Appendix 2

INDUSTRY SECTOR PI ROADMAPS

2.1 PETCHEM ROADMAP

Heat limited reactions

2050: 15% overall energy efficiency increase through Process Intensification

Mass transfer limited fast reactions

2050: 20% overall energy efficiency increase through Process Intensification

Cracking

2050: 5% overall energy efficiency increase through Process Intensification

PETCHEM processes - PI Roadmaps

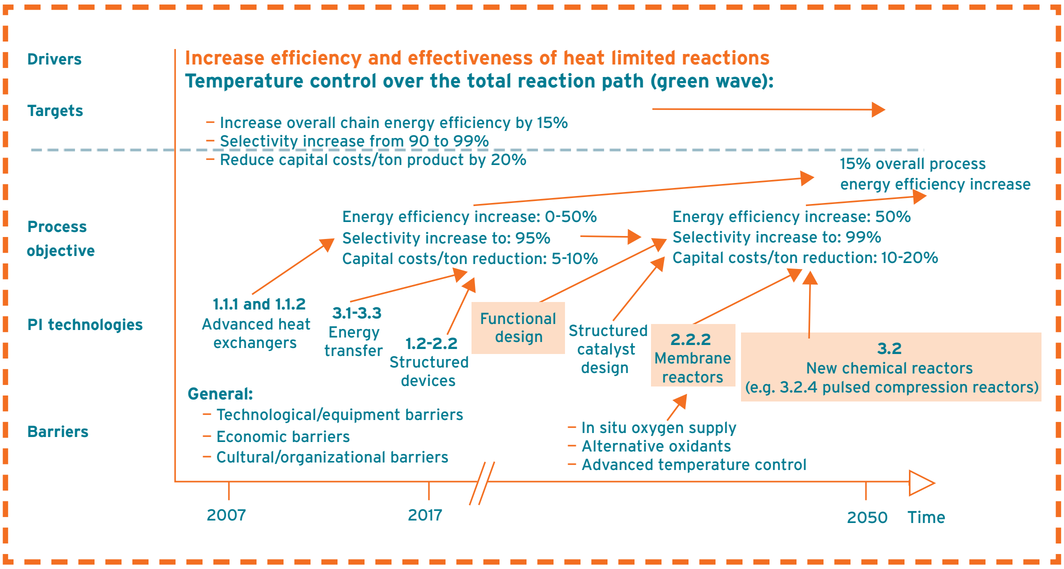
Ammonia

2050: 30% overall energy efficiency increase through Process Intensification

Energy efficient separation

2050: 20% overall energy efficiency increase through Process Intensification

HEAT LIMITED REACTIONS ROADMAP



Description of the current process

Selected process

All PETCHEM processes with high heat production or consumption in the reaction section (majority of processes)

State of the art

For example, shell and tube reactors

Needs

- Increase in energy efficiency
- Temperature control (increased safety and selectivity)
- Capital cost reduction

Main technological limitations/bottlenecks

Radial and axial temperature gradients by insufficient heat transfer, leading to lower selectivity and more by-products. Green wave will lead to an unblocked, smoothly controlled high way for the desired reaction path by guiding the introduction and optimum mixing of reactants and maintaining optimum temperature control in the reaction environment

Improvement potential

	Within 10 years	Within 30-40 years
Increase in process energy efficiency	0-50%[1]	50%[2]
Selectivity increase (from 90%)	95%	99%
Reduction in capital costs per ton of product	5-10%	10-20%

Promising PI technologies

PI technologies	Energy efficiency potential	
	Within 10 years	Within 30-40 years
1.1.1 Advanced plate-type heat exchangers	4%	10%
1.2.2 Micro Reactors (including Micro Mixers)		
3.1 - 3.3 Energy transfer		
1.2 - 2.2 Structured devices		
Functional design		
Structured catalyst design		
2.2.2 Membrane reactors	0%	10%
2.2.8 Reactive distillation	2%	5%
3.2.4 New chemical reactors	0%	10%

Possible combinations

- 1.1.1 Advanced plate-type heat exchangers and 1.2.2 Micro Reactors (including Micro Mixers)
- 2.2.1 Heat exchange or milli reactors, 2.2.8 reactive distillation and 1.2.1.4 advanced structured packings

Barriers, required research, timing and actions

1.1.1 Advanced plate-type heat exchangers

Barriers: Customer confidence

Time until implementation: 0-10 years

1.2.2 Micro Reactors (including Micro Mixers)

Barriers: Experience and fouling

Research required: Applied

Time until implementation: 0-10 years

---

[1] Overall chain energy efficiency increase: 0-10%

[2] Overall chain energy efficiency increase: 15%

2.2.8 Reactive distillation

Barriers: Catalyst development and lack of expertise
Research required: Applied
Time until implementation: 0-10 year

1.2 – 2.2 Structured devices

Barriers: Selection, catalyst application/loading in situ regeneration, costs of structural elements and design rules
Research required: Fundamental and applied
Time until implementation: 0-20 years

2.2.2 Membrane reactors

Barriers:

- Role of O2 in oxidation reactions
- Controlled introduction of oxidants (oxygen)
- Temperature control
- Up-scaling of membranes and reactor concepts
- Immobilization (e.g. fouling, mechanical strength, safety and catalyst)
- Retrofitting (e.g. use of current reaction heat)
- Catalytic cracking with PI
- Knowledge/design base

Research required: Applied and fundamental materials, manufacturing and chemical process technology
Time until implementation: 10-25 years

3.2.4 New chemical reactors

Barriers: Opportunities unknown, knowledge insufficient
Research required: Fundamental and applied
Time until implementation: > 20 years

3.3 Energy transfer

Barriers: Window of operation, design rules, engineering
Research required: Fundamental and applied
Time until implementation: 10-20 years

Functional design

Research required: Applied

Structured catalyst design

Barriers: Costs, catalyst application, regeneration and loading
Research required: Combined
Time until implementation: 5-15 years

General barriers

- Capital expensive technologies for large scale applications
- Capital investments
- Financing of PI pilots (“lack of technology providers and sponsors”)

- Centralized vs. decentralized thinking throughout the organization
- Lack of knowledge about economic evaluations
- No-change mentality
- Retrofitting discipline
- Interaction between R&D and manufacturing departments

HEAT LIMITED REACTIONS ROADMAP
EXAMPLE – TBA DEHYDRATION

Description of the current process

Selected process

- Reaction: TBA à i-C4= + H_2O using catalyst
- Water removal
- C4= purification
- Water de-hydrocarbonizing

The reaction is in the vapor phase and endothermic with pressure at about 7 bar and a temperature between 270 and 370 oC. Several reactors operate in the series

- Selectivity is about 90%
- Fouling, by-products and temperatures are high
- Efficient heat input

State of the art

There are reactors with pre-heating furnaces in the series. Product washing and purification is in several distillation columns and water is cleaned by distillation

Main technological limitations/bottlenecks

- Heating is done by furnaces with limited efficiency
- Catalyst needs to be changed frequently
- Fouling creates high pressure drops
- Capacity of current unit is limited
- Purification takes place in two steps

Improvement potential

	Within 10 years	Within 30-40 years
Selectivity increase (from 90%)	> 95%	

Promising PI technologies

PI technologies		
Moving bed reactor		
Reactive distillation		
Liquid phase reaction		
Direct integration with exothermic reaction		
Membrane reactor		

Possible combinations

- Heat integrated reactor and reactive distillation

Barriers, required research, timing and actions

Moving bed reactor

Barriers: Uncertainty and high cost for an expected low return
Research required: Applied/combined
Time until implementation: > 20 years

Reactive distillation

Barriers: Fouling and long term
Research required: Fundamental and applied
Time until implementation: 10 years

Liquid phase reaction

Barriers: Testing
Research required: Fundamental and applied
Time until implementation: 10 years

Direct integration with exothermic reaction

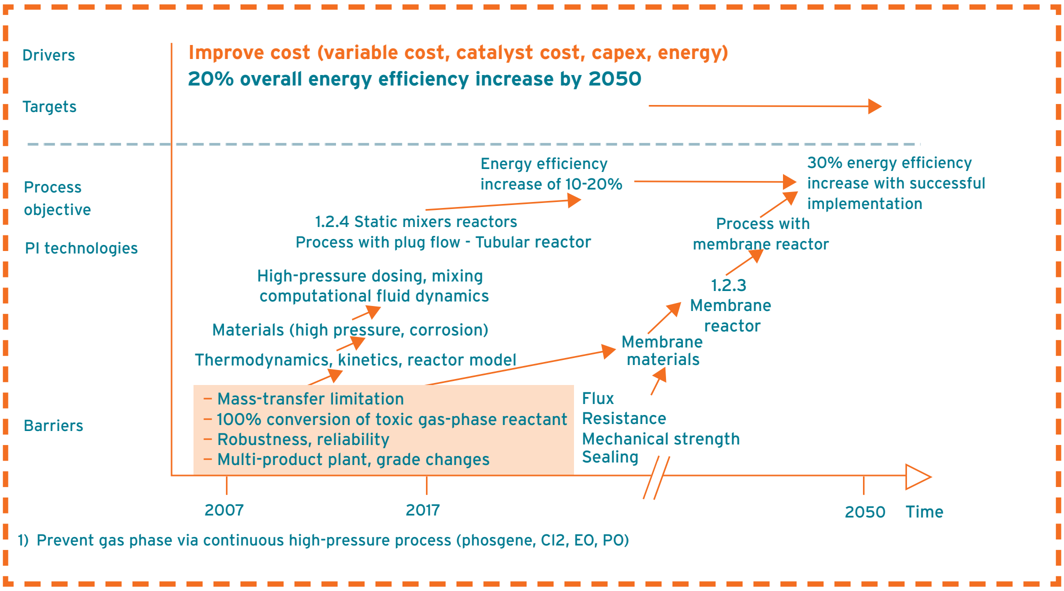
Barriers: Uncertainty
Research required: Fundamental and applied
Time until implementation: 6 years

General barriers

- Reliability
- Fouling
- Dependency of concurrence of reactions
- Only in turnaround periods
- Limited CAPEX, for profitable investment
- Market for the product is changing
- Priority for development

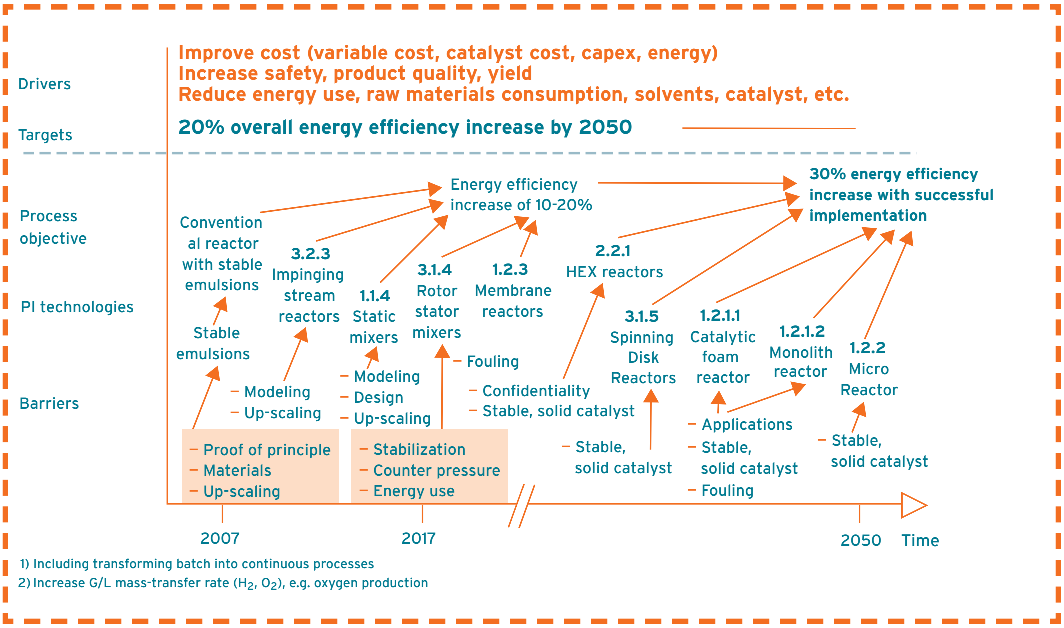
MASS-TRANSFER-LIMITED FAST REACTIONS ROADMAP

Continuous high-pressure process roadmap[3]



1) Prevent gas phase via continuous high-pressure process (phosgene, Cl2, EO, PO)

Increase G/L mass-transfer rate roadmap[4+5]



1) Including transforming batch into continuous processes

2) Increase G/L mass-transfer rate (H_2, O_2), e.g. oxygen production

---

3 Including transforming batch into continuous processes

4 Prevent gas phase via continuous high-pressure process (phosgene, Cl_2, EO, PO)

5 Increase G/L mass-transfer rate (H_2, O_2), e.g. oxygen production

SHORT/MID TERM

Description of the current process

Selected process

- Prevent gas phase via continuous high-pressure process (phosgene, Cl_2, EO, PO)
- Increase G/L mass-transfer rate (H_2, O_2) including transforming batch to continuous processes

Needs

- Increase product quality (e.g. better control of chain length in polymerization reactions)
- Selectivity (side-reactions) must equal variable cost and feed cost. Generally, there is a loss of selectivity due to a slow mass transfer rate. Also, for selectivity reasons, sometimes there is a need for some controlled mass transfer limitation
- Feedstock and catalyst yield/cost: incomplete catalyst utilization due to mass transfer limitation
- CAPEX (e.g. reactors that are too large due to mass transfer limitation)
- Process stability: instability due to mass transfer limitation
- Reduce energy use – Energy loss due to batch reactions (no possibility for heat integration)
- Increase safety and reduce the effort required for safe operation

Main technological limitations/bottlenecks

- Mass transfer rate (G/L) and mixing (L/L)
- Batch reactions in several cases
- Need for full conversion of toxic reactants (poor mixing, particularly in micro-mixing)
- Multi-product plants: need for grade changes
- Wide residence time distribution

Improvement potential

	Within 10 years	Within 30-40 years
Increase in process energy efficiency	10-20%	
Improved operating equipment within the batch process	10%	
Integrating continuous operating elements/units with batch reactors (structured reactors, etc.)	40%	
Reduced use of chemical (i.e. solvents)		

Promising PI technologies

PI technologies		
1.2.4 Static mixers reactors – Tubular high-pressure reactor with multiple feed injection and efficient heat removal via evaporative coolant		
Reactor with stable emulsion (small gas bubbles and high kLa)		
1.1.4 Static mixers		
3.1.4 Rotor stator mixers		
3.2.3 Impinging stream reactors		
1.2.3 Membrane reactors		

Possible combinations

The above mentioned technologies cannot directly be combined, however there are possibilities in:

- Combining with hybrid operation (e.g. separations): 2.2.2 membrane reactors, 2.2.3 reactive adsorption and 2.2.8.reactive distillation
- Combining with alternative energy transfer: 3.2.5 sonochemical reactors, 3.3.3.4 microwave reactors and 3.3.4 photochemical reactors

Barriers, required research, timing and actions

1.2.4 Static mixers reactors – Tubular high-pressure reactor with multiple feed injection and efficient heat removal via evaporative coolant

Barriers: Mass-transfer limitation, 100% conversion of toxic gas-phase reactant, robustness, reliability and changes in multi-product plant grade

- We need to understand the thermodynamics, kinetics and reactor model
- We need to research materials (e.g. high pressure and corrosion)
- We need to learn about high-pressure dosing and mixing computational fluid dynamics

Research required: Applied

Time until implementation: < 5 years (technology is ready for implementation)

3.2.3 Impinging stream reactors

Barriers: Modeling and up-scaling

Research required: Applied

Time until implementation: < 5 years

Reactor with stable emulsion (small gas bubbles and high kLa)

Barriers: Proof of principle, materials and up-scaling

- We need to create stable emulsions

Research required: Applied

Time until implementation: 5-10 years

1.1.4 Static mixers

Barriers: Modeling, design and up-scaling
Research required: Applied
Time until implementation: 5-10 years

3.1.4 Rotor stator mixers

Barriers: Stabilization, counter pressure and energy use (no increase in energy efficiency)
Research required: Applied
Time until implementation: 5-10 years

1.2.3 Membrane reactors

Barriers: Modeling and up-scaling

- We need to research membrane materials (high pressure, fouling, flux, etc.)

Research required: Fundamental
Time until implementation: 10-15 years

General barriers

- Robustness and reliability
- Lack of tools available to design (partially) continuous process
- Need to reinvent processes (i.e. safety procedures)
- Sufficient mixing (L/L) (high pressure reactor) and a need for full conversion of toxic reactants
- Avoid risk of production/quality loss – Realizing grade change in multi-product plants (fate of twilight material)

LONG TERM

Description of the current process

Selected process

Product and process development based on thinking in terms of continuous processes – No or hardly new products in petrochemicals

- Process design (incl. catalyst development) focused on “real” chemistry instead of “apparent kinetics” determined in stirred vessels
- All steps in the life-cycle of processes (from chemistry development to process development to operational know-how) based on continuous processing

Vision

The processes mentioned under “short-term” might be sufficient already; otherwise, processes should be based on:

- Membrane reactor with a feed of gaseous reactant via membrane in liquid-full reactor
- Milli reactor (with high kLa and good heat removal)
- Production of chemicals currently produced in batch processes in a fully continuous mode

Main technological limitations/bottlenecks

- Fundamentally different approach is necessary in some aspects: i.e. to replace passive temperature control by evaporation (current batch process) with active temperature control in the heat exchanger
- Operation knowledge of the batch reactor is an accumulation of decades of experience in specific processes. Therefore, experience with continuous reactors is often limited
- Membrane development (selectivity, flux and fouling)
- Membrane reactor development (stability, sealing, high-pressure and plug flow)
- Development of milli reactors with good kLA (e.g. monoliths and foams) but also with good heat removal
- Development of stable catalysts, fixed to the milli reactor walls: stable activity and selectivity

Improvement potential

- Energy efficiency increase of 30% for a successful implementation from reduced energy for stirring to increased heat recovery potential in continuous processes
- Reducing the use of chemicals, including feedstock (higher yield) to less solvents

Promising PI technologies

PI technologies		
1.2.3 Membrane reactor		
2.2.1 HEX reactors		
1.2.1.1 Catalytic foam reactor		
1.2.1.2 Monolith reactor		
3.1.5 Spinning Disk Reactors		
1.2.2 Micro reactor		

Possible combinations

• Above mentioned technologies cannot be directly combined. However, we can use possibilities similar to the short term:

- Combining with hybrid operation (e.g. separations): 2.2.2 membrane reactors, 2.2.3 reactive adsorption and 2.2.8.reactive distillation
- Combining with alternative energy transfer: 3.2.5 sonochemical reactors, 3.3.3.4 microwave reactors and 3.3.4 photochemical reactors

Barriers, required research, timing and actions

1.2.3 Membrane reactor

Barriers: Mass-transfer limitation, 100% conversion of toxic gas-phase reactant, robustness, reliability, multi-product plant, grade changes, flux, resistance, mechanical strength and sealing

- We need to research membrane materials

Research required: Fundamental

Time until implementation: 10-15 years

2.2.1 HEX reactors

Barriers: Confidentiality and stable, solid catalyst
Research required: Applied
Time until implementation: 5-10 years

3.1.5 Spinning Disk Reactors

Barriers: A stable and solid catalyst
Research required: Applied (existing technology)
Time until implementation: 5-10 years

1.2.1.1 Catalytic foam reactor

Barriers: A solid, stable catalyst , applications and fouling
Research required: Fundamental
Time until implementation: 10-15 years

1.2.1.2 Monolith reactor

Barriers: A solid, stable catalyst, applications and fouling
Research required: Applied
Time until implementation: 10-15 years

1.2.2 Micro reactor

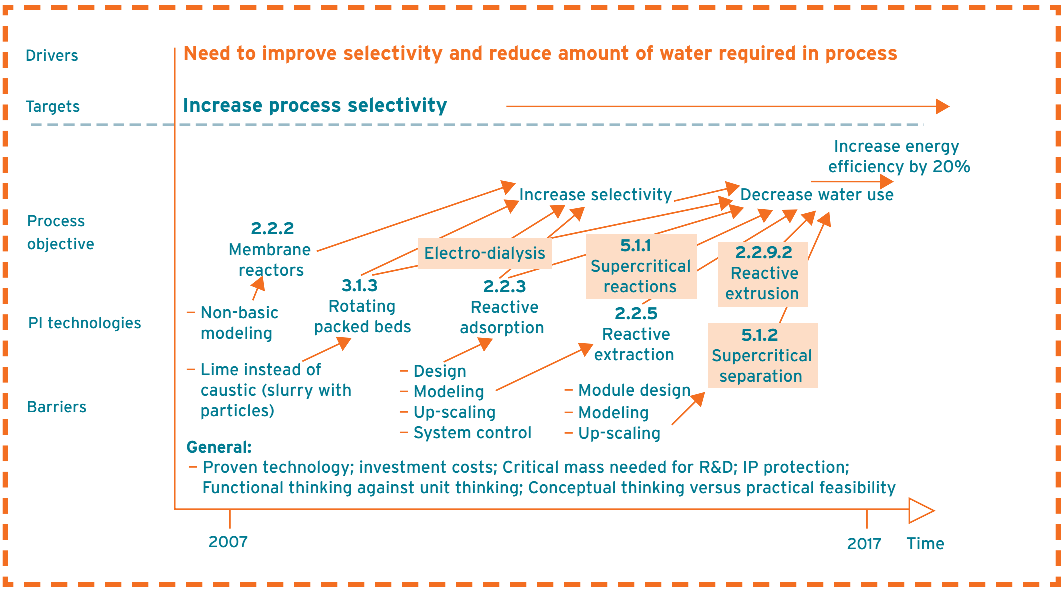
Barriers: A stable and solid catalyst
Research required: Fundamental
Time until implementation: > 15 years

General barriers

- Lack of process design tools for continuous processes
- Achieving sufficient residence time in continuous processes
- Sufficient mass transfer (G/L) (membranes) - This might be a difficult hurdle
- Need for full conversion of toxic reactants - This can be solved
- Robustness and reliability - This will require demonstration
- Realizing grade change in multi-product plants (fate of twilight material) - This can be done and will lead to capex
- Catalyst performance, stability of activity and selectivity (in milli reactor) - This might be a difficult hurdle
- Heat removal in monolith, foam and milli reactors - This requires new designs and might be a difficult hurdle

MASS-TRANSFER-LIMITED FAST REACTIONS ROADMAP
EXAMPLE – ALLYL CHLORIDE (AC) TO DICHLOROHYDRIN (DCH)

SHORT/MID TERM



Description of the current process

Selected process

To improve on the AC to DCH selectivity in order to reduce the amount of water needed for this conversion

State of the art

Make use of the 3.1.3 rotating packed beds or electro-dialysis

Main technological limitations/bottlenecks

Low selectivity and high amounts of water are required

Improvement potential

A 20% increase in energy efficiency through selectivity increase and decrease in water use

Promising PI technologies

PI technologies		
2.2.2 Membrane reactors		
3.1.3 Rotating packed beds		
Electro-dialysis		
2.2.3 Reactive adsorption		
2.2.5 Reactive extraction		
5.1.1 Supercritical reactions		
5.1.2 Supercritical separation		
2.2.9.2 Reactive extrusion		

Possible combinations

Faster and better dispersion of AC and Chlorine via 3.2.7 ultrasound with enhanced phase dispersion/mass transfer

Barriers, required research, timing and actions

2.2.2 Membrane reactors

Barriers: Complicated (non-basic) modeling
Research required: Fundamental
Time until implementation: > 15 years

3.1.3 Rotating packed beds

Barriers: Use lime instead of caustic (slurry with particles)

2.2.3 Reactive adsorption

Barriers: design, modeling, up scaling and system control
Research required: Combined/fundamental
Time until implementation: 5-15 years

2.2.5 Reactive extraction

Barriers: Design, modeling, up-scaling and system control
Research required: Combined
Time until implementation: 5-10 years

5.1.2 Supercritical separation

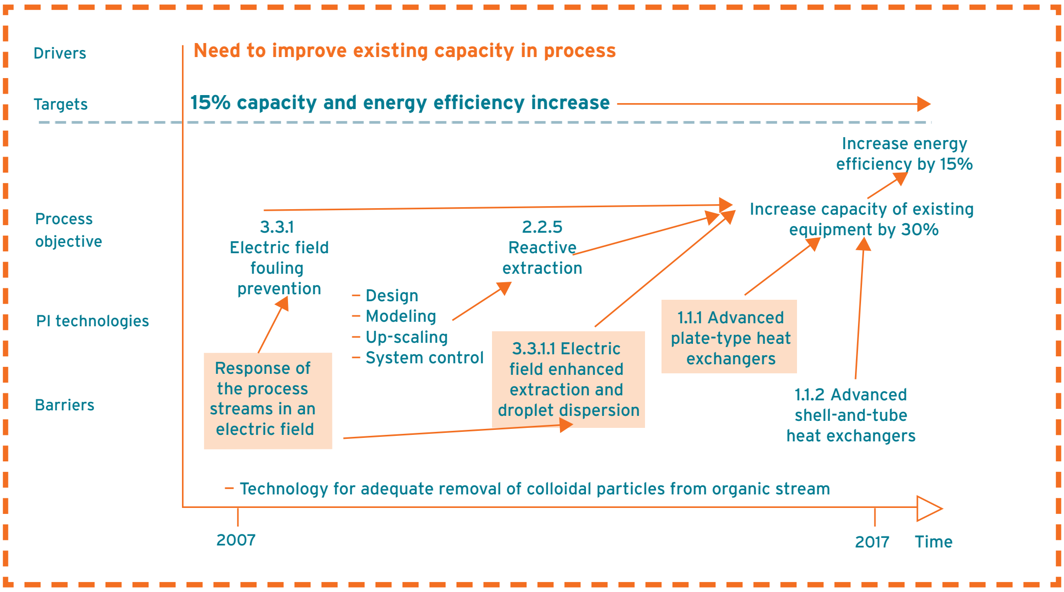
Barriers: Module design, modeling and up-scaling
Research required: Combined
Time until implementation: < 5 years

General barriers

- Proven technology versus new technology
- CAPEX versus pay back time
- Critical mass needed for R&D (basic data, kinetics and mass transfer studies)
- IP protection
- Functional thinking versus unit thinking
- Conceptual thinking versus practical feasibility

MASS-TRANSFER-LIMITED FAST REACTIONS ROADMAP
EXAMPLE – LIQUID EPOXY RESIN PRODUCTION

SHORT/MEDIUM TERM



Description of the current process

Selected process

Liquid epoxy resin production process

State of the art

Capacity increase and energy reduction of the existing plants

Improvement potential

Increase in energy efficiency of 15-30% capacity with existing equipment

Promising PI technologies

PI technologies		
3.3.1 Electric field fouling prevention		
2.2.5 Reactive extraction		
3.3.1.1 Electric field enhanced extraction and droplet dispersion		
1.1.1 Advanced plate-type heat exchangers (i.e. plate-and-shell)		
1.1.2 Advanced shell-and-tube heat exchangers		

Barriers, required research, timing and actions

3.3.1 Electric field fouling prevention

Barriers: Design, modeling, up-scaling, system control and operating safety

Research required: combined

Time until implementation: <5 years

2.2.5 Reactive extraction

Barriers: design, modeling, up-scaling and system control

Research required: combined

Time until implementation: 5-10 years

3.3.1.1 Electric field enhanced extraction and droplet dispersion

Barriers: Design, modeling, up-scaling, system control and safe operation

Research required: Combined

Time until implementation: < 5 years

1.1.1 Advanced plate-type heat exchangers (i.e. plate-and-shell)

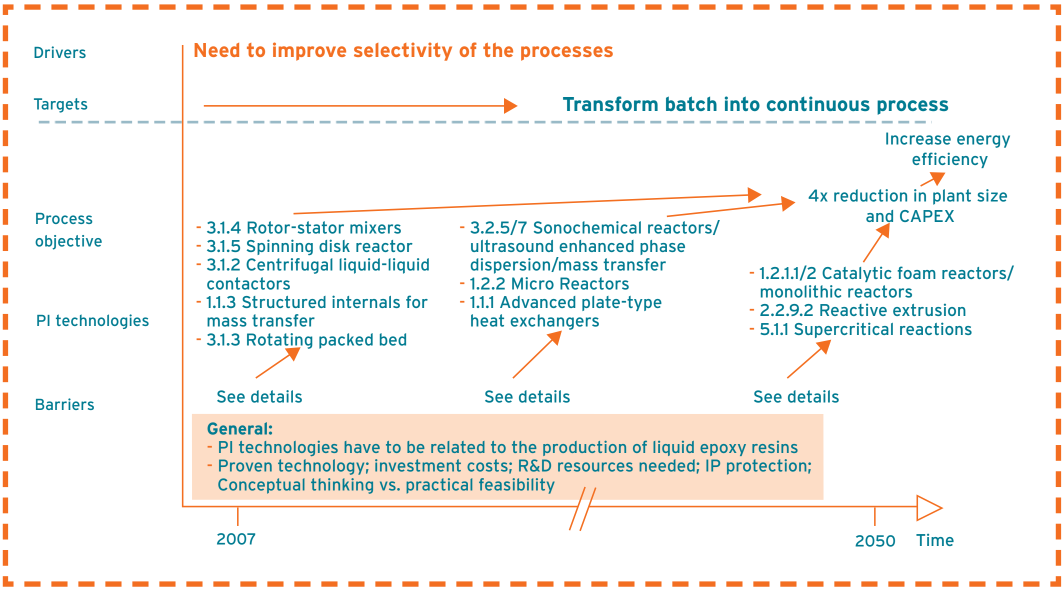
Research required: Applied

Time until implementation: < 5 years

General barriers

- Technology for adequate removal of colloidal particles from organic stream has to be developed
- The response of the process streams in an electric field has to be studied

LONG-TERM



General:
- PI technologies have to be related to the production of liquid epoxy resins
- Proven technology; investment costs; R&D resources needed; IP protection; Conceptual thinking vs. practical feasibility

Description of the current process

Selected process

Liquid epoxy resin production

Vision

The epikote process that is now primarily performed in the batch reactors will be transferred to a continuous reactor operation. Reactor types are most likely of the SDR type, i.e. static mixers reactors, rotor stator mixers, etc. We must develop new epoxy resin routes that are cheaper (CAPEX) and simpler

Main technological limitations/bottlenecks

Batch reactors need to be replaced by continuous reactors (i.e. 3.1.5 spinning disk reactor)

Improvement potential

A liquid epoxy resin plant should be reduced in size and CAPEX with at least factor 4

Promising PI technologies

PI technologies		
3.1.4 Rotor-stator mixers		
3.1.5 Spinning disk reactor		
3.1.2 Centrifugal liquid-liquid contactors		
1.1.3 Structured internals for mass transfer		
3.1.3 Rotating packed bed		
3.2.5/7 Sonochemical reactors/ultrasound enhanced phase dispersion/mass transfer		
1.2.2 Micro-reactors		
1.1.1 Advanced plate-type heat exchangers		
1.2.1.1/2 Catalytic foam reactors/monolithic reactors		
2.2.9.2 Reactive extrusion		
5.1.1 Supercritical reactions		

Barriers, required research, timing and actions

3.1.4 Rotor-stator mixers

Barriers: Stabilization, counter pressure and energy use (no increase in energy efficiency)

Research required: Applied

Time until implementation: 5-10 years

3.1.5 Spinning disk reactor

Barriers: A stable and solid catalyst

Research required: Applied (existing technology)

Time until implementation: 5-10 years

3.1.2 Centrifugal liquid-liquid contactors

Barriers: System design, process control and investment costs
Research required: Applied
Time until implementation: < 5 years

3.1.3 Rotating packed bed

Barriers: Corrosion and fouling

3.2.5/7 Sonochemical reactors/ultrasound enhanced phase dispersion/mass transfer

Barriers: System design, up-scaling, process control and investment costs
Research required: Fundamental
Time until implementation: 10-15 years

1.2.2 Micro-reactors

Barriers: A solid, stable catalyst
Research required: Fundamental
Time until implementation: >15 years

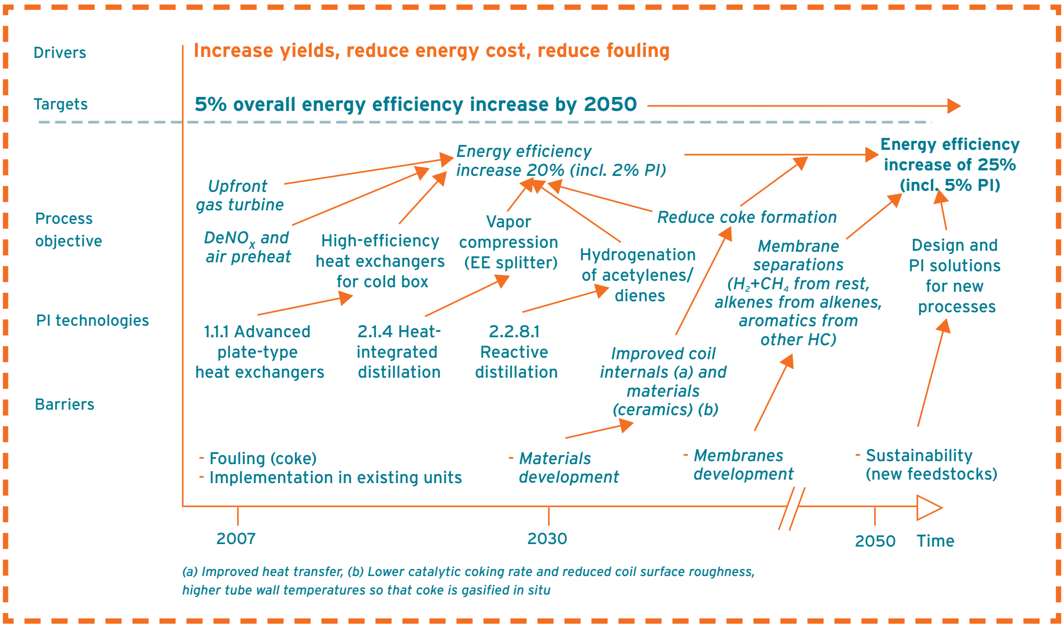
1.2.1.1/2 Catalytic foam reactors/monolithic reactors

Barriers: Applications, fouling and a solid, stable catalyst
Research required: Fundamental and applied
Time until implementation: 10-15 years

General barriers

- Proven technology versus new technology
- CAPEX versus pay back
- Resources needed for R&D
- IP protection
- Conceptual thinking versus practical feasibility

ETHYLENE CRACKING ROADMAP



(a) Improved heat transfer, (b) Lower catalytic coking rate and reduced coil surface roughness, higher tube wall temperatures so that coke is gasified in situ

SHORT/MID-TERM

Description of the current process

Selected process

Largely more or less “conventional“ solutions (not PI):

- Use of gas turbines upfront of furnaces
- Use de-NOX with NH_3 (SCR) in combination with air preheated by flue gas and a move away from less energy-efficient, low-NOx burners
- Optimize emissivity of furnace walls and coils
- Optimize coil inlet temperature (cracking reactions are just beginning)
- Some PI elements:
- Use of high-efficiency heat exchangers for cold box (lower temperature approach) or reboilers (less fouling), if fouling will permit
- Use of heat pumps (e.g., vapor compression), especially for EE splitters
- Use of dividing wall column internals
- Use of reactive distillation for hydrogenation of acetylenes/dynes

State of the art

Largely existing

Main technological limitations/bottlenecks

- Ethylene plants are complex, highly integrated and capital-intensive processes that are optimized towards the yield of high-value chemicals and the use of energy. A significant part of the energy is required as heat reaction (endothermic cracking reactions). Speaking short-term, there are no clear alternatives to the current method for producing ethylene, which is done via radical reactions at extremely high temperatures with low selectivity (many products) requiring a.o. cryogenic separations

- Fouling by coke and poly-aromatics reduces heat transfer with effects on selectivity/yield (less ethylene, more acetylene, aromatics and coke)

Improvement potential

No increase in energy efficiency is expected from PI

Promising PI technologies

PI technologies		
1.1.1 Advanced plate-type heat exchangers (hex)		
2.1.4 Heat-integrated distillation		
2.2.8.1 Reactive distillation		

Possible combinations

None

General barriers

- Fouling occurs mainly in the reaction section, but also plays a role in downstream sections (e.g. prefractionator and distillation). In the reaction section, fouling:
  - Limits heat transfer rate
  - Sets a minimum to tube diameters via pressure drop and plugging
  - Sets a maximum for reaction temperature, and consequently a minimum for residence time
  - Requires cleaning (e.g. coils 1x/50 days and exchangers 2x/year)
- Ethylene crackers are complex and expensive existing installations. In existing crackers, there will only be opportunity-driven changes and only gradually over time (up to 2030):
  - Only in turnaround periods
  - Limited capex, for profitable investment - A de-bottlenecking incentive is needed to justify the investment in energy efficiency
  - Retrofitting PI technologies in existing unit operations/process schemes will enhance the opportunity
- A high level of energy integration
  - Some heat waste is efficiently used for separations (PP splitter), but there is a need for steam balance
  - If energy is saved on the ethylene cracker side, e.g. generating excess MP steam production, there should be a good alternative use for this MP steam

LONG-TERM

Description of the current process

Selected process

- We assume that, even in 2050, there will still be a strong demand for ethylene and propylene as building blocks of the petrochemical industry
  - If we could prevent the need for the lowest temperatures, significant compression energy could be saved (-150 oC for evaporative H_2/CH_4 separation)
  - A significant part of the compression could be prevented if there were an upfront alkane/alkene separation or separation of aromatics from other hydrocarbons
- Alternative feedstocks and processes: In an environment with higher cost of crude oil (naphtha), and higher cost of CO_2, new routes (some based on other feeds such as natural gas, coal and biomass) might be used. Moreover, the competition between the use of fossil feedstock for chemicals (e.g. naphtha for ethylene) and fuels may change in the favor of chemicals production at higher oil prices and increased energy costs
- The existing alternative routes are:
  - Production of syngas from natural gas, coal or biomass followed by production of lower olefins from syngas, e.g. via methanol (MTO, MTP) or via synthetic naphtha (MTG or Fischer-Tropsch), and conventional cracking of such feed
  - Deep catalytic cracking (FCC with new catalysts giving lower olefins than gasoline, especially C3-C4)
  - Production of ethanol from biomass, followed by production of ethylene and PE (e.g. Dow announcement for j.v. in Brazil in 2011)

Vision

Increase use of sustainable feedstock

Main technological limitations/bottlenecks

- Reduce fouling/coke formation via improved heat transfer (lower wall temperatures, or higher temperatures in combination with shorter residence times)
  - Use of new coil materials (to be identified, incl. ceramics; attention to ceramics/metal material transitions)
  - Use of internals giving increased turbulence but without concomitant higher pressure drop
- Reduce coke adhesion to walls and improve run-off of condensates
  - Use smoother materials (materials to be identified, e.g. ceramics) or energy (e.g. ultrasound)
- Separation of H_2, CH_4 and CO from ethylene,via membranes, and for only H_2 via adsorption or reaction
- Separation of alkenes from alkanes via membranes or adsorption
- Separation of aromatics from alkanes/alkenes via membranes or adsorption
- Design and use for PI in new process routes

Improvement potential

Ethylene cracker technology: ca. 25% energy efficiency in 2030, including a contribution of PI technologies of 5%. Currently, no quantification is possible for alternative processes. Research is required to determine the energy/CO_2 efficiency of alternative processes, including those using bio feeds

Promising PI technologies

Membrane separations will help, but are not PI (link to DSTI roadmap for development of membrane materials). Perhaps membrane adsorption (2.1.5.2) or membrane extraction (2.1.5.6) could occur in a later stage. Use of PI techniques will depend on the character of new process routes for alternative feeds

Possible combinations

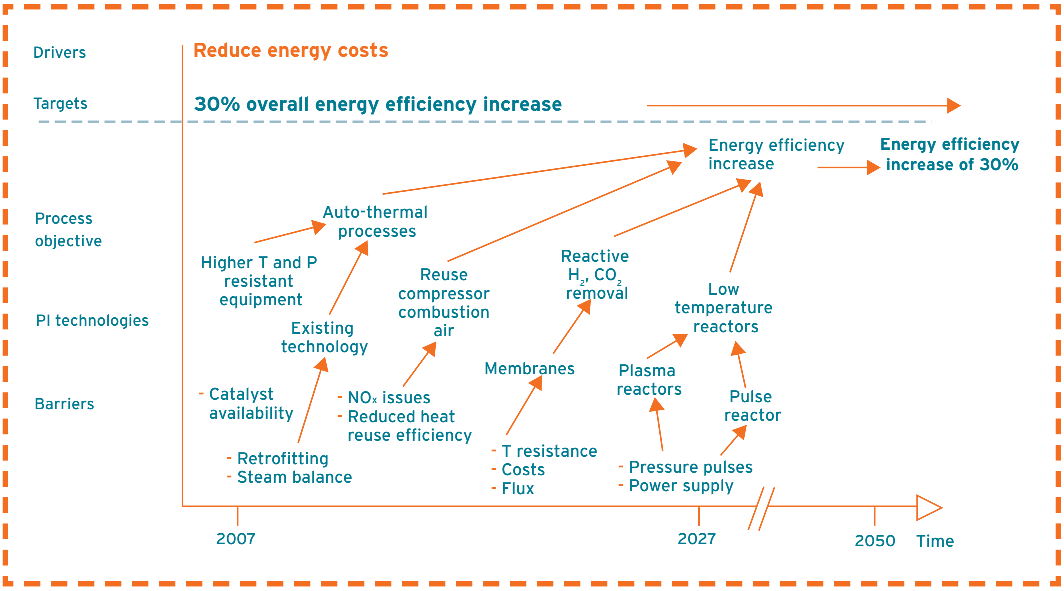
None

General barriers

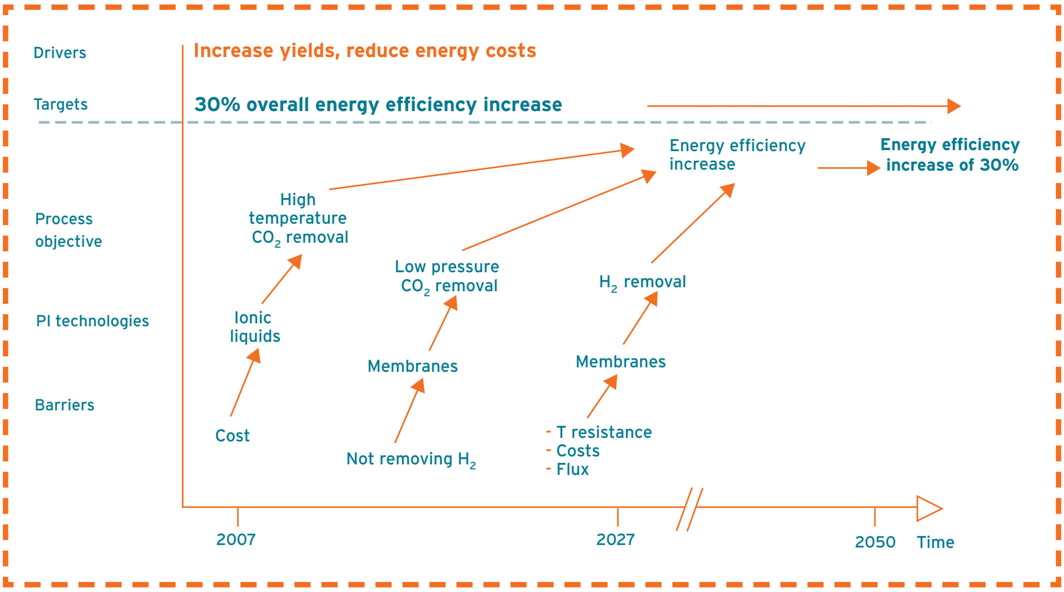
See short/mid-term

AMMONIA ROADMAP

Ammonia reforming roadmap[6]



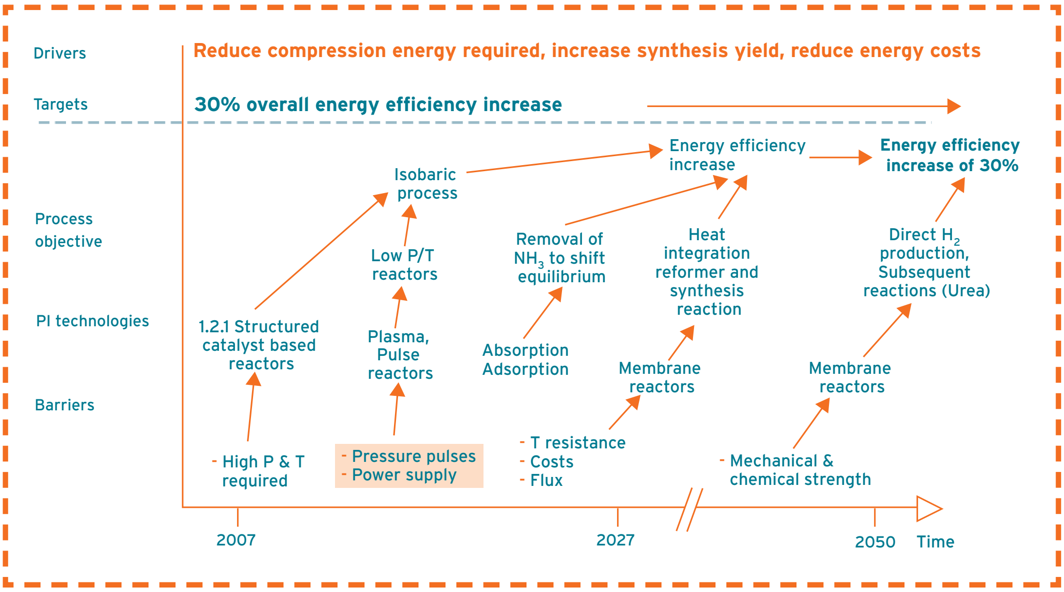
Ammonia CO_2 removal roadmap



---

[6] Also applicable for hydrogen production

Ammonia synthesis roadmap



SHORT/MID-TERM

Description of the current process

Selected process

Reformer: $CH_4 + H_2O \longrightarrow CO + 3 H_2$

CO shift: $CO + H_2O \longrightarrow CO_2 + H_2$

CO_2 removal: Removal of CO_2 from the H_2, N_2, H_2O and CH_2 mixture by liquid absorption

Methanation: $CO + CO_2 + H_2 \longrightarrow CH_2 + H_2O$ to remove traces of CO and CO_2 in the H_2

Compression: Increase system pressure from 30 to about 200 bar

Synthesis: $3 H_2 + N_2 \longrightarrow 2 NH_3$

State of the art

The theoretically minimum energy demand for ammonia production with regards to feedstock consumption is 20,65 GJ/ton NH_3. Current operated units are at about 30 GJ/ton NH_3. The Best Available Technology (BAT) processes are at about 28-29 GJ/ton NH_3.,so the potential for energy reduction is 7-30% BAT (theoretical minimum)

Main technological limitations/bottlenecks

- Steam reforming (endothermic) is the major energy consumer and equipment design is at metallurgy limits
- It seems inefficient to produce pure high pressure H_2 in five-steps
- Compression is a major energy consumer (however, it reuses steam from other stages)
- Synthesis process has a 15-20% yield per pass

Improvement potential

Implementing BAT can potentially yield a 7% increase in energy efficiency

Promising PI technologies

Reformer step

- Higher T and P resistant equipment to shift the equilibrium
- Auto-thermal reforming to limit loss of flue gas - This is the existing technology
- Reuse compressor combustion air in the reformers
- H_2 or CO removal with membranes
- Low-temperature reactors with plasma or pulsed compression reactors

CO shift & CO_2 removal steps

- High temperature CO_2 removal with ionic liquids
- Low pressure CO_2 removal with membranes
- H_2 removal with membranes

Synthesis step

- Structured catalysts to allow for lower T&P conditions (isobaric process enabler)
- Smart heat removal from synthesis reaction by integration with the reformer step in one counter flow reactor/heat exchange system
- Removal of NH_3 to shift equilibrium with adsorption, absorption and subsequent reactions (Urea)

Possible combinations

Membrane integration with new reactor designs

Barriers, required research, timing and actions

Reformer step

- Auto-thermal processes: Retrofitting and steam balance
- Reuse compressor combustion air: NOx issues and reduced efficiency for heat reuse
- Membranes: T resistance, costs and flux (no fouling issues)
- Plasma and pulsed compression reactors: Use of a catalyst in these systems and design and control issues

CO_2 removal steps

- Membranes: Removal of CO and CO_2 without the removal of H_2 and mechanical strength at high T&P

Synthesis step

- New reactor designs
- Membranes: Removal of NH_3 without the removal of N_2 or H_2 and mechanical strength at high T&P

General barriers

In existing facilities, there will only be opportunity-driven changes:

- Units are highly integrated so the total energy system has to remain in balance
- Only in turnaround periods
- Limited CAPEX for profitable investment - Generally, there must be a de-bottlenecking incentive to justify investment in energy efficiency

- Retrofitting PI technologies in existing unit operations/process schemes will enhance the opportunity

LONG-TERM

Description of the current process

Vision

We envisioned three scenarios

- Biomass-based fertilizer or melamine production eliminating large-scale ammonia facilities. Direct production of urea, nitric acid or even nitrates from direct oxidation of N_2 are developed. Then, no new ammonia facilities would be required. This scenario was not further considered for this PI Roadmap

For the two other scenarios we assumed that in 2050, there will still be a strong demand for ammonia (e.g. an ammonia based fuel economy combined with higher agricultural demands and ammonia for chemicals)

- Ammonia synthesis from direct Hydrogen production routes, i.e. nuclear electrolysis of water reacting. These processes, which involve fuel cells, will require separation techniques for oxygen removal from hydrogen
- The current feedstock basis is methane or coal based processes. However, coal based routes will produce more CO_2. Smart combination of the heat effects of the reforming and synthesis reactions lead to direct energy savings. A counter current single reactor combined with a membrane for smart transfer of the H_2 from the reforming side to the synthesis side will drive the equilibrium reactions to higher levels
- Production of hydrogen (through syngas) from biomass fits well in the current systems

Main technological limitations/bottlenecks

As all process steps are equilibrium reactions, it will be beneficial to design better catalysts that operate at milder conditions to drive the equilibrium reactions to completion. This will benefit the ammonia production significantly. Systems to separate H_2, CO_2 or NH_3 from the reaction/reactors (membranes, adsorption, ionic liquids or reaction)

Improvement potential

A 25% increase in energy efficiency through direct H_2 production, with the energy required for making Hydrogen en heat input for the endothermic synthesis will remain. Additionally, there will be a 50% increase in energy efficiency through selective increase in the synthesis step

Promising PI technologies

PI technologies		
1.2.3 Membrane reactors		
2.1.5.x Membrane technologies		
2.2.2 Catalytic membrane reactors		
2.2.5 Reactive extraction		
2.2.6 Reactive adsorption		
3.2.4 Pulsed compression reactors		
3.3.5 Plasma (GlidArc) reactors for direct oxidation		

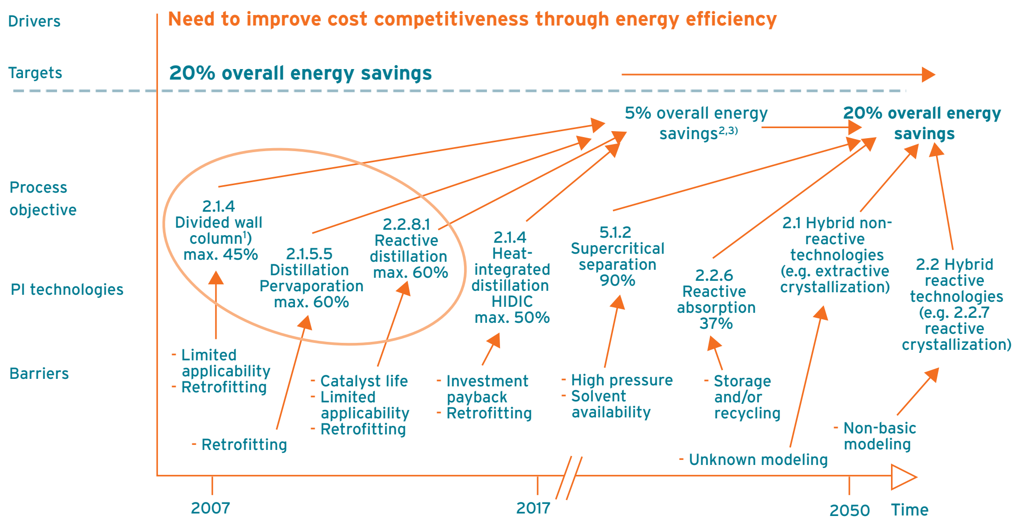
Possible combinations

Various technologies, as given above, to influence the equilibrium reactions

General barriers

Ammonia production facilities are expensive, existing installations, which limits improvement potential. The chance that significant capacity from recently constructed facilities will come on-stream in Europe

ENERGY EFFICIENT SEPARATION ROADMAP



1) Already applied by BASF
2) A number of technologies are already applied
3) Convincing management is a general barrier

Note: Replace last distillation step (for 95 to 99% purity) by a filtration step (5% energy savings increase)

Description of the current process

Selected process

The current separation processes require large amounts of steam energy. Every sequential process step needs steam and will waste this energy content by cooling

Main technological limitations/bottlenecks

In general, the implementation of new technologies is only possible if it concerns retrofitting in existing processes

Improvement potential

Over-all energy saving potential compared to present process: 5-10% in 10 years and 20% in 30-40 years

Promising PI technologies

PI technologies	Energy efficiency potential	
	Within 10 years	Within 30-40 years
2.1.4 Divided wall column³	Max. 45%	
2.1.5.5 Distillation/Pervaporation	Max. 60%	
2.2.8.1 Reactive distillation	Max. 60%	
2.1.4 Heat-integrated distillation (HIDIC)	Max. 50%	
5.1.2 Supercritical separation	Max. 90%	
2.2.6. Reactive absorption	Max. 37%	
2.1... Hybrid non-reactive technologies		
2.2... Hybrid reactive technologies		

Possible combinations

2.1.5.5 Distillation/pervaporation, 2.1.4 heat-integrated distillation (HIDIC) and 2.2.8.1 reactive distillation might be combined in specific cases

Barriers, required research, timing and actions

2.1.4 Divided wall column

Barriers: Limited applicability and retrofitting
Research required: Applied (already commercially available)
Time until implementation: < 5 years

2.1.5.5 Distillation/Pervaporation

Barriers: The applicable current membrane technology is limited due to membrane instability in applications other than methanol or water pervaporation
Research required: Applied (already commercially available)
Time until implementation: < 5 years

2.2.8.1 Reactive distillation

Barriers: The short life of the catalyst, which is only for exothermic and equilibrium reactions and retrofit difficult
Research required: Applied (already commercially available)
Time until implementation: < 5 years

2.1.4 Heat-integrated distillation (HIDIC)

Barriers: Long payback on investment, limited applicability
Research required: Combined
Time until implementation: 10 years

5.1.2 Supercritical separation

Barriers: High-pressure techniques and, other than CO_2, limited solvent availability
Research required: Fundamental
Time until implementation: 15 years

2.2.6 Reactive absorption

Barriers: Storage and recycling of solvents
Research required: Applied (since the 1980‘s by Lurgi, BASF)
Time until implementation: < 5 years

2.1… Hybrid non-reactive technologies

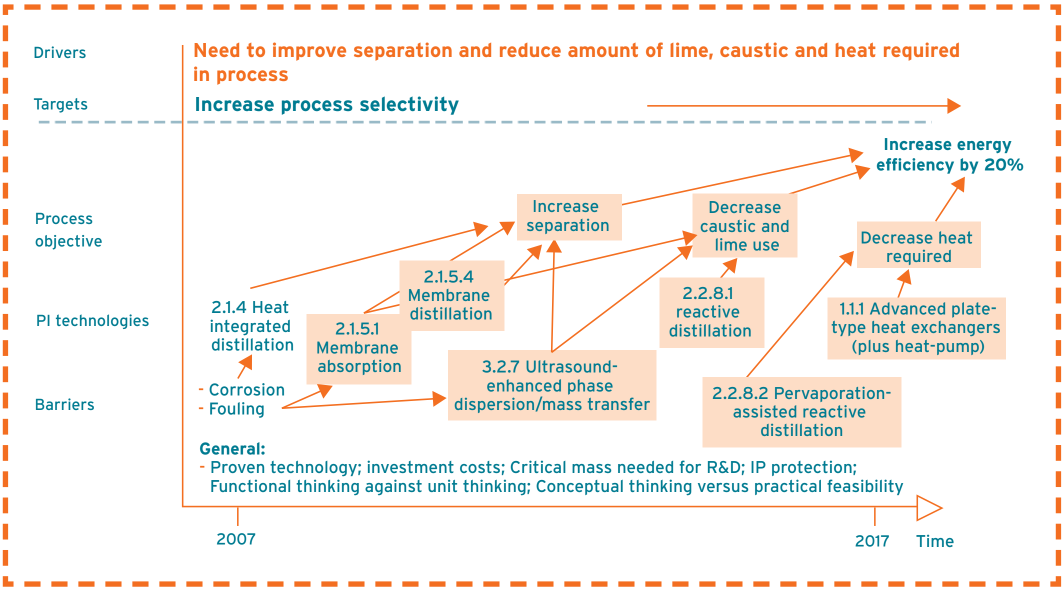
Barriers: Unknown modeling
Research required: Fundamental
Time until implementation: > 15 years

2.2… Hybrid reactive technologies

Barriers: Complicated (non-basic) modeling
Research required: Fundamental
Time until implementation: > 15 years

ENERGY EFFICIENT SEPARATION ROADMAP
EXAMPLE – DICHLOROHYDRIN (DCH) TO EPICHLOROHYDRIN (ECH) SELECTIVITY

SHORT/MEDIUM TERM



Description of the current process

Selected process

To improve the reactive stripping process in which DCH is converted into ECH by the use of caustic or lime, and at the same time stripped from the liquid phase. ECH is lost either via hydrolysis, a failure to convert DCH or a failure to strip ECH completely from the liquid

State of the art

Technology that intensifies the contact between hydroxide and DCH, while effectively separating ECH

Main technological limitations/bottlenecks

- Overcome mass transfer limitations, and subsequently reduce holdup
  - to prevent hydrolysis reaction of ECH
  - as a prerequisite to be able to separate ECH as effectively as possible
- Reduce caustic and lime consumption
- Integrate heat or heat recovery from effluent stream

Improvement potential

A 20% increase in energy efficiency through

- Separation increase
- Decrease in caustic and lime use
- Decrease in heat use

Promising PI technologies

PI technologies		
2.1.4 Heat integrated distillation		
2.1.5.1 Membrane absorption		
2.1.5.4 Membrane distillation		
3.2.7 Ultrasound-enhanced phase dispersion/-mass transfer		
2.2.8.1 Reactive distillation		
2.2.8.2 Pervaporation-assisted reactive distillation		
1.1.1 Advanced plate-type heat exchangers (plus heat-pump)		

Possible combinations

Process improvements are linked to the improvements in the AC to DCH process

Barriers, required research, timing and actions

2.1.4 Heat-integrated distillation (HIDIC)

Barriers: Long payback on investment and limited applicability
Research required: Combined
Time until implementation: 10 years

2.1.5.1 Membrane absorption

Barriers: Corrosion, fouling, up-scaling and module design
Research required: Combined
Time until implementation: 5-10 years

2.1.5.4 Membrane distillation

Barriers: Corrosion, fouling and costs
Research required: Combined
Time until implementation: 10 years

3.2.7 Ultrasound-enhanced phase dispersion/mass transfer

Barriers: Corrosion, fouling, up-scaling and cavitations
Research required: Combined
Time until implementation: 10 years

2.2.8.1 Reactive distillation

Barriers: Short life of catalyst, only for exothermic and equilibrium reactions and difficult retrofit
Research required: Applied (already commercially available)
Time until implementation: < 5 years

2.2.8.2 Pervaporation-assisted reactive distillation

Barriers: Short life of catalyst, only for exothermic and equilibrium reactions and difficult retrofitting for membrane stability

Research required: Applied (already commercially available) for limited applications
Time until implementation: 5 years

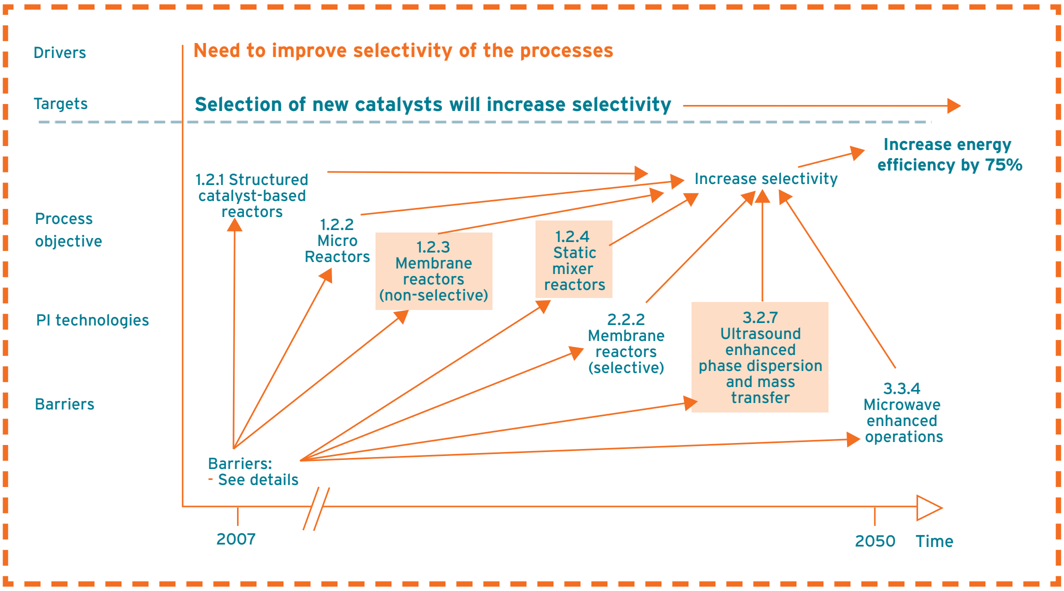
1.1.1 Advanced plate-type heat exchangers (plus heat-pump)

Barriers: Corrosion and fouling
Time until implementation: 10 years

General barriers

- Proven technology versus new technology
- Capex versus pay back time
- Critical mass needed for R&D (basic data, kinetics and mass transfer studies)
- IP protection
- Functional thinking versus unit thinking
- Conceptual thinking versus practical feasibility

LONG-TERM



Description of the current process

Selected process

AC to DCH and DCH to ECH selectivity

Vision

Select the corresponding reactor and separation line-up based on the right homogeneous/heterogeneous catalysts

Improvement potential

A 75% increase in energy efficiency through increase of selectivity

Promising PI technologies

PI technologies		
1.2.1 Structured catalyst-based reactors		
1.2.2 Micro-reactors		
1.2.3 Membrane reactors		
1.2.4 Static mixer reactors		
2.2.2 Membrane reactors		
3.2.7 Ultrasound enhanced phase dispersion and		
3.3.4 Microwave enhanced operations		

Possible combinations

None

Barriers, required research, timing and actions

1.2.2 Micro-reactors

Barriers: A solid, stable catalyst, fouling and up-scaling
Research required: Fundamental
Time until implementation: > 15 years

1.2.3 Membrane reactors

Barriers: Mass-transfer limitation, 100% conversion of toxic gas-phase reactant, robustness, reliability, multi-product plant, grade changes, flux, resistance, mechanical strength and sealing

– We need to research membrane materials

Research required: Fundamental
Time until implementation: 10-15 years

1.2.4 Static mixer reactors

Barriers: Mass-transfer limitation, 100% conversion of toxic gas-phase reactant, robustness, reliability and multi-product plant grade changes

– We need to understand the thermodynamics, kinetics and reactor model
– We need to research materials (e.g. high pressure and corrosion)
– We need to learn about high-pressure dosing and mixing computational fluid dynamics

Research required: Applied
Time until implementation: < 5 years (technology is ready for implementation)

2.2.2 Membrane reactors (selective)

Barriers: Complicated modeling, cost and robustness
Research required: Fundamental
Time until implementation: > 15 years

3.2.7 Ultrasound enhanced phase dispersion and mass transfer

Barriers: Design, modeling, up-scaling, system and applications control and cavitations

Research required: Fundamental
Time until implementation: 15 years

3.3.3 microwave enhanced operations

Barriers: Design, modeling, up-scaling, system control and safe operation
Research required: Combined
Time until implementation: 10-15 years

2.2 FINEPHARM ROADMAP

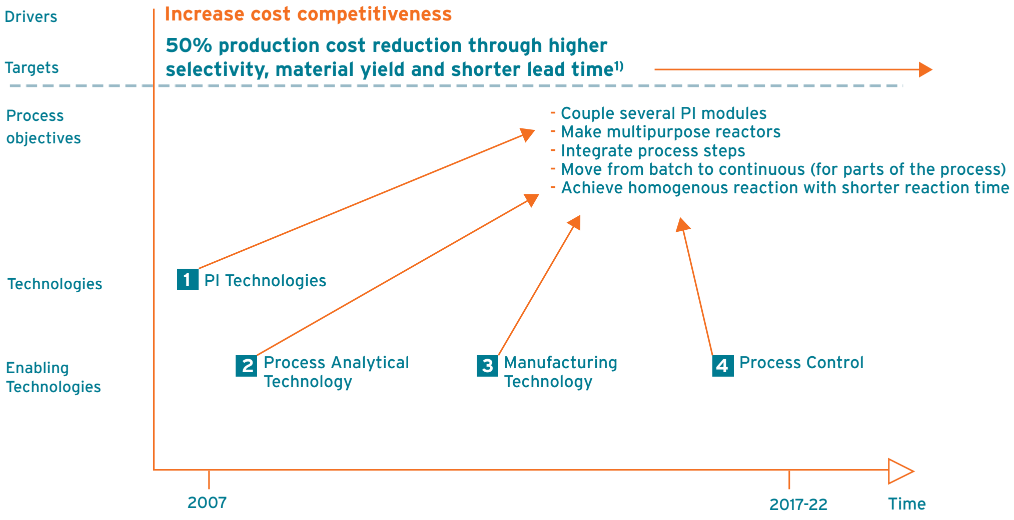
PI Technologies
Reduction in production costs
through higher selectivity,
material yield and shorter lead time.
– 5-10 years: 20% reduction
– 10-15 years: 50% reduction

FINEPHARM processes - PI Roadmaps

Proces Analytical Technology - enabling
– Full control of production and downstreamprocessing

Manufacturing Technology enabling
– Full inductrial scale-up and piloting of novel PI equipment within two years after lab scale proof -of-concept

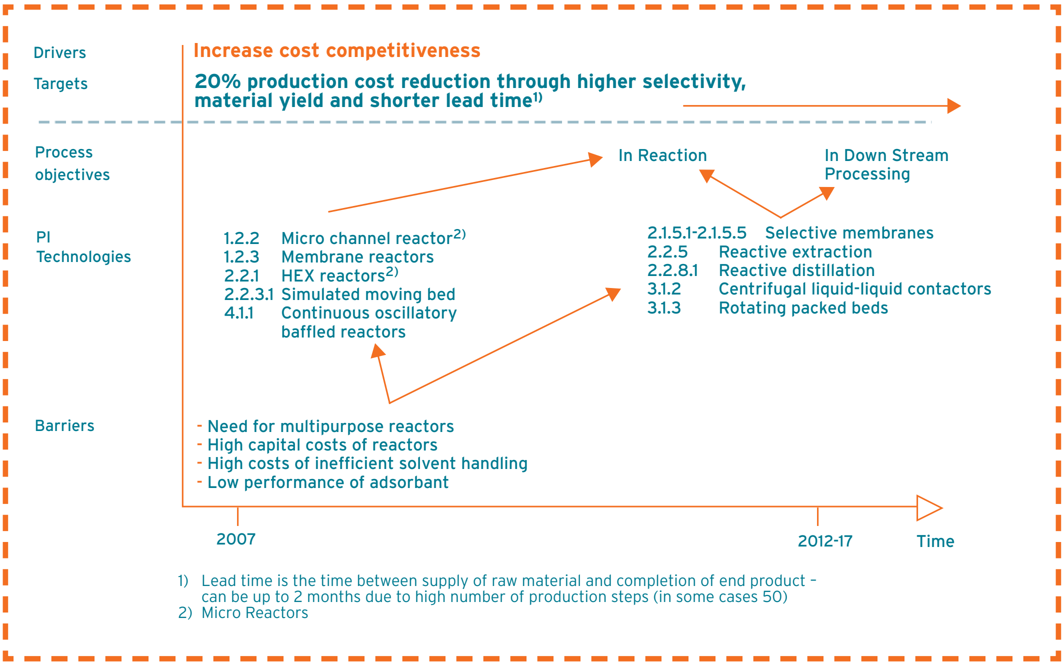
Proces Control - enabling
– Full controllable continuous multi-step processes on inductrial scale within six years



1) Lead time is the time between supply of raw material and completion of end product – can be up to 2 months due to high number of production steps (in some cases 50)

PI TECHNOLOGIES ROADMAP
TOWARDS A MULTIPURPOSE SERIAL PRODUCTION TRAIN

SHORT/MID TERM



Drivers: Increase cost competitiveness

Targets: **20% production cost reduction through higher selectivity, material yield and shorter lead time**[1]

Process objectives: In Reaction; In Down Stream Processing

PI Technologies:

1.2.2 Micro channel reactor[2]
1.2.3 Membrane reactors
2.2.1 HEX reactors[2]
2.2.3.1 Simulated moving bed
4.1.1 Continuous oscillatory baffled reactors

2.1.5.1-2.1.5.5 Selective membranes
2.2.5 Reactive extraction
2.2.8.1 Reactive distillation
3.1.2 Centrifugal liquid-liquid contactors
3.1.3 Rotating packed beds

Barriers:

- Need for multipurpose reactors
- High capital costs of reactors
- High costs of inefficient solvent handling
- Low performance of adsorbant

1) Lead time is the time between supply of raw material and completion of end product - can be up to 2 months due to high number of production steps (in some cases 50)
2) Micro Reactors

Description of the current process

Needs

Production cost reduction through higher selectivity, material yield and a shorter lead time

Main technological limitations/bottlenecks:

Limited heat and mass transfer of batch reactor and low batch operation productivity

Improvement potential

20% reduction of production cost through higher selectivity, material yield and a shorter lead time, resulting in a 20% reduction in energy consumption.

Promising PI technologies

Reaction part	**Production cost reduction**	
	Within 5-10 years	**Driver**
1.2.2 Micro channel reactor	40-80%	Space-time yield
1.2.3 Membrane reactors	20-50%	In situ product removal
2.2.1 HEX reactors	30-70%	Space-time yield
2.2.3.1 Simulated moving bed	30-70%	Separation and equilibrium shift
4.1.1 Continuous oscillatory baffled reactors	20-50%	Space-time yield

Reaction and down stream processing part	**Production cost reduction**	
	Within 5-10 years	
2.1.5.1. - 2.1.5.5 Selective membranes	50%	
2.2.5 Reactive extraction	50%	
2.2.8.1 Reactive distillation	50%	
2.2.8.2 Pervaporation-assisted reactive distillation	50%	
3.1.2 Centrifugal liquid-liquid contactors	50%	
3.1.3 Rotating packed beds (incl. rotating foam reactors)	50%	

Possible combinations

PI unit operations are modular units - The process is reconfigurable using these modular units

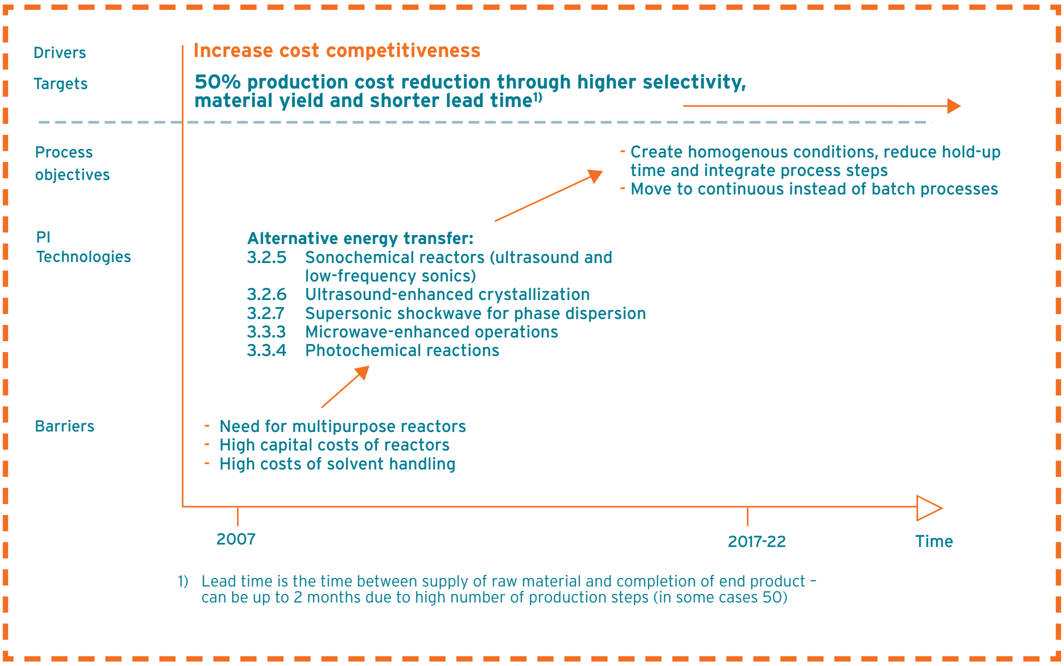
Barriers, required research, timing and actions

All listed PI technologies have achieved proof-of-concept on the lab scale

Barrier: Development of multi-purpose, lower capital cost reactors
Research required: Applied
Time until implementation: 5 years

Barriers: Up-scaling and piloting
Research required: Applied
Time until implementation: 5 years

LONG TERM



Drivers: **Increase cost competitiveness**

Targets: **50% production cost reduction through higher selectivity, material yield and shorter lead time[1)]**

Process objectives:
- Create homogenous conditions, reduce hold-up time and integrate process steps
- Move to continuous instead of batch processes

PI Technologies:

Alternative energy transfer:
3.2.5 Sonochemical reactors (ultrasound and low-frequency sonics)
3.2.6 Ultrasound-enhanced crystallization
3.2.7 Supersonic shockwave for phase dispersion
3.3.3 Microwave-enhanced operations
3.3.4 Photochemical reactions

Barriers:
- Need for multipurpose reactors
- High capital costs of reactors
- High costs of solvent handling

1) Lead time is the time between supply of raw material and completion of end product – can be up to 2 months due to high number of production steps (in some cases 50)

Description of the current process

Vision

Intrinsically safe, fully continuous, multi-purpose production trains with a lead time of days instead of months

Main technological limitations/bottlenecks:
Limited heat and mass transfer of batch reactor and low productivity of batch operation

Improvement potential

50% reduction of production cost through higher selectivity, material yield, and a shorter lead time, resulting in a 50% reduction of energy consumption

Promising PI technologies

Reaction part	**Production cost reduction**	
	Within 10-15 years	
3.2.5 Sonochemical reactors (e.g. ultrasound and low-frequency sonics)	50%	
3.2.6 Ultrasound-enhanced crystallisation	50%	
3.2.7 Supersonic shockwave for phase dispersion	50%	
3.3.3 Microwave reactors for heterogeneous catalyzed processes	50%	
3.3.4 Photochemical reactions	50%	

Reaction and down stream processing part	**Production cost reduction**	
	Within 10-15 years	
2.1.5.1 – 2.1.5.5 Selective membranes	30-70%	
2.2.5 Reactive extraction	20-50%	
2.2.8.1 Reactive distillation	20-50%	
3.1.2 Centrifugal liquid-liquid contactors	30-60%	
3.1.3 Rotating packed beds (incl. rotating foam reactors)	30-60%	

Possible combinations

PI unit operations are modular units - The process is reconfigurable using these modular units

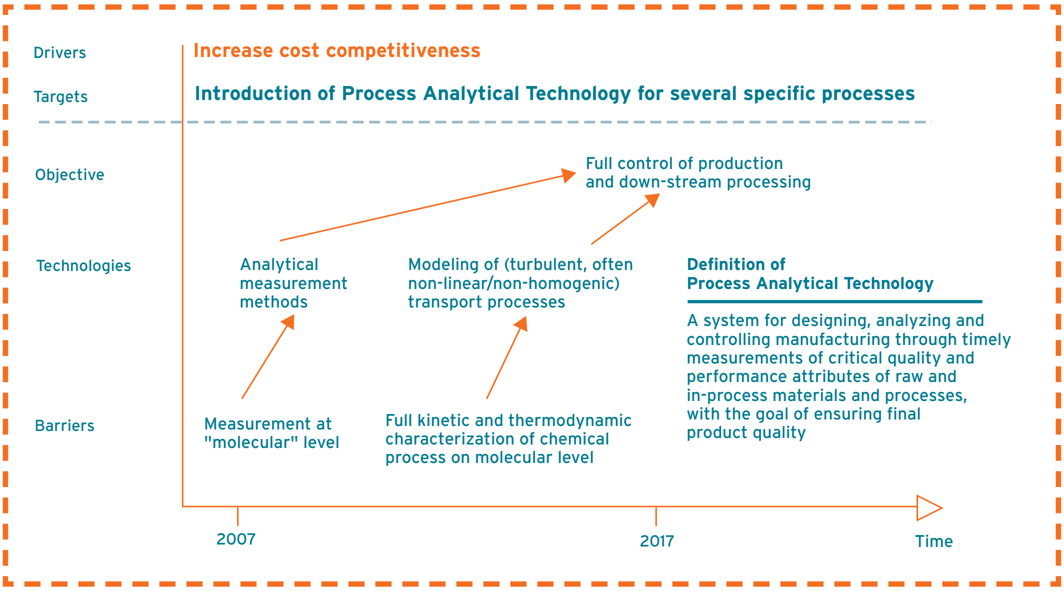
Barriers, required research, timing and actions

Barriers: Proof-of-concept validation on a lab scale is necessary for listed PI technologies
Research required: Fundamental
Time until implementation: 10-15 years

Barriers: Switch from batch to continuous production
Research required: Applied
Time until implementation: 5 years

Barriers: Up-scaling and piloting
Research required: Applied
Time until implementation: 5 years

PROCESS ANALYSIS TECHNOLOGY
ENABLING ROADMAP



A system for designing, analyzing and controlling manufacturing through timely measurements of critical quality and performance attributes of raw and in-process materials and processes, with the goal of ensuring final product quality

Description of the current process

State of the art

- Measurement technology
  - Methods for in situ measurement of reactions are not readily available. The most common methods are able to measure bulk compositions at some equilibrium point. Development of in situ measurement technology is necessary
- Modeling
  - Detailed models of flow and chemical reaction exist. These models need to be more robust and much faster
  - Proper identification of reaction schemes is cumbersome and must be improved
  - Quick introduction of detailed reaction schemes in models is possible, but must be further developed to increase calculation speed and robustness
- Process knowledge is insufficient

Needs

Higher selectivity and control of process leads to higher raw materials yield, which results in higher cost competitiveness

Main technological limitations/bottlenecks:

Kinetic and thermodynamic characteristics of chemical processes are insufficiently understood at the molecular level

Barriers, required research, timing and actions

Barriers: Fundamental process knowledge
Research required: Fundamental
Time until implementation: 5-10 years

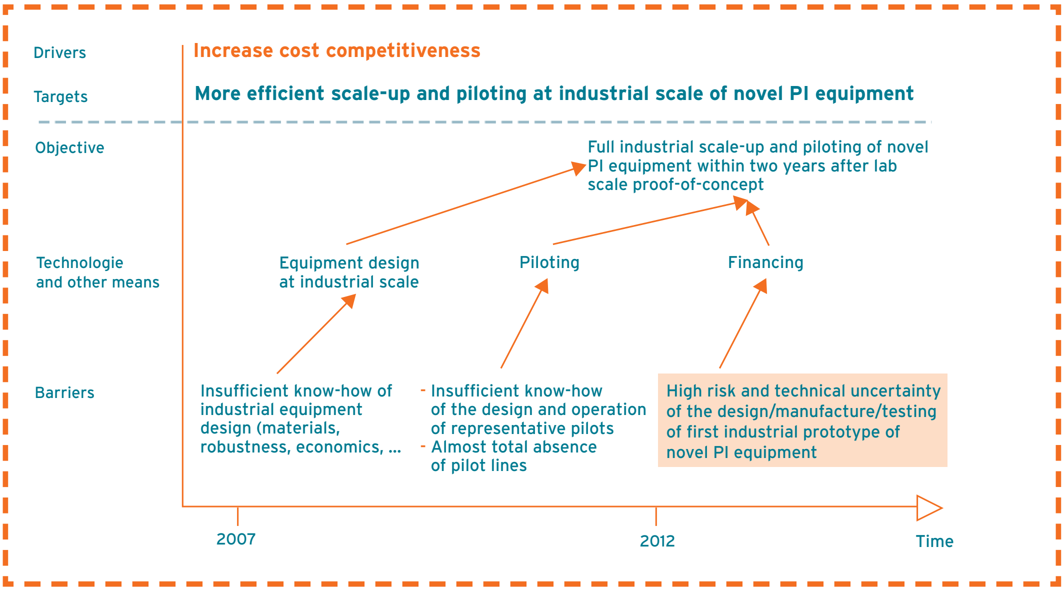
Barriers: Adequate diagnostic analytical methods to measure kinetic and thermodynamic reactions at the molecular level
Research required: Fundamental
Time until implementation: 5 years

Barriers: Non-linear numerical models and model reduction technology to derive fast models from detailed models
Research required: Applied
Time until implementation: 2-3 years, per specific process application

General barriers

- Measurement at the molecular level
- Development of representative (non-linear) numerical models
- Very divergent chemistry

MANUFACTURING TECHNOLOGY
ENABLING ROADMAP



Description of the current process

Needs

Up-scaling and testing at industrial scale of novel PI equipment

Main technological limitations/bottlenecks:

- Systems engineering (e.g. uniform design of industrial chemical equipment/ process systems) is only available for proven technology (the typical providers are engineering consultants). There is insufficient know-how for the up-scaling of novel equipment (e.g. technologies, materials, analysis of production economics, etc.). This skill is only available among the larger equipment providers such as Siemens and Sulzer GTI's could be a logical focal point for this knowledge, but they have insufficient opportunities to develop the skill at the moment
- Insufficient practical experience in the development of efficient, representative piloting programs (e.g. efficient design and operation of pilot lines, translation of pilot program resulting in reliable forecasting of full-scale production)
- Pilot facilities are almost completely absent, therefore testing is dependant on infrequent piloting possibilities on industrial production lines
- Financing of the design, manufacture and testing of a first industrial equipment prototype is very difficult due to high risk and technical uncertainty
- Insufficient integration of the manufacturing knowledge and process knowledge. This leads to process designs that are too expensive to manufacture. Integration in the chain from product development through process development to equipment manufacturing is essential

Actions, required research, timing and actions

Action: Develop know-how for the design of full-scale PI equipment and integrate this with the applied research for production lines
Research required: Applied
Time until implementation: 4 years

Action: Develop know-how for the planning and execution of efficient and representative pilot programs for applied research
Research required: Applied
Time until implementation: 5 years

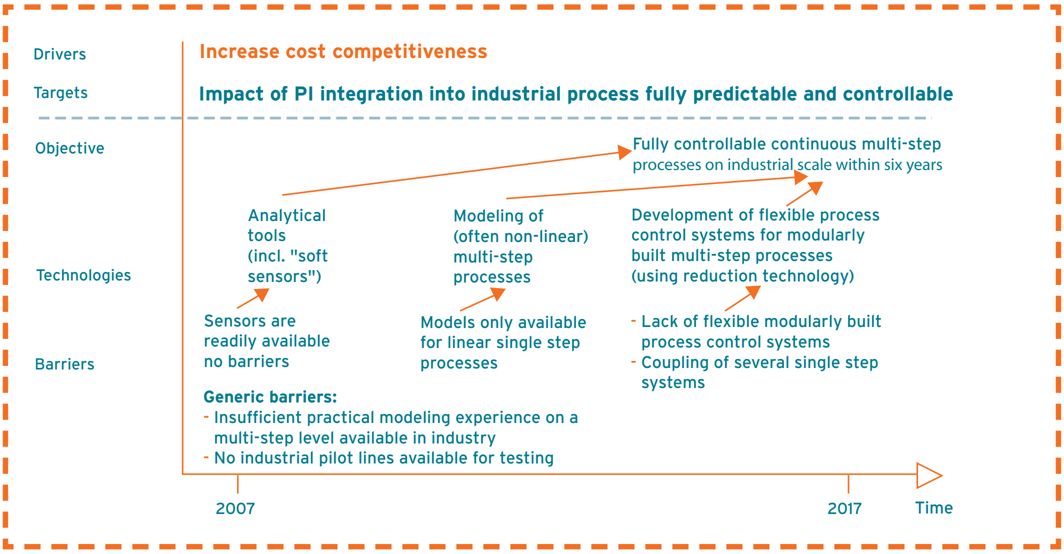
Action: Make pilot facility (e.g. building, utilities, PLC systems, line operators, etc.) available for a consortium of FINECHEM companies, equipment suppliers and knowledge infrastructure partners
Research required: Investment and applied
Time until implementation: 1-2 years

Action: Work on standardization of PI process equipment, defining the proper interfaces between units
Research required: Applied
Time until implementation: 3 years

Action: Build an engineering tool kit that assists with selecting the proper materials, proper geometries and the right manufacturing technology for a given process. This may take the form of an expert system and engineering principles or guidelines
Research required: Applied
Time until implementation: 4 years (in close coordination with the pilot facility)

Action: Build a consortium between several FINECHEM companies and one equipment supplier to finance the design, manufacturing and piloting of PI technology for industrial equipment prototypes
Research required: Financing
Time until implementation: 3 years

PROCESS CONTROL
ENABLING ROADMAP



Description of the current process

State of the art

- Necessary sensor technology is readily available
- Numerical models for modeling are available when using reduction technology. However, models are only available for linear, single-step processes, not for coupling of several single-step systems. There is also a lack of flexible process control systems
- Translation from numerical model to process control system has already been completed by TNO
- Fully operational, flexible modularly build systems for multi-step process control are not available yet

Needs

Higher selectivity leads to higher raw materials yield, which results in higher cost competitiveness

Main technological limitations/bottlenecks:

It is difficult to predict the impact of new PI module on process stability and product quality, e.g. continuous PI modules lead to buffers on interface with batch modules, which can have significant impact on process stability and product quality

Improvement potential

Fully controllable, continuous multi-step processes on an industrial scale, equipped with flexible modularly build systems, within six years

Barriers, required research, timing and actions

- Numerical process modeling: Not yet readily available for non-linear multi-step processes
    - Lack of flexible modularly build process control systems
    - Coupling of several single-step systems
- Process control: Non-linear optimization is not yet robust and generally applicable
- Generic barriers:
    - Practical modeling experience on a multi-step level is insufficient in the industry
    - No lines available to pilot

Action: Develop non-linear numerical models
Research required: Fundamental
Time until implementation: 5 years

Action: Develop non-linear optimization, suitable for model predictive control
Research required: Fundamental
Time until implementation: 5 years

Action: Make product development data available for process modeling
Research required: Applied
Time until implementation: 4 years

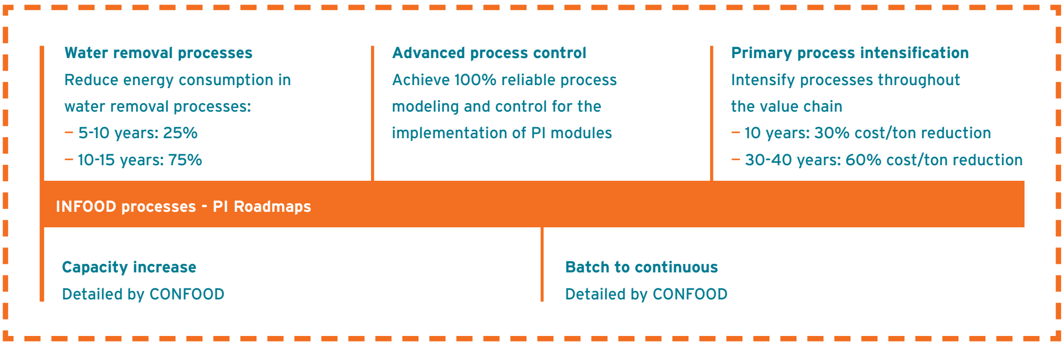
Action: Make model reduction technology applicable at a general level
Research required: Fundamental
Time until implementation: 5 years

Action: Develop and test process models and control systems on an industrial scale
Research required: Applied
Time until implementation: 4 years

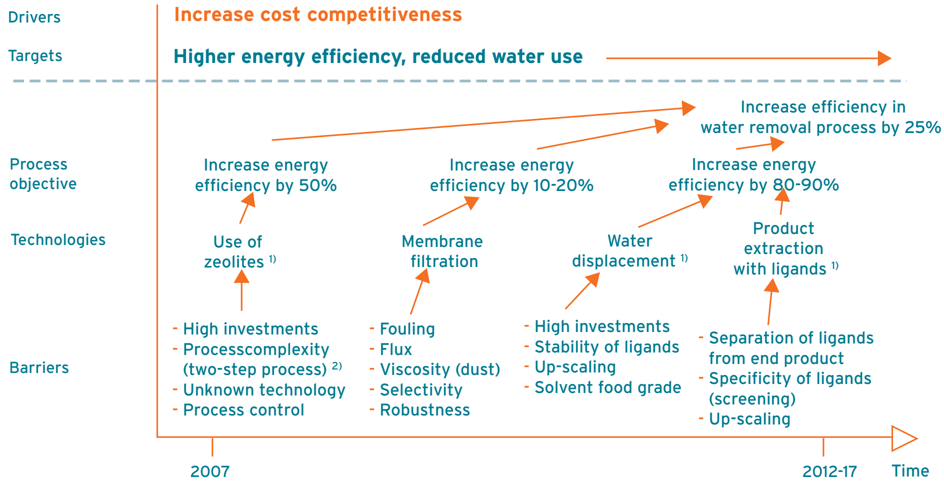
Action: Make facility available for the installation of pilot lines
Research required: Applied
Time until implementation: within 3 years

Action: Develop know-how for the development of representative pilot lines
Research required: Applied
Time until implementation: within 2 years

2.3 INFOOD ROADMAP

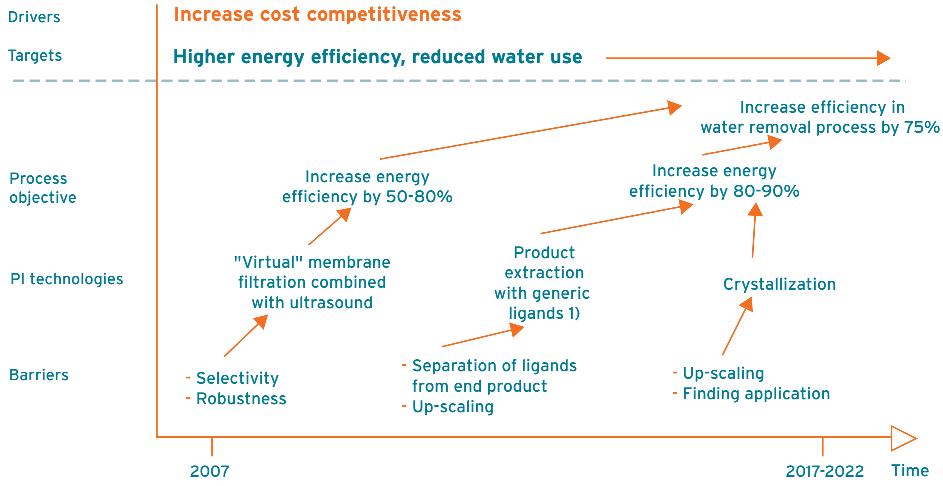


WATER REMOVAL PROCESS ROADMAP



1) Additional benefits are milder processes due to lower temperatures

2) First step is the use of zeolites, remaining water needs to be removed (e.g. by microwave technologies) in order to reach quality/purity requirements



1) Additional benefits are milder processes due to lower temperatures

Description of the current process

Selected process

Water removal processes in INFOOD's process

State of the art

Waterless processes throughout the value chain

Main technological limitations/bottlenecks:

Inefficient reaction due to heat (energy) and water use throughout the various steps in the water removal process in the value chain.

Improvement potential

	Within 5-10 years	Within 10-15 years
Increase in process energy efficiency	25%	75%

Reduction of water use by using other solvents or less water

Promising PI technologies

PI technologies	Energy efficiency potential	
	Within 5-10 years	Within 10-15 years
Membrane filtration	40%	
Filtration with "virtual" membranes/ultrasound		50-80%
Zeolites (in water removal when low temperatures are required(< 60oC))	50%	
Water displacement	80-90%	
Product extraction with specific ligands	80-90%	

Possible combinations

Not applicable

Barriers, required research, timing and actions

Membrane filtration

Barriers: Fouling, flux, viscosity (dust), selectivity and robustness; applied research
Time until implementation: 5-10 years

"Virtual" membrane filtration/ultrasound

Required research: Fundamental research
Time until implementation: > 15 years

Zeolites

Barriers: Complex process (two-step process: remaining water needs to be removed by e.g. microwave technologies in order to get quality/purity requirements), high investment costs and unknown technology; technology has been proven, pilots are available; combined research; additional benefit: milder processes due to lower temperatures (lower temperatures lead to better product quality)
Time until implementation: 5-10 years

Water displacement

Barriers: High investment costs, limited low-scale applications known in Germany and South Africa, up-scaling (current pilots achieve max. 3-4 liters) and solvent food grade (e.g. per-chloride as a solvent is not feasible)
Research required: Combined
Time until implementation: 5-10 years

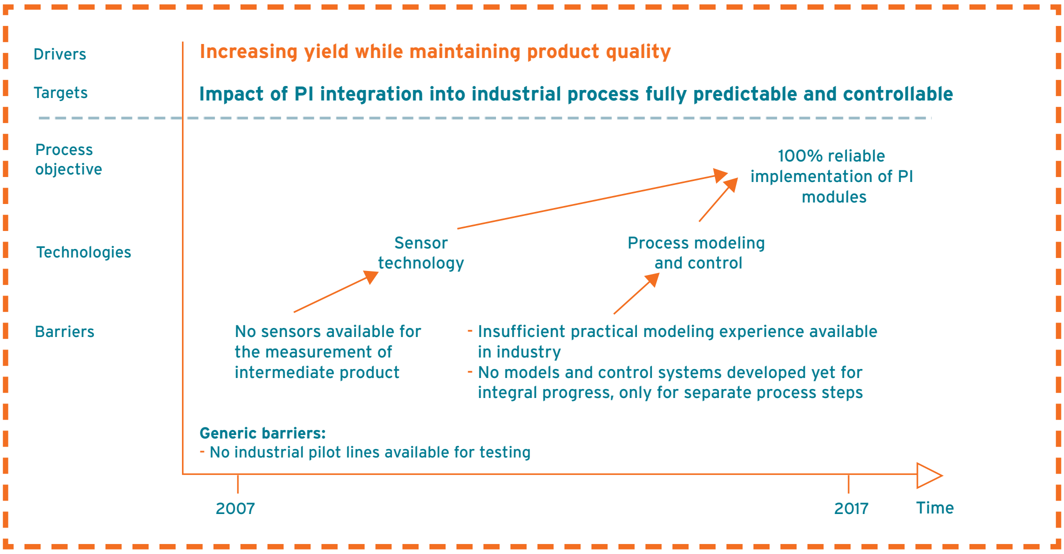
Product extraction with ligands

Barriers: Separation of ligands from end product, specificity of ligands and up-scaling the pilot processes; application: separate large volumes of proteins from fats/water
Research required: Fundamental
Time to implementation: 5-10 years (for generic ligands this will take 10-15 years)

Crystallization (at low temperatures)

Barriers: Up-scaling and finding application
Research required: Fundamental and applied

ADVANCED PROCESS CONTROL
ENABLING ROADMAP



Description of the current process

State of the art

- Necessary sensor technology: partly available, but new sensors are needed
- Numerical models for modeling: mostly available (6-sigma, Neural networks, etc.)
- Systems for process control: several software tools for off-, at- and in-line process control available

Needs

- Robust processing (100% control of process, fast adaptation to deviations)
- Constant quality (> 99% products in spec)
- Higher yield and capacity

Main technological limitations/bottlenecks:

- Many processes have large fluctuations and are not well in control, resulting in a decreased capacity for utilization (10-20%) and part of the end product falling outside of specifications (10-20%)
- Generally, there is a lack of knowledge about which parameters influence the process/product (yield, capacity, quality)
- Fluctuations in raw material (seasonal effect/ different suppliers)
- Each step of the process is optimized and controlled separately (i.e. no integral optimization of complete process and lack of knowledge of how deviations in previous steps influence the following step s)
- Lack of information whether intermediate product is within end specification

Barriers, required research, timing and actions

Sensors

Barriers: New sensors for extra in-line control (i.e. in-line measurement of intermediate products based upon taste or other “soft” criteria that are important for the end product)
Research required: Develop new sensors to check intermediate product on end specs

Numerical process modeling

Barriers: Industry awareness of the available state-of-the-art tools
Research required: Developed and tested on an industrial scale

Process control

Barriers: Lack of experience with available tools
Research required: Developed and tested on an industrial scale

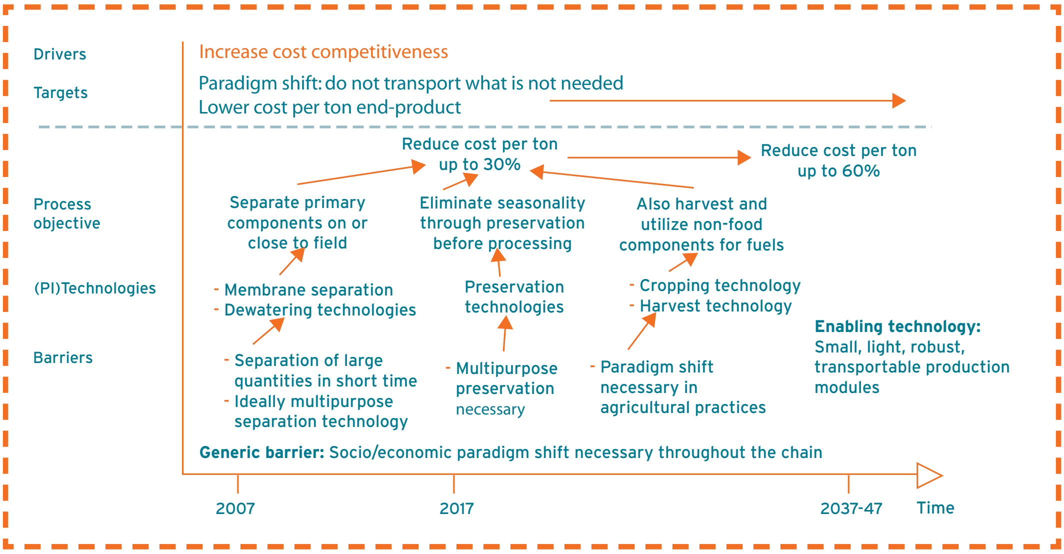
Process knowledge

Barriers: Lack of experience with the integral process (i.e. how do deviations effect next step)

General barriers

- Industrial pilot lines need to be available for testing

PRIMARY PROCESS INTENSIFICATION
GENERIC ROADMAP



Description of the current process

Needs

Lower cost per ton through:

- Higher yield per ha land
- Higher dry solids yield per ton
- Lower transportation costs
- Heat integration in small CHP units

Main technological limitations/bottlenecks:

- Reduce transportation costs through separation of intermediate product streams, remaining soil (e.g. minerals and organic matter) and water during the beginning stages of the process
- Remove water during harvest with light equipment
- Eliminate seasonal impact on capacity utilization through separation and preservation during the beginning stages of the process
- Utilize non-food crops as feedstock for biofuels that will replace fossil fuels – Utilization of multi crop input technology to valorize all crop components
- Use of low-value components for biogas generation for small scale CHP with heat integration

Improvement potential

	Within 10 years	Within 30-40 years
Costs/ton product reduction	30%	60%

Promising PI technologies

PI technologies	Energy efficiency potential	
	Within 10 years	Within 30-40 years
Membrane filtration		
Other dewatering technologies		
Separation technologies for specific crops		

Enabling technology

Small, light and robust transportable production modules, which can separate at the farmers' location without damaging the soil

General barriers

- Social/economical paradigm shift necessary in agro food chain – Social/economical study of entire agro food chain, with development of optimal transition path

2.4 CONFOOD ROADMAP

Preservation process
– 2020: Increase energy efficiency by 10-15%
– 2050: Increase energy efficiency by 30-40%

Increased capacity of food production equipment
– 2050: 20% capacity increase and 60% energy reduction in food processing

Making batch processes continuous
– 2050: 20% capacity increase and 30% energy reduction in food processing

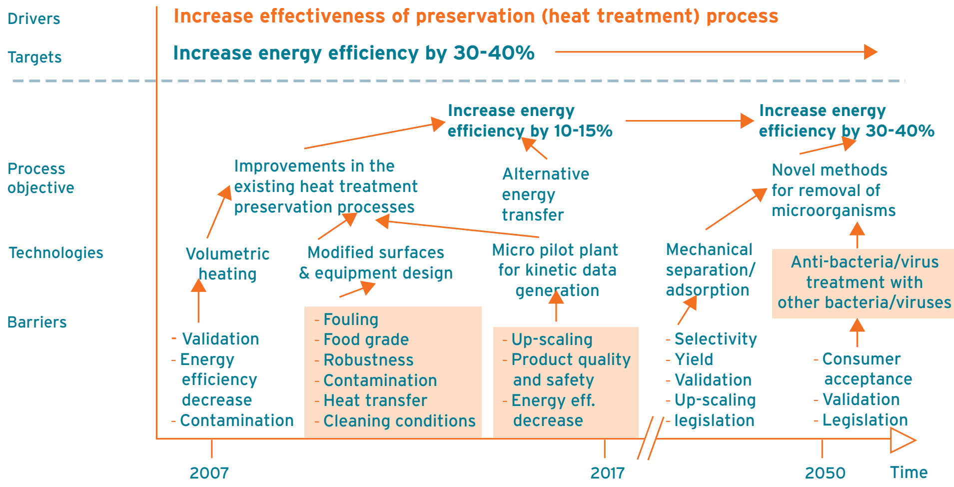
INFOOD processes - PI Roadmaps

Emulsions and dispersions
– 2050: 5% energy efficiency increase

High throughput product/process development
– Technology enabler

Water removal process
– Detailed by INFOOD

PRESERVATION ROADMAP



Split stream processing will enable all improvement potential mentioned to be more selective and efficient
High throughput process & product development will enable fast and more efficient sustainable processes to be developed

Description of the current process

Selected process

Food preservation process in CONFOOD

State of the art

Novel methods for removal of microorganisms

Needs

- Milder techniques requiring less energy and leading to better product quality
- More selective treatment of ingredients
- More effective removal of micro traces
- Increased flexibility in processing (e.g. less cleaning after batch run)

Main technological limitations/bottlenecks:
Energy efficiency decrease, processing of part streams and economic reasons (business case)

Improvement potential

	Within 10 years	Within 30-40 years
Increase in process energy efficiency	10-15%	30-40%

SHORT/MID TERM

Promising PI technologies

PI technologies	Energy efficiency potential	
	Within 30-40 years	
Volumetric heating to reduce product contact with	10%	Better yields
Improve equipment surface	20%	
Alternative energy transfer (e.g. ultrasound, UV light, radio frequency and pulse electric fields)	15-30%	
Improve module design (e.g. in membranes processes)	20%	

Possible combinations

Split-stream processing will enable the noted improvement potential to be more selective and efficient

Barriers, required research, timing and actions

Volumetric heating to reduce product contact with equipment

Barriers: Validation (e.g. homogeneous treatment and treatment time), decrease in energy efficiency and contamination
Research required: Applied (already commercially available)
Time until implementation: 5 years

Improve equipment surface

Barriers: Fouling, food grade (e.g. no corrosion), robustness (e.g. removal of all bacterial traces), contamination (lotus effects, e.g. glassy carbon) and heat transfer, including various expansion coefficients and sealing
Research required: Fundamental (mainly developing new surface materials)
Time until implementation: 10 years

Alternative energy transfer (e.g. ultrasound, UV light, radio frequency and pulse from electric fields)

Barriers: Upscaling (depth of penetration and throughput time, which is currently 2m every 3 hours), product quality and decreases in energy efficiency
Research required: Applied
Time until implementation: 5-10 years

LONG TERM

Promising PI technologies

PI technologies	**Energy efficiency potential**	
	Within 30-40 years	
Mechanical separation/adsorption	50%	Including indirect energy savings through e.g. less cooling and easier transportation
Anti-bacteria/virus treatment with other bacteria/ viruses (e.g. pro-biotic and lactic acid treatments)	70%	

Possible combinations

Split-stream processing (enabling targeted processing) will enable all improvement potential mentioned to be more selective and efficient

- Ohmic heating and micro reactors (split-stream processing)
- Heating and ultrasound

Barriers, required research, timing and actions

Mechanical separation/adsorption

Barriers: Selectivity, yield, validation, Up-scaling and legislation (long negotiation processes with food authorities)

Research required: Fundamental

Time until implementation: > 15 years (approval of new technology alone requires 3-5 years)

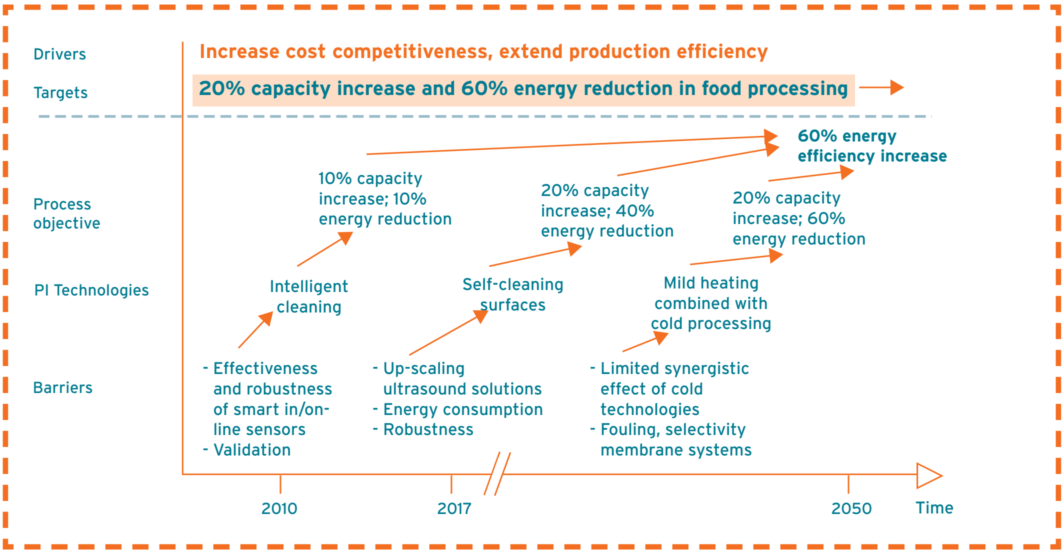
Anti-bacteria/virus treatment with other bacteria/viruses

Barriers: Consumer acceptance (marketing issues), validation and legislation (long negotiation processes with food authorities)

Research required: Fundamental

Time until implementation: > 15 years (approval of new technology alone requires 3-5 years)

INCREASED CAPACITY OF FOOD PRODUCTION EQUIPMENT ROADMAP



Description of the current process

Selected process

Increased capacity of food production equipment in CONFOOD

State of the art

In/on-line fouling and cleaning control and optimization

Needs

Reduce bio-fouling of food processing equipment and increased cleaning efficiency

Main technological limitations/bottlenecks:

- Product losses
- Product contamination by micro-organisms released from bio-film
- Toxin formation
- Reduced heat transfer

Improvement potential

	Within 10 years	
Increase in process energy efficiency	60%	
Capacity increase	20%	

Promising PI technologies

PI technologies	Energy efficiency potential	
	Within 30-40 years	
Self-cleaning surfaces (by pulsed ultrasound)		
Mild heating combined with emerging cold processing technologies (i.e. high pressure, pulsed electric fields and membrane separation)		
Intelligent cleaning (clean-on-demand with smart sensors and self-learning software)		

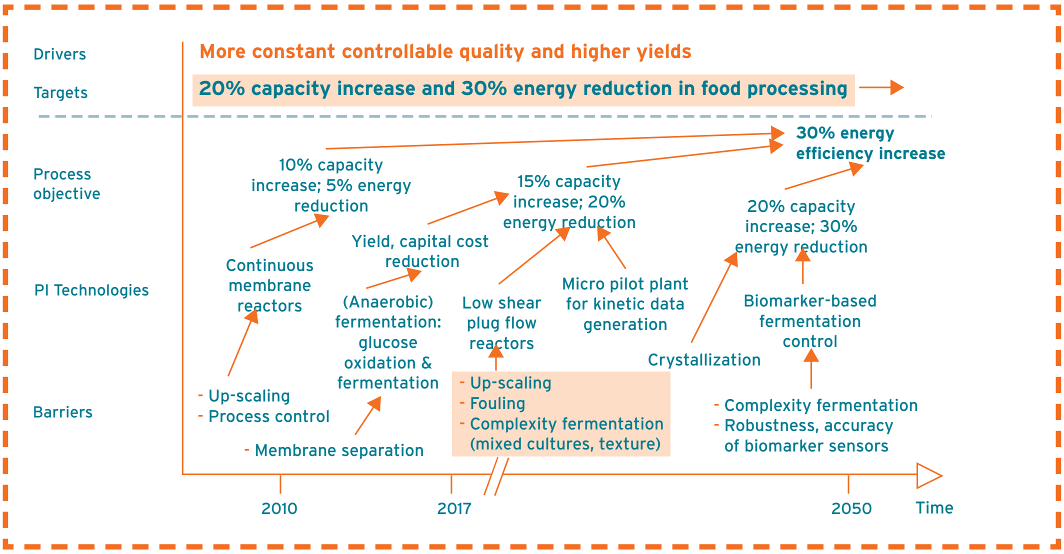
Possible combinations

All PI technologies can be combined

General barriers

- Up-scaling ultrasound solutions and energy consumption
- Limited synergistic effect of cold processing technologies
- Effectiveness of membrane systems: fouling and selectivity (> 99,9999%)
- Effectiveness and robustness of smart sensors
- Validation of cleaning

MAKING BATCH PROCESSES CONTINUOUS ROADMAP



Description of the current process

Selected process

Continuous fermentation/crystallization of food products in CONFOOD

State of the art

Reactor technology (design, membrane)

Needs

Constant quality of fermented products, more effective heating/cooling and mixing, higher yields, higher capacity and simultaneous oxidation and fermentation (membrane reactors)

Main technological limitations/bottlenecks:

- Control of product properties
- Less efficient heat and mass transfer of nutrients
- High volumes
- Limited flexibility
- Diversity in raw materials
- Aseptic product separation

Improvement potential

	Within 10 years	
Increase in process energy efficiency	30%	
Capacity increase	20%	

Promising PI technologies

PI technologies		
Continuous membrane reactors (e.g. continuous removal of growth limiting fermentation products)		
Model-based control of fermentation using advanced sensors (e.g. biomarkers based on DNA technologies)		
Plug-flow reactors with low shear rates to process structured fermented products		
Crystallizers		

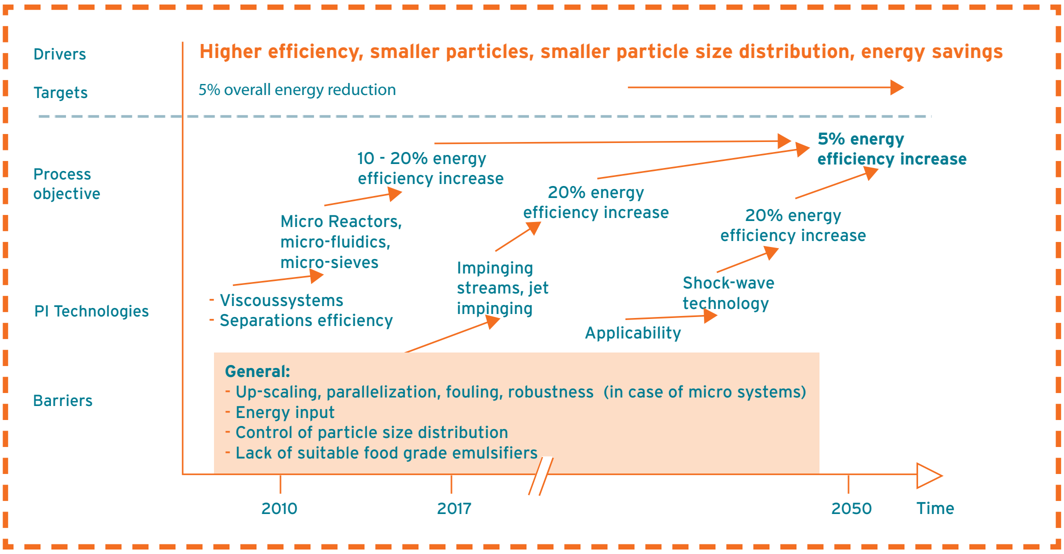
Possible combinations

All PI technologies can be combined

General barriers

- Complexity of fermentation (aerobic/anaerobic, mixed cultures and texture formation)
- Robustness and accuracy of biomarker sensors
- Up-scaling

EMULSIONS AND DISPERSIONS PRODUCTION ROADMAP



Description of the current process

Selected process

Production of emulsions and dispersions in CONFOOD

State of the art

Use of homogenizers, rotor-stator mixers and high shear mixers

Needs

Higher efficiency, smaller particles, smaller particle size distribution and energy saving

Main technological limitations/bottlenecks:

- Limited control of particle size distribution
- High power input
- Construction/investment to create high homogenization pressure (> 1000 bar)
- Suitability for high viscous materials and materials with solid particles

Improvement potential

	Within 10 years	
Increase in process energy efficiency	5%	

Promising PI technologies

PI technologies		
Micro-reactors, micro-fluidics and micro-sieves		
Impinging streams and jet impinging		
Shock-wave technology		

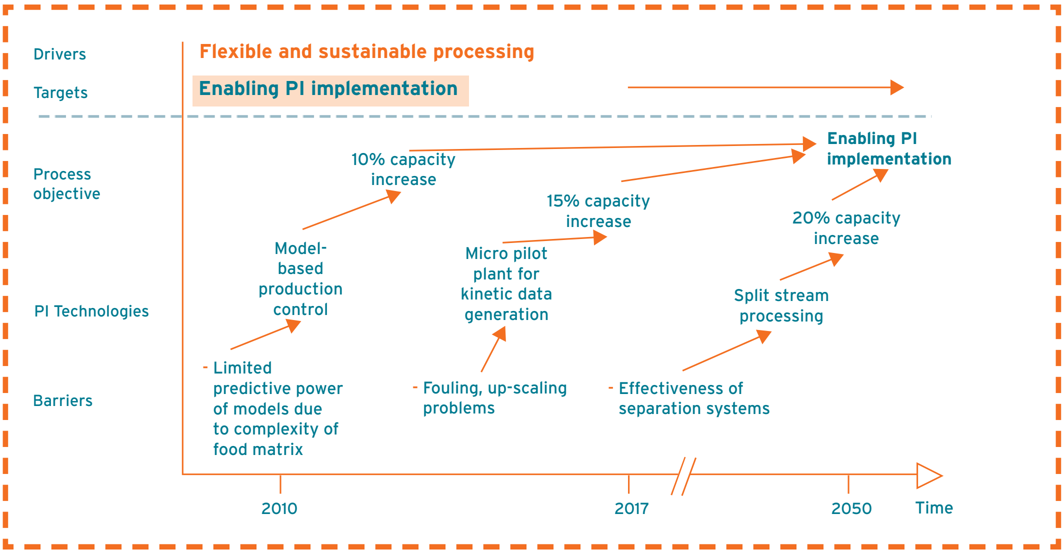
Possible combinations

Combinations with ultra-sound

General barriers

- Up-scaling, parallelization, fouling and robustness (in case of Microsystems)
- Energy input
- Control of particle size distribution
- Lack of suitable food grade emulsifiers

HIGH THROUGHPUT PRODUCT/PROCESS DEVELOPMENT ROADMAP



Description of the current process

Selected process

Multifunctional, self-developing production lines in CONFOOD

Needs

Flexible process configuration for many different products, up-scaling that is accurate from the start, no product loss due to off-spec and sustainable design

Main technological limitations/bottlenecks:

- Equipment design focused on one product category
- Variation raw materials
- Limited knowledge on process-product interactions
- Time-consuming experiments needed for new product formula

Improvement potential

	Within 10 years	
Capacity increase (less product loss)	20%	

Promising PI technologies

PI technologies		
Model-based control of production lines leading to co-current process product development that is		
Micro-pilot plant for high throughput determination of kinetic product data		
Split-stream processing (e.g. recombination of half-products just before packaging)		

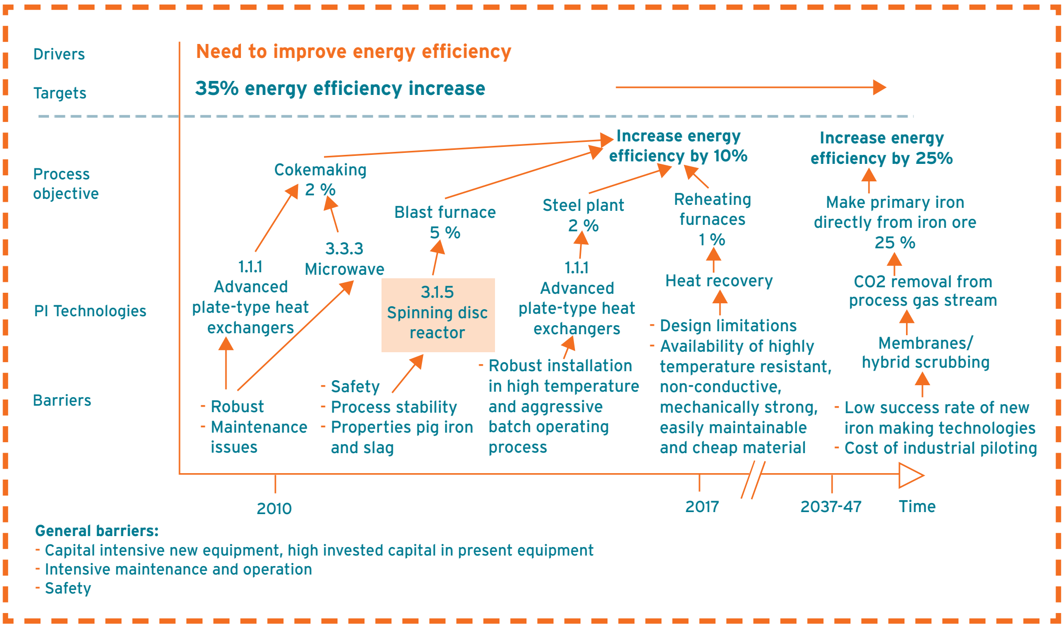
Possible combinations

Model-based control of production lines leading to co-current process product development that is based on product specs (input) and predictive models and micro-pilot plant for high throughput determination of kinetic product data

General barriers

- Fouling and up-scaling problems with the micro-pilot plant
- Predictive power of models due to complexity of food matrix
- Effectiveness of separation (membrane) systems for split-stream processing

2.5 STEEL PRODUCTION ROADMAP



General barriers:
- Capital intensive new equipment, high invested capital in present equipment
- Intensive maintenance and operation
- Safety

Description of the current process

Selected process

Coke making – short term

Needs

- Controlled coal moisture control before coke making
- Waste heat recovery from coke
- Waste heat recovery from coke oven gas

Improvement potential

	Within 10 years	Within 30-40 years
Increase in process energy efficiency	2%	

Promising PI technologies

PI technologies		
Advanced heat exchanger		
Microwave technology		

Barriers, required research, timing and actions

Barriers: Capital intensive technology (need 2); intensive maintenance and operation (need 3); and heat exchangers suitable for dirty (and potentially corrosive) gas

Research required: Applied

Time until implementation: 5 years

Description of the current process

Selected process

Blast furnace – short term

Needs

- Reduction coke consumption per ton pig iron
- Enhanced heat recovery

Main technological limitations/bottlenecks:

With current installations and processes the limits of coke consumption reduction seems to be reached

Improvement potential

	Within 10 years	Within 30-40 years
Increase in process energy efficiency	5%	

Promising PI technologies

PI technologies		
Spinning disk reactor		

Barriers, required research, timing and actions

Barriers: Safety issues; Blast furnace process stability; Required properties of pig iron and slag (need 2); Capital intensive technology; and Intensive maintenance and operation

Research required: Fundamental and applied

Time until implementation: 5 years

Description of the current process

Selected process

Reheating furnaces – short term

Needs

- Heat and slab resistant slab support
- Heat recovery from support cooling
- Integration (direct hot connection with caster can bypass reheating furnace)

Main technological limitations/bottlenecks:

Develop material with above mentioned properties

Improvement potential

	Within 10 years	Within 30-40 years
Increase in process energy efficiency	2%	

Promising PI technologies

PI technologies		
Spinning disk reactor		

Barriers, required research, timing and actions

Barriers: Design limitations; highly temperature resistant, non-conductive, mechanically strong, easily maintainable and cheap material is not available; and logistics of different qualities combined with need to follow rolling program (need 3)

Research required: Fundamental and applied

Time until implementation: 5 years

Description of the current process

Selected process

primary iron making from iron ores – long term

Needs

A new iron making process using raw materials directly as mined, avoiding the ore agglomeration and coking stages. The waste gasses from this process should allow capture and storage of CO_2 (preferably "capture ready" off gas). It should be possible to use renewable carbon as fuel and reductant

Main technological limitations/bottlenecks:

Capture and storage of CO_2

Improvement potential

PI technologies		
Reduction of CO_2 emissions and primary energy usage		25% energy efficiency
Use of low cost raw materials, non coking coals and lower grade iron ores.		
The process must "fit" with existing steelmaking facilities.		
Low operating and capital costs.		
Low environmental impact (emissions, dust, noise, skyline)		

Promising PI technologies

PI technologies		
CO_2 removal from process gas stream		
Hybrid membrane/scrubbing CO_2 removal		

Barriers, required research, timing and actions

Barriers: High level of invested capital in present blast furnace route; high risk of development (low success rate of new iron making technologies); high costs of demonstrating new technologies on industrial scale (international cooperation required); and global competition (demanding cost competitive production)

Research required: Fundamental and applied

Time until implementation: 10 years