and Verification of Logic Controllers

- Interaction of continuous dynamics with logic (discrete event) controllers leads to complex behavior (even chaotic behavior possible).
- Correct function is difficult to assess
- Critical logical controllers should be verified (proof of correctness), Inspection and common sense is not enough!
- Application of techniques from computer science
  - Abstraction of the continuous dynamics into (timed) discrete systems
  - Formal models of the controller and of the specifications
  - Composition and formal verification (UPPAAL, PHAVER) that controller and plant together do not violate the specifications

✓ Formal models of logic controllers described by SFC

!! Abstraction of continuous models to automata models

!! Completeness and correctness of the specification

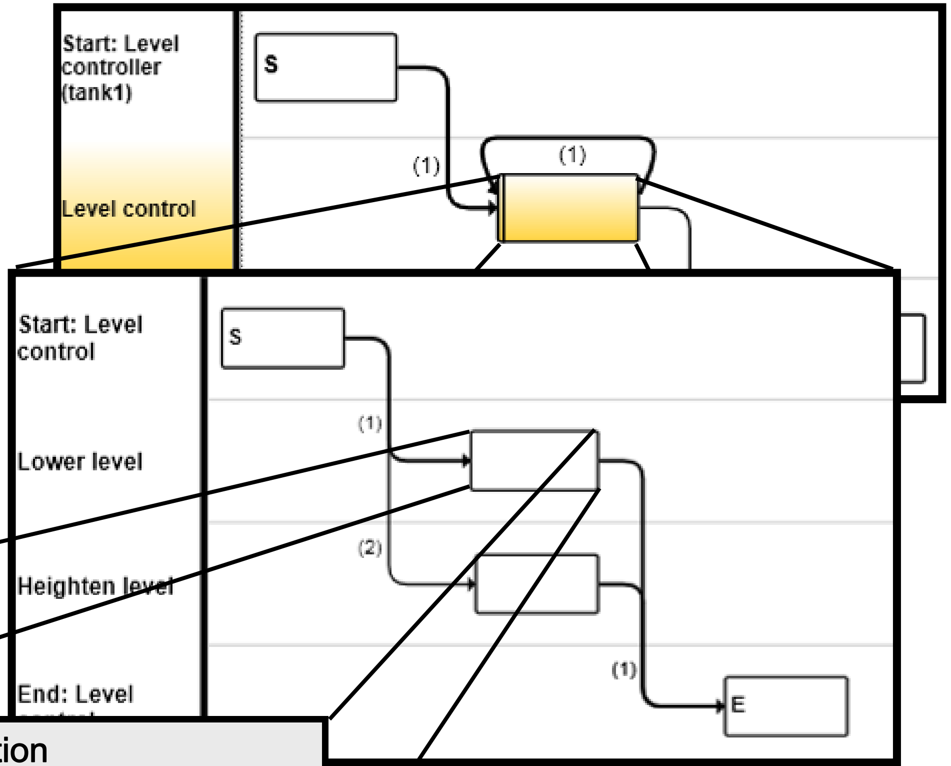
Current Projects in Hybrid Control

- EU Project Multiform (Coordinated by TU Dortmund / DYN Christian Sonntag, Martin Hüfner, Stephan Fischer)
  - Design support for complex controlled systems using different model formalisms and computer tools
  - Tool transformations to the Compositional Interchange Format
  - Logic controller specification and verification (DC/FT Formalism)
  - Robust verification based on approximate models
  - Systems design framework
  - Case study: Pipeless plant demonstrator

- Optimal start-up of processing plants with switching controls (NN)
- Synthesis of switching controllers (Thanh Ha Tran)

Logic Controller Design by Refinement

- Systematic and hierarchical approach
  - Dependency Chart (DC)
    - Conceptional design
    - Similar to Gantt chart
    - Hierarchy – DCs may contain DCs
    - On the lowest level, a DC is specified by a Function Table
  - Function Table (FT)
    - Detailed description
    - List of sequential actions
    - Documentation of design decisions

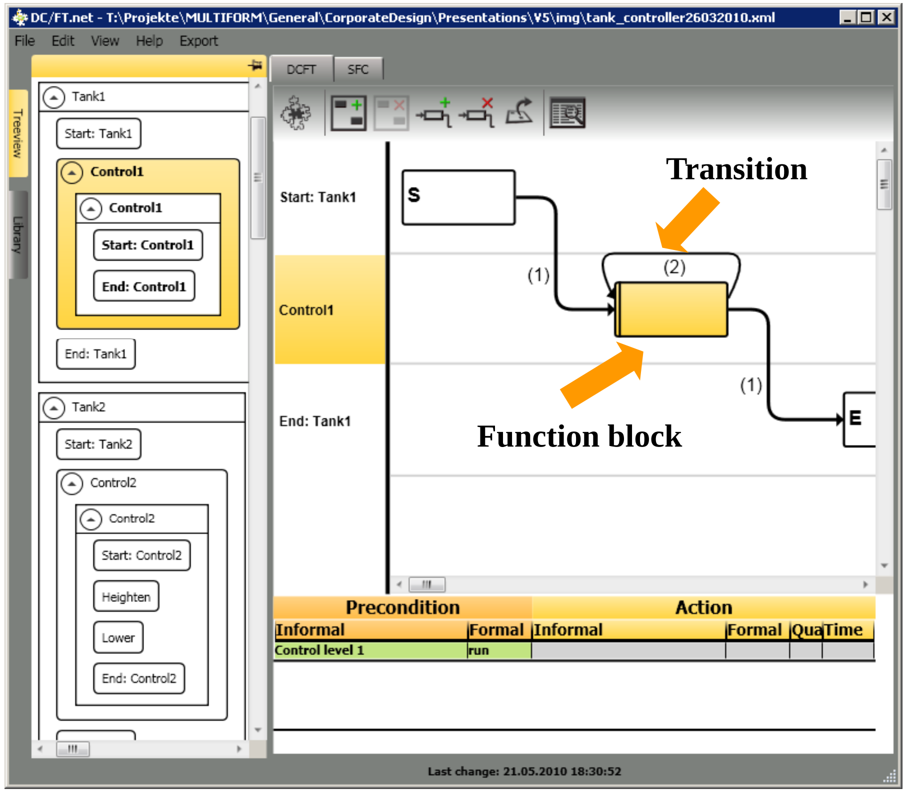


Precondition		Action		
Informal	Formal	Informal	Formal	Qualifier
Tank level is to high	H> H_max	*Open drain valve*	V1:=1	S

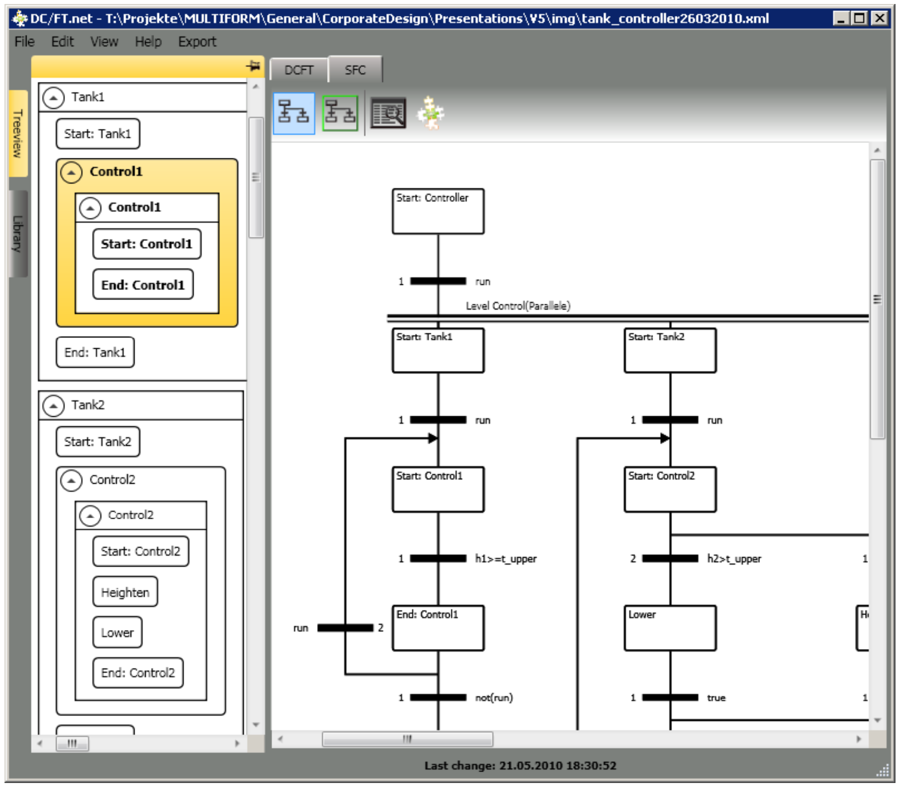
Logic Controller Design by Refinement (2)

- Systematic refinement of informal specifications into logic controllers

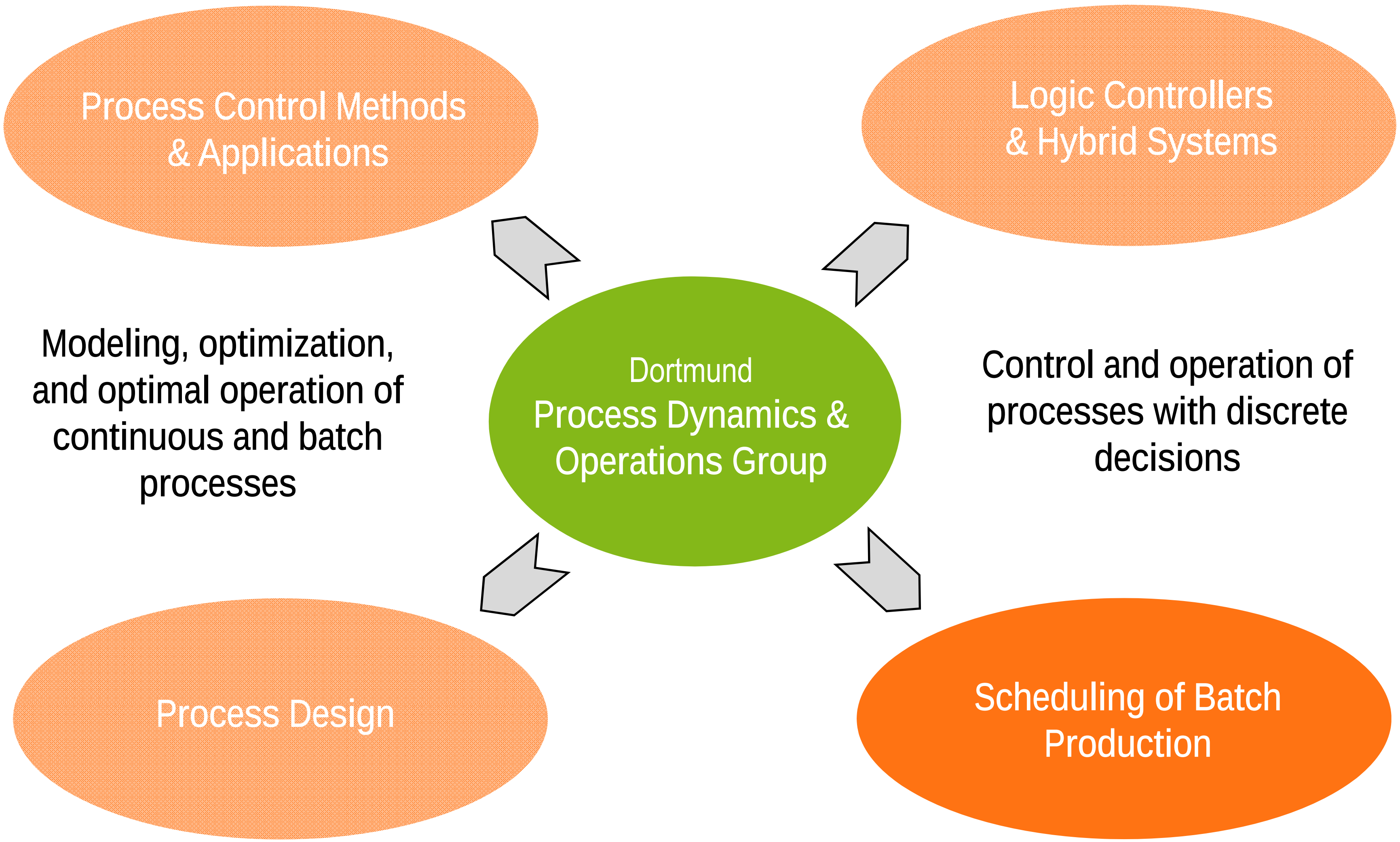
DC/FT view



SFC view



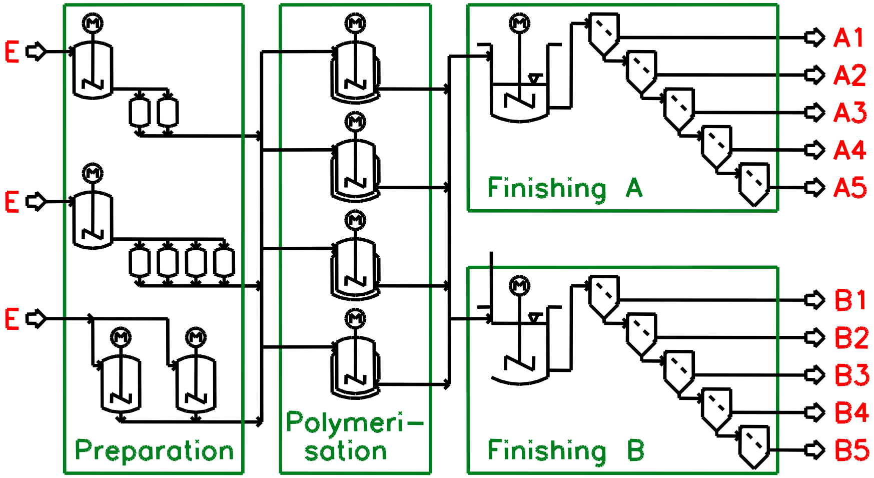
DYN@TUDO: Fields of Research

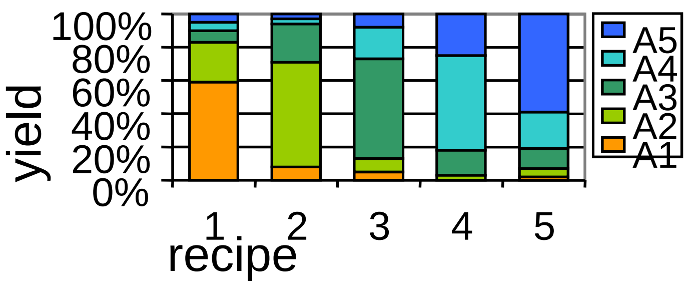


Production Planning and Scheduling in Batch Plants

Focus of our research:

- Online (reactive) planning and scheduling
- Dealing with uncertainties



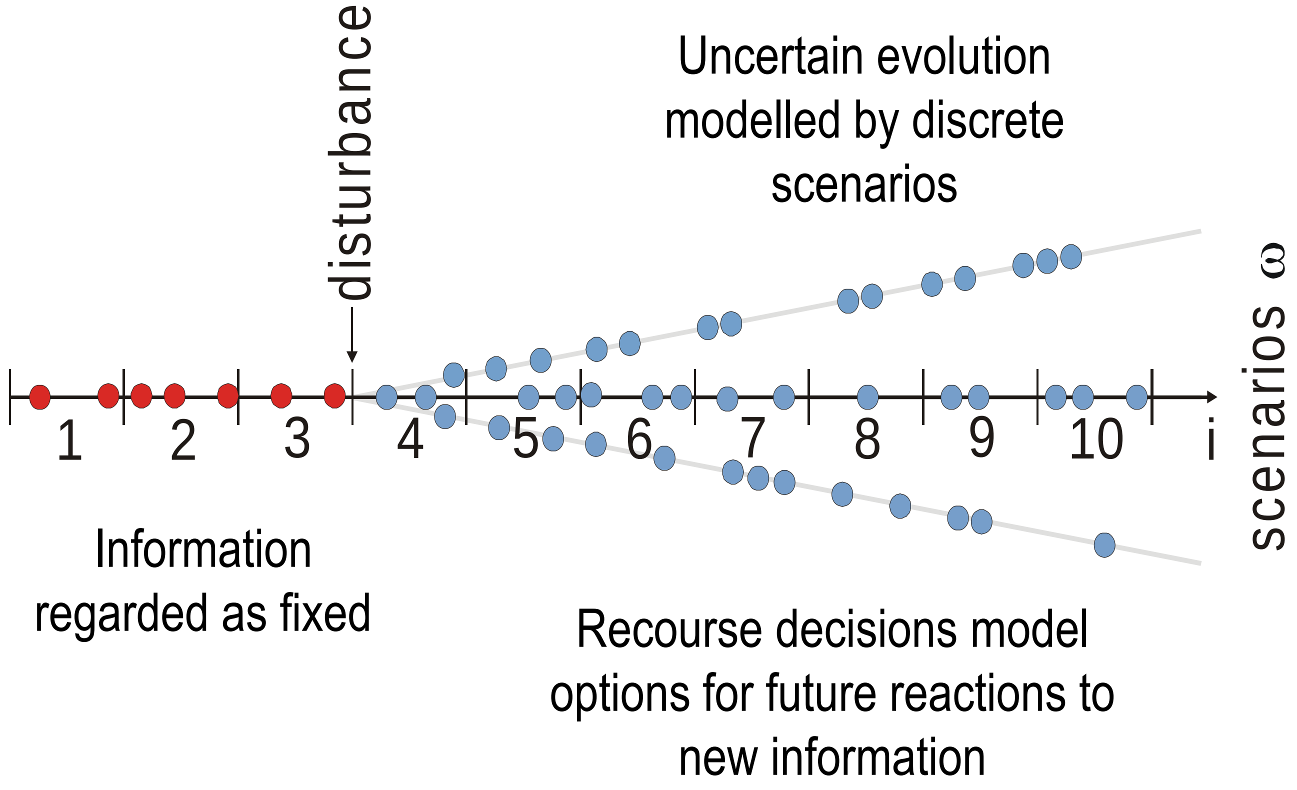


Example EPS Process

- Decisions
  - Assignment of the recipes and timing of the batches (batching and batch scheduling)
  - Operation state finishing line
- Constraints
  - Capacity of the polymerization stage
  - Capacity of the finishing stage
  - Start-up / shut-down of the finishing stage
- Objective: maximize the profit
- Uncertainties
  - Future demands
  - Future capacity (reactor availability)
  - Yields

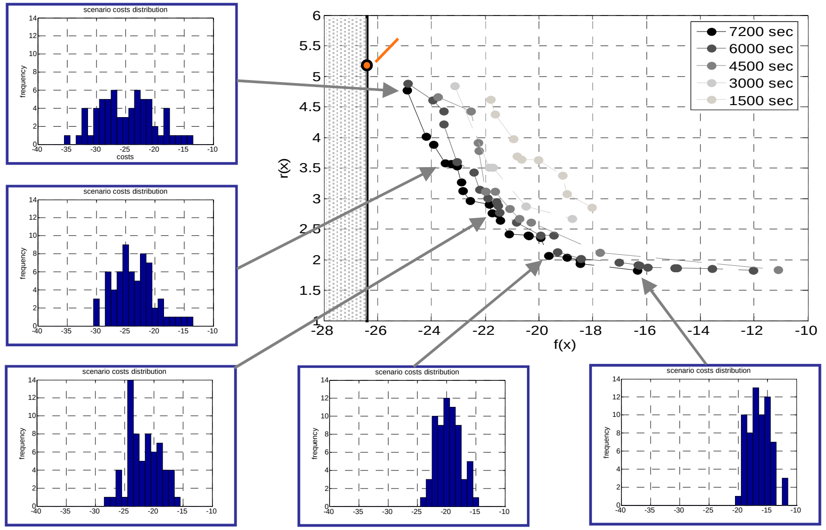
Two-stage Decision Problem

- Information and decision-structure
  - First stage decisions $x \neq f(\omega)$ (here and now)
  - Second stage decisions $y = f(\omega)$ (recourse)



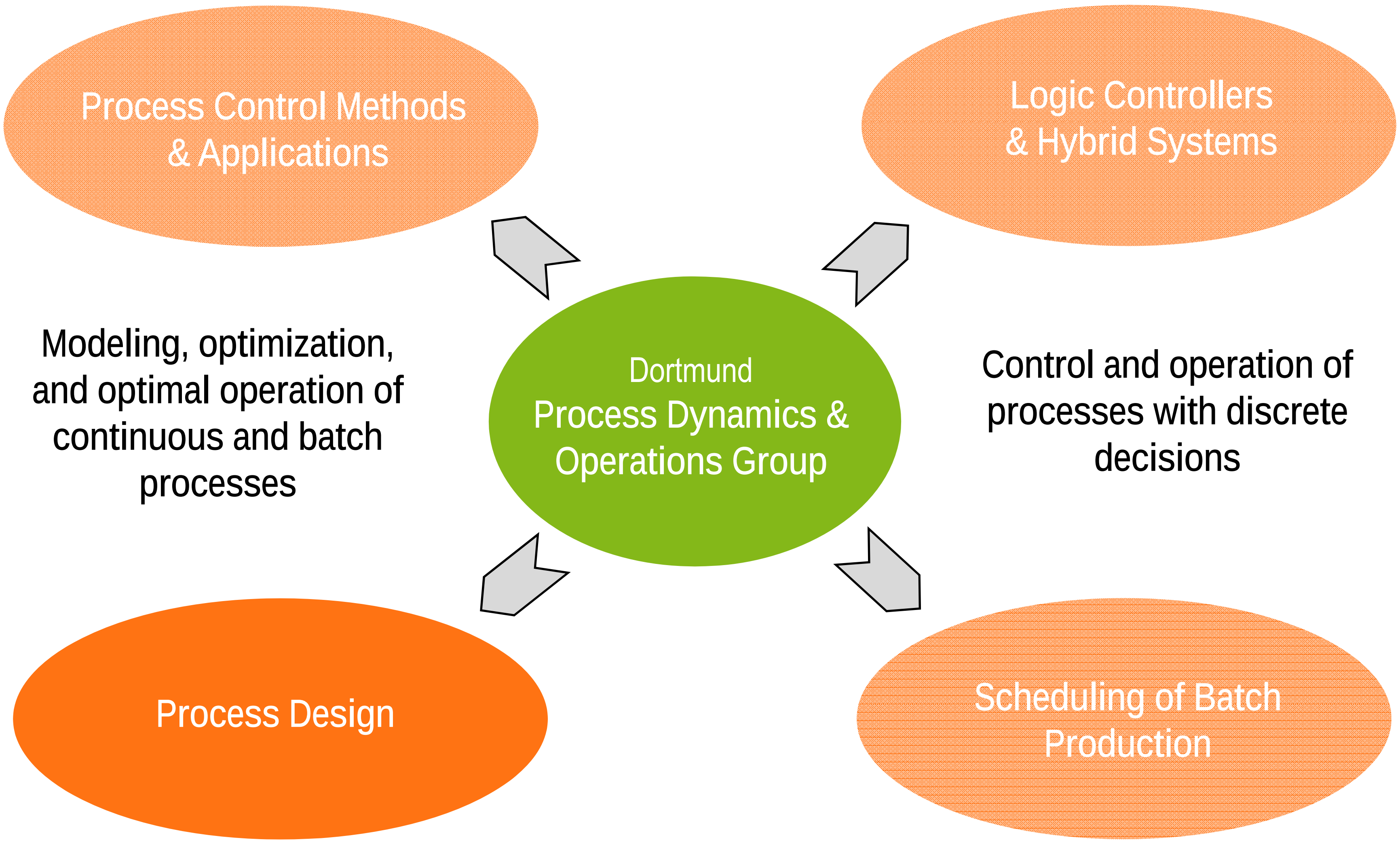
Approaches

- Two-stage stochastic programming (Sand and Engell, C&CE 2004)
- Decompostion strategies – EA/MILP algorithms
  - Pareto front of average profit and risk (Tometzki and Engell, Comp. & Chem. Engg., in press)

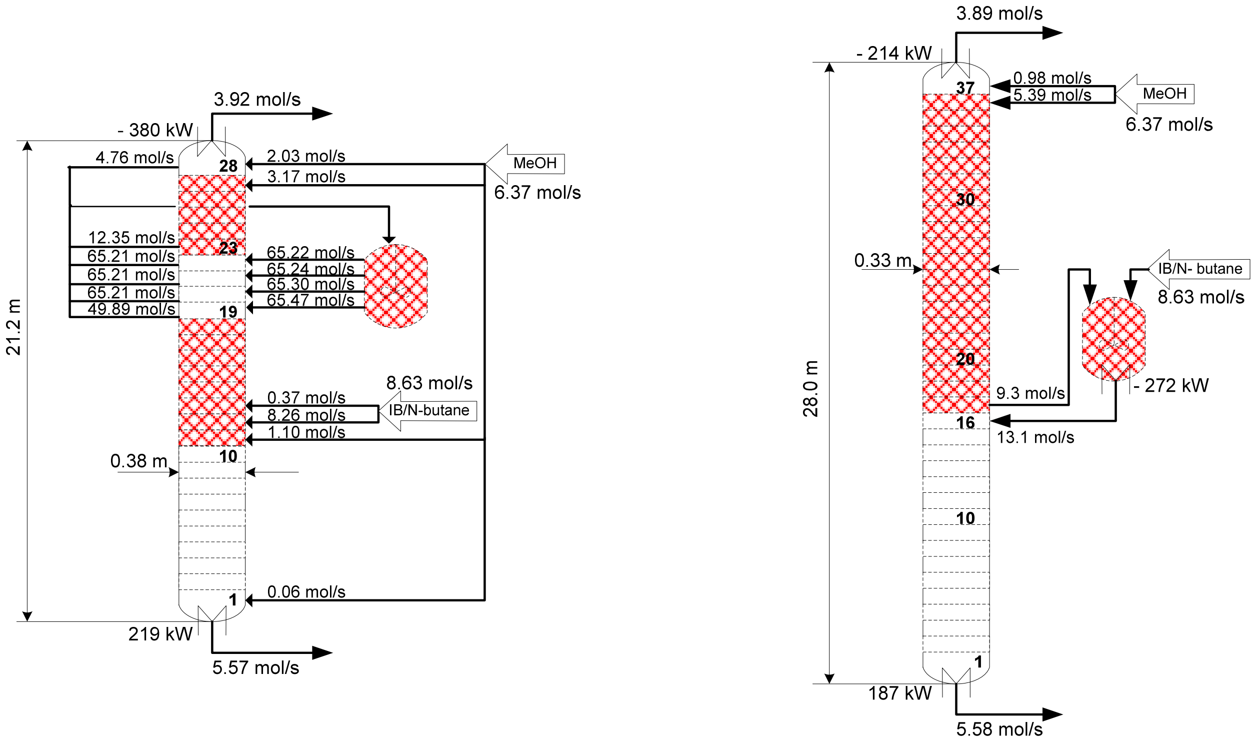


- Moving horizon scheduling based upon two-stage stochastic solution (Cui and Engell, Comp. & Chem. Engg., 2010)
- Fast scheduling using timed-automata models (Subbiah, Panek, Engell)

DYN@TUDO: Fields of Research



Locally Optimal Column Designs with External Reactor



- Knowledge-based initialization
- Profit: 1,089 $\cdot 10^3$ € p.a.

- Initialization by scatter search
- Profit: 1,102$\cdot 10^3$ € p.a.

Algorithmic Challenge: Large number of local optima!

Current Projects in Process Design

- Memetic (EA/NLP) algorithms for complex design problems with many local optima (Maren Urselmann)
- Detection and manipulation of cycles in biological systems (Tobias Neymann/ Sven Wegerhoff)
- Model-based coordination of the development of new production processes (SFB TR 63, Jochen Steimel)