Reverse Process Synthesis for PI

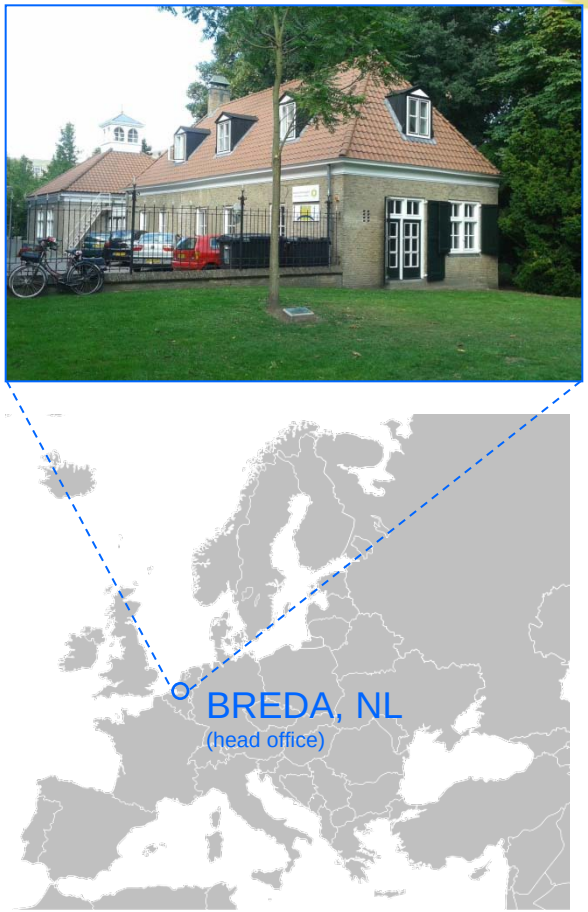
NL GUTS & PIN-NL meeting / 9 April 2014 – Nijkerk (NL)

Outline

1. Introducing Process Design Center (PDC)
2. Structured Conceptual Process Design - PROSYN®
3. Idea to use reverse **Pro**cess **Syn**thesis
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

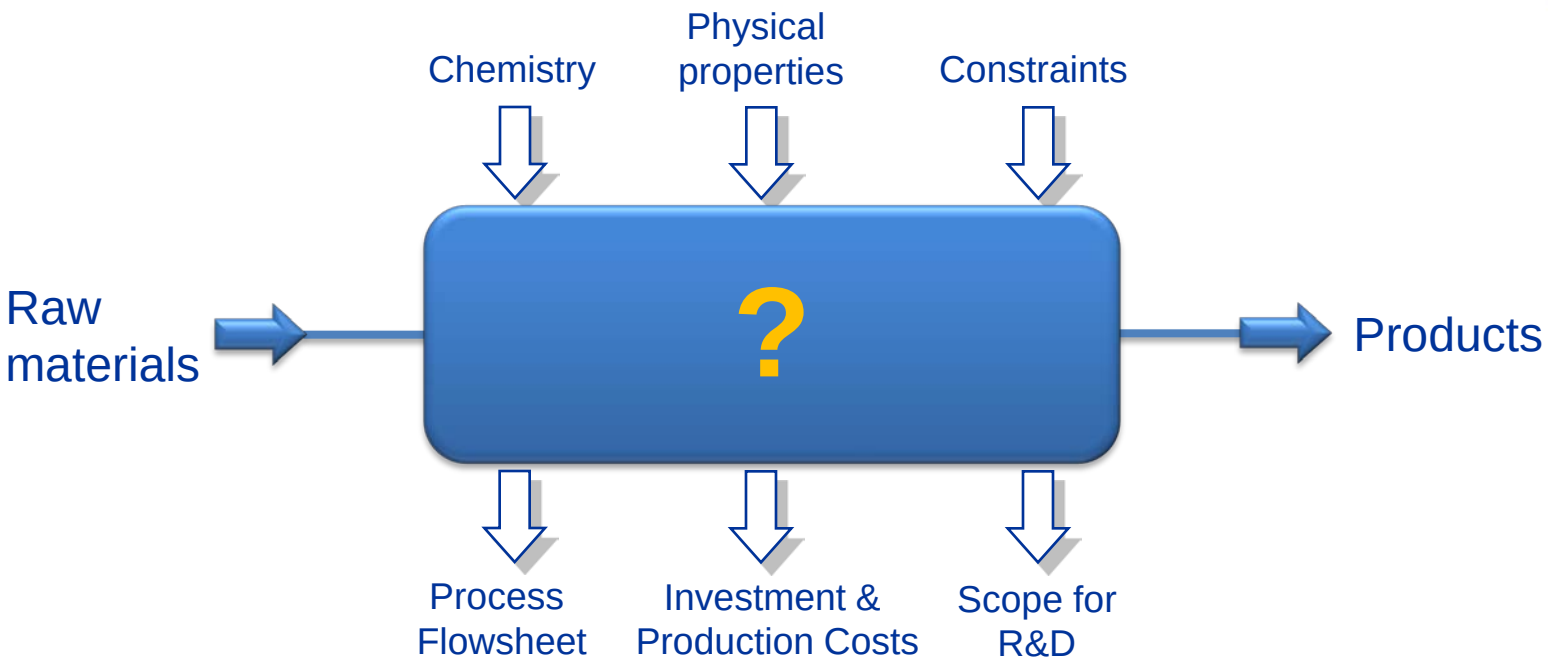
More than 50 leading companies worldwide (Europe, USA, and Asia)

- 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)

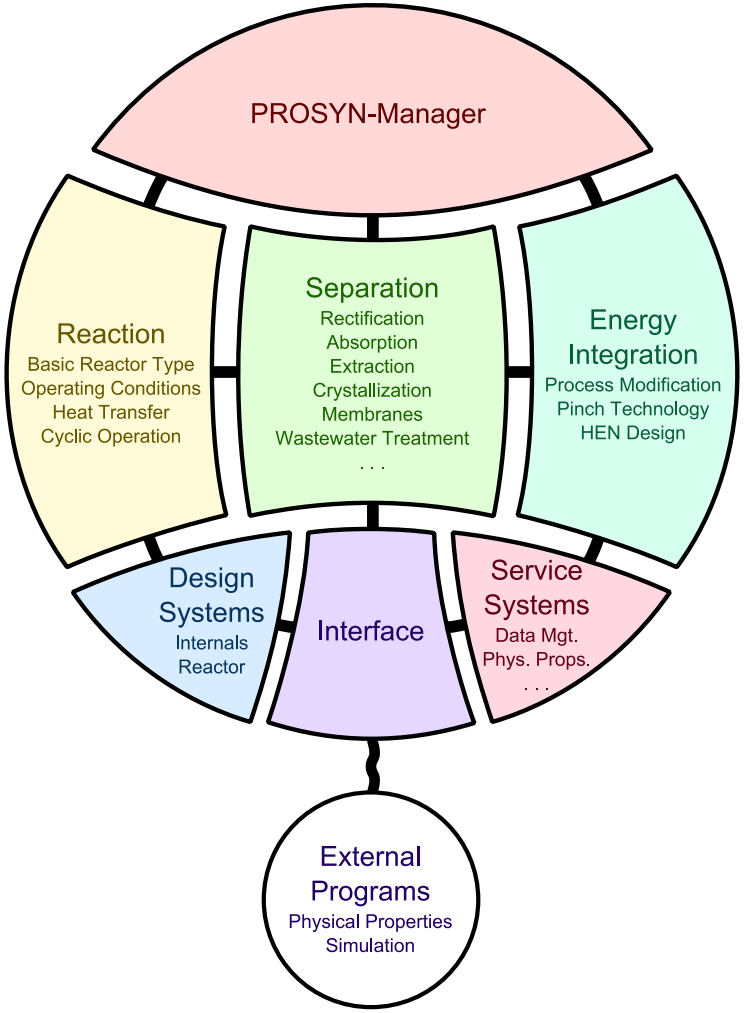
FP5		
• CYCLOP	cyclic operation of trickle-bed reactors	2000 – 2003
FP6		
• INSERT	reactive distillation	2004 – 2007
• NEPUMUC	microreactors	2005 – 2008
• CACHET	CO_2 precombustion capture	2006 – 2009
FP7		
• F^3 Factory	flexible, fast and future production processes	2009 – 2013
• EuroBioRef	integrated biorefinery	2010 – 2014
• CARENA	catalytic membrane reactors	2011 – 2015
• CAPSOL	CO_2 post-combustion capture	2011 – 2014
• BISIGODOS	algae derived chemicals and bioresins	2013 – 2016
• FASTCARD	fast industrialisation by catalysts R&D	2014 – 2017
Horizon 2020		
• SPIRE	Sustainable Process Industry through Resource and Energy Efficiency	2014 –

Conceptual Process Design (CPD)



- Based on fundamentals — physical properties, chemistry
- Use of design heuristics — engineering rules of thumb
- Check of alternatives — highest driving force for reaction/separation
- Hierarchical approach — black box | process functions | unit operations | integrated design
- Multiple target functions — capital investment, production cost, carbon footprint, …

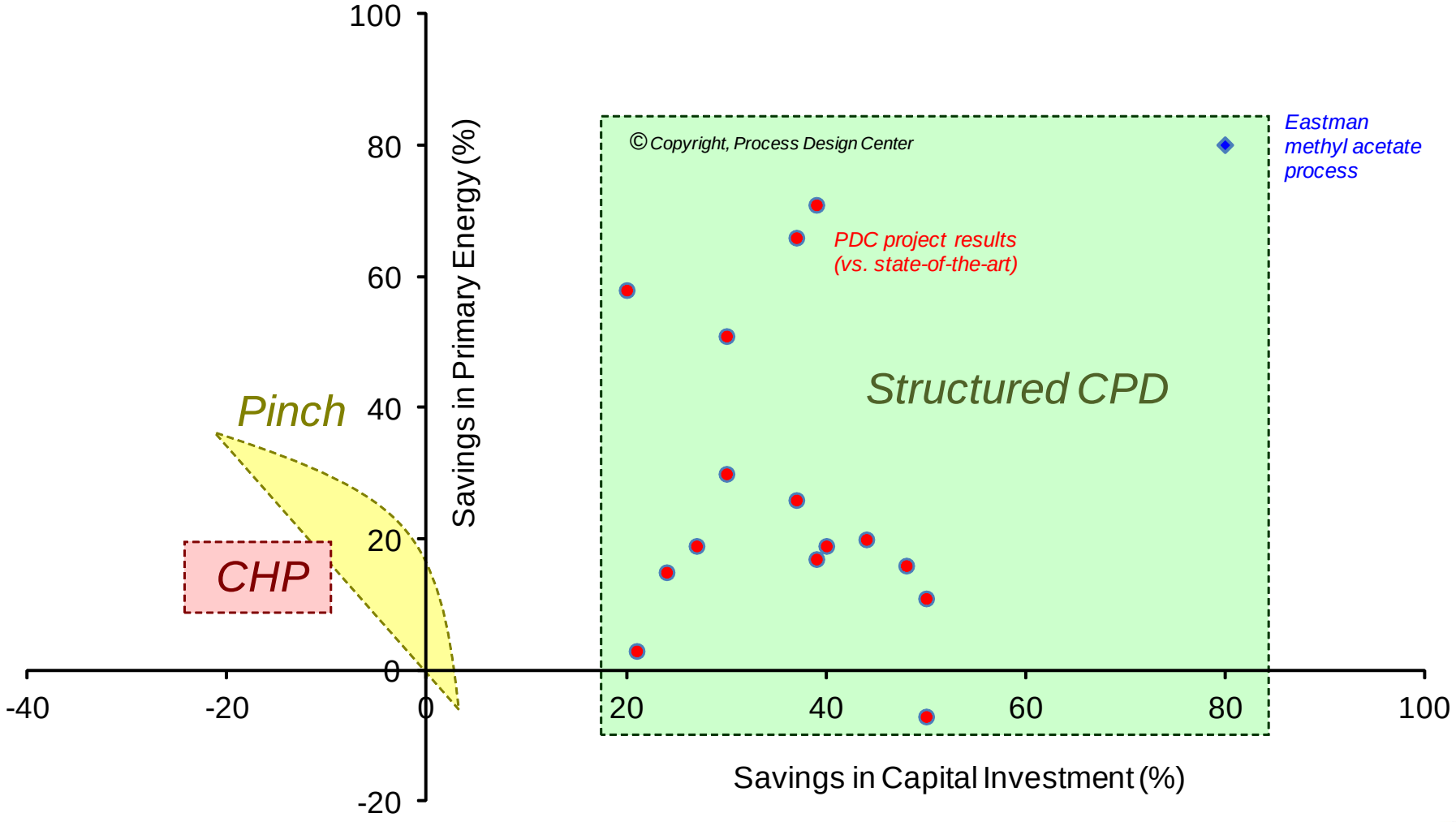
PROSYN®: Structure of the System



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



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
- Development of Expert Systems
  - Extraction of knowledge rules
  - Building of PROSYN® expert systems
  - Dedicated expert systems (for partners/clients)
- Energy efficiency and sustainability
  - Pinch analysis
  - Heat integration / HEN design
  - Energy audits
  - Energy permits
  - Carbon footprint reduction
  - Resource efficiency
- Benchmarking
  - >50 Energy and CO_2 benchmarks
  - Approved by governments, EU legislation (ETS)

Process Design Center B.V.

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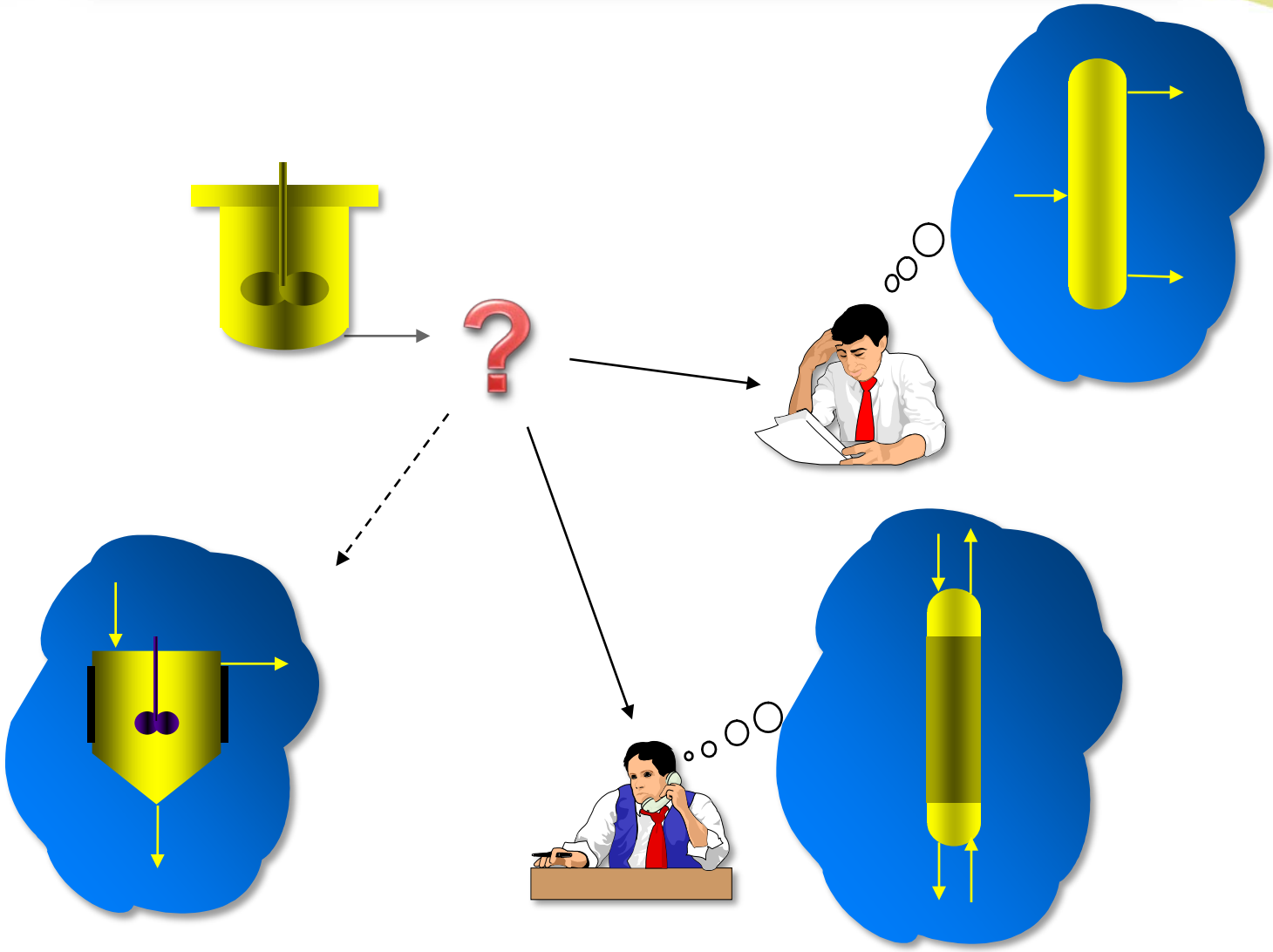
PROSYN® - timeline

- 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

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

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 Delft University of Technology

PDC

technische universität dortmund

Horizon 2020 – SPIRE 5 proposal

- **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**

www.process-design-center.com

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