1. Introducing Process Design Center (PDC)
2. Structured Conceptual Process Design - PROSYN®
3. Idea to use reverse Process Synthesis
4. IT and PI projects
Process Design Center

- Independent consultant for the process industry
- Highly qualified experts in chemical engineering (PhD/MSc)
  - Conceptual process design
  - Techno-economic evaluation
  - Energy efficiency
- Proprietary tools and methods - PROSYN®
  - Expert system for conceptual process design
  - 300 man years invested (since 1980s)
  - Ongoing development
- Profound experience
  - Proven capability to come up with better solutions
  - Wide international experience
  - Well recognized by the major companies
Our clients

More than 50 leading companies worldwide (Europe, USA, and Asia)

- Air Liquide
- Air Products
- AkzoNobel
- Amyris
- Arkema
- Avantium
- Aventis
- BASF
- Bayer
- Borealis
- BP
- Cargill
- Dow
- DSM
- Eastman
- ENI
- Evonik
- ExxonMobil
- Grolsch
- Haldor Topsoe
- Ineos
- LanzaTech
- Lyondell
- Mitsubishi Chemical
- PETRONAS
- SABIC
- Shell
- Shin-Etsu
- Solvay / Rhodia
- Total
- Syral
- Tessenderlo Chemie
- Unilever
- YARA
- …
Joint Research Projects (EU)

- **FP5**

- **FP6**

- **FP7**
  - BISIGODOS: algae derived chemicals and bioresins (2013 – 2016)

- **Horizon 2020**
Conceptual Process Design (CPD)

- Based on fundamentals
- Use of design heuristics
- Check of alternatives
- Hierarchical approach
- Multiple target functions

flowsheet | constraints | scope for R&D

physical properties, chemistry engineering rules of thumb highest driving force for reaction/separation black box | process functions | unit operations | integrated design capital investment, production cost, carbon footprint, …
**PROSYN®: Structure of the System**

PROSYN = **PROcess SYNthesis**

- **Expert system for structured conceptual process design**
  - Heuristic rules
  - Numerical methods

- **Application**
  - Broad range, from first idea to retrofit design
  - Very suitable in data-lean environment

- **Development effort**
  - 250-300 man years (since 1980s) with German chemical industry
  - 800,000 lines of code - estimated rebuild value 60 MM$
  - Continued effort
    - *new expert systems, e.g. membrane reactors*
    - *transfer to new platforms (web browser)*
Track record and potential of CPD

Savings in Primary Energy (%) vs. Savings in Capital Investment (%)

- Pinch
- CHP
- Structured CPD
- Eastman methyl acetate process

PDC project results (vs. state-of-the-art)

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Summary of PDC Expertise

- **Conceptual Process Development**
  - Structured conceptual design using expert systems
  - Idea generation and validation
  - Process simulation
  - Process optimization
  - Physical properties
  - Mass and energy balance
  - Technical and economic evaluation
  - R&D guidance

- **Energy efficiency and sustainability**
  - Pinch analysis
  - Heat integration / HEN design
  - Energy audits
  - Energy permits
  - Carbon footprint reduction
  - Resource efficiency

- **Benchmarking**
  - >50 Energy and CO₂ benchmarks
  - Approved by governments, EU legislation (ETS)

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**Process Design Center B.V.**
Catharinastraat 21F, NL-4811 XD Breda, The Netherlands
☎: +31 (0)76 5301 900
✉: www.process-design-center.com

**Contact:**
- Ir. Hans Keuken, managing director
  keuken@process-design-center.com
- Dr. Hank Vleeming, CTO
  vleeming@process-design-center.com
PROSYN® - timeline

• Started in 1980s
  - Prof. Simmrock (TU Dortmund)
  - Consortium with German Chemical Industry (BASF, Bayer, Degussa, Hoechst, Hüls)
  - PhDs (TUD, TUHH, RWTH Aachen, TU Berlin, TU Bochum)

• PROSYN from TUD to GHN in 1996

• GHN merged with K&K in PDC (1999)
  - PDC successfully applied PROSYN in industrial consultancy

• Continuous development effort
  - New expert systems (e.g. CRYSPERT, SYNTHESIZER, membrane reactors)
  - Transfer to new platforms (Windows, web-browser)
  - Increased IT development effort after 2010
# PROSYN® – modules

<table>
<thead>
<tr>
<th>Name</th>
<th>Description of expert system</th>
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<tbody>
<tr>
<td>Absopert</td>
<td>Absorber design</td>
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<tr>
<td>Azeopert</td>
<td>Azeotrope systems</td>
</tr>
<tr>
<td>Bikom</td>
<td>Treatment of industrial waste water</td>
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<tr>
<td>Ciscon</td>
<td>Column internals selection</td>
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<tr>
<td>Cryspert</td>
<td>Crystallization</td>
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<tr>
<td>Heatpert</td>
<td>Heat integration (based on pinch analysis)</td>
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<td>Hen</td>
<td>Heat exchanger networks</td>
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<tr>
<td>KK</td>
<td>Complex distillation columns</td>
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<tr>
<td>Lilex</td>
<td>Liquid-liquid extraction</td>
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<tr>
<td>PROSYN-M</td>
<td>Process Synthesis Manager</td>
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<tr>
<td>Mempert</td>
<td>Membrane separation</td>
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<tr>
<td>P3</td>
<td>PROSYN physical properties</td>
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<tr>
<td>Readpert</td>
<td>Reactor selection and design</td>
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<tr>
<td>Rekpert Plus</td>
<td>Rectification</td>
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<tr>
<td>Sequencer / Synthesizer</td>
<td>Reactive separation (reactive distillation)</td>
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<tr>
<td>Solpert</td>
<td>Solvent selection</td>
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<tr>
<td>Teagpert</td>
<td>Separation of close-boiling components</td>
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</tbody>
</table>
Idea generation and check of alternatives
Reverse Process Synthesis for PI

• IT project
  - to enable heuristic & numeric algorithms to go in reverse.

• Partners:
  - PDC
  - KU Leuven
  - vrije Universiteit amsterdam

• PI project
  - to target the most suitable applications for new and existing PI solutions

• Current Partners:
  - TU Delft
  - TU Dortmund
• We target the SPIRE 5 call (2015, R&I): New adaptable catalytic reactor methodologies for Process Intensification

  - The project is about finding the most suitable applications for individual **proven Process Intensification (PI) solutions** by **structured reverse process synthesis** in reactions

  - Quantify opportunities (benefits) for **novel PI solutions**, in early stage of development, as function of system properties (thermodynamic, kinetic, hydrodynamic, electromagnetic, etc), operating windows and hardware (integration) limitations
**Impact**

- Integrating the value chain by bridging the gap between PI researchers & developers, technology providers, and end-users.

- Reducing the time to market of PI technologies: Find the most promising applications for several PI technologies.

- Automating PI targeting by reverse process synthesis and extending PROSYN® expert system with PI solutions.

- Envelop novel PI technologies.

- Advance state-of-art technology from SME’s (e.g. trays, membranes, process analytical technology).
Looking for partners…

- PI technology providers that are interested to embed their technology solutions in conceptual design expert systems and to identify their process applications

- Process industries that are keen to improve their processes by PI

- Academic partners that are interested in identification of novel PI process concepts