In the framework of
- Globalization of markets,
- Sustainability
- Environmental protection,
- Green Products "first on the market" with the "desired end-use property",
- ...
- chalenging demands for new sustainable processes and technologies

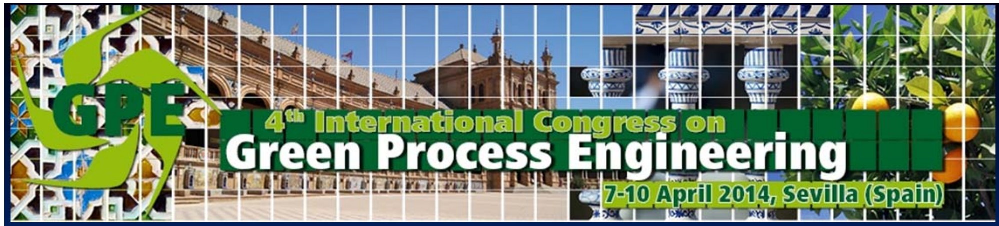
What kind of Modern "green" "sustainable" Chemical Engineering for the design of the "Factory of Future"

(How to transform molecules into money)
(Towards a plant in a shoe box or a banana container?)

Jean-Claude Charpentier

Laboratoire Réactions et Génie des Procédés CNRS/ENSIC
Université de Lorraine, Nancy, France.

jean-claude.charpentier@univ-lorraine.fr



A Strong message:

Green Chemistry needs process extension to Green Engineering to cover multiscale issues beyond molecular-scale reaction: purification, heat integration, Verbund, …to consider full-chain chemical manufacturing: "from cradle to the grave …"

Green Process Engineering (GPE) is more than Engineering Green Chemistry

The aim of Green Process Engineering is

to appropriately and successfully bring a green product to market and ensure that it is done in sustainable fashion

This requires **the multiscale length and time approach** of the **couple « green product/green process »** aiming and

targetting process intensification

As it was presented with the content of GPE4: Indeed

outline

- Some recalls on chemical engineering, its evolution and on process intensification

- The world of chemistry and related industries at the heart of a great number of scientific and technological challenges due to
    - the Rapid increase of knowledge in chemistry and biochemistry
    - the 21th century demands clearly focalized on societal exigencies
    - the non-sustainable mankind

- What are we waiting from chemical and process engineering and WHY?
(product with required end-use properties first on the market, sustainable clean product and process design,…)
The answer:

- The today chemical and process engineering approach:
    Did you say "The triplet molecular Process-Product-Processes Engineering (3PE)"

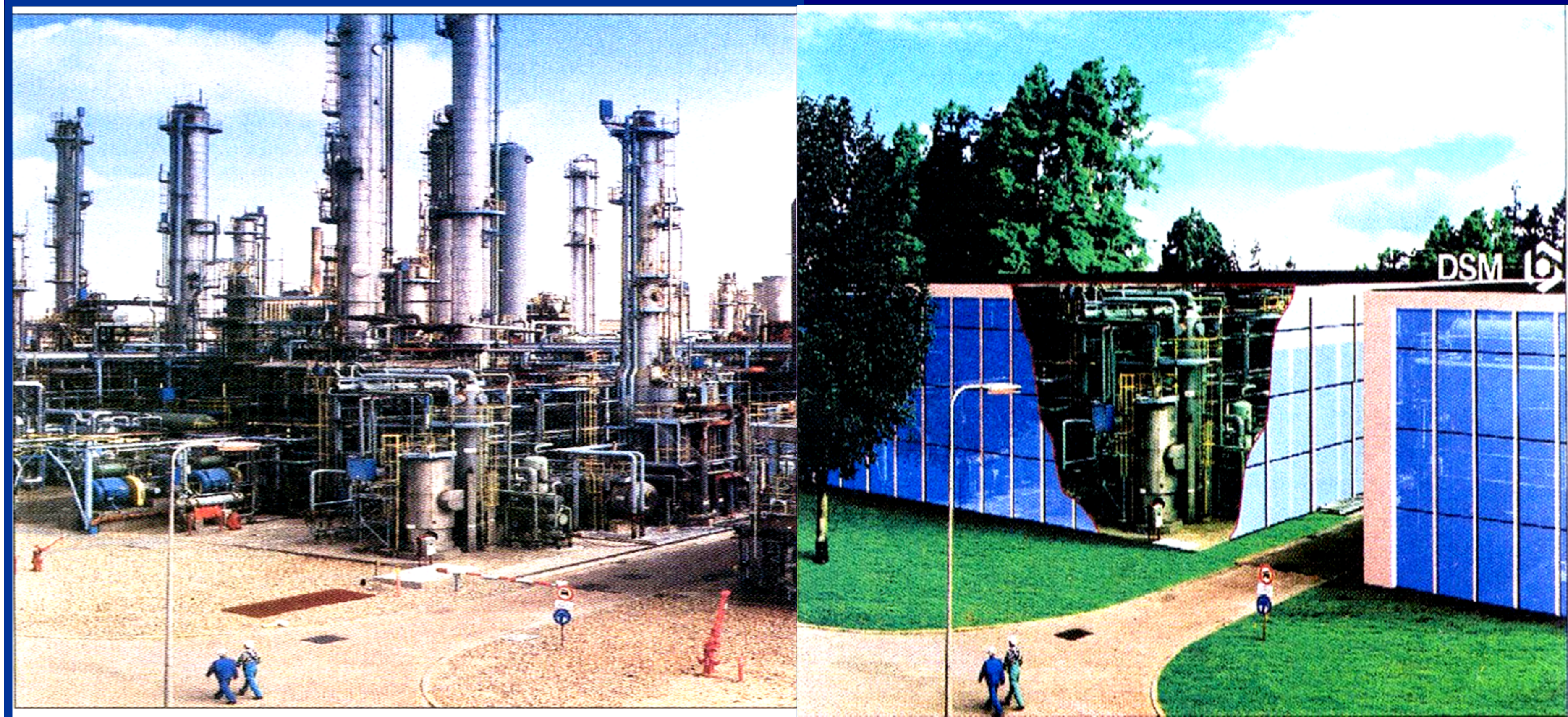
- Chemical Engineering: QUO VAMUS ?
    With the multidisciplinary and multiscale integrated approach for a necessary key-technology serving a great number of mankind needs,

i.e. (towards a green process engineering thanks to process intensification for the factory of future)
but how?

4 proposed tracks

One vision of how a future plant employing new sustainable green chemical engineering may look (right) vs. a conventional plant (left).

(Rendering courtesy of DSM)



OPERATING with NON POLLUTING and VERY EFFICIENT PROCESSES SUSTAINABLE involving PROCESS INTENSIFICATION for the production of products with required end-use properties

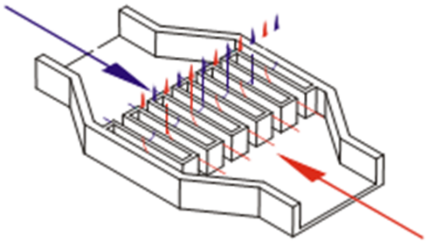
SAVINGS ABOUT 30 % (RAW MATERIALS + ENERGY + OPERATING COSTS)

4 proposed tracks

N.-T. Nguyen, Z. Wu, J. *Microm. Microeng.* **15** (2005) R1-R16
Hessel, V., Löwe, H., Schönfeld, F. *Chem. Eng. Sci.* **60** (2005) 2479 – 2501

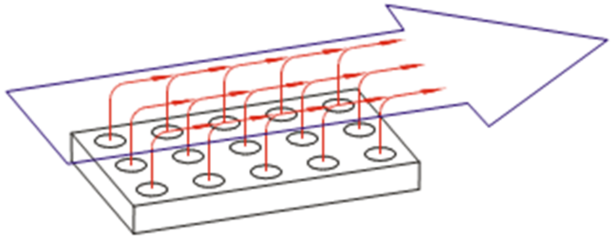
MIXING PRINCIPLES AND CORRESPONDING IMM MICROMIXERS

Lamination for hydro-dynamic or shear decay



Bas-relief induced recirculation flow

Injection in turbulent flow



Interdigital Micromixers

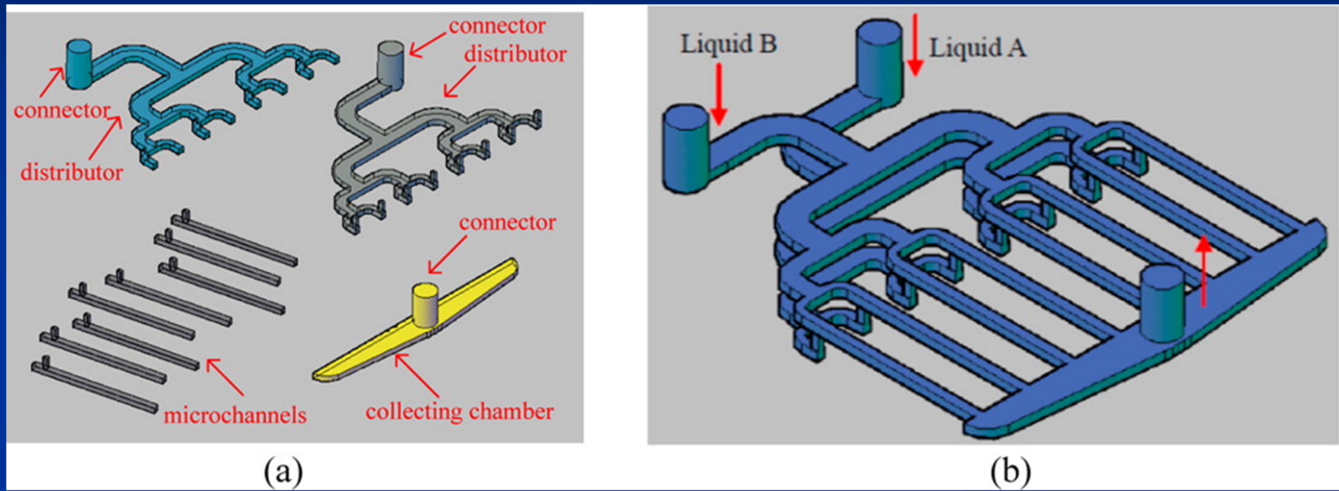
SIMM-V2
SSIMM
…

Caterpillar Micromixers

CPMM-R300-V1.2, CPMM-R600-V1.2
CPMM-R1200-V1.2, CPMM-R2400-V1.2
…

Star Laminator Micromixers

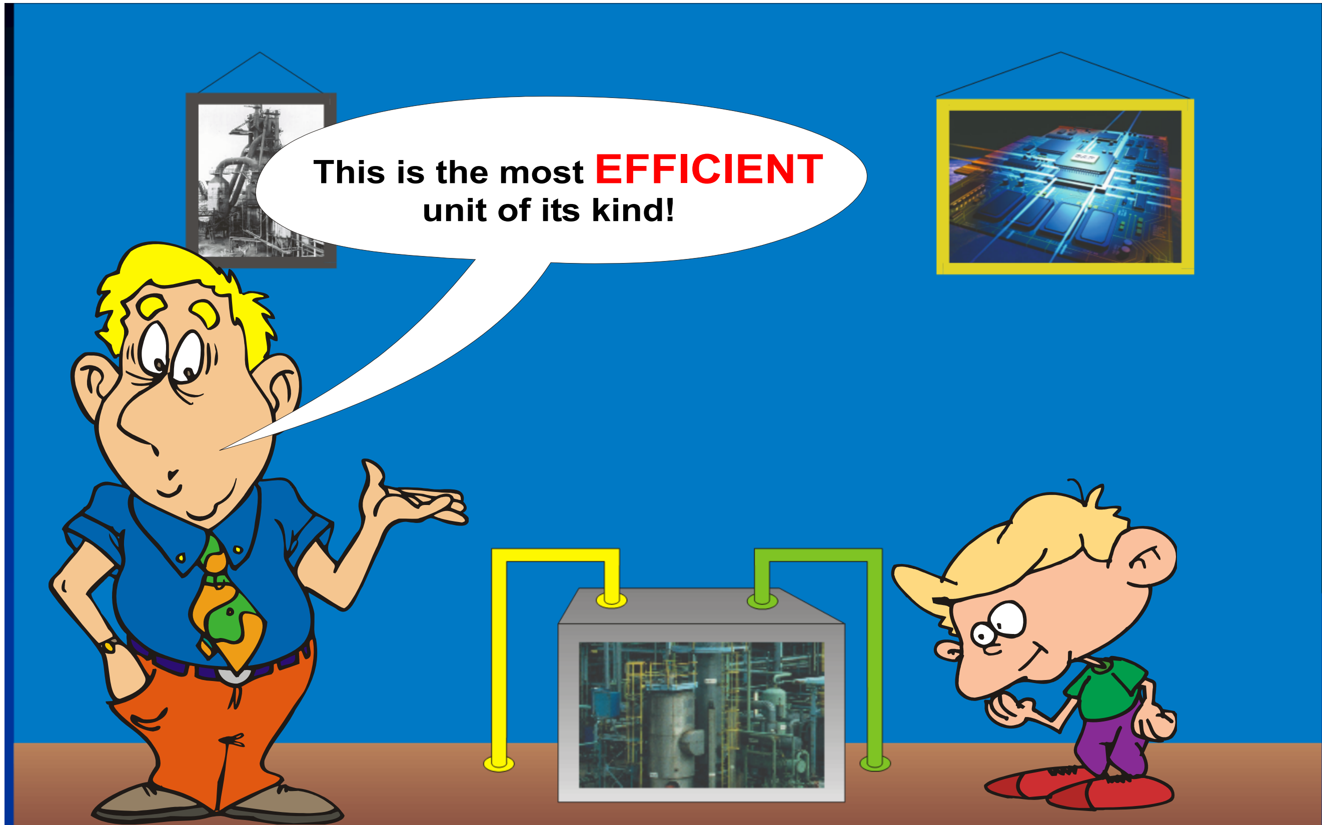
StarLam 15
…



Multichannel micromixer design: components (a), assembly (b).

Published in: Yuanhai Su; Anna Lautenschleger; Guangwen Chen; Eugeny Y. Kenig; *Ind. Eng. Chem. Res.* **2014,** 53, 390-401.

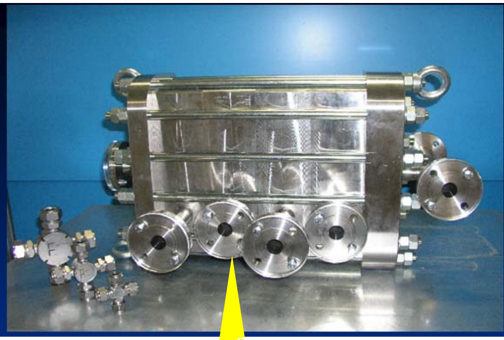
Copyright © 2013 American Chemical Society



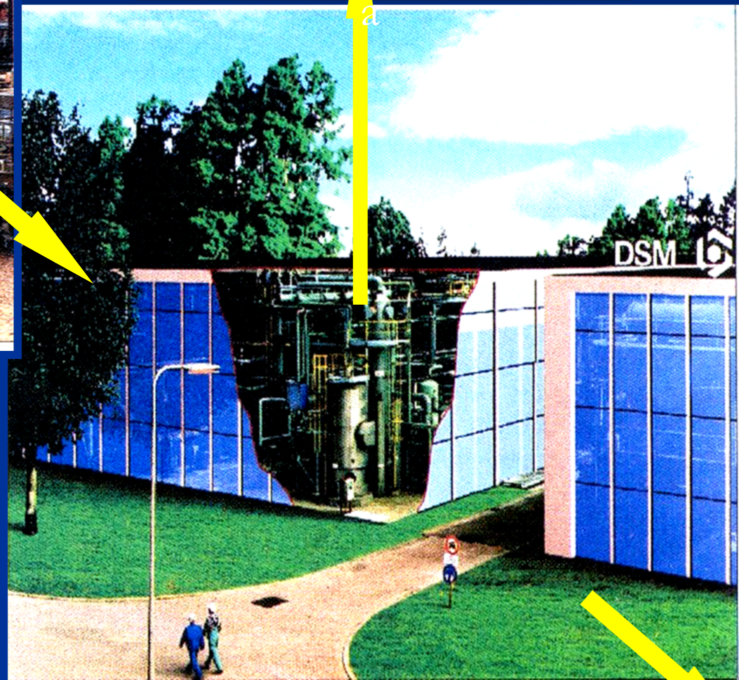
Process Intensification: towards a Plant in a Shoe Box or in Banana container?

WHY and HOW Process Intensification and Process Intensification Reactors?

The necessary Evolution of Chemical and Process Engineering



Modern Chemical Engineering involving process intensification for the Plant of Future



Sustainable Dévelopment
A plant in a
- Shoe box or
- Banana Container

4 Simultaneous tracks for the future of Green Process Engineering with a multiscale approach for the design of the factory of future

1-To increase productivity and selectivity through intelligent operations and multiscale control of processes: i.e. Molecular information engineering
Micro and-Nano and Micro tailoring of porous and cristalline Materials (nanotechnology) ← Green Process Engineering with multiscale approach

2- Design of novel equipment based on scientific principles and new modes of production: process intensification with multifunctional reactors or microstructured reactors (microfluidic) ← Green Process Engineering with multiscale approach

3- Manufacturing end-use properties: development of a multidisciplinary product-oriented engineering i.e. product design and engineering with special emphasis on solids technology and complex fluid processing ← Green Process Engineering with multiscale approach

4- Implement multiscale and multidisciplinary computational chemical engineering modeling and simulation to real-life situations: from the molecule scale up to the overall complex production scale.
Automation, control and safety , LCA ← Green Process Engineering with multiscale approach

Charpentier J. C., Oil & Gas Science and Technologies, 2013, 68, 952-964

outline

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The domain of chemical engineering consists of chemical, physical and biological transformations of starting materials to products

Raw Materials

Non Renewable:
- Petroleum
- Coal
- Ores
- Minerals

Renewable:
- Plants
- Animals

Chemical, Physical and Biological Transformations → **Pollution**

Products

Fuels
Materials
Plastics
Pharmaceuticals
Food
Feed
etc.

CHEMICAL ENGINEERING is the profession in which a knowledge of mathematics, chemistry and other natural sciences gained by study, experience and practice is applied with judgment to develop economic and environmentally acceptable ways of using materials and energy for the benefit of mankind.

S3

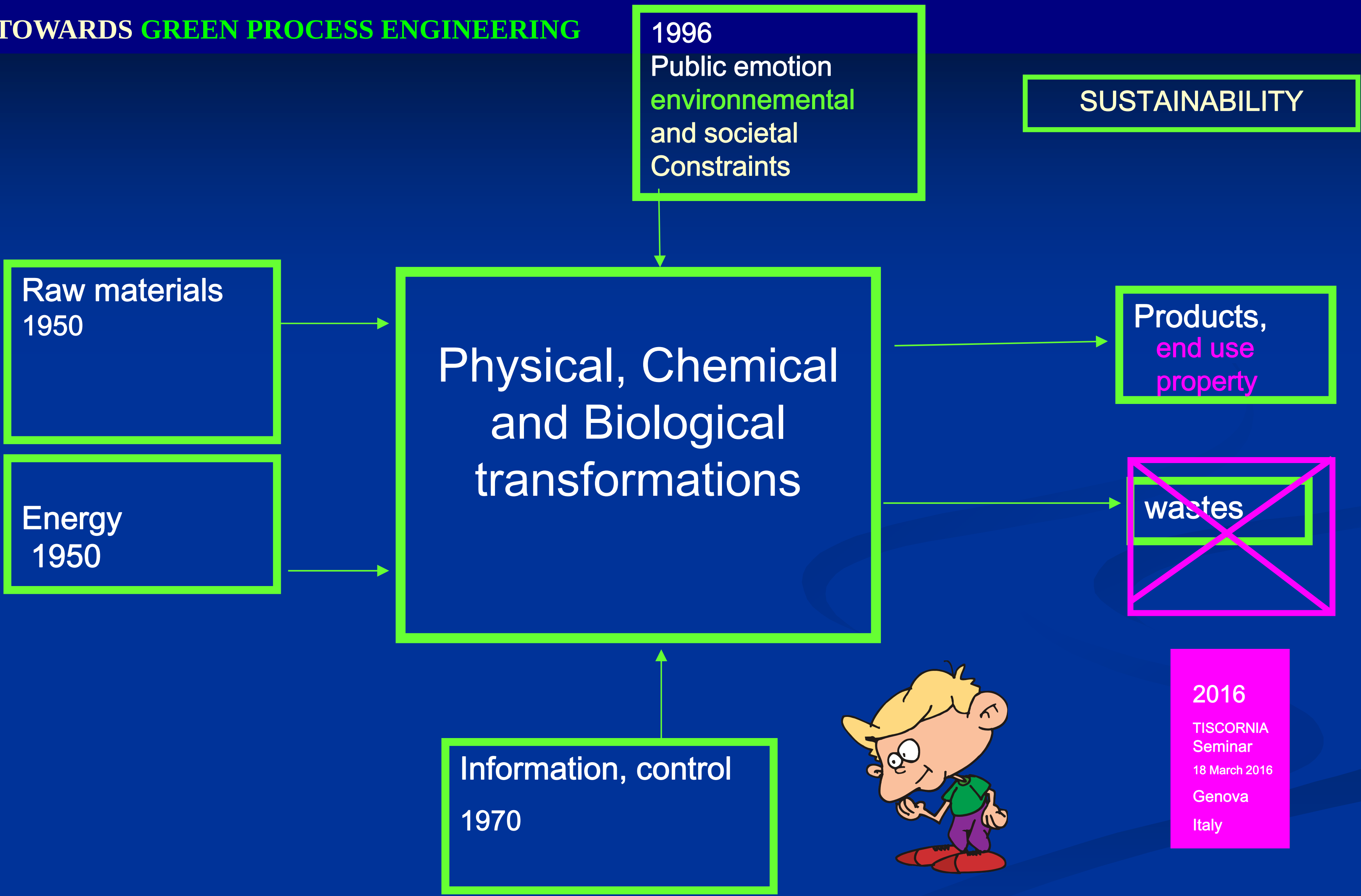
Chemical Engineering is a multidisciplinary Engineering Science which integrates the concepts of the following basic sciences:

-Thermodynamique chimique et biologique,
-Catalyse et cinétique chimique,
-Cinétique physique (transfert de chaleur, de masse et de quantité de mouvement),
-Mécanique des fluides et des milieux poreux et dispersés,
-Dynamique des systèmes,
-Optimisation, Simulation, Automatique, Contrôle, Sécurité
-Sciences économiques.

* Engineering Science : science under constraints with obligation of successìììì

EVOLUTION of CHEMICAL ENGINEERING SINCE LAST 66 YEARS

TOWARDS GREEN PROCESS ENGINEERING



REQUIRED END-USE PROPERTY of PRODUCTS

Shape
Color
Touch
Handling
Cohesion
Friability
Soft after hydratation

Aptitude to dissolution

Size
Rugosity
Taste, Succulence
Flavour
Aesthetics
Sensory properties
Drug-encapsulated controlled release
(Pico, nano, micro) mono disperse emulsion
Catalysts nano -µstructure
Powders (nano,micro…..) mechanic. acoustic properties
Green solvents, Ils..
……

Conditioned by
Mastering SOLIDS MORPHOLOGY, GRANULOMETRY POROSITY
(powder and divided solids technology)
or GAS and/or LIQUID DROP SIZES
(functionalized surface chemistry and technology)

This concerns products which are much more complex, in terms of molecular structure, than traditional industrial high-bulk-volume chemicals

Examples of Product Forms (Prof Ka M Ng, 2013)

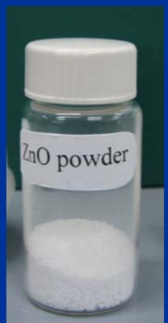
Transdermal patches

Creams

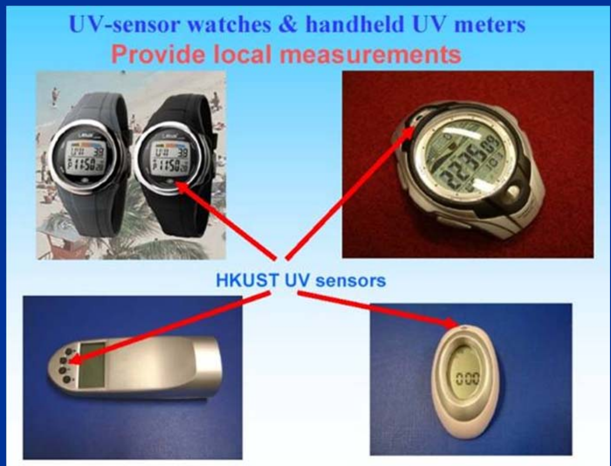
LCD Display

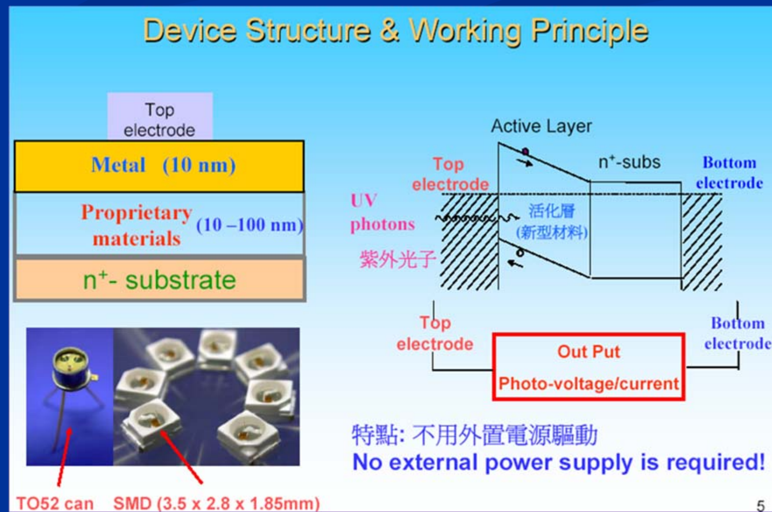
Granules/ Capsules

Powder/ Composite solids



UV Sensor

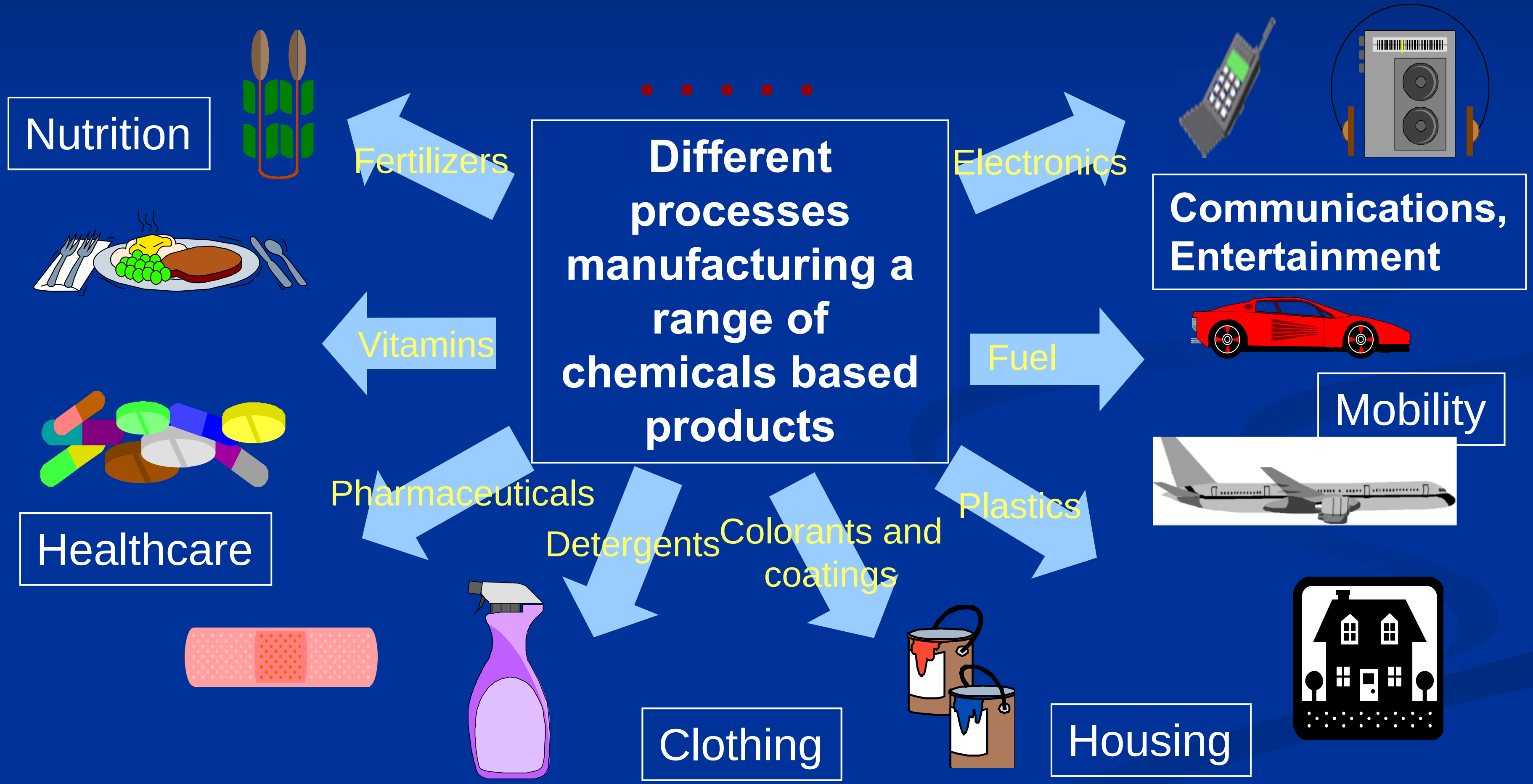




Contribution of Chemical Engineering

How to supply the many needs (products with required end-use property) of the modern society from a limited number of resources in the factory of future?

The answer: **Need of Process Intensification**



PROCESS INTENSIFICATION

refers to complex technologies that replace large, expensive energy intensive and polluting equipment or process with

- ones that combine multiple operations into a single apparatus (ex: reactive distillation) or into fewer devices,

- or ones that are smaller, less costly, less polluting, less energy requiring, safer, more efficient (i.e. microfluidic)

- or ones with new operating modes with neoteric solvents (supercritic fluids,ionic liquids) or with the application of external driving (energy alternative sources et forms)

i.e. **«Producing much more and better with much less»**

- producing more targetted products and better in smaller volumes, with a better efficiency and selectivity, in using less raw materials and energy, less solvents, with reduced transport costs,..and more secure
- More sustainable production with innovative technologies

SUSTAINABILITY related dimensions

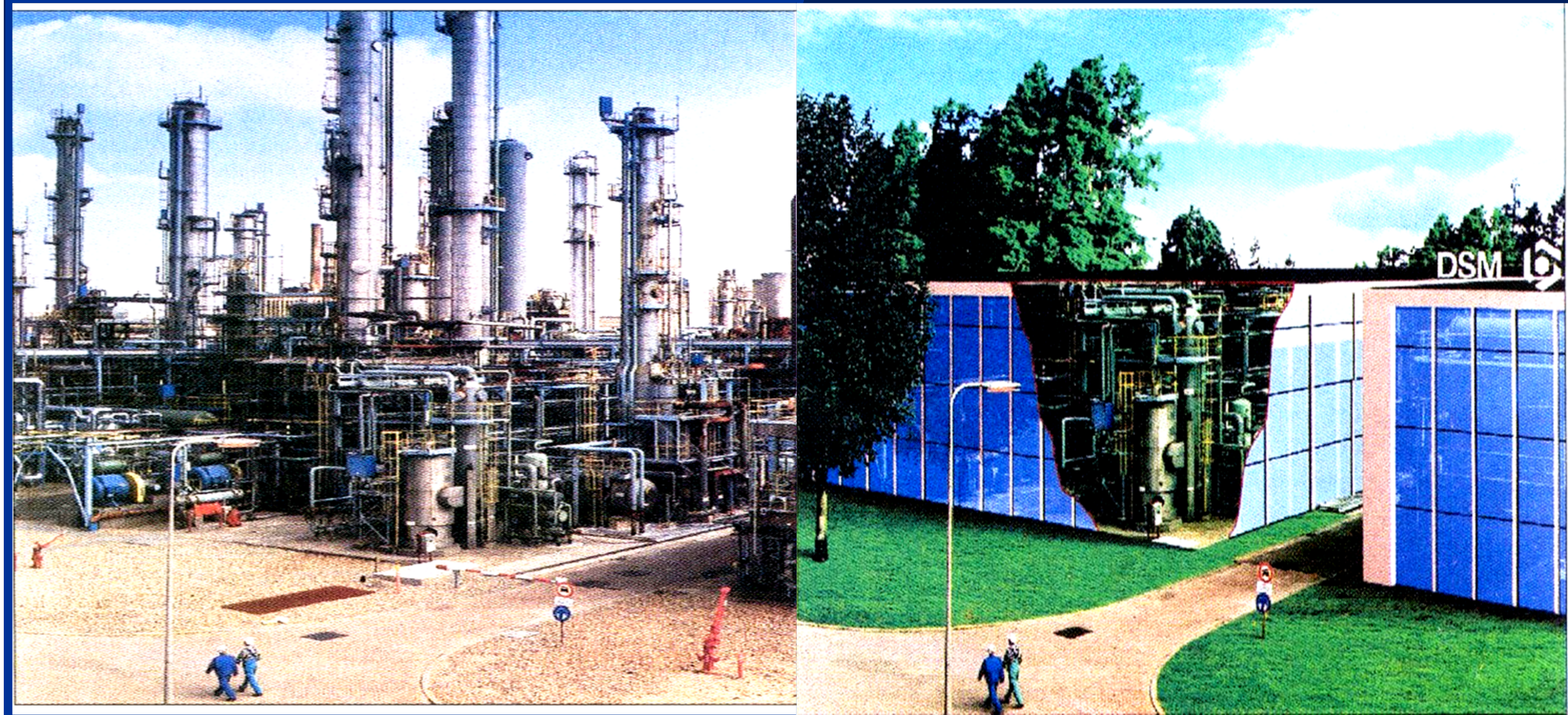
thus

Enhancing Corporate Image (in clean and efficient process design)

a future plant in a dream….

One vision of how a future plant employing Process Intensification may look (right) vs. a conventional plant (left).

(Rendering courtesy of DSM)



OPERATING with NON POLLUTING and VERY EFFICIENT PROCESSES SUSTAINABLE involving PROCESS INTENSIFICATION for the production of products with required end-use properties

SAVINGS ABOUT 30 % (RAW MATERIALS + ENERGY + OPERATING COSTS)

But sustainable-mankind not always a dream!...

To design clean and very efficient processes in refining and petrochemicals

FCC unit for the valorization of heavy crude oil to produce gazoline (deep conversion) 16,000 bpsd

TAMOIL (CH)

Esterfip H process

First industrial unit : Sète in France (startup 03/2006)

To design clean and very efficient processes in refining and petrochemicals

(Diesel Oil from Biomass 1G)

Glycerin purety > 98.5% with no purification step

Catalyst activity stable for 9 months

outline

- Some reminds on chemical engineering, its evolution and on process intensification

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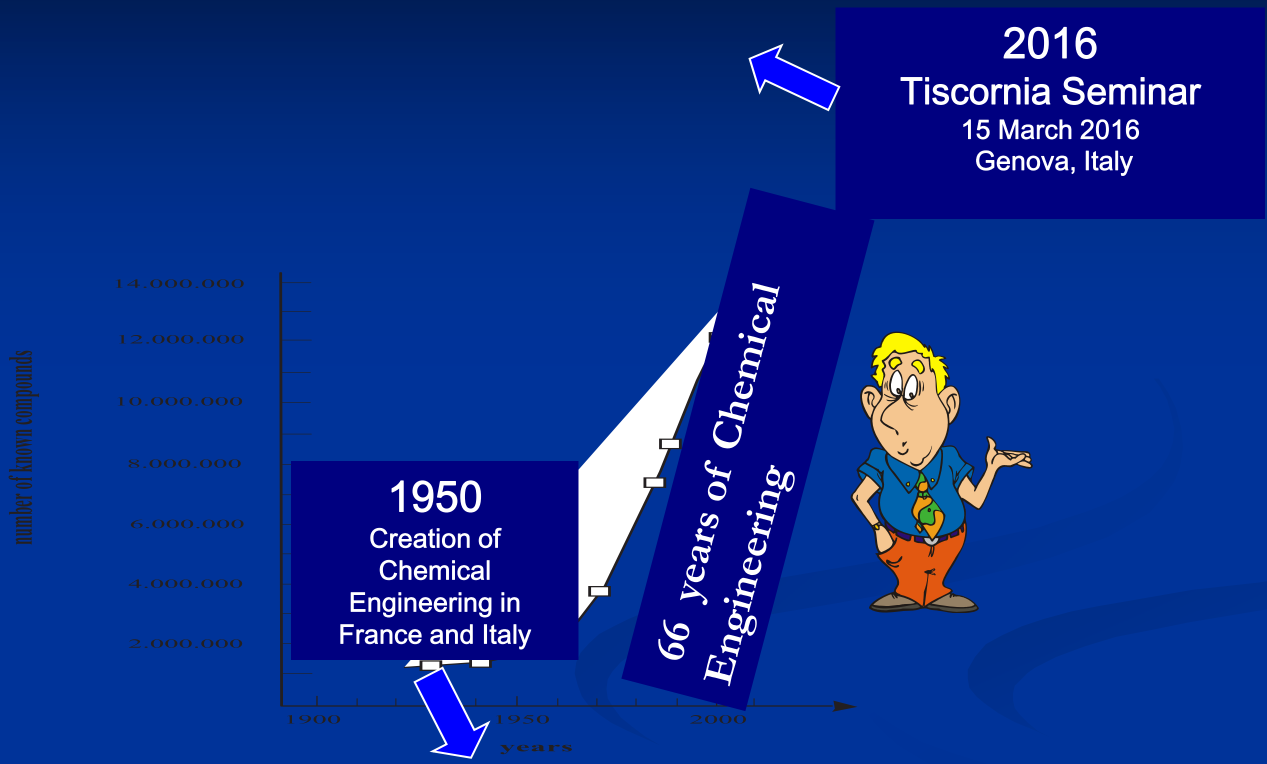


Rapid knowledge in chemistry and biochemistry

- more than 14 million molecular compounds have been synthesized in 2015
- **only a small number of them is found in nature**
- **others are and will be conceived and manufactured by scientists and engineers to meet the needs of man and to satisfy his quest for knowledge (i.e., post-genomic era)**

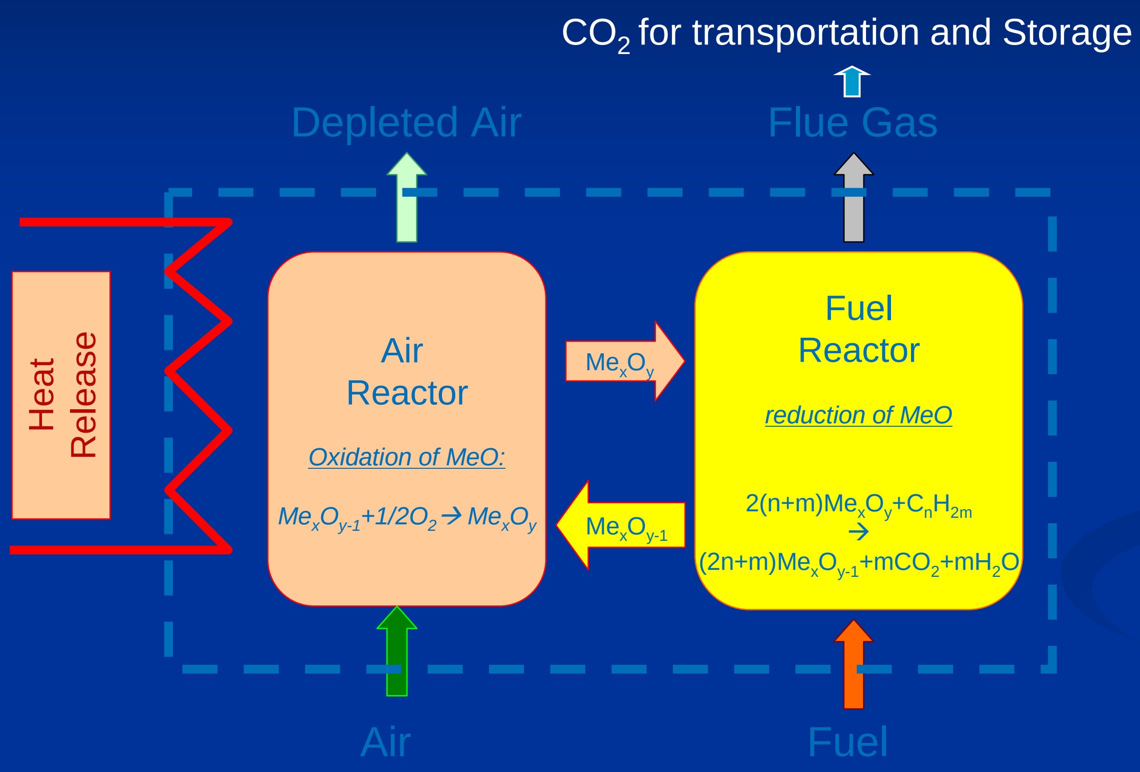
21st century demands concern

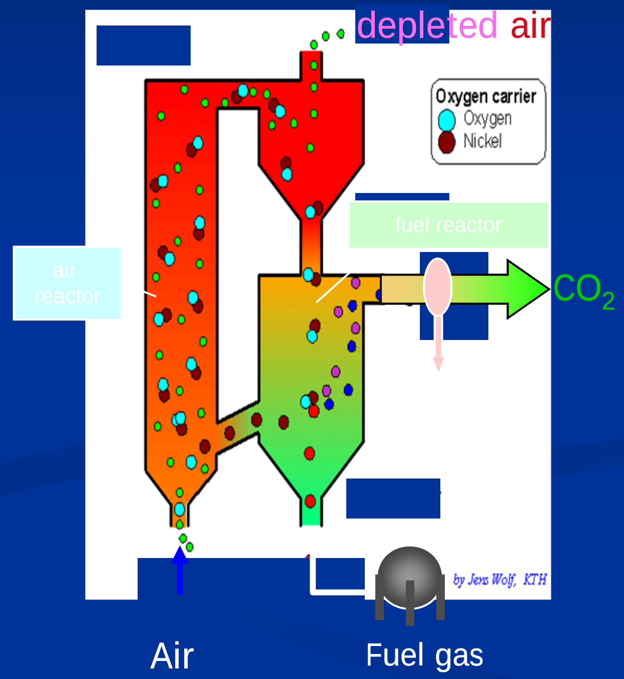
- Energy and environmental engineering
- Biomass conversion
- Matérials engineering (biomaterials, inorganic nanostructured materials)
- Nanotechnology: preparation of nanoparticles
- Biotechnology and bioprocess engineering
- Controlled drug delivery
- Use of neoteric solvents (ionic liquids, aqueous biphasic systems, (green chemistry))
- Dynamics of relaxation of complex molecular compounds
- Manufacture of polyphasic reactors for selective reactions (green processes)
- etc….

and they are clearly focused on society exigences such as

- Carbon capture from post-combustion flue gas and CO2 sequestration or used as solvent for fine chemistry
- Chemical looping combustion (CO2 capture with limited energy penalties)
- Catalytic reforming and catalytic oxidation natural gas to produce syngas (CO+H2)
- Synthesis of biofuels 1st, 2nd , 3rd generations (gasoline, gasoils, production of H2)
- Water demand and treatment
- Life Cycle Analysis, focus life-cycle design, incorporate by-product synergy and account for ecosystems services if we are to progress towards Sustainability

Chemical Looping Combustion

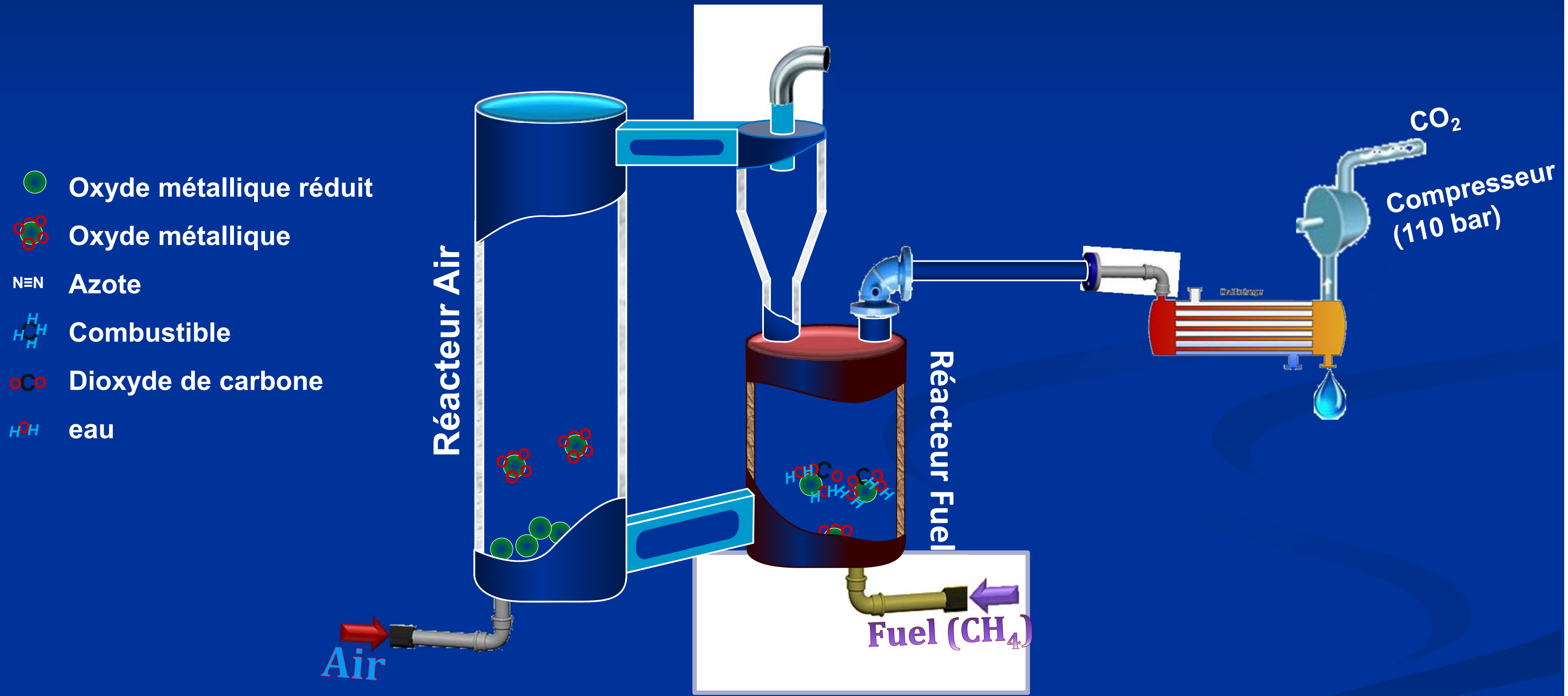




deux types de looping:

- Boucle sur l'oxygène (oxydes métalliques, CaS)
- Boucle sur le CO2 (carbonates)

Chemical Looping Combustion



Séparation du CO_2 avec une pénalité énergétique minimale

Intérêt du CLC pour le captage du CO_2

- **Solution alternative aux Amines, à l'Oxycombustion, à la Gasification**

- **Avantages spécifiques**
  - séparation CO_2 intrinsèque
  - pas d'Unité de Séparation d'Air

  } → Pénalité énergétique limitée:

Un très bon candidat à priori pour capter le CO_2

- Mais...!!!
  - Développement de procédés spécifiques **(pas de retrofit !!)**
  - Mise en oeuvre de procédés complexes (T, lit fluidisé...)
  - Incertitude sur les matériaux

NON-SUSTAINABLE MANKIND

Only 25 wt% of what goes into the pipe comes out as goods and services

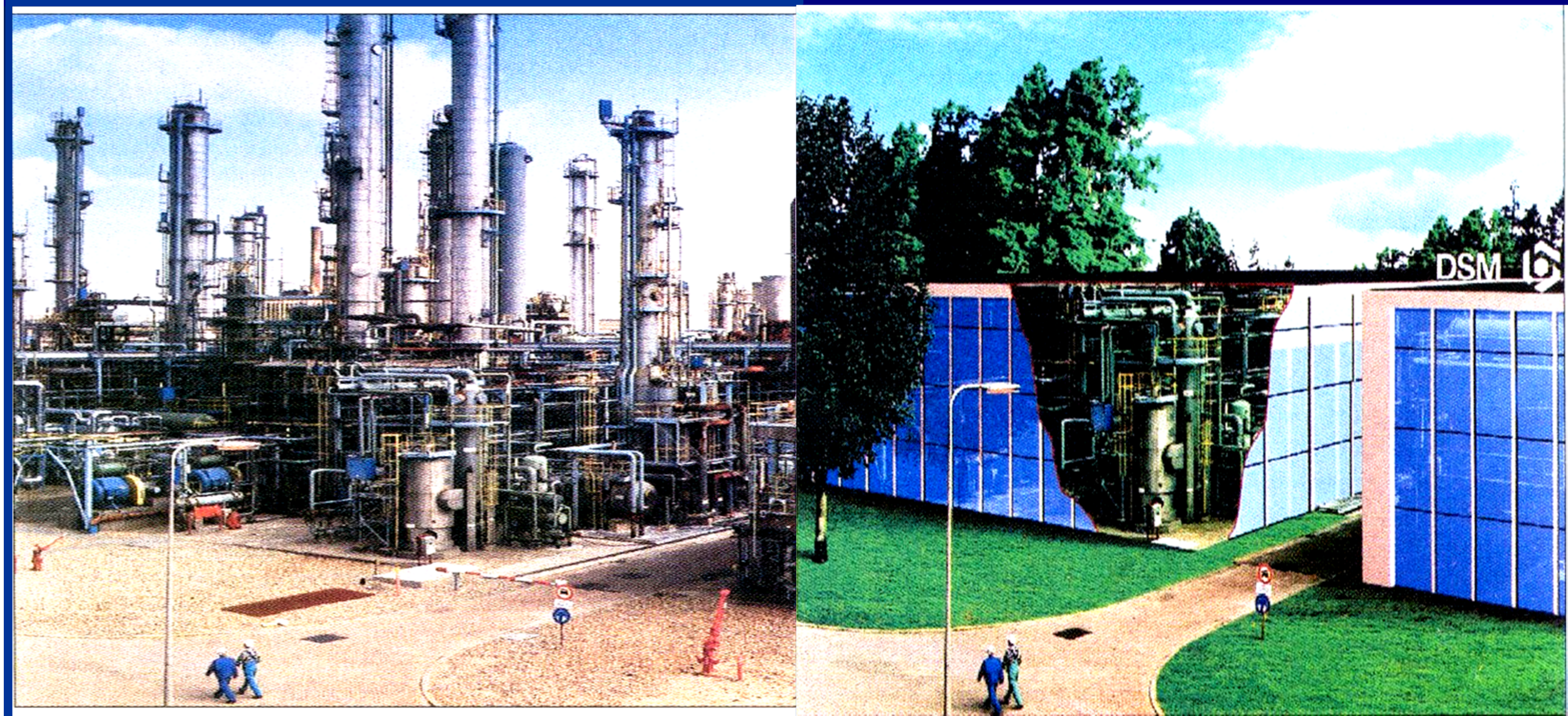
(Source: World Resource Institute)

Improvement needed:

- FACTOR 4 (Von Weizsacker, 1998)
- FACTOR 10 (Schmidt-Bleek, 1993)
- FACTOR 20 (AllChemE, 2001)

One vision of how a future plant employing Process Intensification may look (right) vs. a conventional plant (left).

(Rendering courtesy of DSM)



OPERATING with NON POLLUTING and VERY EFFICIENT PROCESSES SUSTAINABLE involving PROCESS INTENSIFICATION for the production of products with required end-use properties

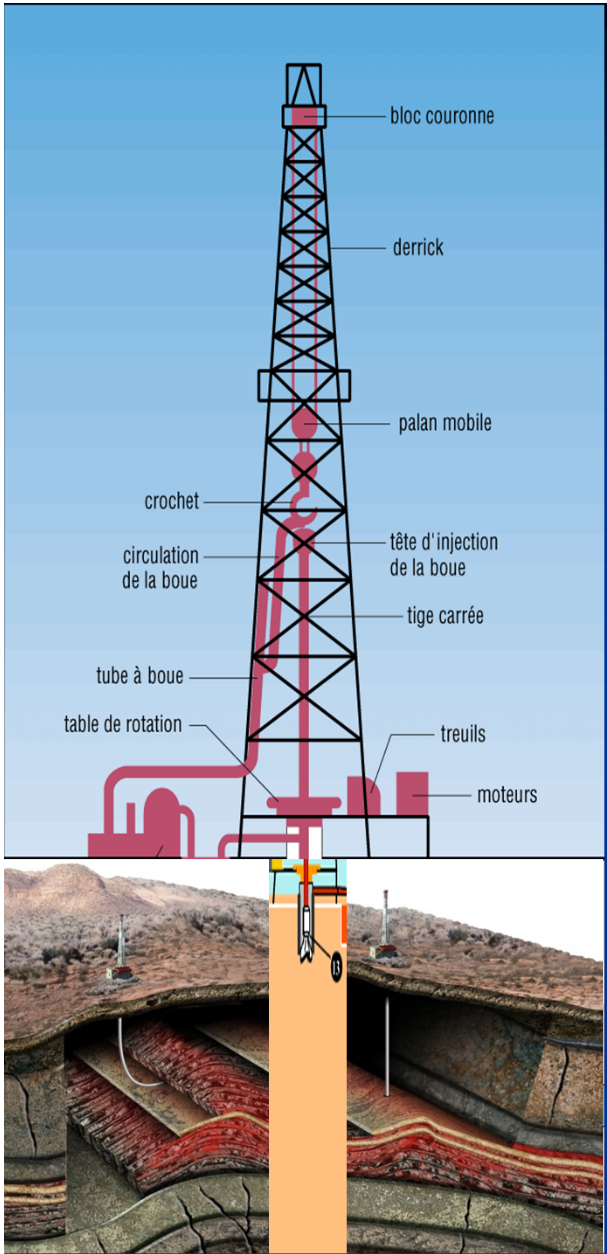
SAVINGS ABOUT 30 % (RAW MATERIALS + ENERGY + OPERATING COSTS)

But sustainable-mankind not always a dream!...

The Old: 1920's El Dorado Field, KS

Les temps changent………….. But imagine and remind

Le forage pétrolier



Pollution

Solide/Eau/Air
CONTAMINATION

Chaleur

Poussière

Odeur

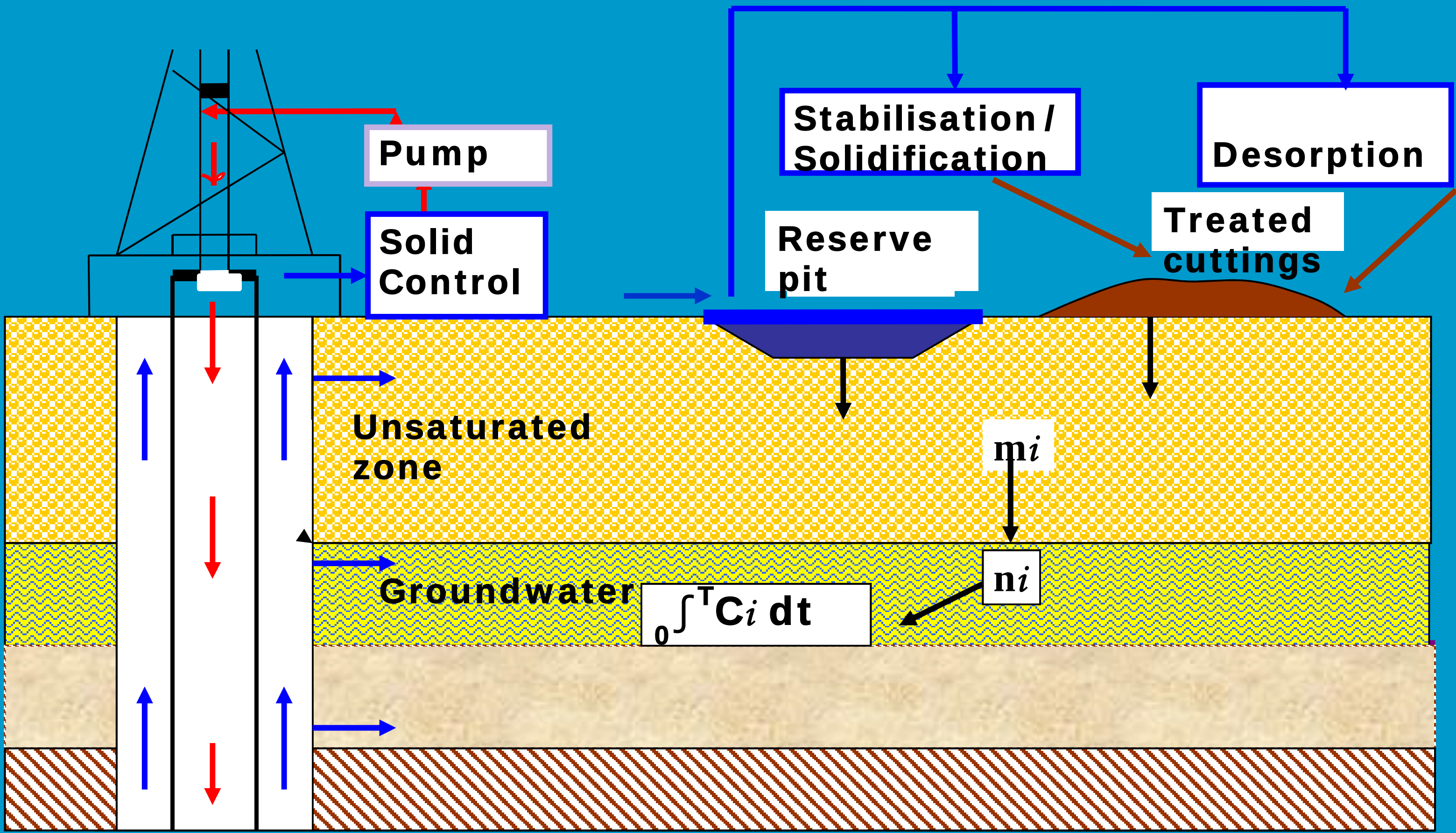
Bruit

Visuelle

Vibration

Des problèmes avant, durant et après forage….

Limites du système



Le volume moyen des rejets

Le volume généré est 5-15 fois le volume foré

SHALE GAS: SUSTAINABLE PRODUCTION

Vikram Rao

Research Triangle Energy Consortium

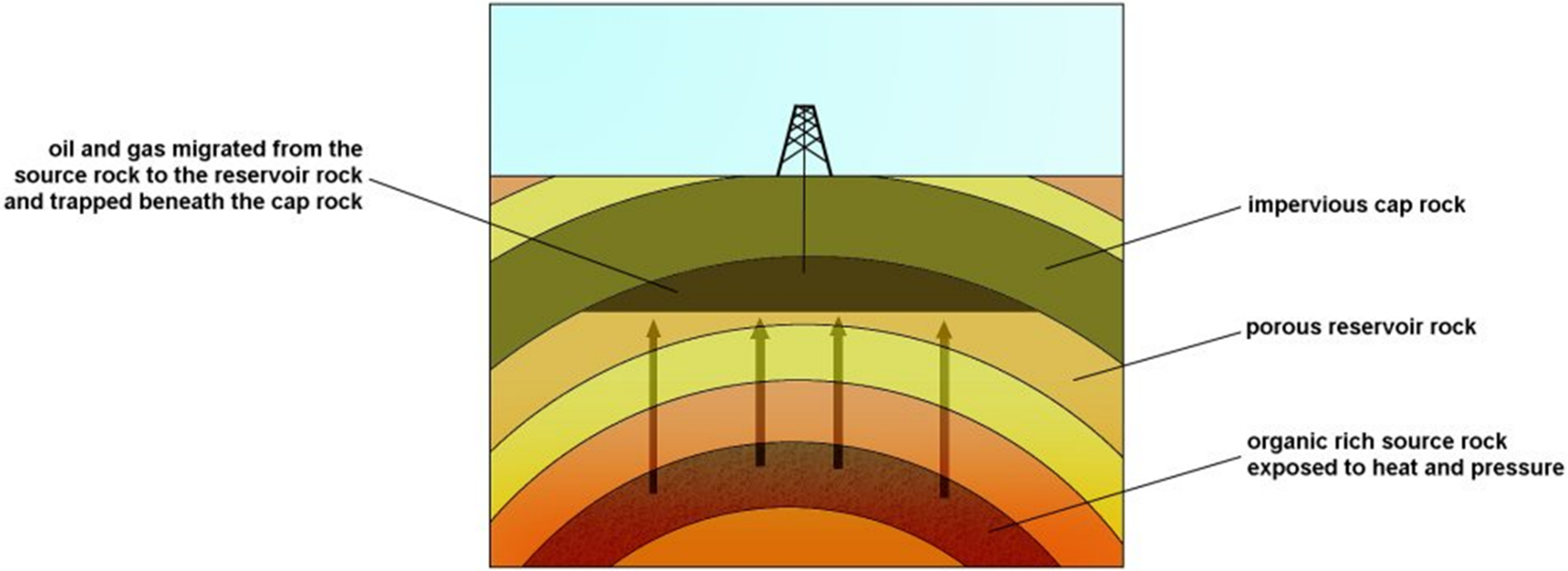
October 7, 2013

NATURAL GAS (Gaz de Schistes, Shale gas)

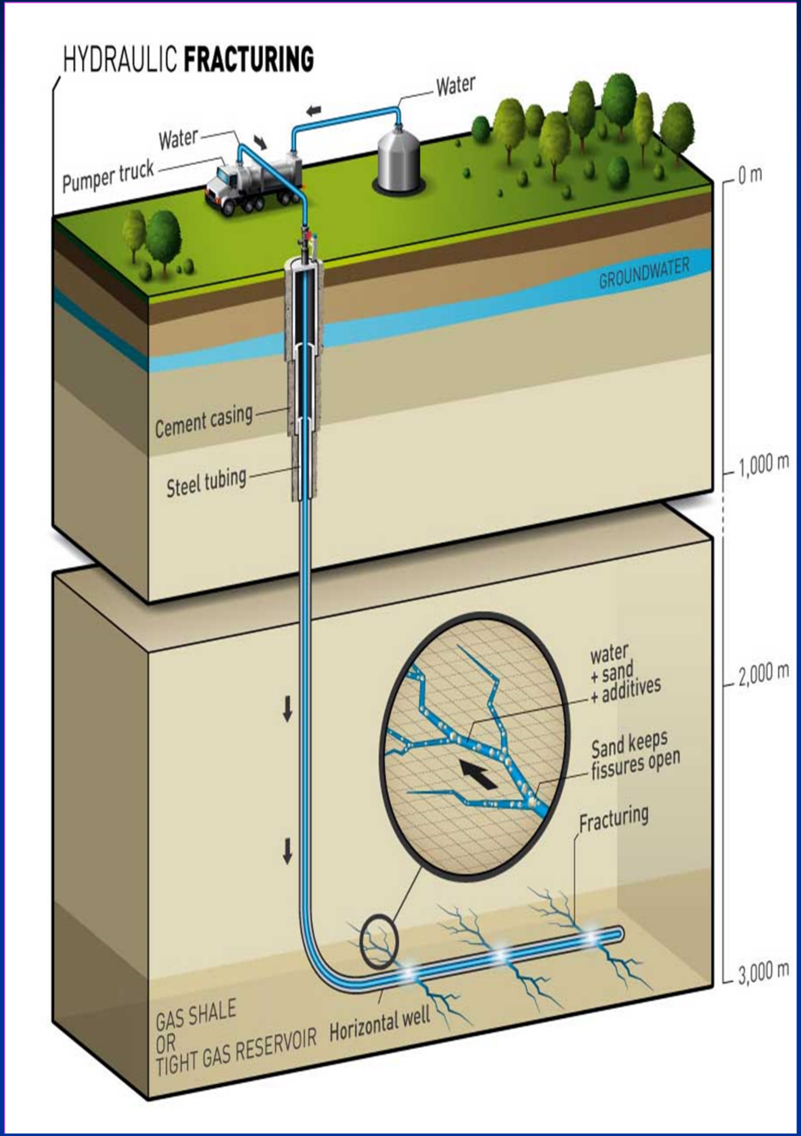
- How it formed
- What makes shale gas different
  - Directly producing from source rock
  - New resource pool: plentiful
  - Low permeability: must be fractured
  - Horizontal wells: why necessary
  - Unique environmental hurdles

PRODUCTION DURABLE DES GAZ DE SCHISTES (SHALE GAS)

Vikram Rao, Research Triangle Energy Consortium, FIM,October 7, 2013



Procédés d'extraction des huiles et gaz de schistes
(Shale Gas Extraction Process)



Horizontal drilling can extend up to 10,000 feet laterally

Questions? Treatment of the waters used for fracking…

Treatment of the fracking waters with membrane processes: UF, RO…

Classical Today Treatment of the waters which have been used for the extraction of shale oils

Gratia, merci to the "Green" modern chemical engineering

J.C. Charpentier LRGP/CNRS/ENSIC/Université de Lorraine, Nancy (F)

NON-SUSTAINABLE MANKIND

Only 25 wt% of what goes into the pipe comes out as goods and services

(Source: World Resource Institute)

Improvement needed:

- FACTOR 4 (Von Weizsacker, 1998)
- FACTOR 10 (Schmidt-Bleek, 1993)
- FACTOR 20 (AllChemE, 2001)

Exemple:

Comportement non durable (Non Sustainable Mankind): Toekomst voor biodiesel is illusie

M Katan, R Rabbinge, W Van Swaaij, Scenario Biomassa, University Twente (Ne) 2007

Accordingly this today NON-SUSTAINABLE MANKIND

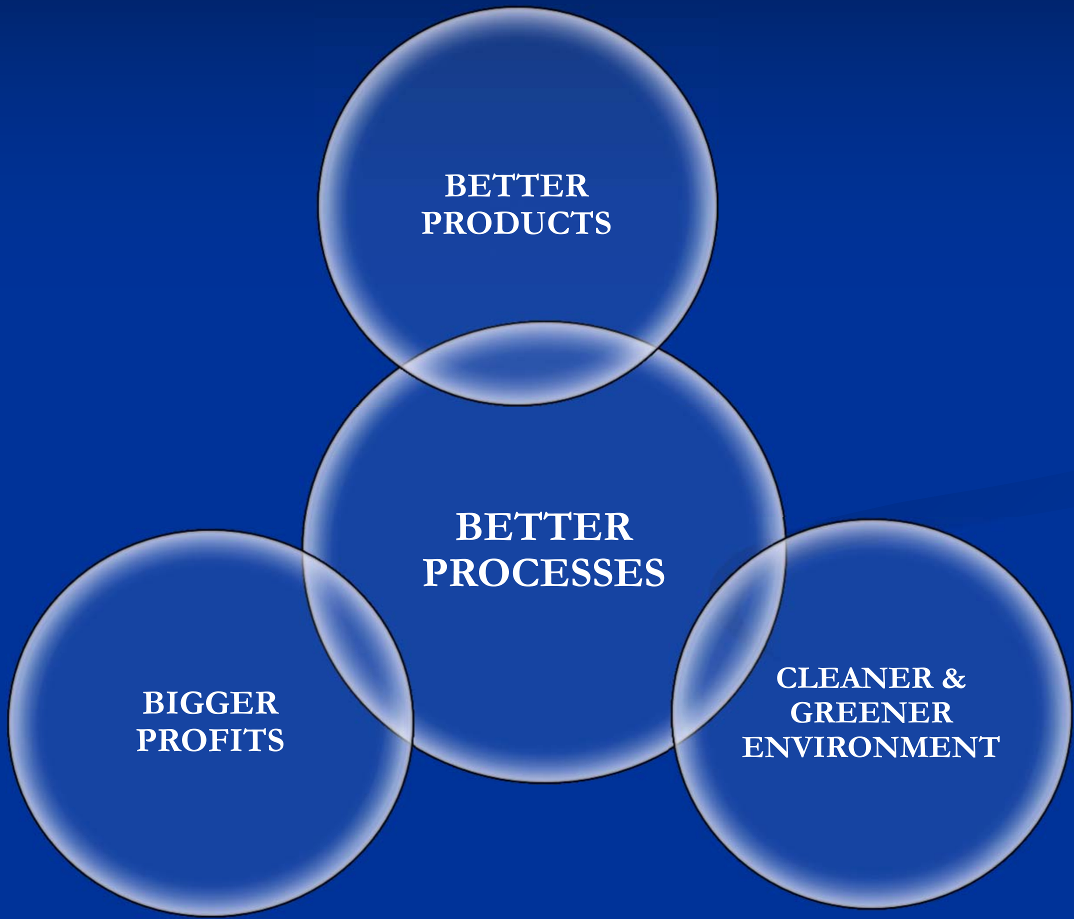
The sustainable-oriented research in chemical and biochemical engineering today and in the coming decennia will need to focus on (but not only on) the:

-Development of technically and economically feasable processes based on renewable feedstocks (i.e. biomass-based processes), and on the

- Development of innovative methods and technologies that could drastically increase the efficiency of chemical and biochemical manufacturing: (i.e. process intensification)

So for a sustainable mankind investigations should focus…

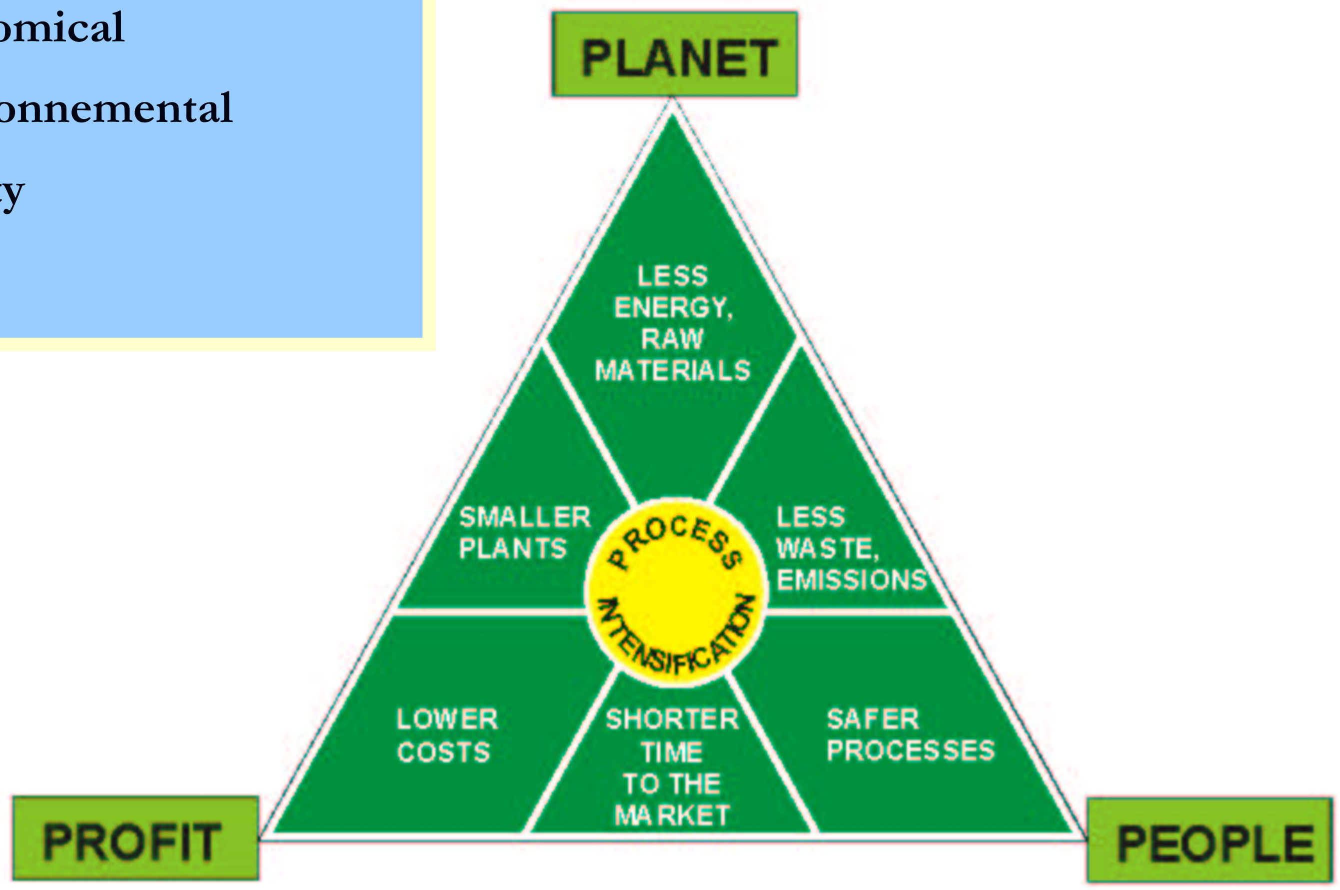
For **Sustainable mankind** our Focus should be on…



A SUSTAINABLE MANKIND MUST BE ASSUMED BY WELL EQUILIBRIED PROGRESSES

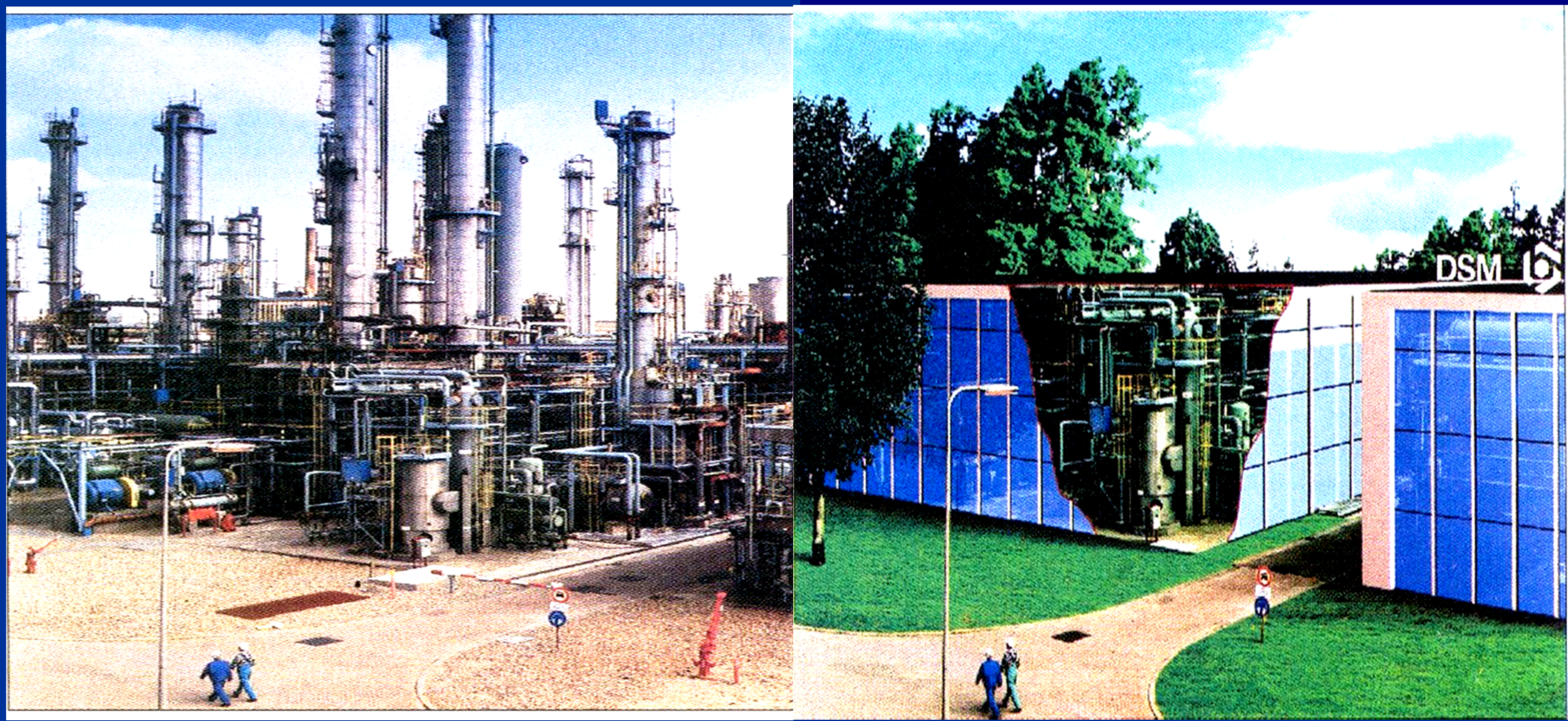
PROGRESSES IN 3 DOMAINS

- Economical
- Environnemental
- Society



One vision of how a future plant employing Process Intensification may look (right) vs. a conventional plant (left).

(Rendering courtesy of DSM)



OPERATING with NON POLLUTING and VERY EFFICIENT PROCESSES involving PROCESS INTENSIFICATION for the production of products with required end-use properties

SAVINGS ABOUT 30 % (RAW MATERIALS + ENERGY + OPERATING COSTS)

But not completely a dream..

Not completely a dream there exists today strong efforts for the radical transferts of technological innovation with changes involving **Micro-process technologies** and **Process Intensification in industry practice**

Financing European Policy

is to « exploit the full potential of microprocess technologies » to the realisation

of « new, intensified process and plant concepts for speeding up market penetration, for

enhancing the product life-cycle and improving sustainable production ».

The European funding policy

- «**Factory of the future** » and « **Flexible Future Production Strategies** » Nanosciences, Nanotechnologies, Materials Calls EU FP7 NMP-2009 and European Commission 2010 Research-Industrial Technologies, Factories of the Future

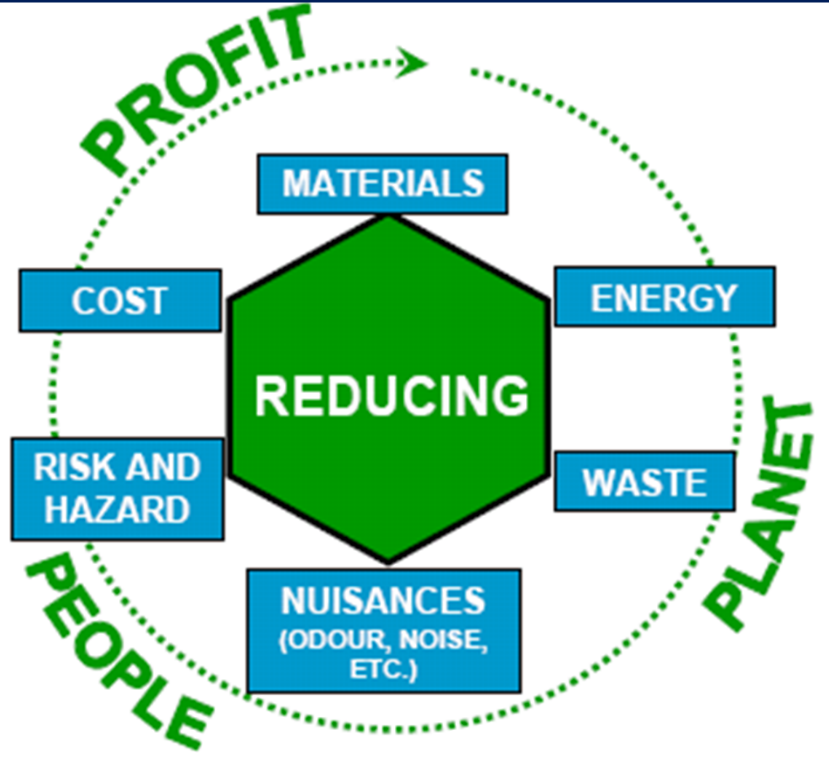
  PILLS 2009 www.fp7pills.eu,- **COPIRIDE 2009** www.copiride.eu,- **F3 FACTORY 2009,** www.f3factory.com

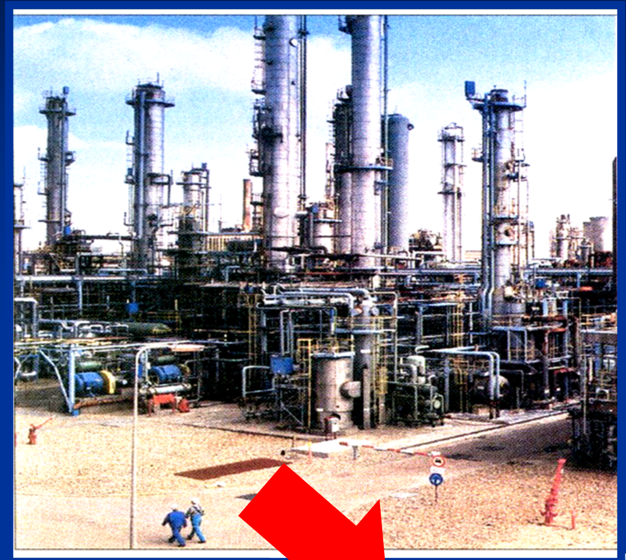
- **H2020….**

- Projet Institut de l'usine décarbonée du futur IEED (Appel à projets « Instituts d'Excellence en Energies Décarbonées (IEED))

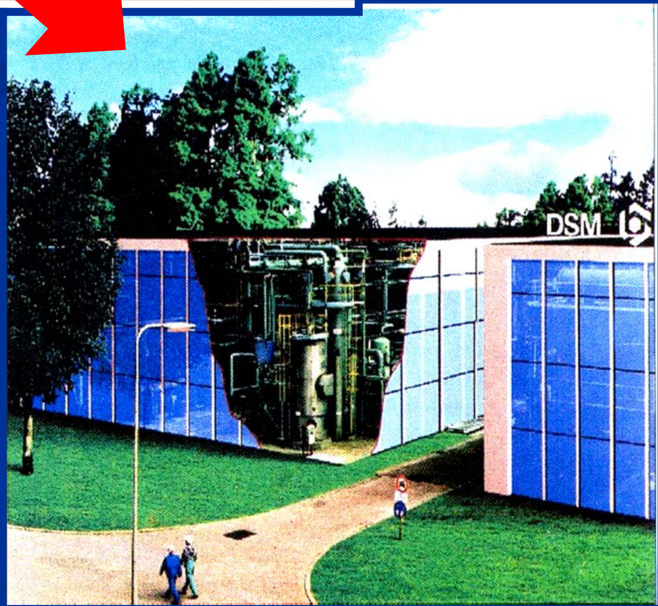
- The consortium of **CARENA** **CAtalytic REactors based on New mAterials**
  Collaborative project to create technologies enabling efficient conversion of light alkanes and CO_2 into higher value chemicals

SUSTAINABILITY and PROCESS INTENSIFICATION





2 CHALLENGES FOR
CHEMICAL ENGINEERING



1st Challenge: Production of COMMODITY AND INTERMEDIATE CHEMICALS
(ammonia, calcium carbonate, ethylene, benzene, butadiene, amines,…) (40% markets demands)

« Supplying high volume bulk chemicals »

Issue: Who can produce large quantities at the lowest possible price?

THE CLIENT BUYS A PROCESS
NON POLLUTING, DEFECT-FREE, PERFECTLY SAFE
(Green Process Engineering) but…

…but the production in the future will increase (X factor 6 in 2050, assuming a growth rate of 4%),

and the plant not any more being built

«JUST A BIT BIGGER»

So the **Challenge** is aiming:

TECHNOLOGY CHANGE (i.e. **process intensification**)
and **INNOVATION (new processes),**

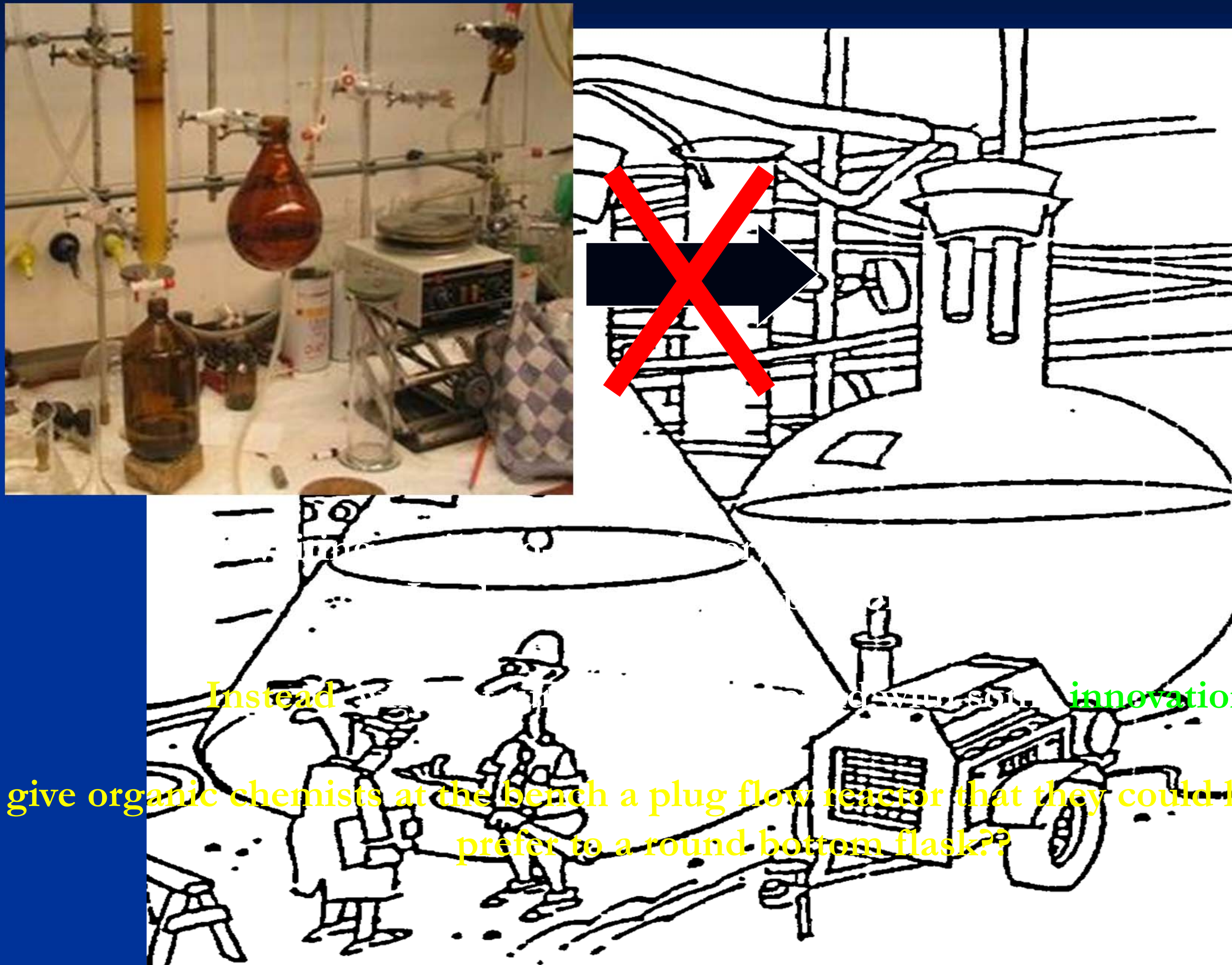
But innovation….

Innovation = Unproven Solutions

("Plant manager never wants to be the first")

"Don't bother me with new ideas, i've got a battle to fight!"

That same old scale-up problem



Instead … innovation:

give organic chemists at the bench a plug flow reactor that they could like – or, even prefer to a round bottom flask??

The IMPULSE Project :
a European response to a global challenge

6th European Framework Programme for Research and Technological Development

Integrated
Multiscale
Process
Units with
Locally
Structured
Elements

Project goal :

Effective **targeted integration of innovative process equipment** (such as microreactors, compact heat exchangers, thin–film devices and other micro and / or meso–structured components) to attain radical performance enhancement for whole process

Industrial leaders : GSK, Degussa, P&G, Siemens

Consortium : **20 partners** from 8 European countries

Project resources : 17 M€ over 4 years
(of which 10,5 M€ from the European Commission)

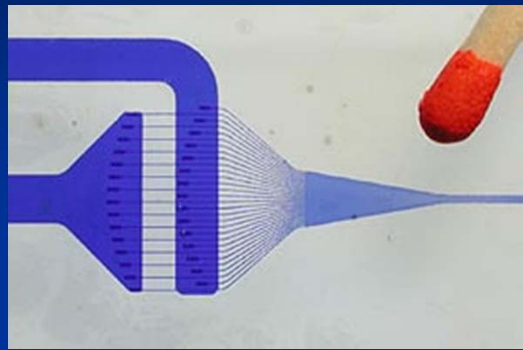
Project duration : February 2005 to January 2009

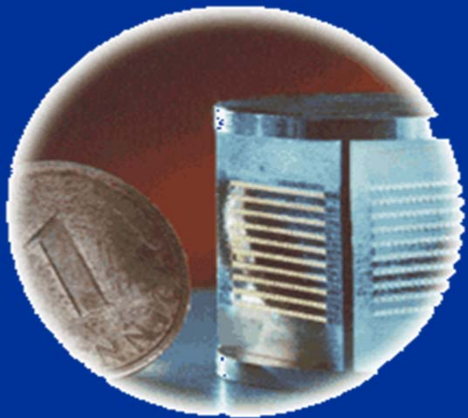
Microstructured components :

an opportunity for the chemical process industries ?

Intensified Process Equipment

- micromixers
- thin–film contactors
- microreactors
- compact exchangers





Essential features →

Controlled topology

(on a sub–millimeter scale : relevant for transfer/mixing)

↓

Diverse materials

(metals, alloys, glass, ceramics, polymers : not only silicon !)

Microstructured components in PRODUCTION :
the concept of Structured Multiscale Design
for PROCESS INTENSIFICATION

A new approach to chemical process design !

STRUCTURED MULTISCALE DESIGN

Principle : construction of large–scale production systems with small–scale inner–structuring at specifically targeted points (= locally structured elements)

Claim : an opportunity for a RADICAL increase in process performance and a MAJOR contribution to process intensification for the chemical industries

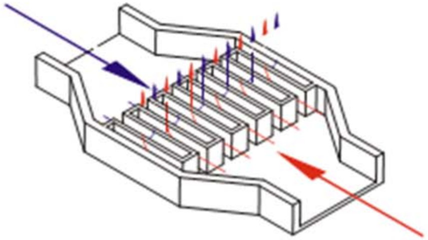
Approach : « put chemistry in the center ! »

rather than adapting chemistry to equipment limitations, adapt the equipment to IMPOSE the local operating conditions required by the desired chemistry !

Answer to the Need of a rational engineering design methodology to put Structured Multiscale Design into practice !

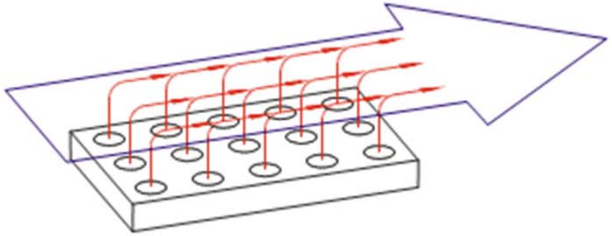
MIXING PRINCIPLES AND CORRESPONDING IMM MICROMIXERS

Lamination for hydro-dynamic or shear decay



Bas-relief induced recirculation flow

Injection in turbulent flow



Interdigital Micromixers

SIMM-V2
SSIMM
...

Caterpillar Micromixers

CPMM-R300-V1.2, CPMM-R600-V1.2
CPMM-R1200-V1.2, CPMM-R2400-V1.2
...

Star Laminator Micromixers

StarLam 15
...

IMPULSE: Résultats en 2009…..and next

(www.impulse-project-net)

Field of Consumer Goods (Procter&Gamble)

Oxydation de SO2 pour fabrication de surfactants, encapsulation de parfums, production d'émulsions contrôlées: faisabilité sur site industriel

Extrapolation par parallélisation d'équipements microstructurés fonctionnant en continu améliorant la qualité des produits et diminuant frais investissements et fonctionnement

Field of Pharmaceuticals (GlaxoSmithKline)

Pour une Hydrogénation continue avec un prototype de démonstration (réacteur microstructuré) fonctionnant en régime chimique avec meilleurs rendement, sélectivité et sécurité qu'en technologie conventionnelle (cuve agitée en discontinu)

Field of Chemical Specialties (Solvent Innovation, Evonik-Degussa)

Pour fabrication de liquides ioniques, avec réactions très exothermiques en milieu liq/liq, un réacteur microstructuré fonctionnant en continu a amélioré la sécurité et la qualité des produits en réduisant l'emploi de solvants.

Synthesis of Ionic Liquids

Fast and highly exothermic reaction

Today

Batch process in stirred vessels

- Temperature increase
- Yellowish to brownish product

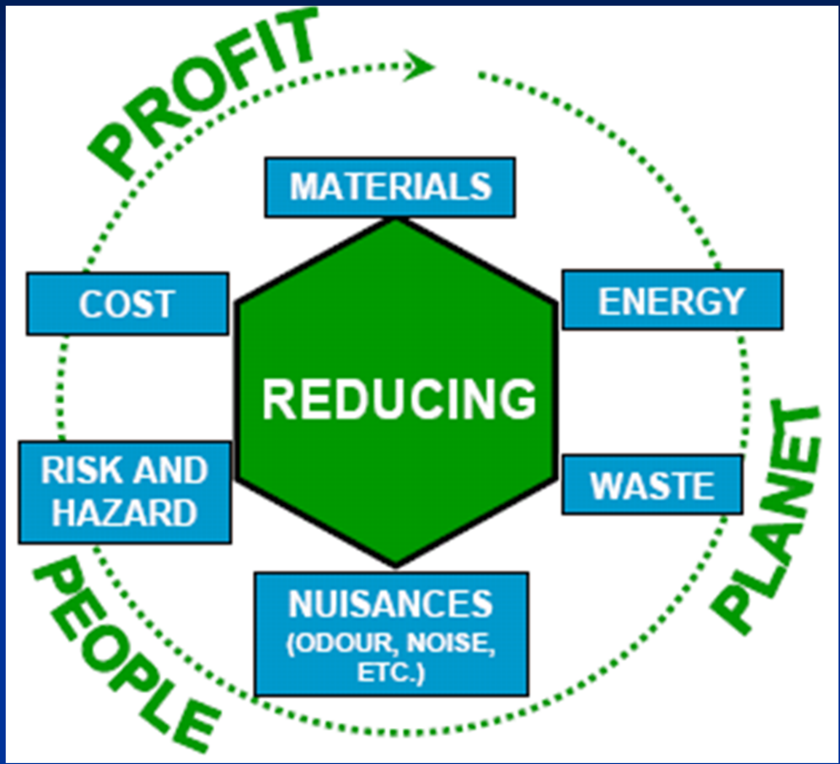
IMPULSE

Continuous process in micro structured devices

- No temperature increase
- Colorless product

Increased product quality

SUSTAINABILITY and PROCESS INTENSIFICATION



2 CHALLENGES FOR
CHEMICAL ENGINEERING

2nd Challenge: NEW SPECIALTIES and ACTIVE MATERIALS CHEMISTRY

(60% markets demands)

Concerns products characterized by new market objectives, sales, competitiveness, and by the end-use property (pharmaceutics, cosmetics, agro food….industries) which are

- CRYSTALLINE, POLYMERIC or AMORPHOUS SOLIDS

need to have a clearly defined physical shape in order to meet the desired quality standards

- PAST-LIKE and EMULSION PRODUCTS

The end-product is a microstructure of disperse phases held together by binding forces leading to the desired product texture

SHORT LIFE-TIME and HIGH MARGIN PRODUCTS

The client buys the PRODUCT MOST EFFICIENT and FIRST ON THE MARKET
(He pays high prices but expects large benefit)

(this requires a Green Product Design and Engineering emphasizing required end-use property)
(i.e. with flexible production, small batches, fast switch over, varying formulation in the same equipment),

Donc

Taking into account the 2 previous challenges imposed either at the process industries (Commodities et intermédiaries) or at the fine chemistry and spécialties industries (pharma, health, cosméto, food…)

The modern green sustainable chemical engineering has to satisfy

- the market demands for green specific products with required end-use properties at the nano and microstructures scales
- and the social and environmental constraints for sustainable green processes at the meso and macro production scales

This requires a multidisciplinary multiscale approach of the different physical-(bio)chemical, non-linear, non- equilibried processes and the transport phenomena processes at the different scales of the (bio)chemical supply chain

i.e.,

INTEGRATED PLURIDISCIPLINARY SYSTEM APPROACH

AT THE DIFFERENT TIME AND LENGTH SCALES OF THE BIOCHEMICAL SUPPLY CHAINNE DE PRODUCTION CHIMIQUE

Time scales : 10^{-15} à 10^{8} seconds

Length scales : 10^{-8} à 10^{6} meters

for a good undestanding of the relations which exist between the phenomena occuring at a lower scale with the properties and the behaviour at higher scale of the supply chain

(from the molecular scale up to the process scale at the industry site)

The time and length scales encountered in the multiscale approach

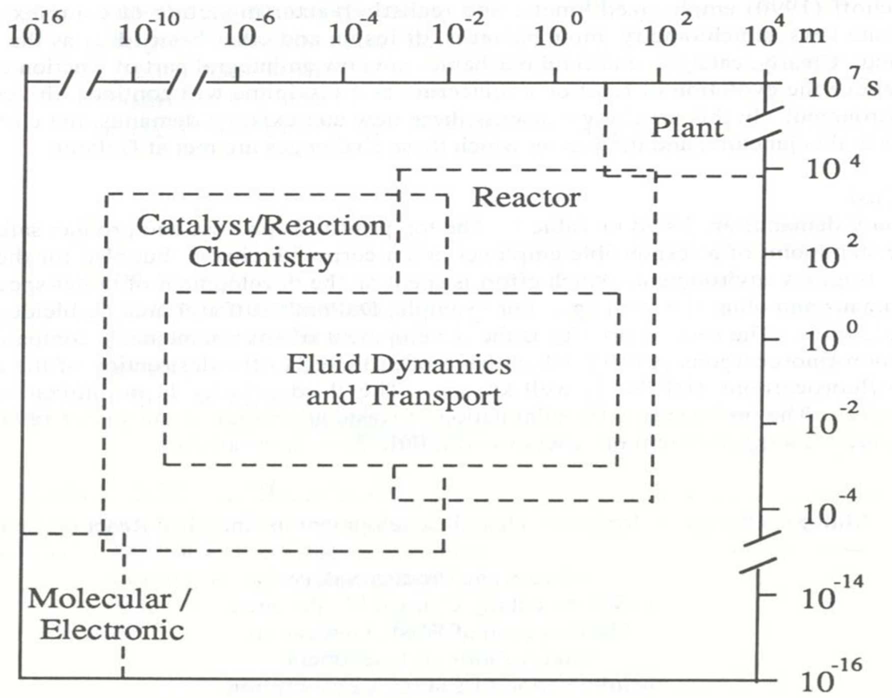
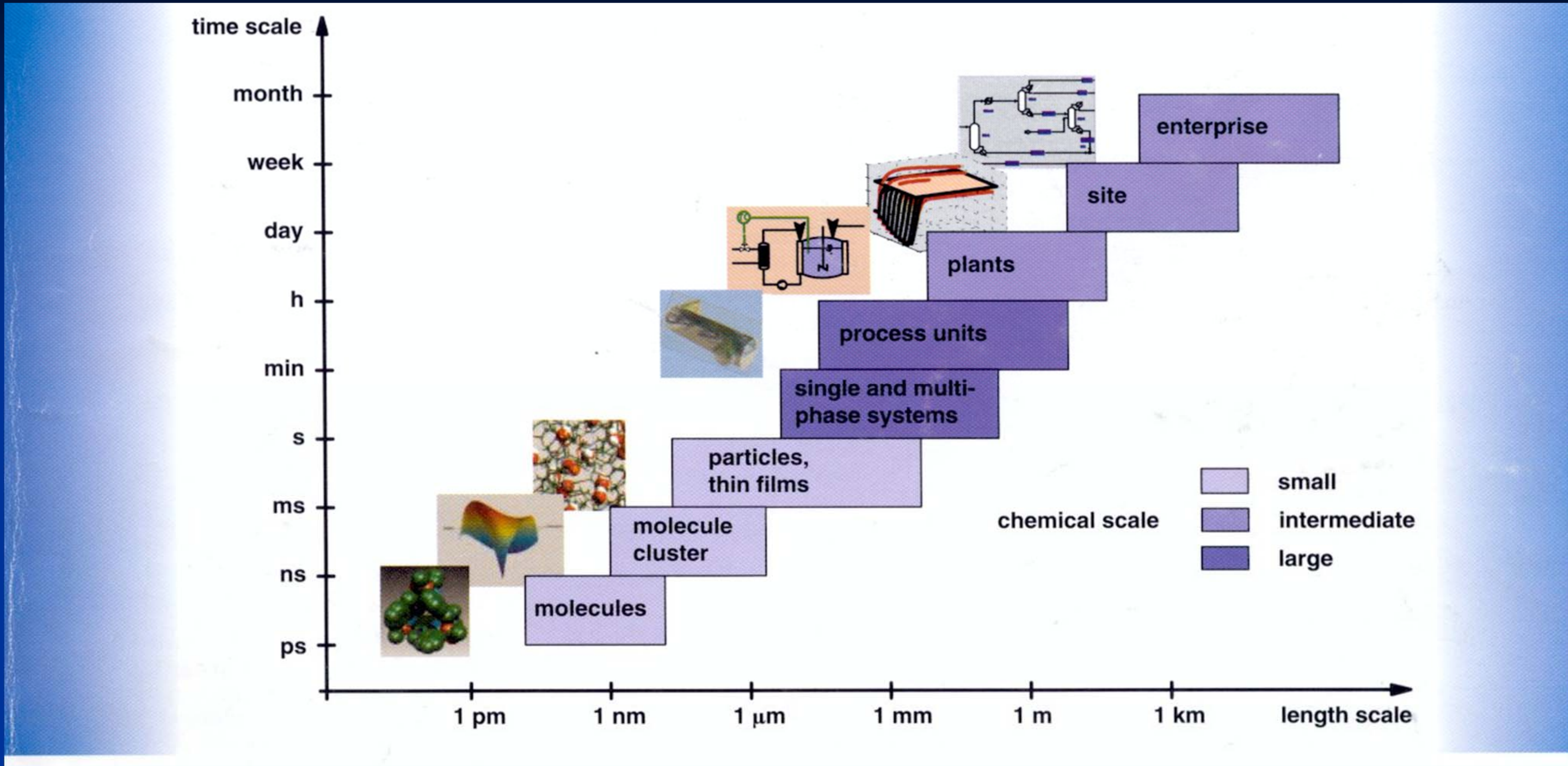


Figure 1. The Length and Time Scales Covered in the Multiscale Approach.

……Organizing the complexity levels

The multi time and length scales of the CHEMICAL SUPPLY CHAIN

(Grossmann & Westerberg, 2000; Marquardt et al, 1998)



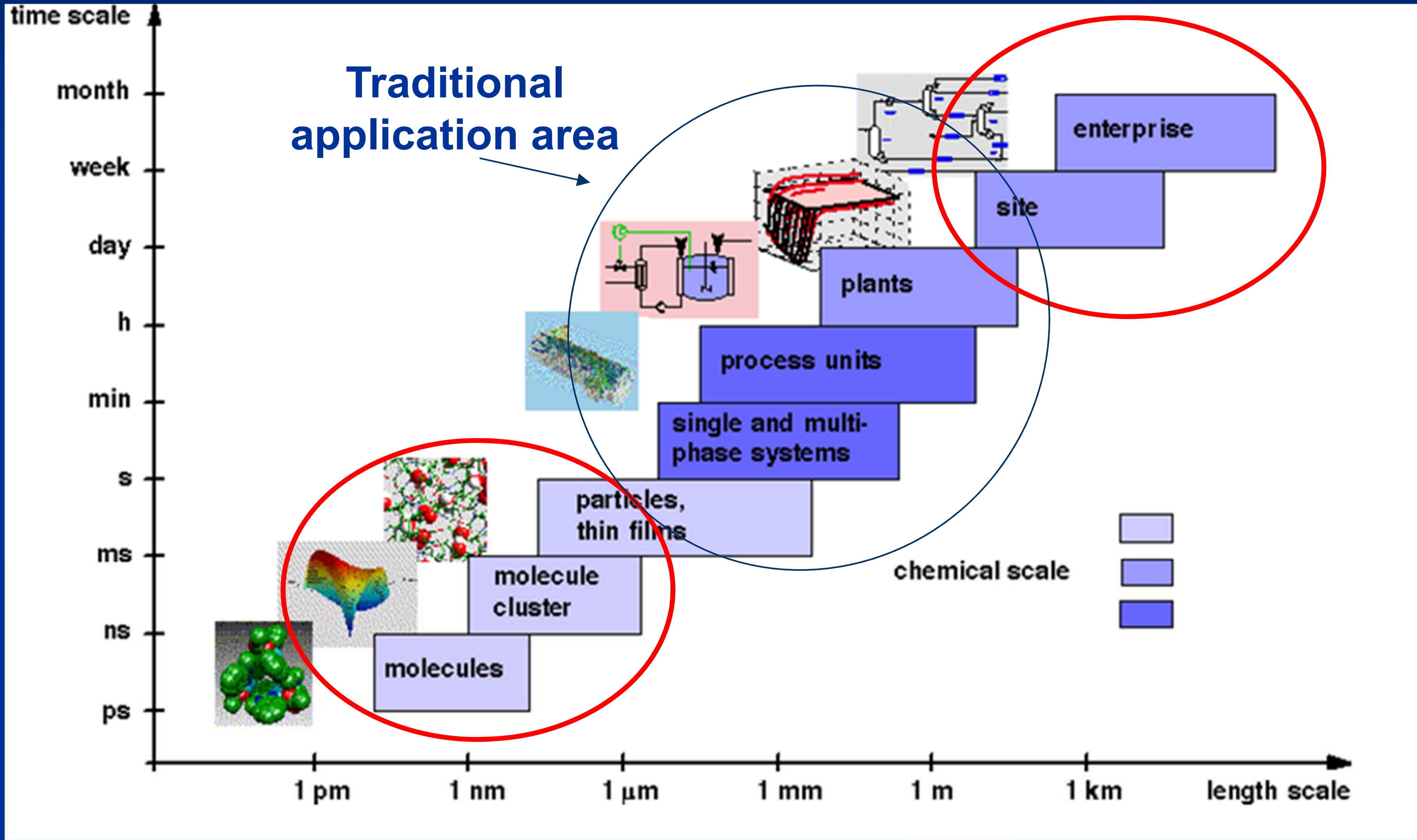
Green Chemistry and Green Chemical and Process Engineering are now concerned with the understanding and development of systematic procedures for the design and operation of chemical process systems, ranging :

FROM nano and microsystems-scales where chemicals have to be synthesized and characterized at the molecular-level

TO industrial-scale continuous and batch processes

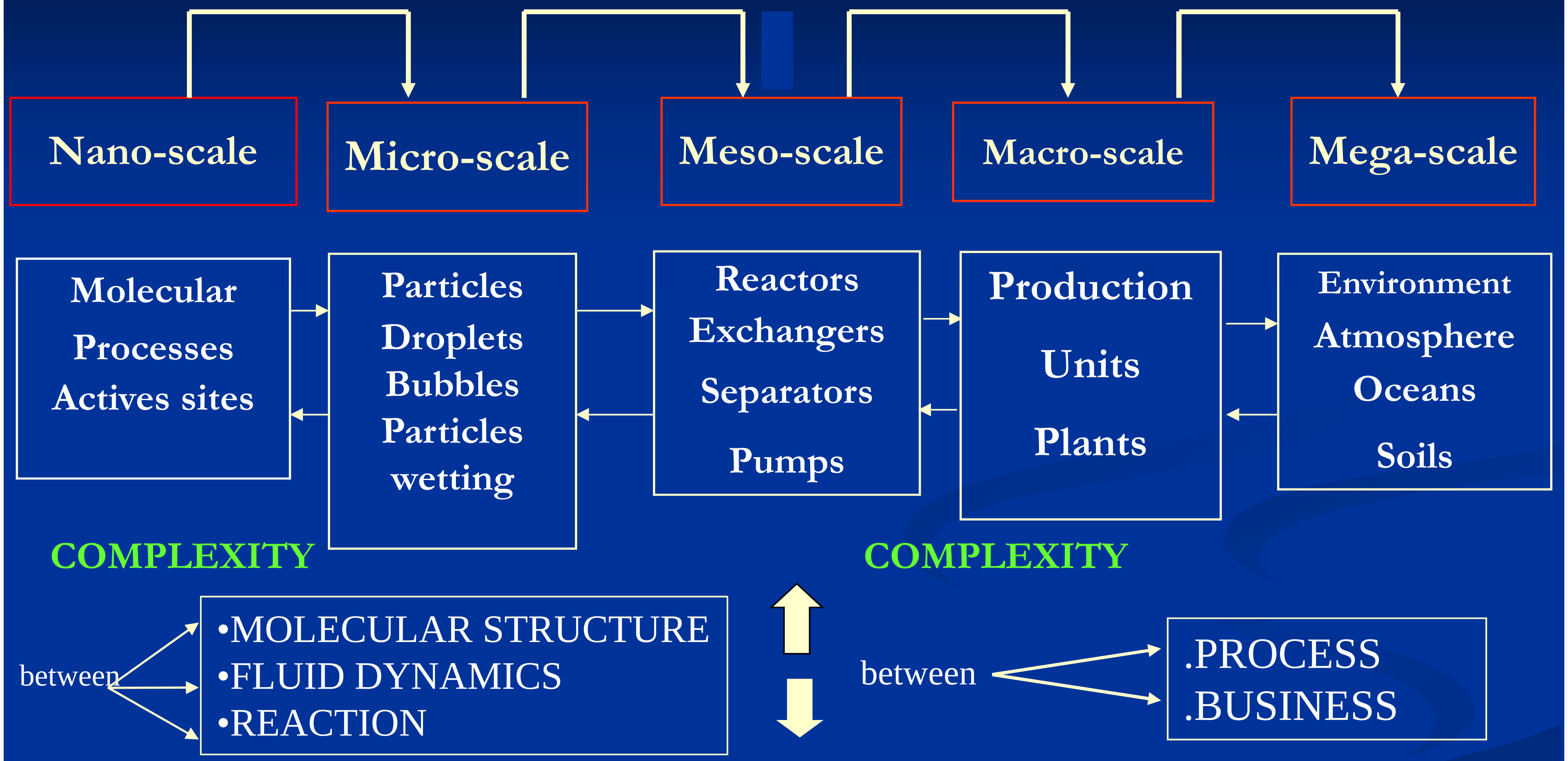
Green modern chemical engineering: The multi-scale time and length approach of the chemical products supply chain

Dimension: Scale; Disciplines; Time, Modelling



J.C. Charpentier LRGP/CNRS/ENSIC/Université de Lorraine, Nancy (F)

Organizing levels of increasing complexity underlies the present view of chemical engineering

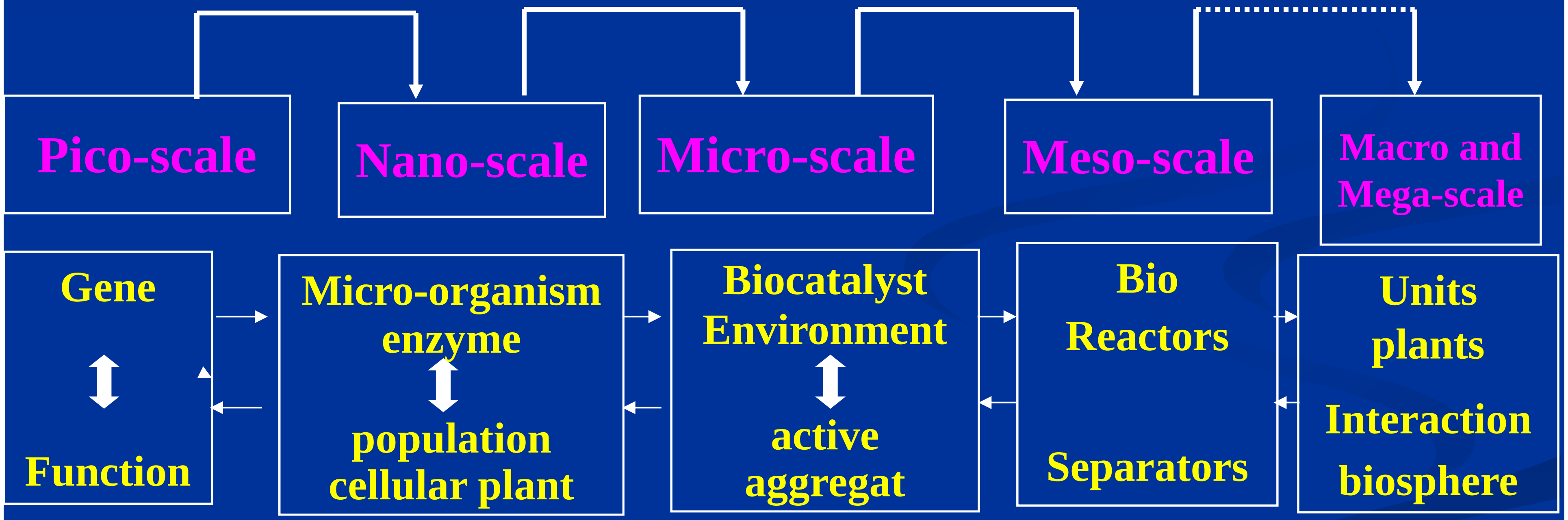


Transforming the MOLECULES INTO MONEY Environmental and Social impact

To understand and to describe the relationship between events at NANO and MICRO-scales to better convert MOLECULES onto USEFUL PRODUCTS at the PROCESS-scales

BIOCHEMISTRY and BIOCHEMICAL ENGINEERING

Organising levels of complexity with an integrated approach of phenomena and simultaneous and coupled processes from the GENE with known structure and function up to the PRODUCT (ecoproduct) with the desired END-USED PROPERTY



Biology's catalysts, the enzymes are proteins molecules that substantially speed up the biochemical reactions in the cell

and

Understanding an enzyme at the molecular level means that it may be tailored to produce a particular end product at the product meso-level, i.e,

again organising levels of complexity……….with the multiscale integrated approach. This gives:

Opportunity to apply genetic-level controls to make better biocatalysts, novel products or developing new drugs, new therapies (social challenges, improvement of the quality of life, customized chemical products…)

Historical paradigms of Chemical Engineering

1st Paradigm: Unit Operations

initiated by Arthur D. Little – ca. 1907 book: "Principles of Chemical Engineering" by Walker, Lewis and McAdams (1923) focus on equipments, construction and performances

2nd Paradigm: Transport Phenomena

appeared in 1960' book: "Transport Phenomena" by Bird, Stewart and Lightfoot (1960) focus on momentum, heat and mass transfer modeling

3rd Paradigm: INTEGRATED SYSTEM TIME and LENGTH MULTISCALE Approach (G3P)

for a modern green sustainable Chemical Engineering

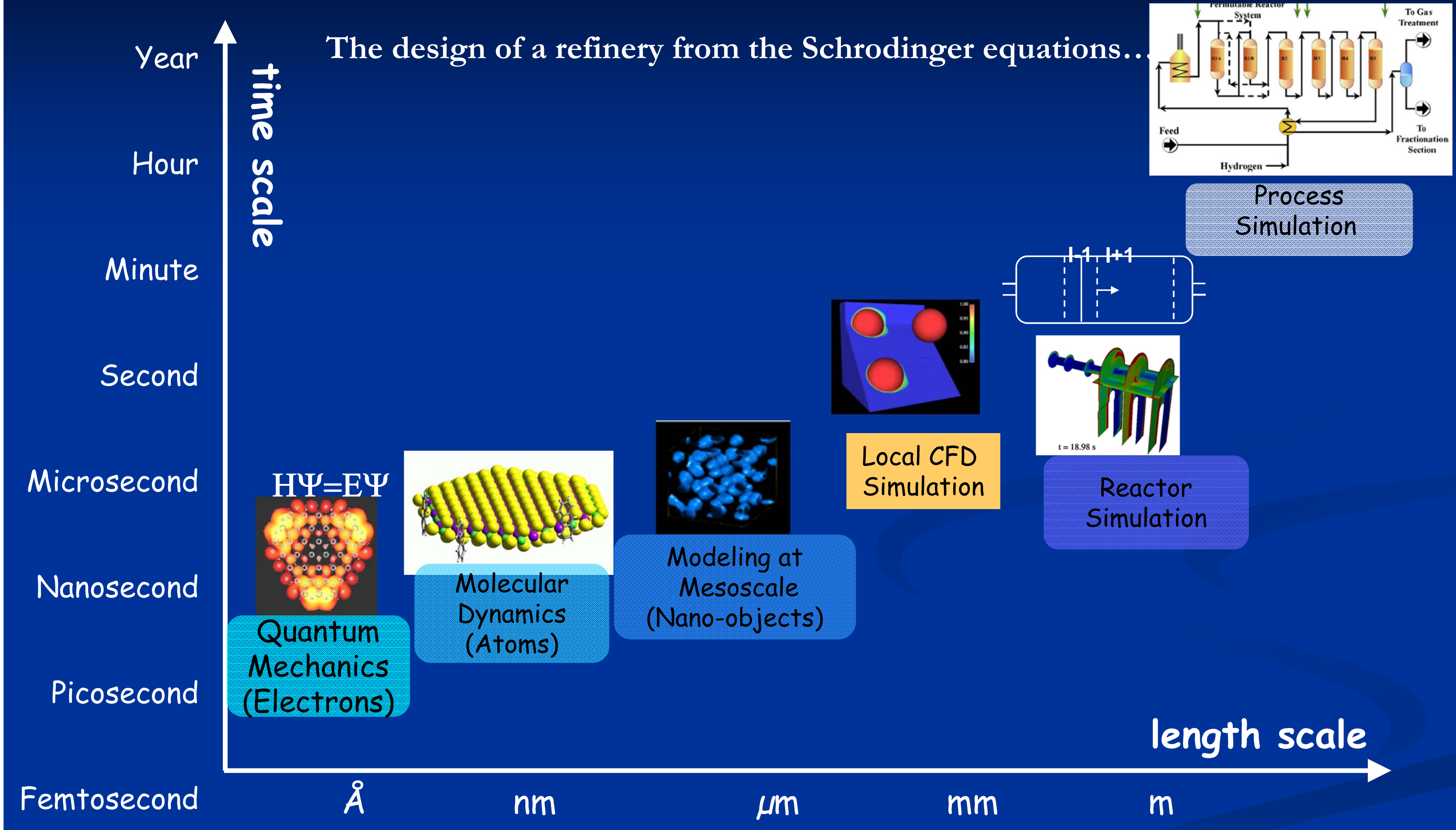
(**involving Process Intensification** for the élaboration of the required end use properties of the green product, etc…)

(vers l'Usine du Futur) (Factory of the Future)

(Charpentier J.C., Chem Eng Res Des, 2010, 88, 248)

Challenges for modeling in chemical engineering

The multiscale approach for the couple green product/process



The integrated multiscale system approach involves to understand how phenomena at a smaller length scale relate to properties and behaviour at a longer length scale of the chemical supply chain.

NEW CONCEPTS and METHODS

requiring a multidiciplinary INTEGRATED SYSTEMS APPROACH

at DIFFERENT TIME and LENGTH SCALE aiming to

PROCESS INTENSIFICATION

to obtain sustainable products (green) with sustainable processes (green)

« The couple Green Products/ Green Process »

are obtained with the

BREAKTHROUGHS in

MOLECULAR MODELING,

Fine non intrusive **SCIENTIFIC INSTRUMENTATION,**

Powerful **COMPUTATIONAL TOOLS**

involving investigations in chemical engineering led in strong collaboration with

physicists, chemists, biologists, ecotoxicologists, instrumentation specialists

Molécular modeling and computer tools

- Nanoscale
  - ♦ to better control catalysis and surface states of catalyst.

    use of molecular modeling
- Microscale
  - ♦ complex and particular systems whose properties are controlled by interfacial phenomena, fractal structure of porous media.

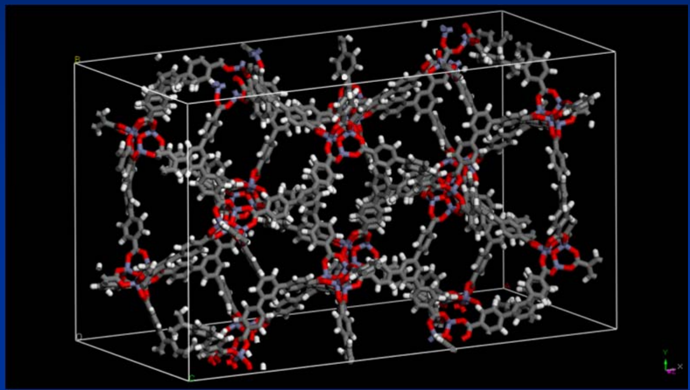
    progress in computational chemistry very useful
- Mesoscale & macroscale
  - ♦ Complex hydrodynamics (GSL catalytic reactor, non newtonian rheology, …) & complex geometries

progress in Computational Fluid Dynamics (CFD)

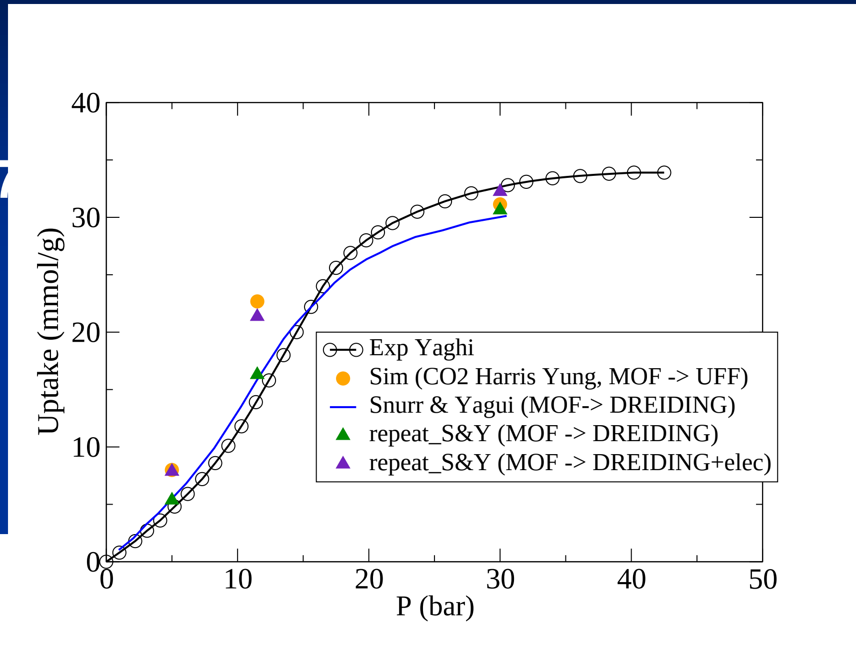
(Mécanique des Fluides Numérique)

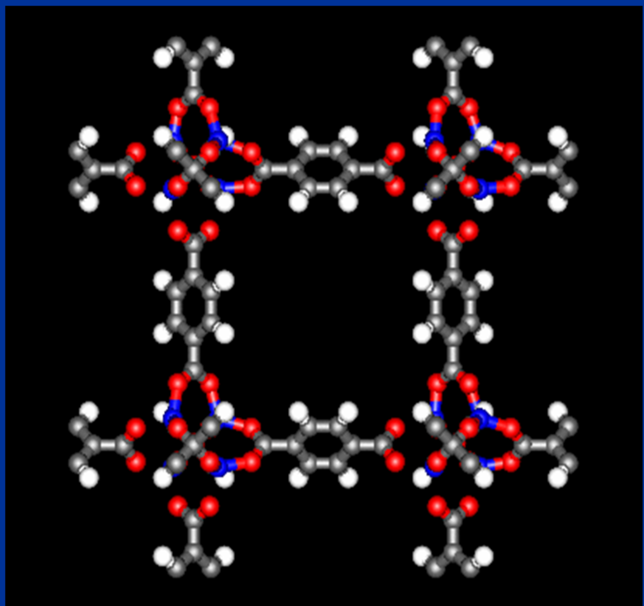
Falk L., Charpentier J. C., Keynote Lecture WCCE 8, Montréal, 2009

MOF-177 et IRMOF-1
Adsorption du CO_2

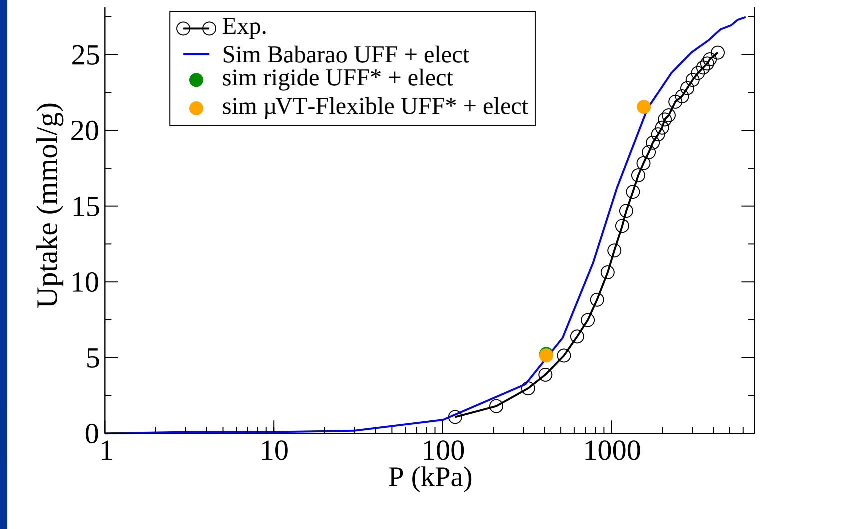


MOF-177

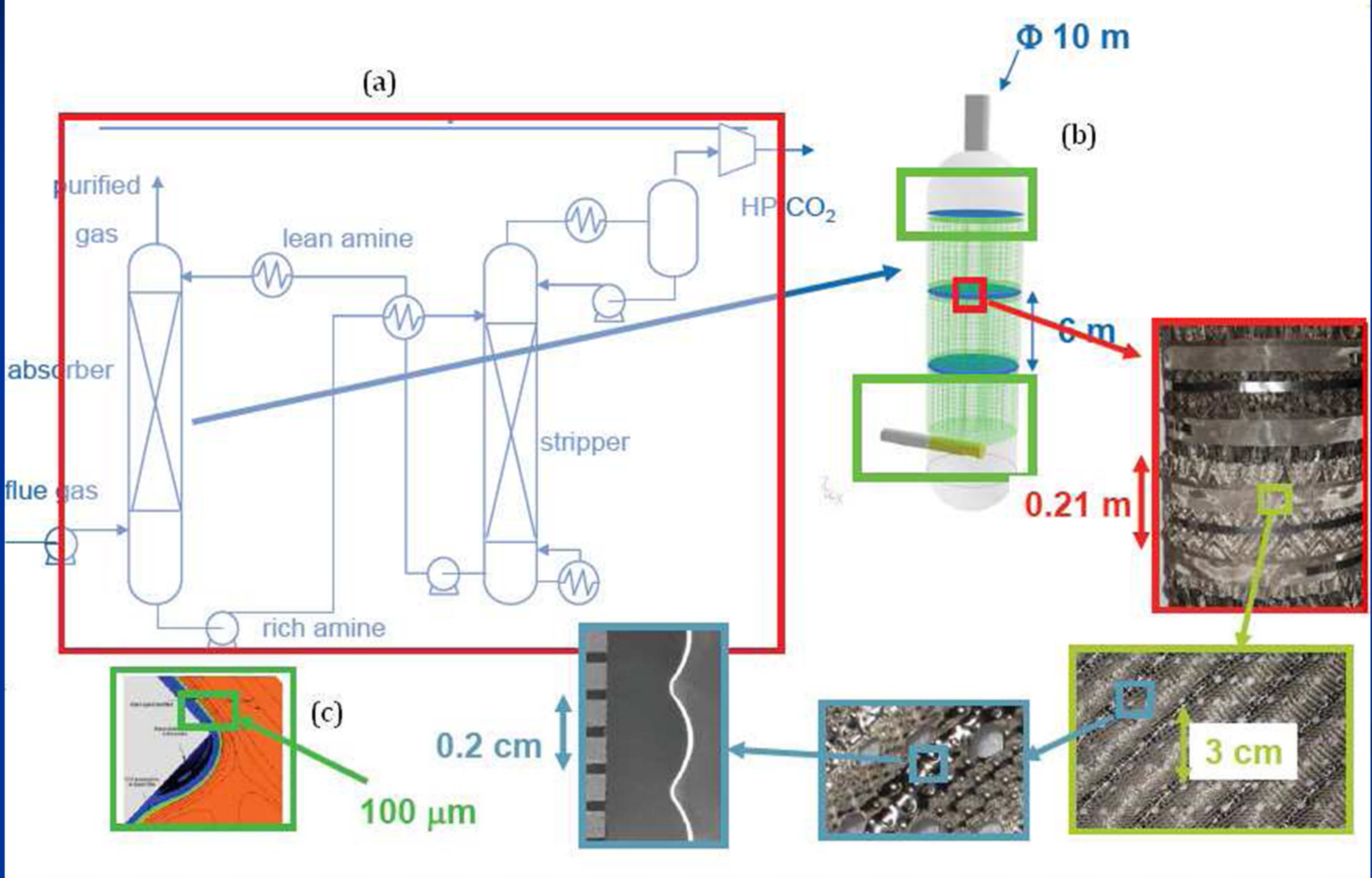




IRMOF-



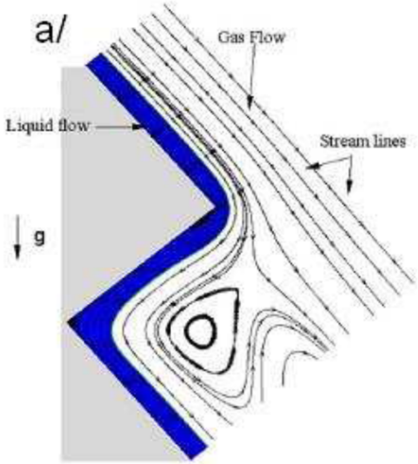
Gas absorption with selective solvents: Capture of CO2 by amines



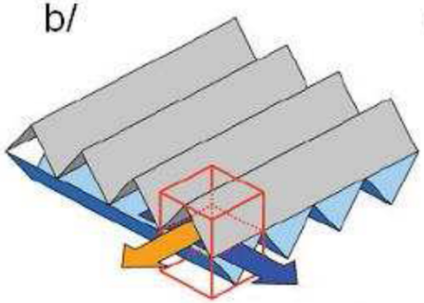
Different simulation scales

- **a/** film de liquide cisaillé par un gaz
- b/ échelle de la cellule élémentaire représentative d'un garnissage structuré
- c/ échelle d'un bloc de garnissage
- d/ échelle d'une colonne (Sulzer Chemtech)

a/



b/

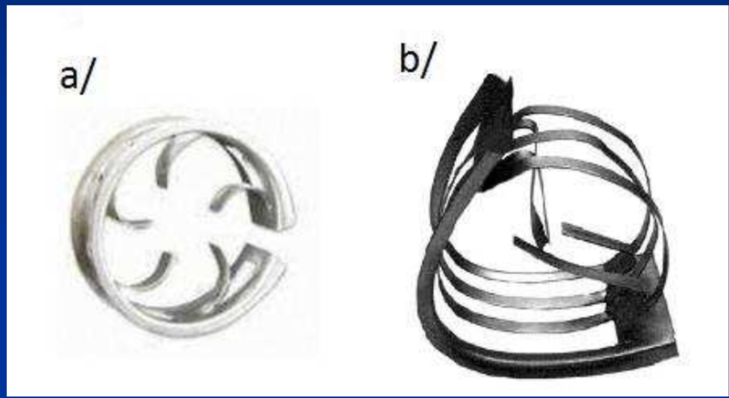


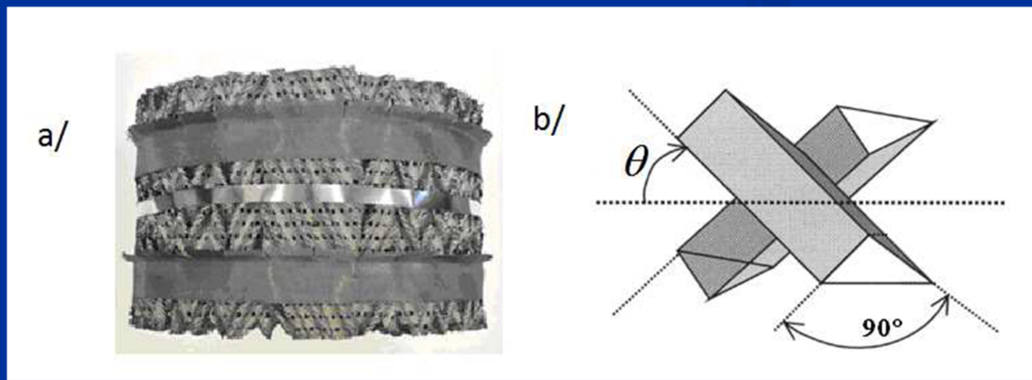
c/

d/

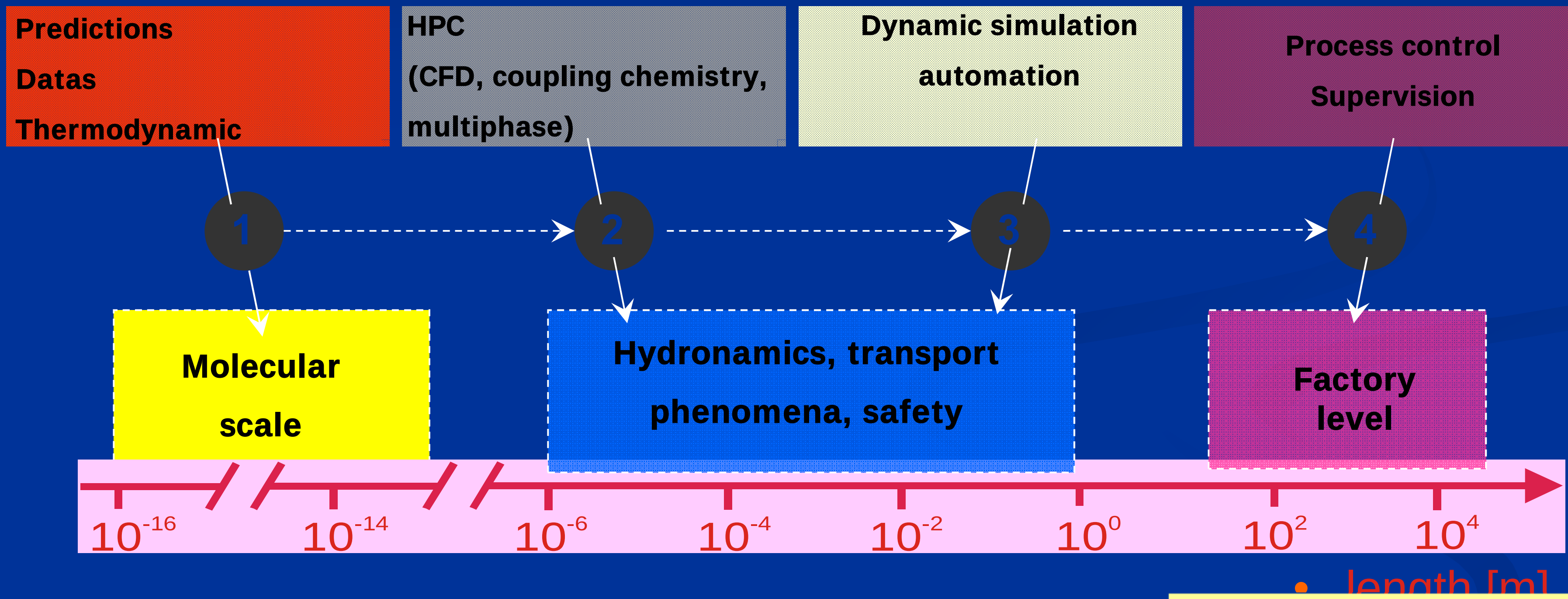
(a) Garnissage cascade Mini Rings (Koch-Glitsh) et (b) garnissage IMTP (Koch-Glitsh)

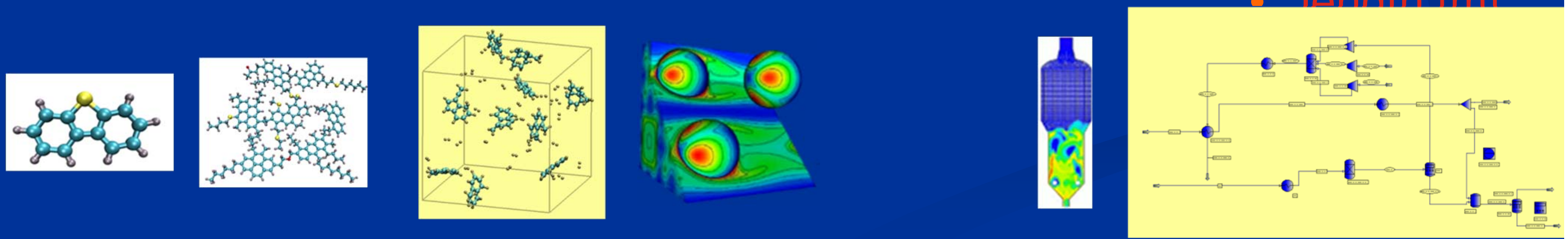
(a) Garnissage structuré M250.X (Sulzer) (b) Structure élémentaire d'un garnissage structuré





Step by step multiscale approach

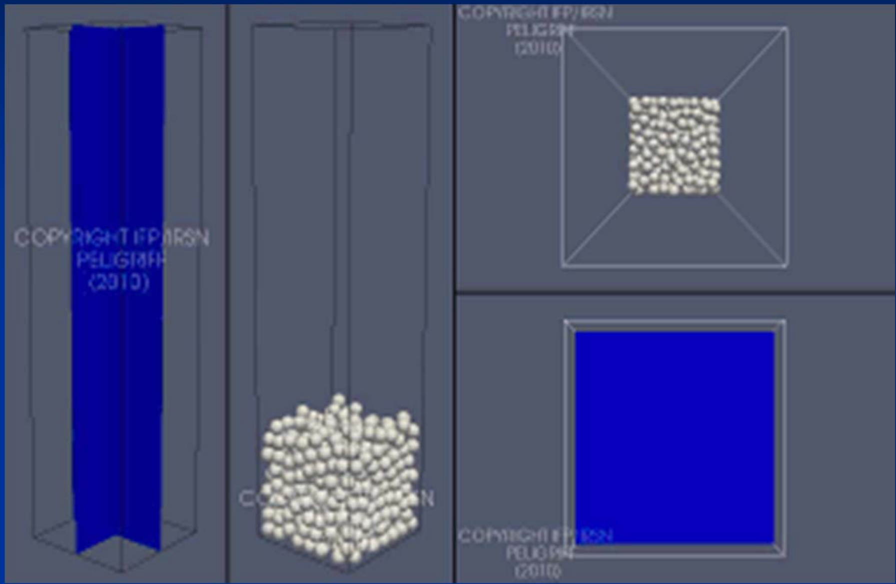




International Conference in

Multiscale Approaches for Process Innovation (MAPI)

(Multiscale Process Innovation)

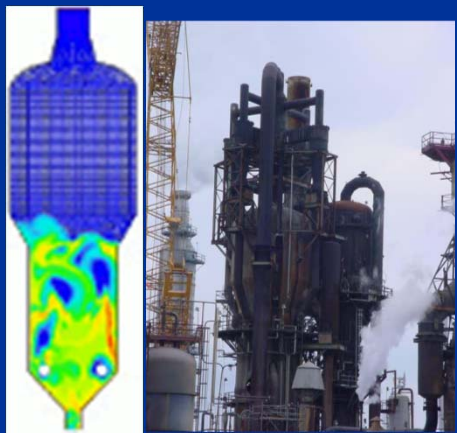


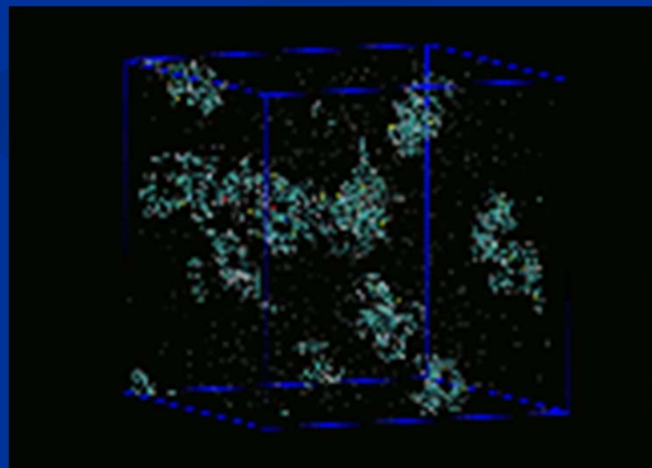
MAPI IFPEnergies nouvelles,

25 – 27 Janvier 2012, Lyon, France

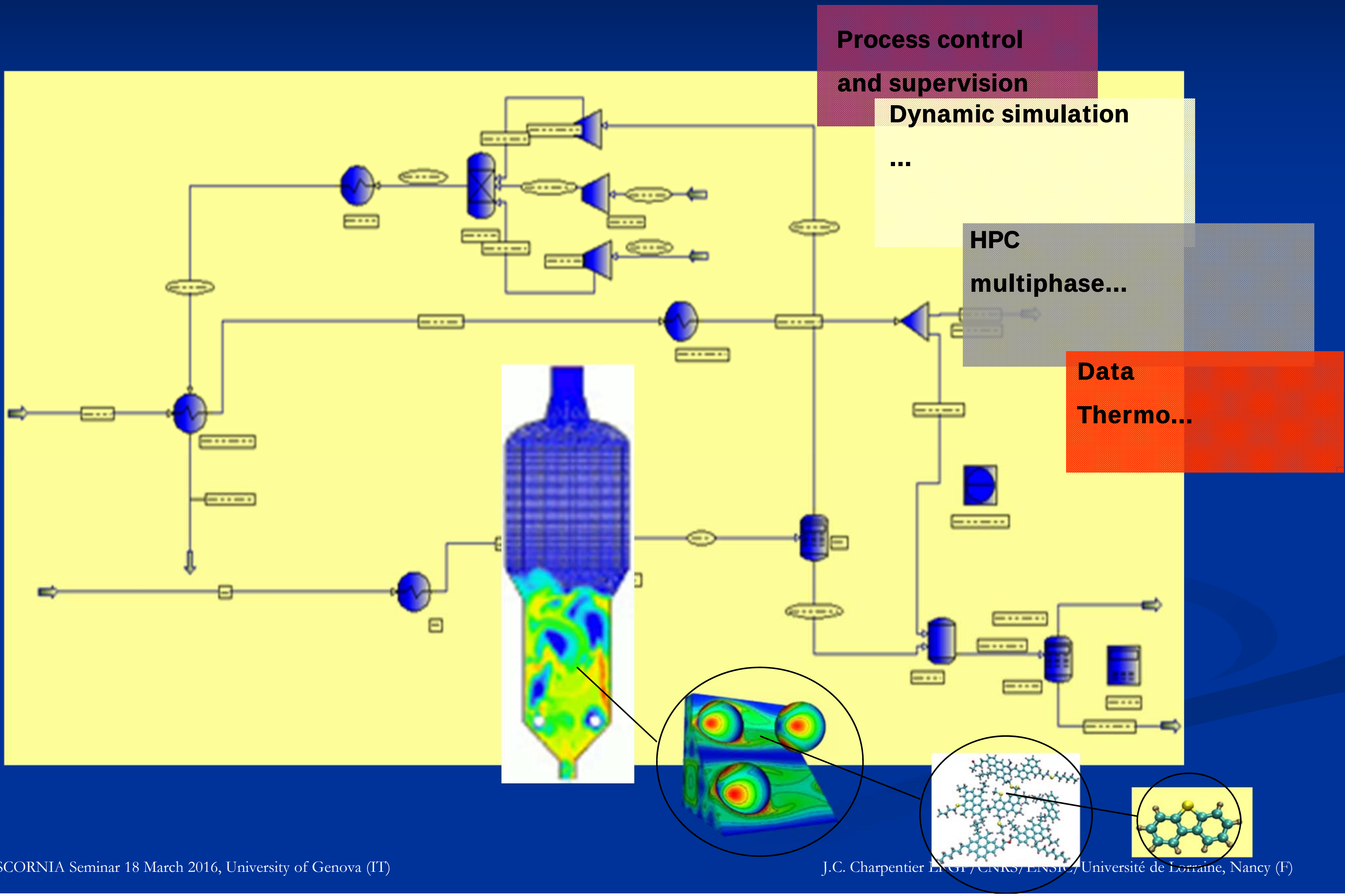
« From detailed feedstock molecular description to multiscale reaction and process modeling »

Oil Gas Science & Technology, 2013, 68, 6, 951-1113





Integrated multiscale approach



REACTION ENGINEERING…

Art *Science*

Past & Present… … Future

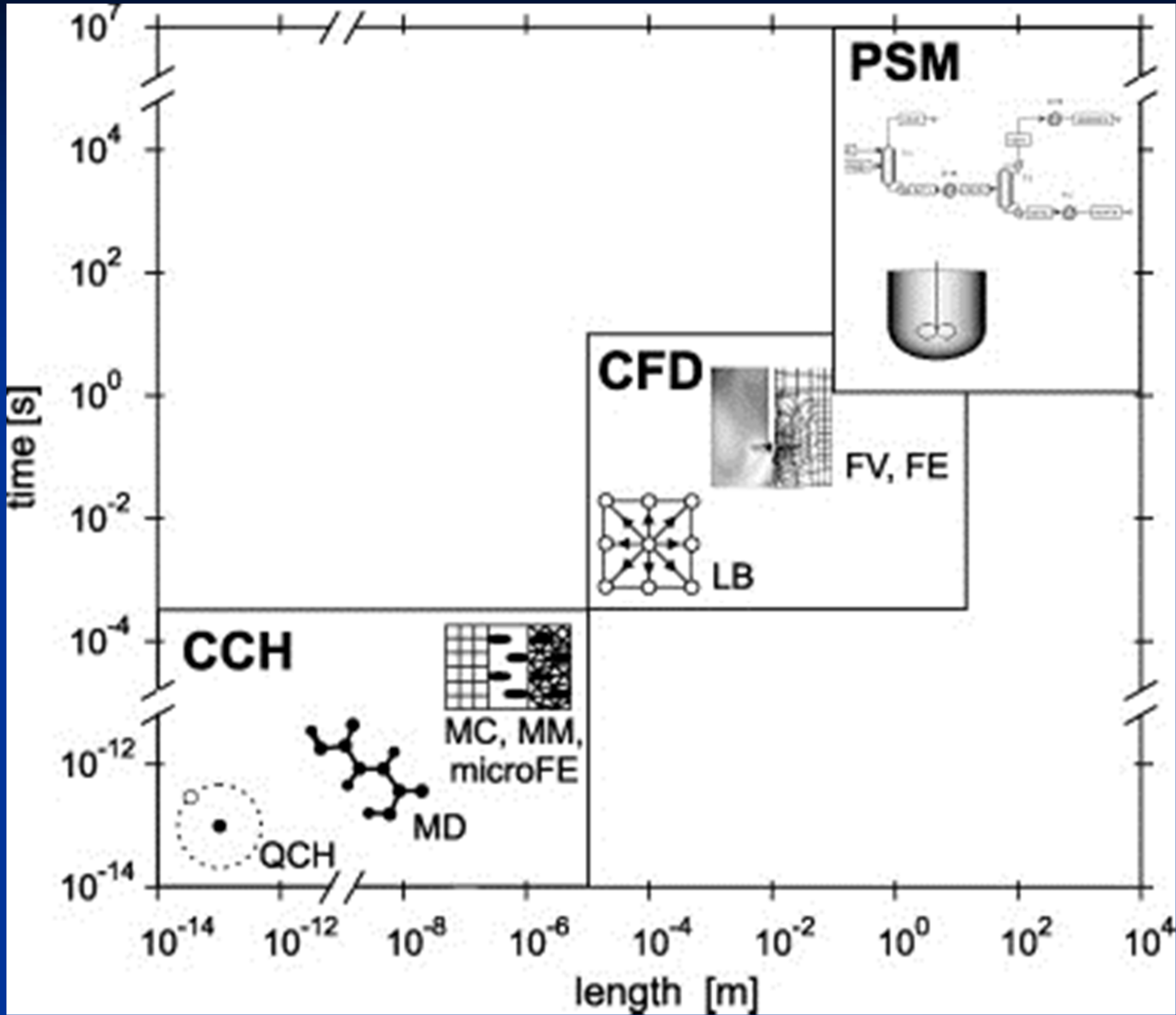
CHEMICAL REACTION ENGINEERING LABORATORY

Washington
WASHINGTON · UNIVERSITY · IN · ST · LOUIS
School of Engineering & Applied Science

S23

But Attention! Attention! Mind!

The modern chemical engineering is not using only simulation and modelization « in silico » for industrial process intensification that produce green products



PSM – process system modeling, CFD – computational fluid dynamics, CCH – computational chemistry, FV – finite volume, FE – finite element, LB – lattice-Boltzmann approach, MC – Monte Carlo,

MM – mesoscale, microFE – micro-finite element, MD – molecular dynamics, QCH – quantum chemistry.

Approaches for Scale-up

Traditional

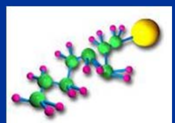
Scale-up in Size →

Emerging (Dream ?)

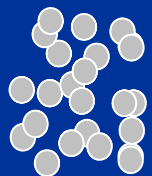
Integration of Knowledge from Catalyst Science and Reaction / Process Engineering

Apply Fundamentals on:

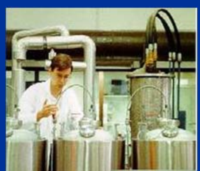
L, m

10^{-12}  Molecular scale

↕

10^{-3}  Eddy / Particle

↕

10^{1}  Reactor Scale

Multi-Scale Analysis

Avancées Advances for multiscale modelisation and simulation in chemical engineering

Actually the bottle necks in simulation and modelization…..

Le goulot d'étranglement pour les bons modèles de systèmes complexes et multiphasiques est la compréhension of physics, chemistry and biology of interactions rather than the refining of mathematics codes

for models, apply EINSTEIN'S citation :

Keep things as simple as possible, but not simpler »

4 Simultaneous tracks for the future of Green Process Engineering with a multiscale approach for the design of the factory of future

1-To increase productivity and selectivity through intelligent operations and multiscale control of processes: i.e. Molecular information engineering
Micro and-Nano and Micro tailoring of porous and cristalline Materials (nanotechnology) ← Green Process Engineering with multiscale approach

2- Design of novel equipment based on scientific principles and new modes of production: process intensification with multifunctional reactors or microstructured reactors (microfluidic) ← Green Process Engineering with multiscale approach

3- Manufacturing end-use properties: development of a multidisciplinary product-oriented engineering i.e. product design and engineering with special emphasis on solids technology and complex fluid processing ← Green Process Engineering with multiscale approach

4- Implement multiscale and multidisciplinary computational chemical engineering modeling and simulation to real-life situations: from the molecule scale up to the overall complex production scale.
Automation, control and safety , LCA ← Green Process Engineering with multiscale approach

Charpentier J. C., Oil & Gas Science and Technologies, 2013, 68, 952-964

1- MODERN CHEMICAL ENGINEERING TO INCREASE PRODUCTIVITY AND SELECTIVITY THROUGH INTELLIGENT OPERATIONS AND MULTISCALE CONTROL OF PROCESSES

a. Intensification of processus

- control local temperature and composition through staged feed and heat supply or removal.

b. Use of microtechnology

- to design synthetic materials with prescribed properties
- to tailor porous materials exhibiting interesting properties
  - for reaction and separation or
  - controlled structure for developing chiral technologies,
  - or for functionalized membranes

...possibility to engineer molecular, microscopic and macroscopic material characteristics i.e.Nanotechnology and functionalised membranes for water treatment application and reaction, for pharmaceutical and biotechnology industry

PROCESS INTENSIFICATION using multifunctionnal reactors

- that couple elementary processus (tranfer - reaction - separation) to increase productivity, selectivity or to facilitate the separation of undesired by-products

➔Catalytic distillation
➔ Absorption with chemical reaction
➔ Chromatographic reactor
➔ Liquid-liquid two phase extractive reaction (or reactive extraction)
➔ Reactive crystallization and distillation
➔ Membrane reactors : MC, MD, membrane emulsification, liquid supported membranes, MOF-based membranes.
➔ Structured packings, monolith, hierarchically structured beds of catalysts

- Or uncoupling elementary processes (nucleation-growth-agglomeration processes, then ad-hoc chemical reaction)

leading to sustainability and society wants i.e., (energy and raw materials savings, safety,…) with

MORE COMPACT, SAFER,
and ENVIRONMENTALLY FRIENDLY SUSTAINABLE TECHNOLOGIES

Hydrocracking : blockbuster HYGO

Process Intensification

with Multi functionnal Reactors

REPSOL Tarragone (Spain)

Hydrocracking : blockbuster HYGO

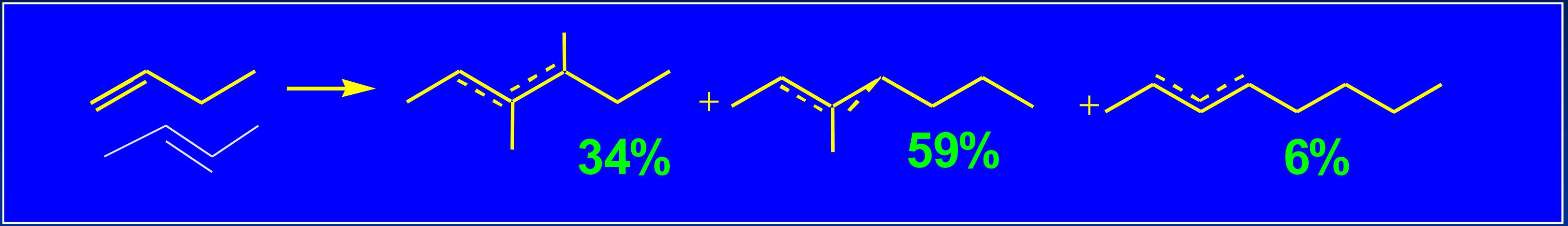
1 catalytic reactor packed with 3 layers of catalysts instead of 3 catalytic reactors

PROCESS INTENSIFICATION USING NEW OPERATION MODES OF PRODUCTION

- operation with new green processes or green media (neoteric solvents:ionic liquids, fluored liquids)

- application of external driving forces (i.e. alternative sources and forms of energy: electromagnetic fields- microwaves, light, plasma technologies…)

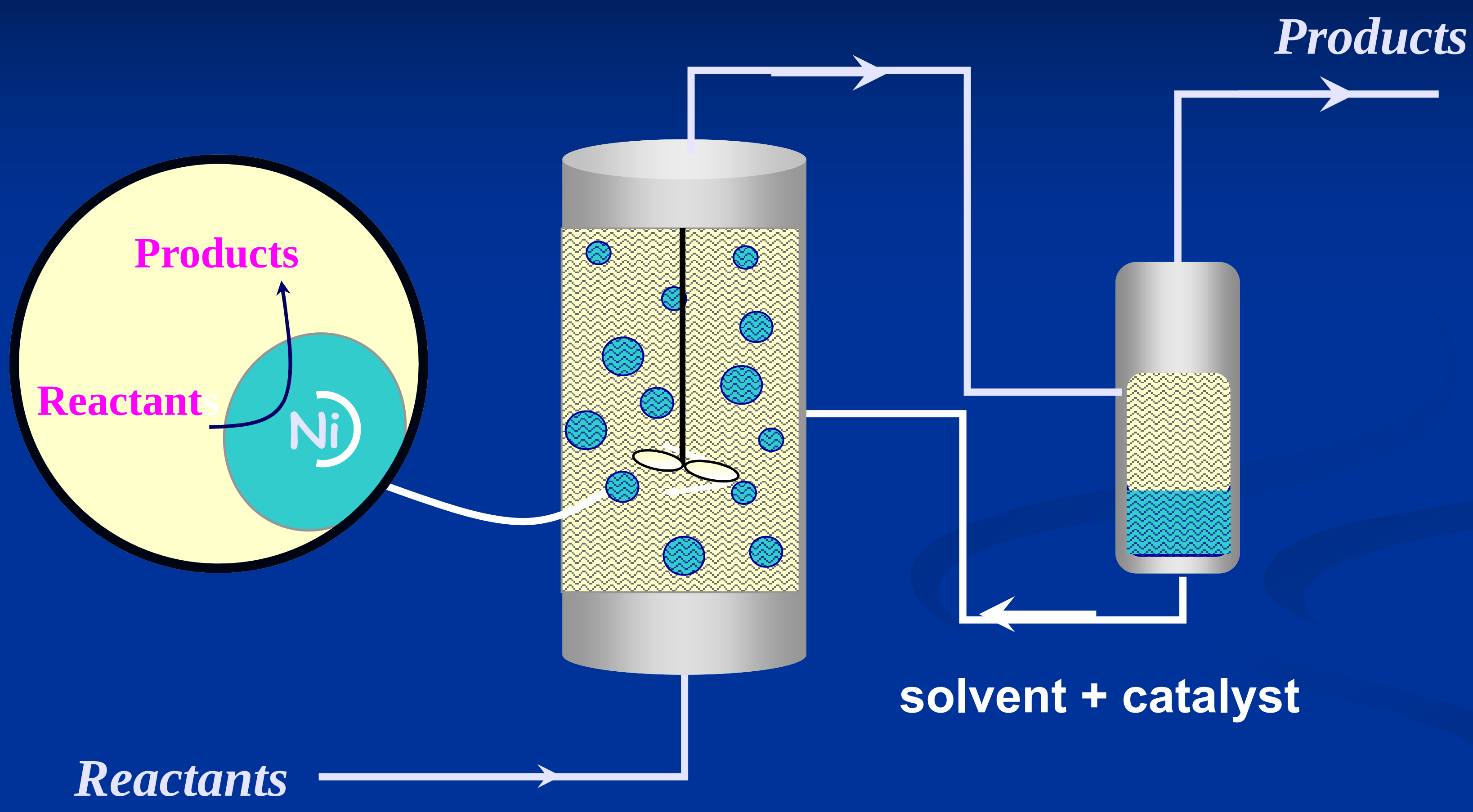
Dimersol Process : for chemistry



Isoctenes (manufactured from **Butene** in using liquid biphasic catalysis with an organic solvent) are used as starting material for PVC plasticizers

0.5 Mt products / year

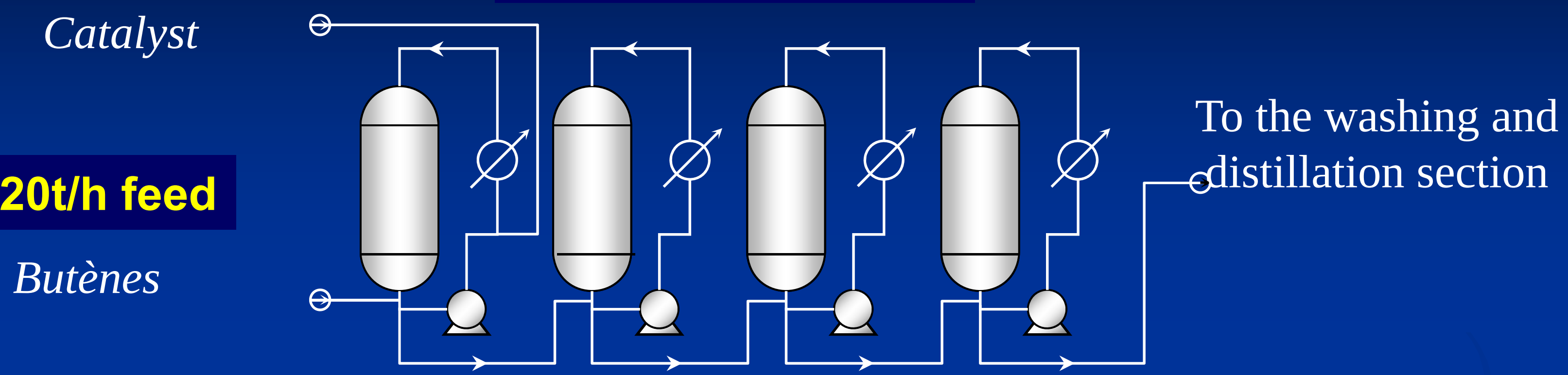
Liquid-Liquid Biphasic Catalysis with non-aqueous ionic liquid



Procédé Dimersol Isooctène (plastifiant PVC) from butène biphasic catalyst (Ni), organic solvant

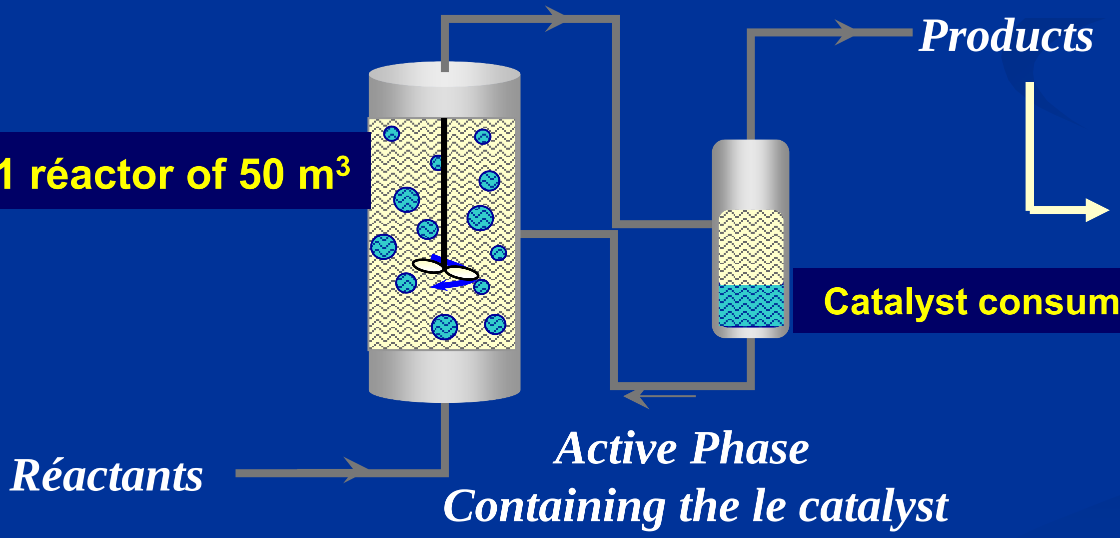
4 reactors of 120 m^3

20t/h feed



Procédé Difasol Isooctène from butène biphasic catalyst (Ni), ionic liquid

1 réactor of 50 m^3



Catalyst consumption (Ni salts) divided by factor 10

Higher yield in dimers

PROCESS INTENSIFICATION

with

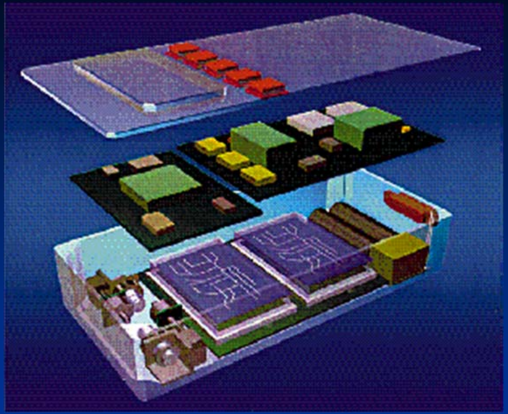
New operating modes

in using

Microengineering and Microtechnololgy

(microstructured mixers and reactors)

J.C. Charpentier LRGP/CNRS/ENSIC/Université de Lorraine, Nancy (F)



Process Intensification with micro structured mixers, separators, analyzers and reactors (microfluidic)

- for the formation of stable emulsions and dispersions

- for the screening of catalyst or pharmaceutical and cosmetic active principles

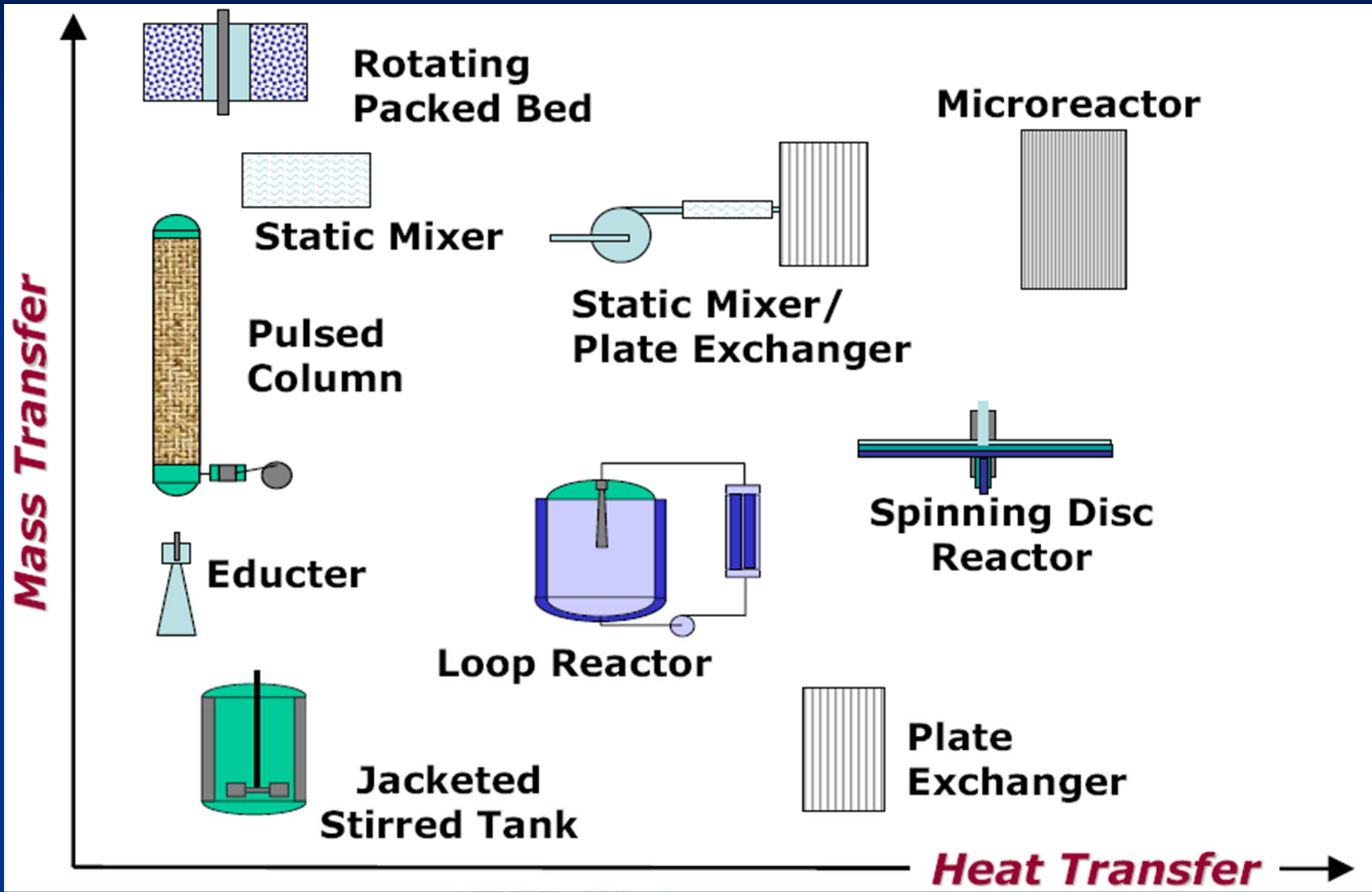
(High throughput Screening)

- and for the Production at laboratory scale and pilot scale

Goals and challenges:

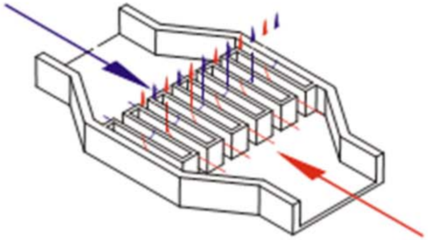
Integration of fluidic, reaction, unit processes, detection, data handling & device control into a single packaged system.

Microstructured reactors for Process Intensification



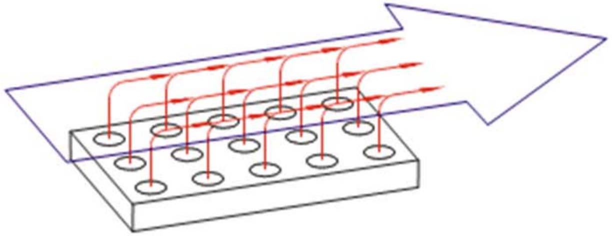
MIXING PRINCIPLES AND CORRESPONDING IMM MICROMIXERS

Lamination for hydro-dynamic or shear decay



Bas-relief induced recirculation flow

Injection in turbulent flow



Interdigital Micromixers

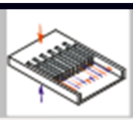
SIMM-V2
SSIMM
...

Caterpillar Micromixers

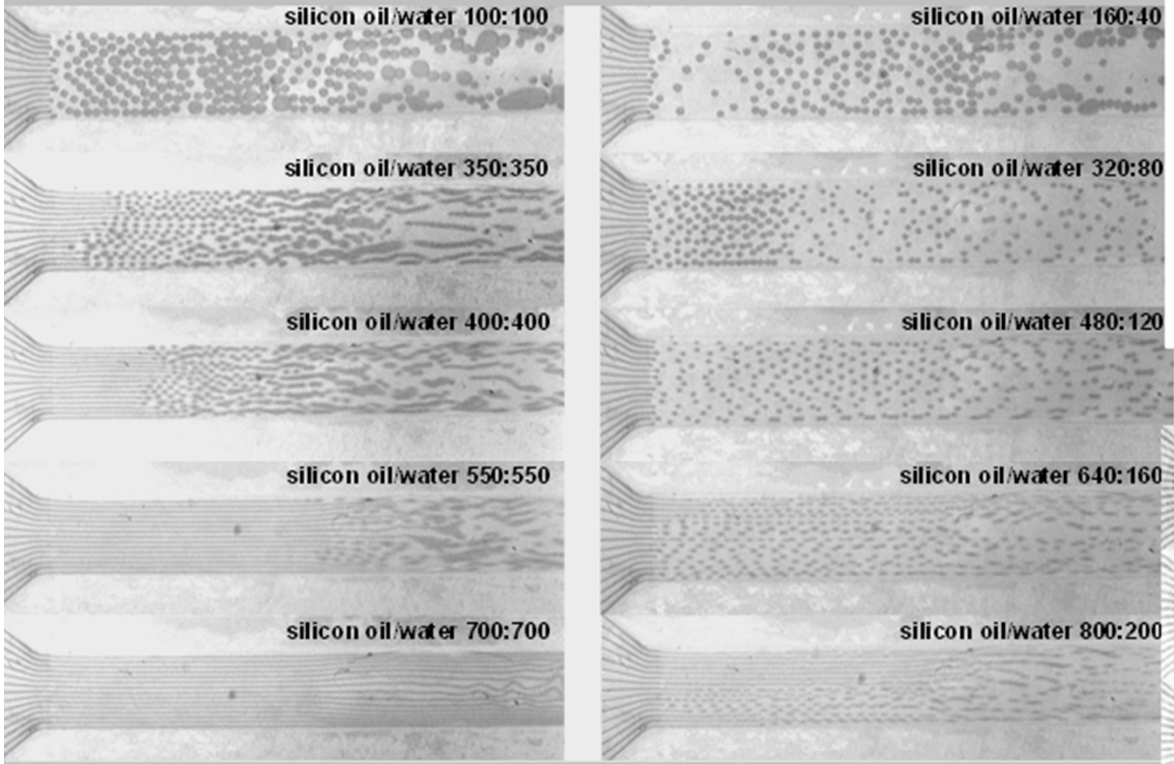
CPMM-R300-V1.2, CPMM-R600-V1.2
CPMM-R1200-V1.2, CPMM-R2400-V1.2
...

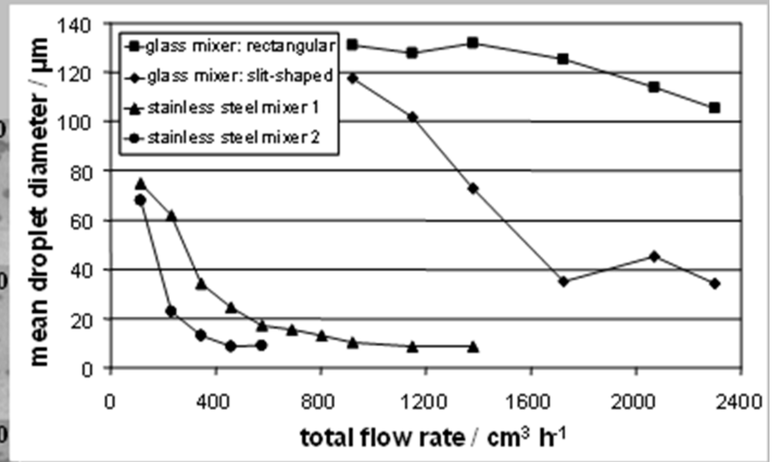
Star Laminator Micromixers

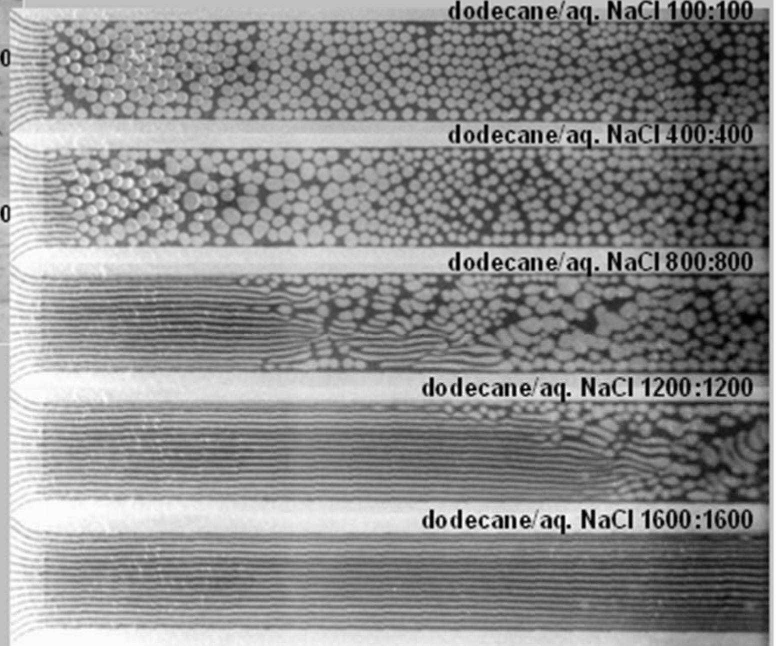
StarLam 15
...



DROPLET FORMATION IN RECTANGULAR INTERDIGITAL MICROMIXERS

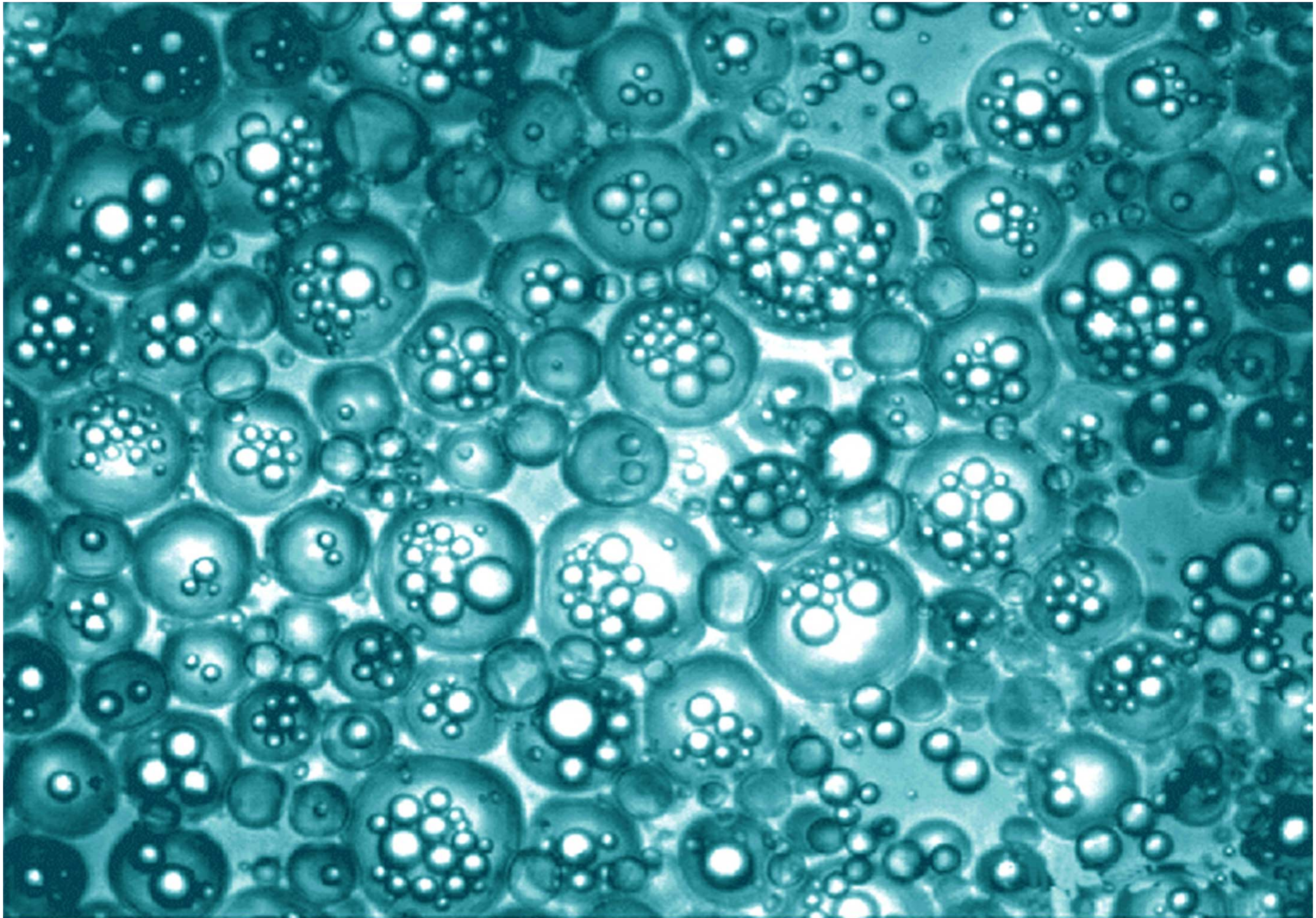






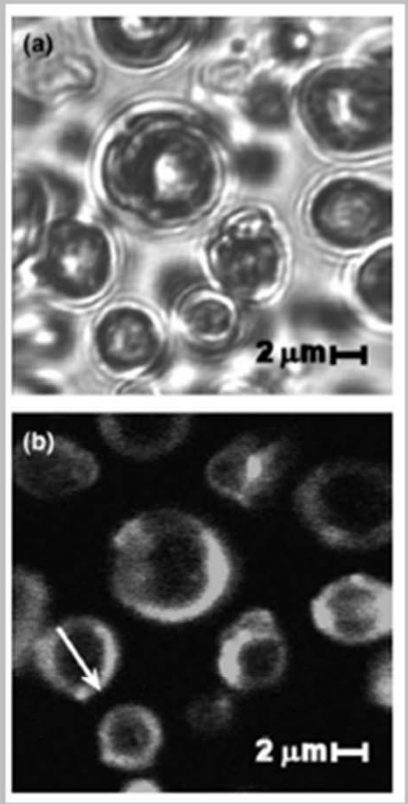
P. Pennemann, S. Hardt, V. Hessel, P. Löb, F. Weise,
Chem. Eng. & Techn. **28**, 3 (2005) 501-508

© IMM, 2006



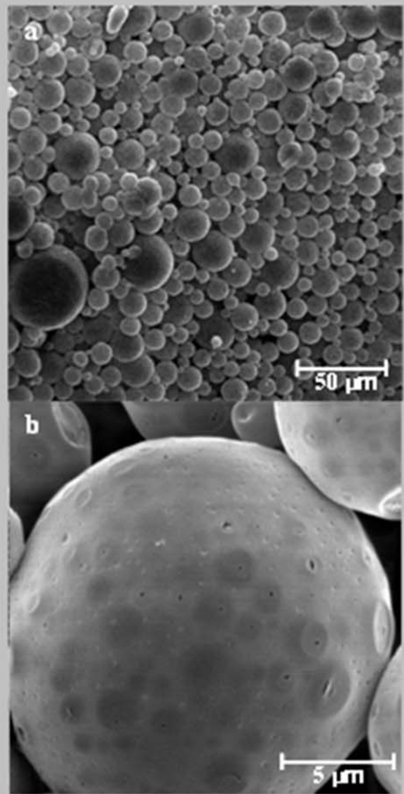
LABORATORY APPLICATIONS OF THE INTERDIGITAL SSIMM MIXER

Microparticles for antigen delivery to dendritic cells



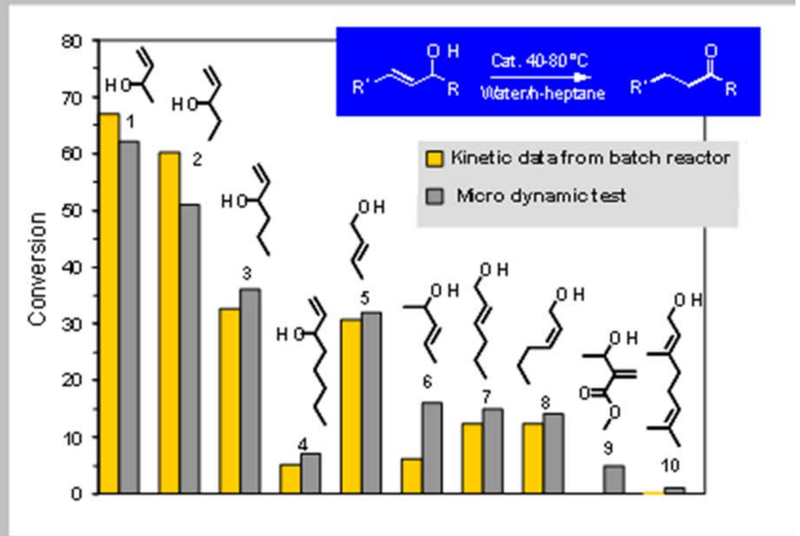
C. Wischke, D. Lorenzen, J. Zimmermann, H.-H. Borchert *Europ. J. Pharmac. Biopharmac.* **62** (2006) 247–253.

Microencapsulation for polymer-loaded particles



S. Freitas, A. Walz, H. P. Merkle, B. Gander, *J. Microencapsulation* **20**, 1 (2003) 67-85.

Transient substrate/catalyst screening of l/l reactions



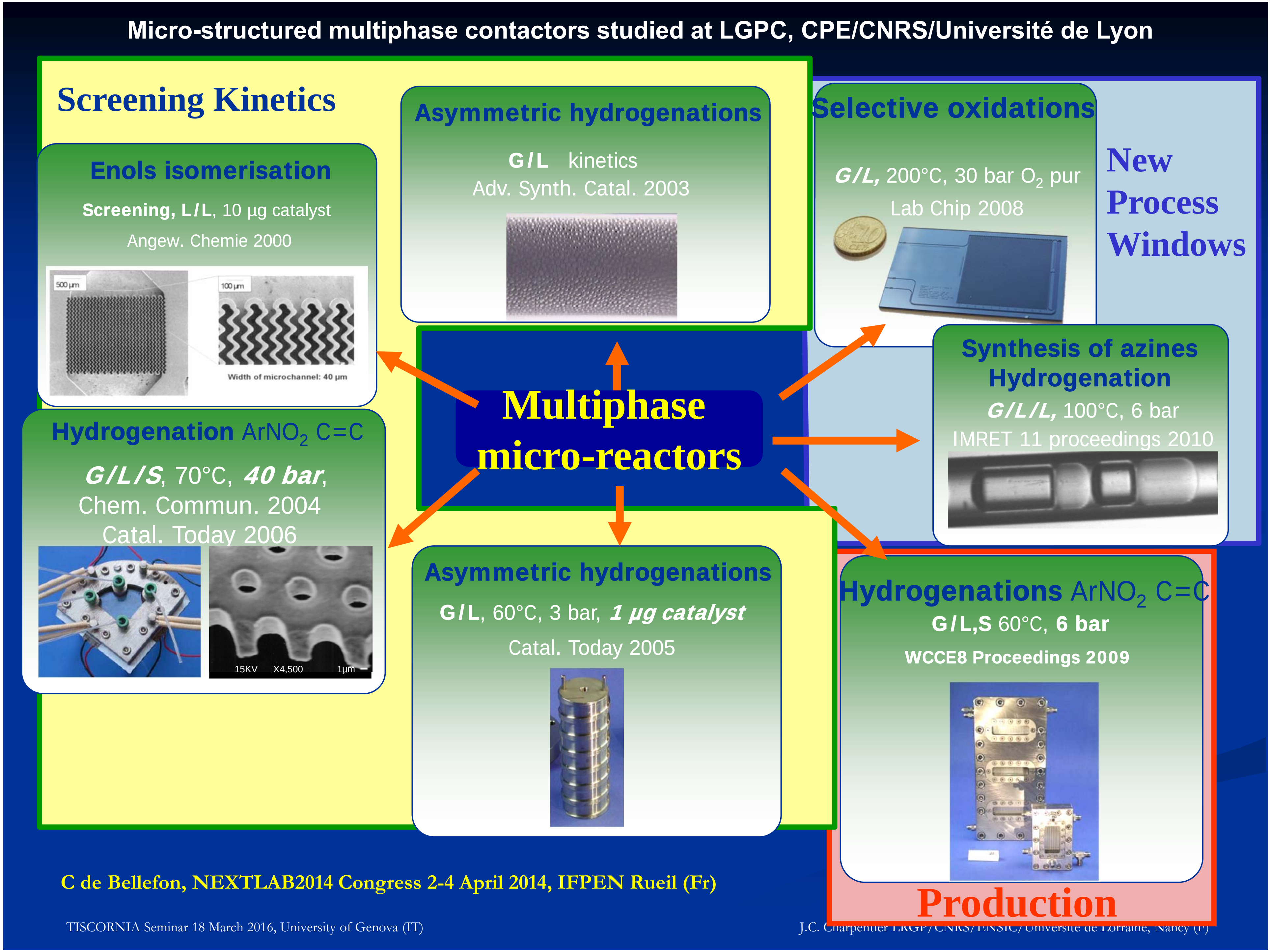
C. de Bellefon, N. Tanchoux, S. Caravieilhes, P. Grenouillet, V. Hessel, *Angew. Chem.* **112**, 19 (2000) 3584-3587.

C. de Bellefon, N. Pestre, T. Lamouille, P. Grenouillet, *Advances in Synthesis and Catalysis* **345** (2003) 190-193.

Réacteur à film tombant avec canal unique pour test de cata

Single channel falling film reactor: Screening of 15 chiral inductors

Single-channel (100*300µm*10cm=3µL) micro-falling film reactor will offer:
- long residence time (30 min)
- very low inventory of material (1-10 µL pulse) for HTS application
- or allow steady-state operations with small inventory of material (50 µL)



Micro-structured multiphase contactors studied at LGPC, CPE/CNRS/Université de Lyon
Screening Kinetics
Enols isomerisation
Screening, L/L, 10 µg catalyst
Angew. Chemie 2000
500 µm
100 µm
Width of microchannel: 40 µm
Asymmetric hydrogenations
G/L kinetics
Adv. Synth. Catal. 2003
Selective oxidations
G/L, 200°C, 30 bar O2 pur
Lab Chip 2008
New Process Windows
Synthesis of azines
Hydrogenation
G/L/L, 100°C, 6 bar
IMRET 11 proceedings 2010
Multiphase micro-reactors
Hydrogenation ArNO2 C=C
G/L/S, 70°C, 40 bar,
Chem. Commun. 2004
Catal. Today 2006
15KV X4,500 1µm
Asymmetric hydrogenations
G/L, 60°C, 3 bar, 1 µg catalyst
Catal. Today 2005
Hydrogenations ArNO2 C=C
G/L,S 60°C, 6 bar
WCCE8 Proceedings 2009
Production
C de Bellefon, NEXTLAB2014 Congress 2-4 April 2014, IFPEN Rueil (Fr)
TISCORNIA Seminar 18 March 2016, University of Genova (IT)
J.C. Charpentier LRGP/CNRS/ENSIC/Université de Lorraine, Nancy (F)

Application de la **technologie microfluidique** (microchannel) non seulement pour le criblage de catalyseurs ou de principes actifs pharmaceutiques ou cosmétiques,

mais

pour la production aux échelles du laboratoire et du pilote industriel

Micro reactors-Current Industrial scenario in 2014

A number of chemical (Clariant, Sweden; SAFC, US; BASF, German; Evonik, German; DSM, US; DuPont, US; Procter and Gamble, US) and pharmaceutical (Schering-Plough, US; Sanofi Aventis, France; Roche, Switzerland; GlaxoSmithKline, UK; Novartis, UK; AstraZeneca, UK) companies are trying to exploit the advantages of microreactors.

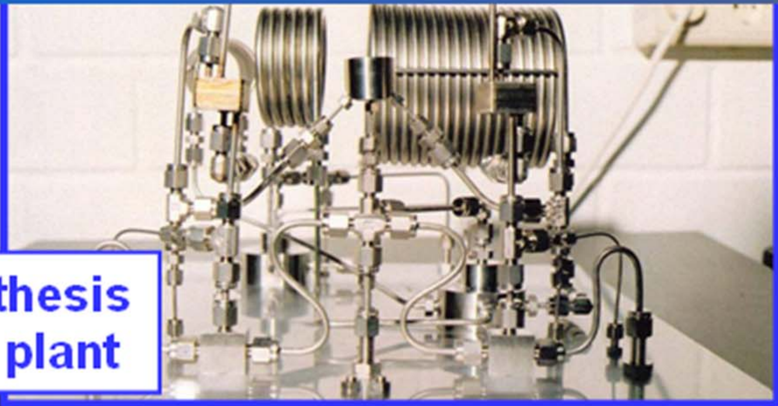
The US-based SAFC uses microreactors to produce about 50 commercial products

US based Corning has developed a microreactor for the production of more than 25 tonnes of a nitration product

Xi'an Huian Chemical, with the help of IMM, Germany, has started producing nitroglycerin in the range of 10 kg/hr at a plant in the middle of China

Recently, Velocys operated a 2 gallon/day BTL microreactor for more than 3,000 hours and achieved productivities of over 1,500kg/m^3/h

TABLE-TOP CMPE PLANTS WITH MICROMIXERS ... FROM LAB TO PILOT ... FROM CHEMISTRY TO CONSUMER GOODS



Organic synthesis bench-scale plant

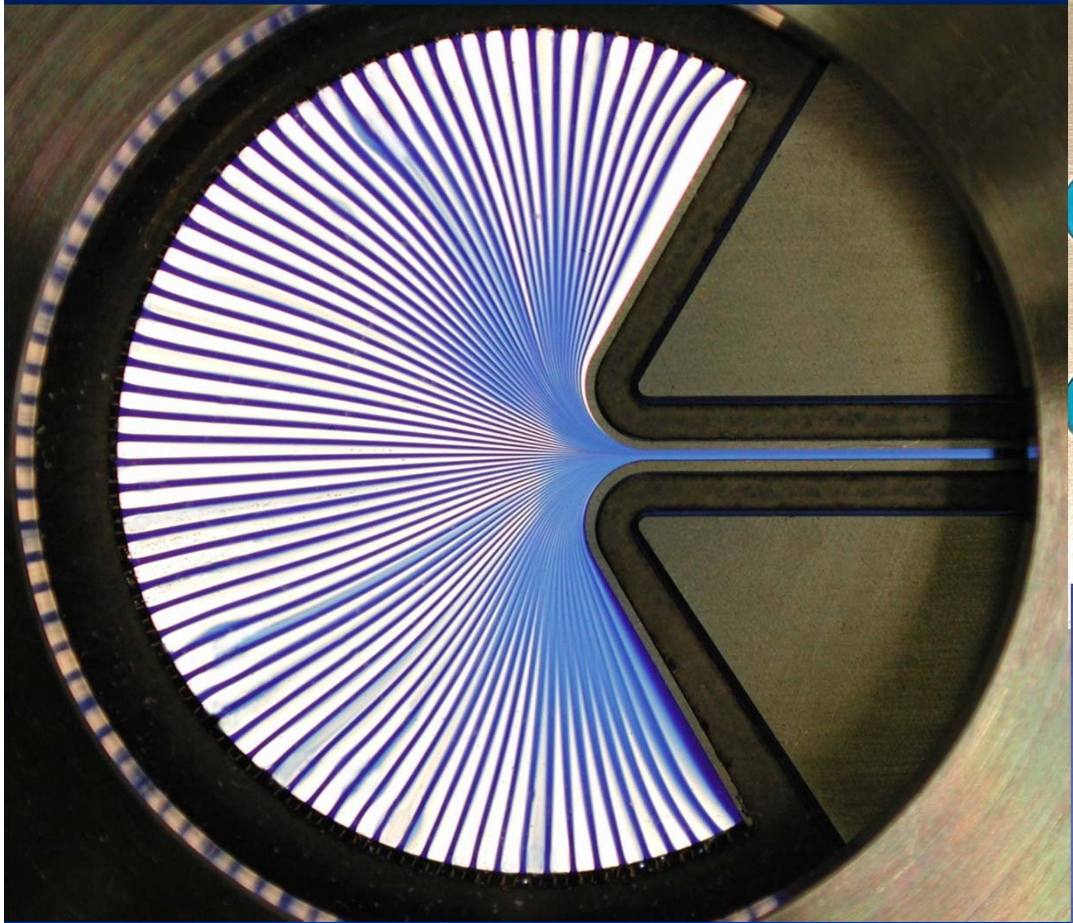
Cream manufacturing plant

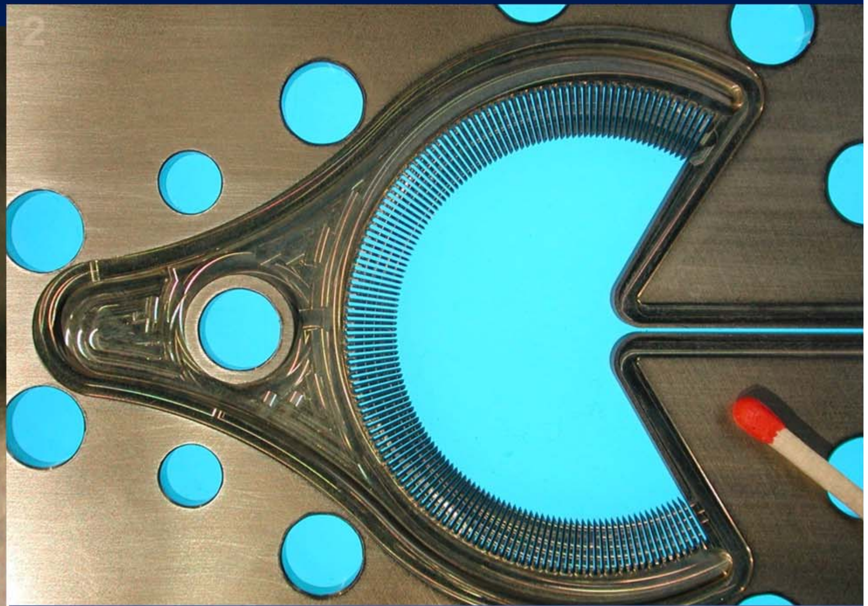
Used by several customers in South Africa, Asia and Europe

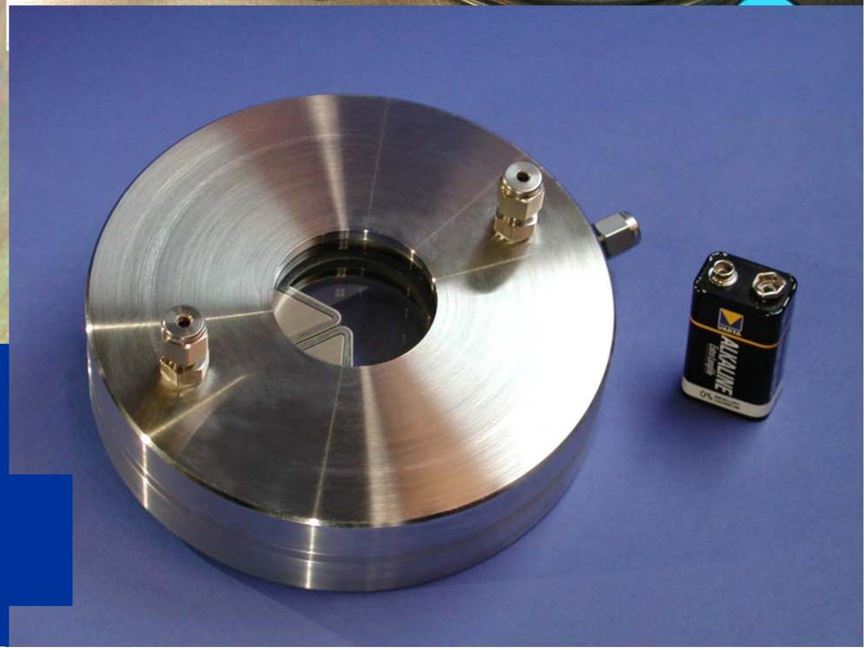
China‘s largest consumer goods producer

MICROMELANGEUR SUPERFOCUS A PLUS LARGE-CAPACITE DE PRODUCTION

(350 l/h; 10 bar)





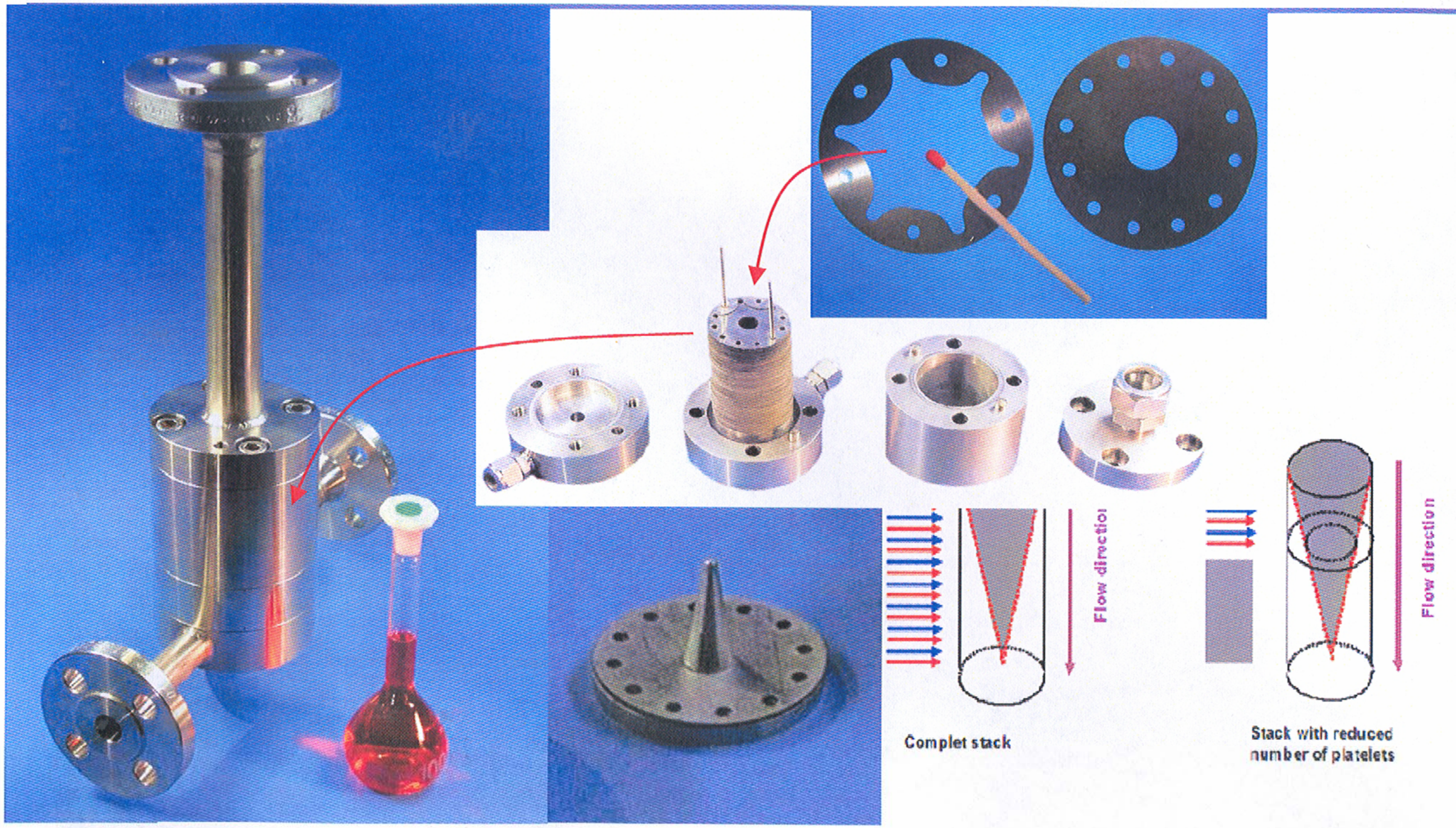


P. Löb et al., *Chem. Eng. Tech.* **27**, 3 (2008) 340-345

Réacteurs Microstructurés: unités de production

avec des Micro réacteurs: technologies micro process

STARLAM MICROSTRUCTURED MIXER – FOR PRODUCTION (≤4000 l/h)



Microstructured mixer part of a production plant at industrial site in Germany and operated at about 3000l/h for some weeks in 2005

B. Werner, V. Hessel, P. Löb,, *Chem. Ing. Tech.* **76**, 5 (2004) 567-574

Chem. Eng. Tech. **78**, 4 (2005) 401-407

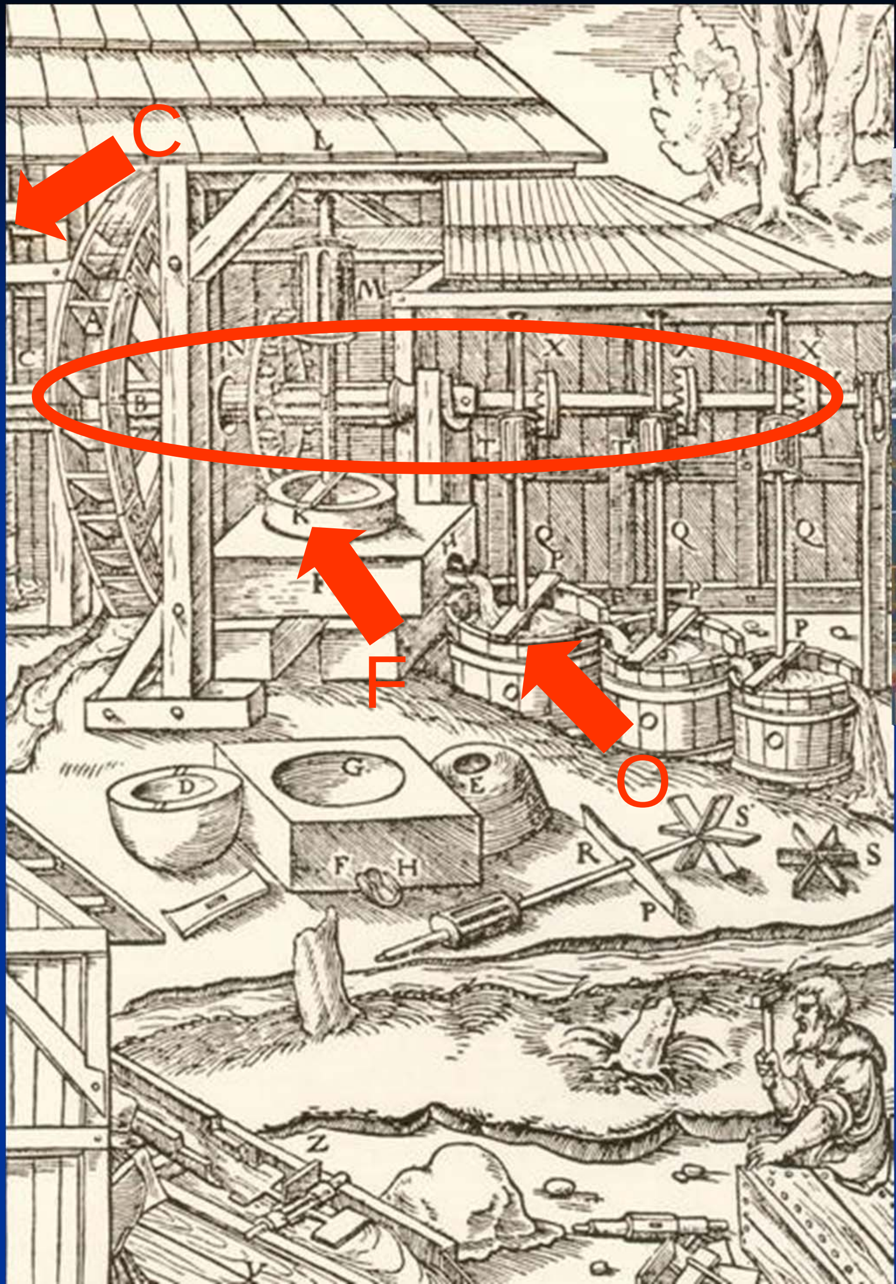
Non seulement aux échelles du laboratoire et du pilote,

mais

Application de la technologie microfluidique (microchannel) à de plus grandes échelles de production

(up to several tons per hours)

WHY?



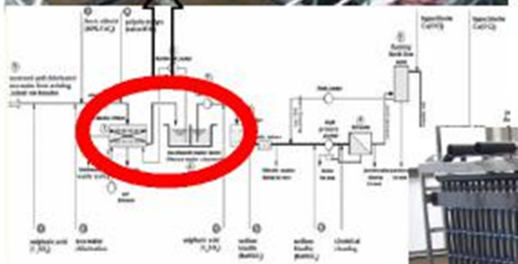
G. Agricola, *De Re Metallica* 1556

Chemical Process Industry, 2006

A CLEAR NEED FOR INNOVATION…

A Stankiewicz (2006)

(a) Une miniature dans G. Agricola, *De Re Metallica,* 1556

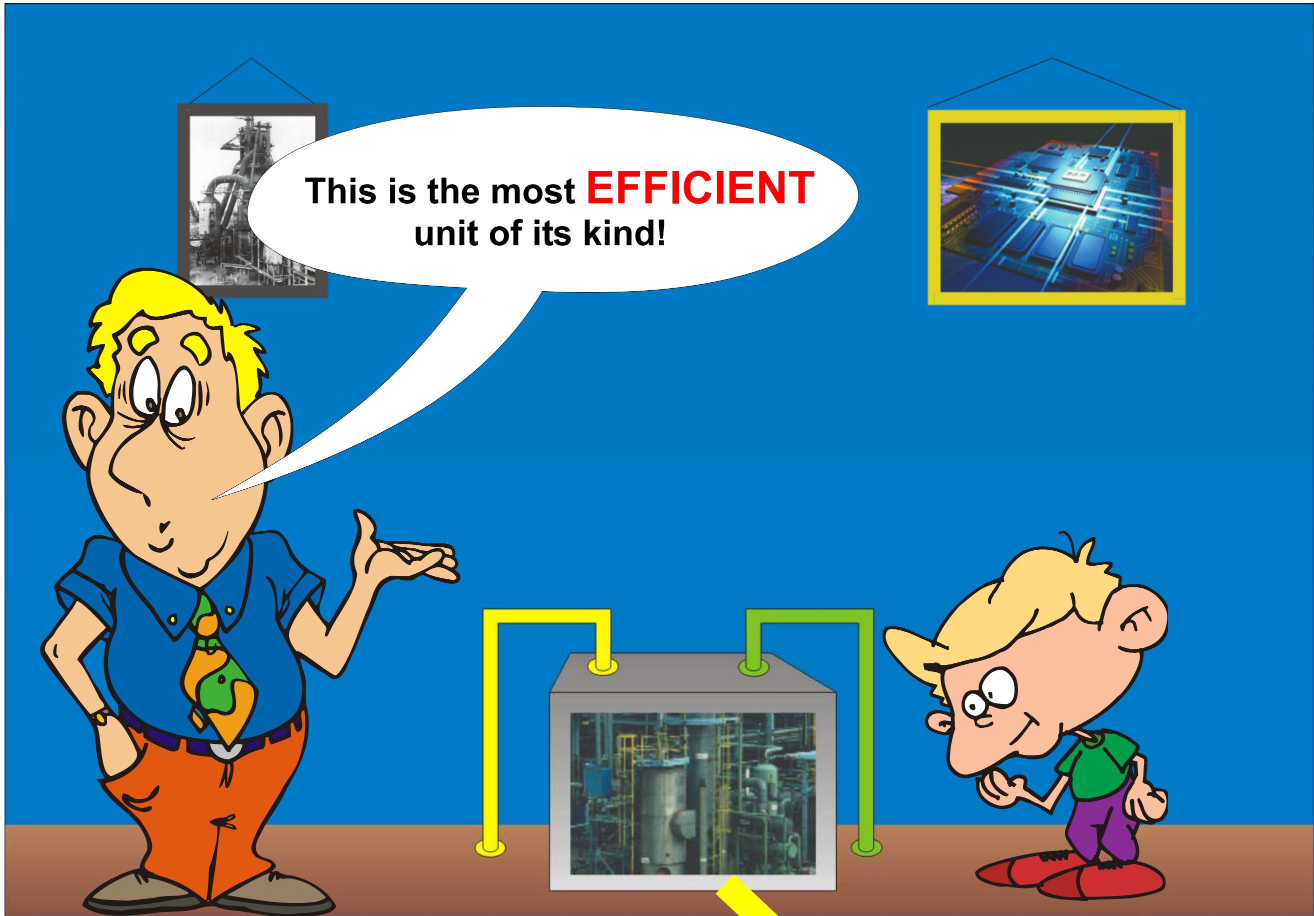


PARADIGM CHANGE: MICROREACTOR BASED PI EQUIPMENT

- 2 l/h
- Research & Education

‘Micro inside’

- 30,000 l/h
- Bulk chemicals within reach



"SHOE BOX" CHEMICAL PLANT

- VISION…

TU Delft 2000

DSM 2005

BECOMING TRUE…

Actually **micromixers and microstructured reactors containing a great number of very sophisticated microstructures are used for production with**

- A few l/h in pharmaceutical, cosmetics, food industries for the synthesis of spécialities or generation of creams, foams and emulsions

- **- Several tens of m3/h for oil and chemical industries, i.e.,**
  - **- Production de polymères**
  - **- Oxydation catalytique partielle du méthane**
  - **- Réformage catalytique à la vapeur avec diminution des émissions polluantes**
  - **- Synthèse Fischer-Tropsch pour convertir la biomasse en carburants**
  - **- Industries de chimie fine en synthèse organique pour la production de produits oxygénés, comme H2O2, Oxyde de Propylène…**

Production with « continuous processes »

.
The intégration of microstructured reactors within existing installations is thus faciliated.

BUT, OBSTACLE!

- **Maturity and economic competitiveness** of these new technologies has to be proven and

- **Conservatism of plant owners** using **BATCH PROCESSES** will not easily accept **CONTINUOUS PROCESSING** solutions offered by **MICROTECHNOLOGY (with microstructured equipments)**

Anyway, miniaturization is one promising approach to achieve this goal !!!

Financing European Policy

is to « exploit the full potential of microprocess technologies » to the realisation

of « new, intensified process and plant concepts for speeding up market penetration, for

enhancing the product life-cycle and improving sustainable production ».

Radical enhancement of the sustainability
of chemical processes is today
technically feasible with **process intensification**
by the development of multifunctional equipment
by using new operating modes,
by application of external driving forces
or by miniaturization of processes

L'Intensification des Procédés pour la Sécurité des Procédés:

SMALLER
is
SAFER!

Bhopal, December 3, 1984

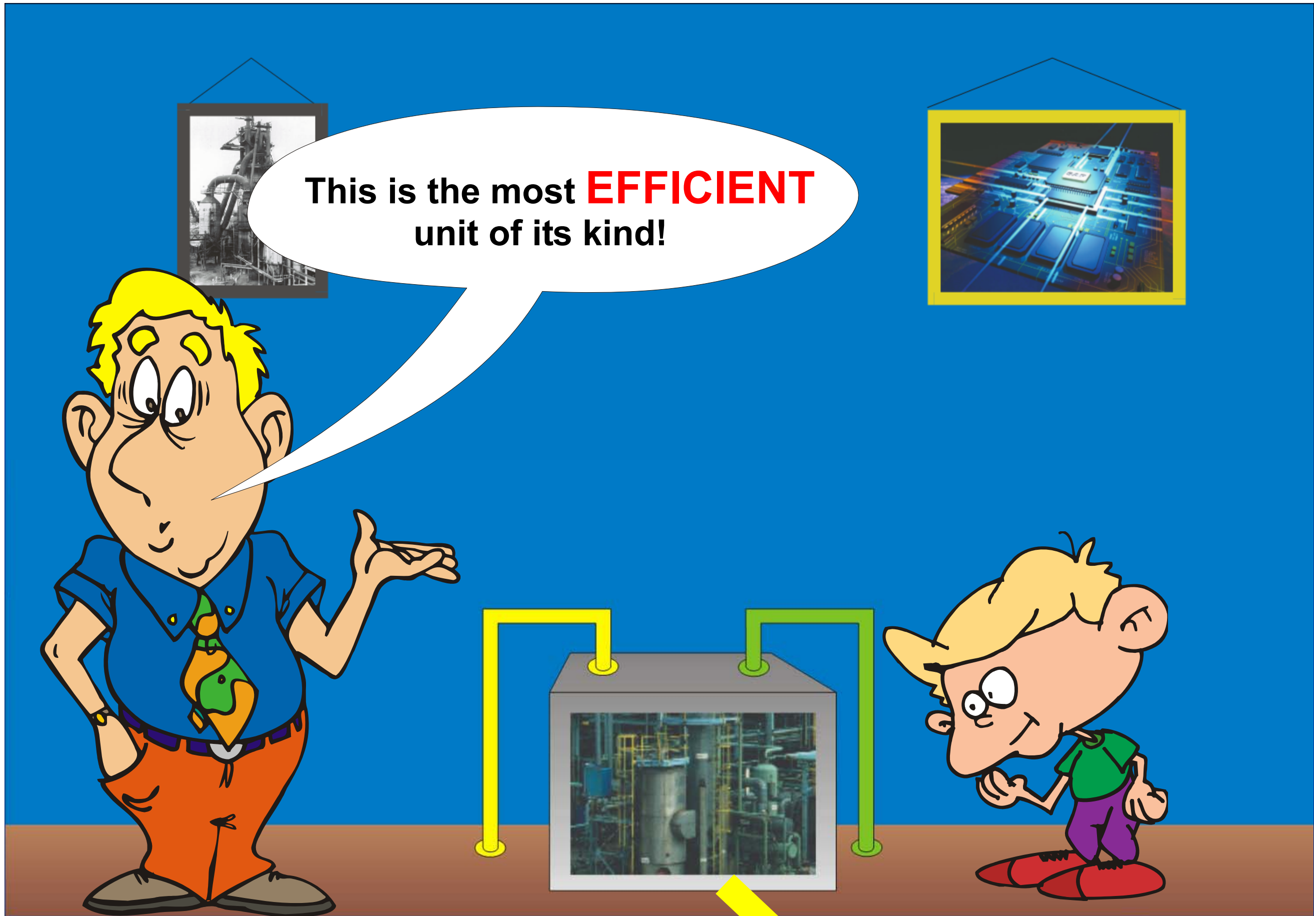
BHOPAL LESSON:

The disaster could have been avoided!

Union Carbide design – 41 tons of methyl isocyanate (MIC)

PI design – less than 10 kg of MIC

(D. Hendershot, CEP, 2000)



“SHOE BOX” CHEMICAL PLANT

- VISION…

TU Delft 2000

DSM 2005

BECOMING TRUE…

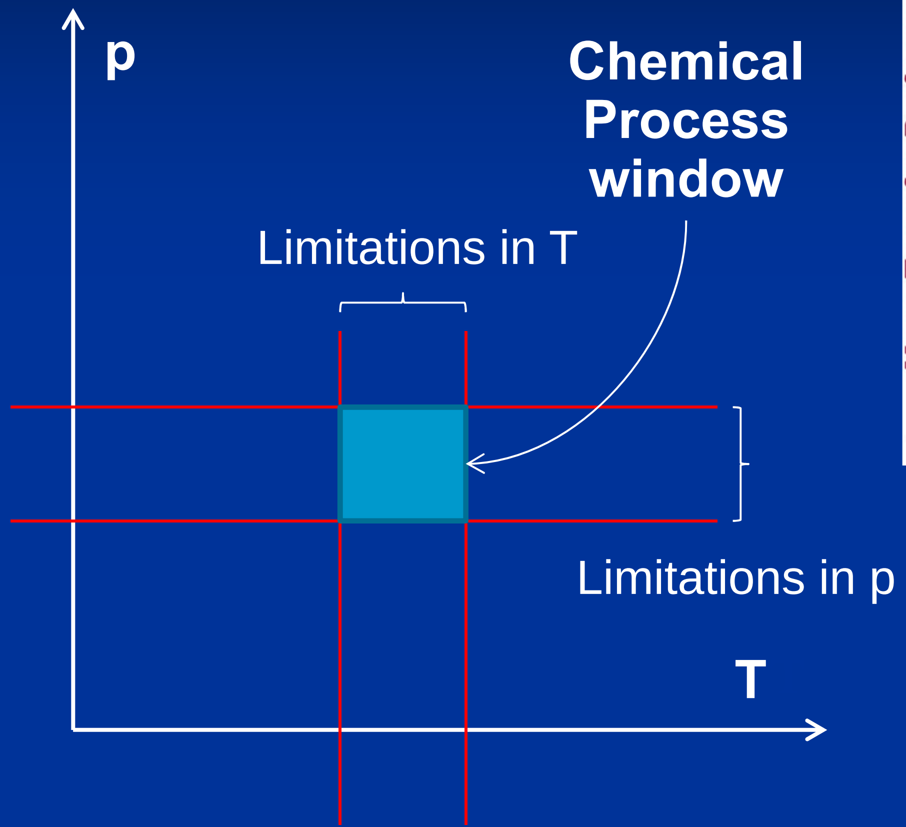
Process Intensification Reactors concerned with Micro Flow Chemistry and Process Technology

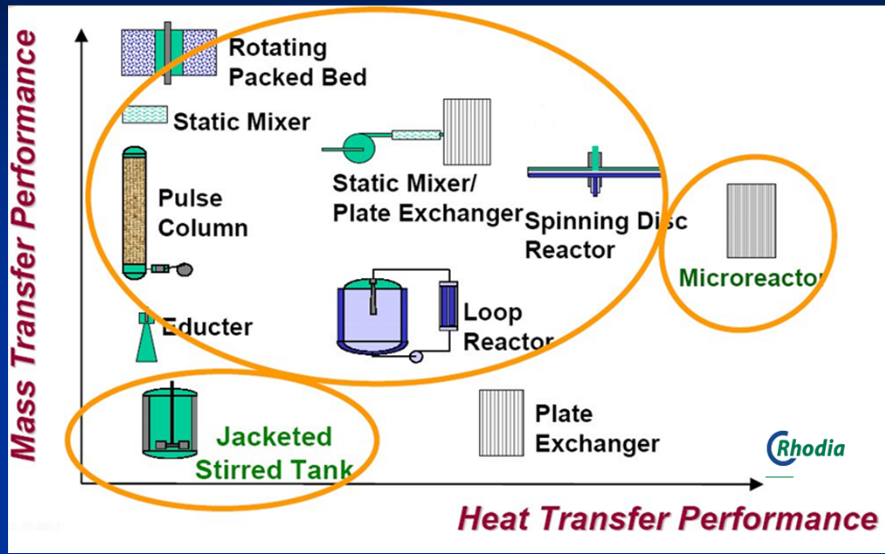
Flow Chemistry Transferred to Industrial Plant Scale

Up to **Modular Compact Container Plant**

PLANT IN A BANANA CONTAINER

WIDENING OF CHEMICAL WINDOWS





Stouten et al. Aust. J. Chem. 66 (2013) 121
Hessel et al. ChemSusChem 6, 5 (2013) 746
Hessel et al. Chem. Eng. Sci. 66 (2011) 1426
Illg et al. Bioorg. Medic. Chem. 18 (2010) 3627
Hessel Chem. Eng. Technol. 32 (2009) 1655
Hessel et al. Energy Environ. Sci. 1 (2008) 467
Hessel Curr. Org. Chem. 9 (2005) 765

- **The microreactor instrumentation has widened engineering windows for process intensification**
- **Question is: can it widen chemical windows? Novel Process Windows (NPW) for process intensification**

Novel Process Windows (NPW)

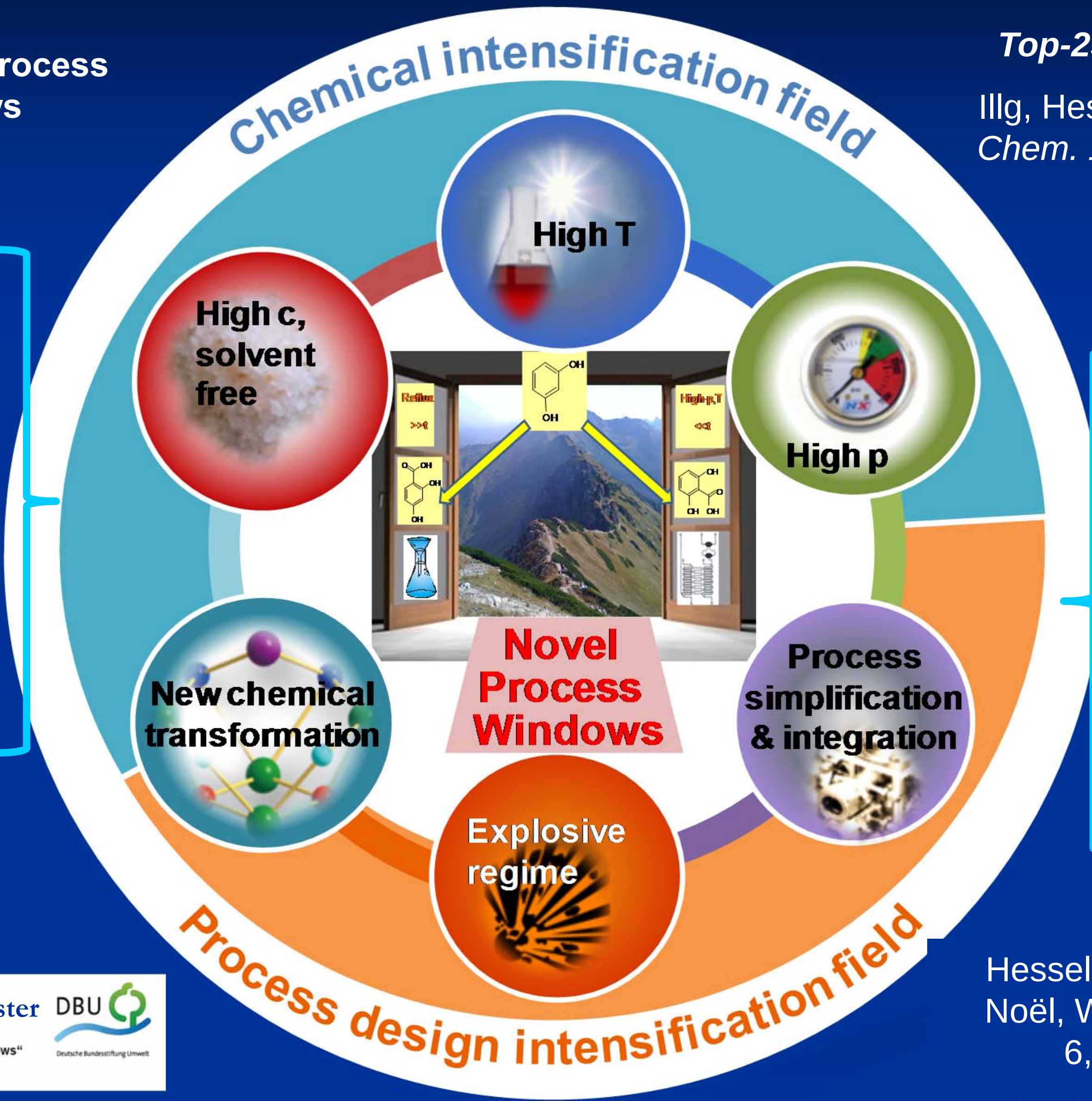
Microreactor-enabled Process Intensification

Novel Process Windows

Top-25 cited paper on NPW

Illg, Hessel, Löb, *Bioorg. Medic. Chem. 18, 11 (2010) 3627-4154*

Activate
Confine
Orient
Boost

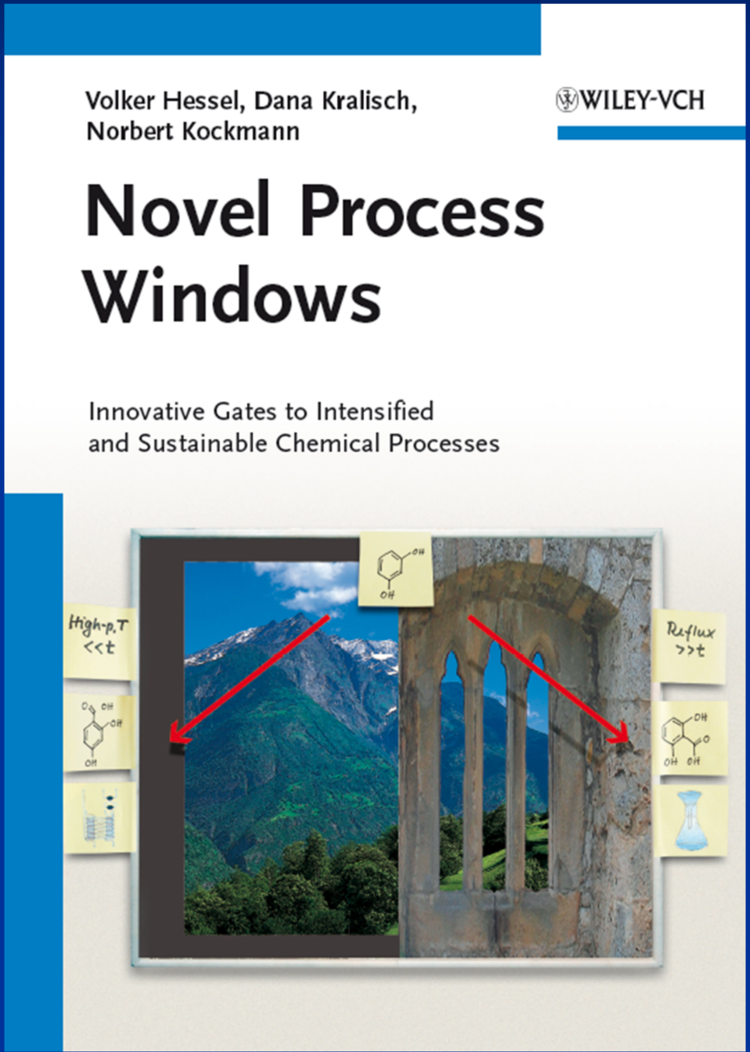


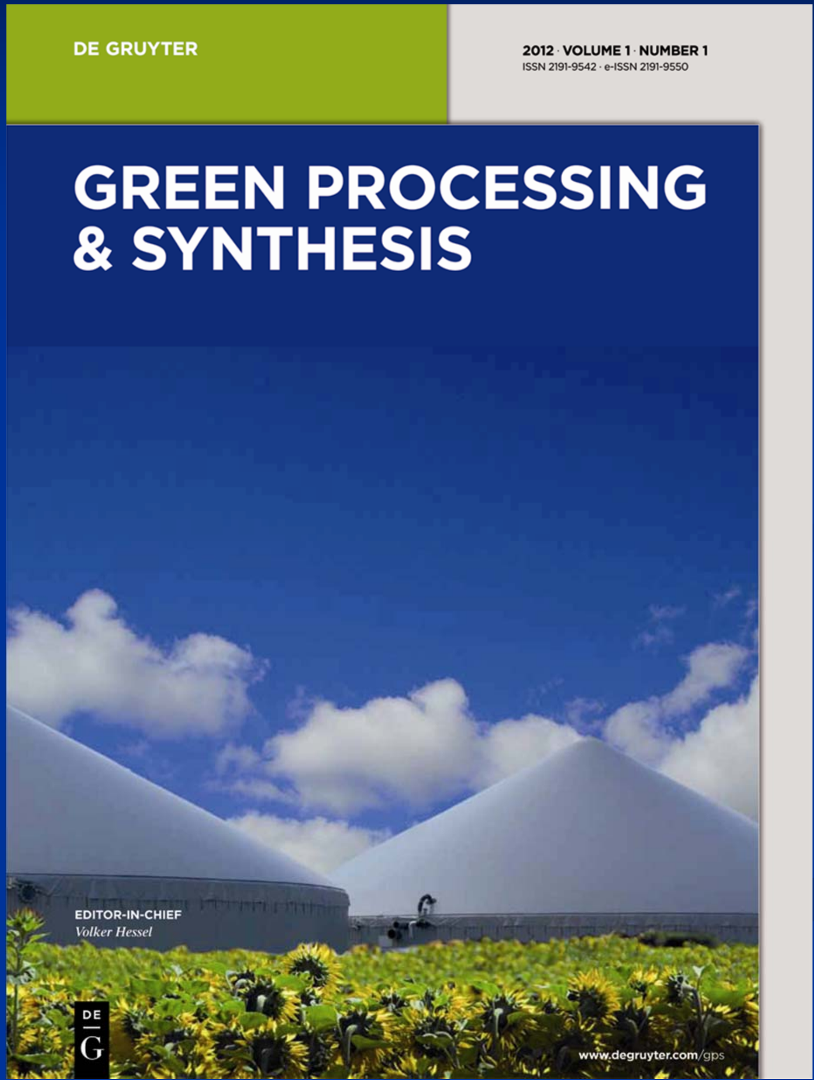
Simplify
Integrate
Synergize
Minimize

Hessel, Kralisch, Kockmann, Noël, Wang, ChemSusChem 6, (2013) 746-789.

NPW Research Cluster
Forschungscluster „Novel Process Windows"

Book Novel Process Windows
Green Processing & Synthesis





Novel Process Windows Generate Opportunities for Coming Projects

• **NPW-Activation for Industrial Demonstration** (EU Future Factory projects)

- **high-T, safety: soybean oil epoxidation (Mythen)**
- **supercritical, cat.: biodiesel conversion (Chemtex)**
- **hydrodynamics, high-c: anionic polymerization (Evonik)**

• **NPW-Process Design for Industrial Demonstration** (EU Future Factory, ERC)

- **process integration: cascaded & telescoped synthesis (Rufinamide, OmniChem)**
- **process simplification: direct synthesis (adipic acid, DSM)**
- **process integration: purification (hydrogenation, Sanofi)**

• **Plants: Standardized production platforms (Evotrainer) and modular plants (F3)**

- **GMP-type Evotrainer**
- **Cash-flow analysis for Evotrainer for 3 business cases**

Process Intensification reactors:
PLANT IN A BOX

Process Intensification:
The first plant in a box

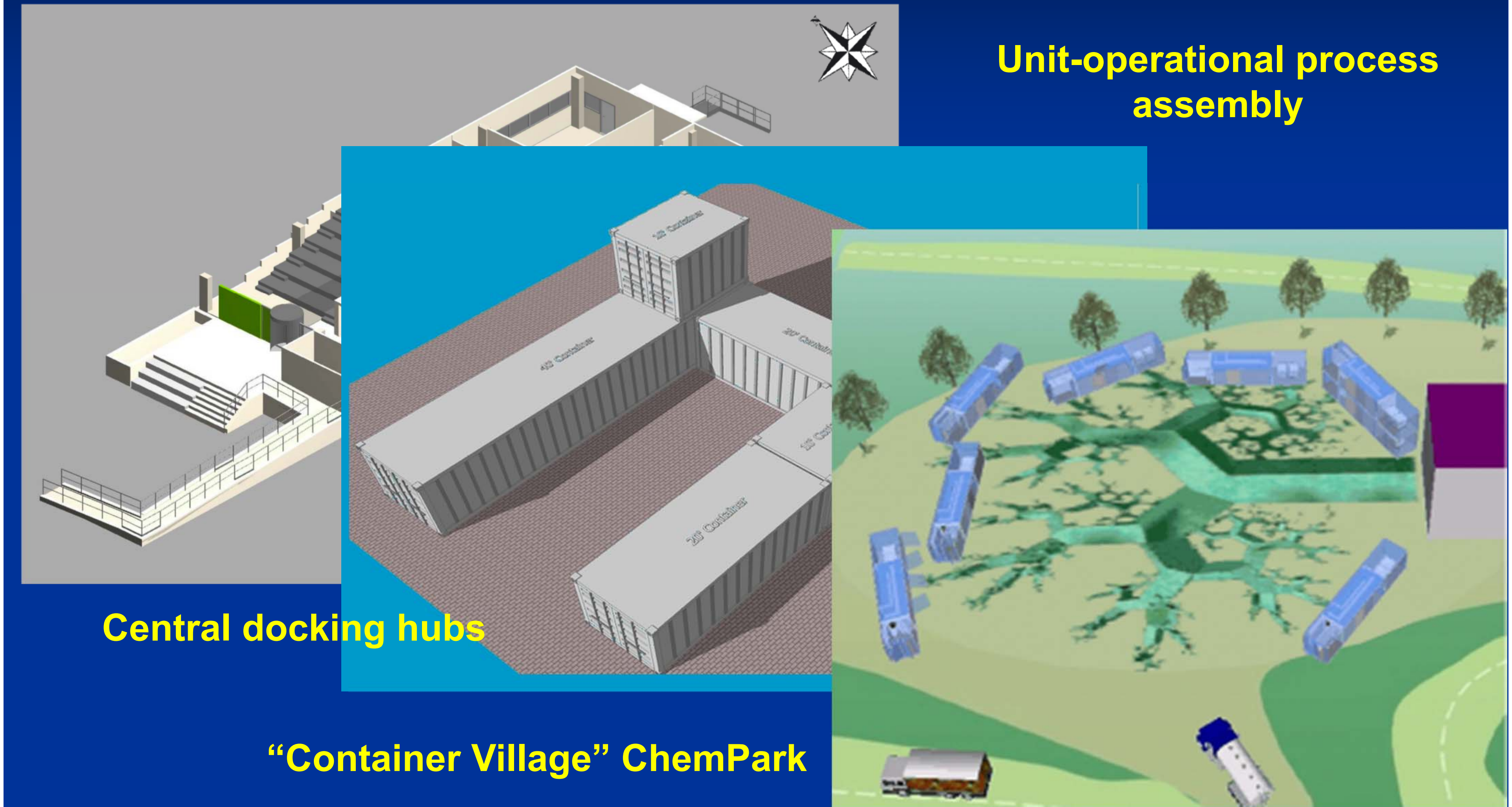
From a simple banana container
to a
multifunctional modular concept

Dr. Juergen Lang
Hanes Richert
Evonik Industries AG

EVONIK INDUSTRIES

Building a Process
or Plants in Boxes ??

Unit-operational process assembly



Central docking hubs

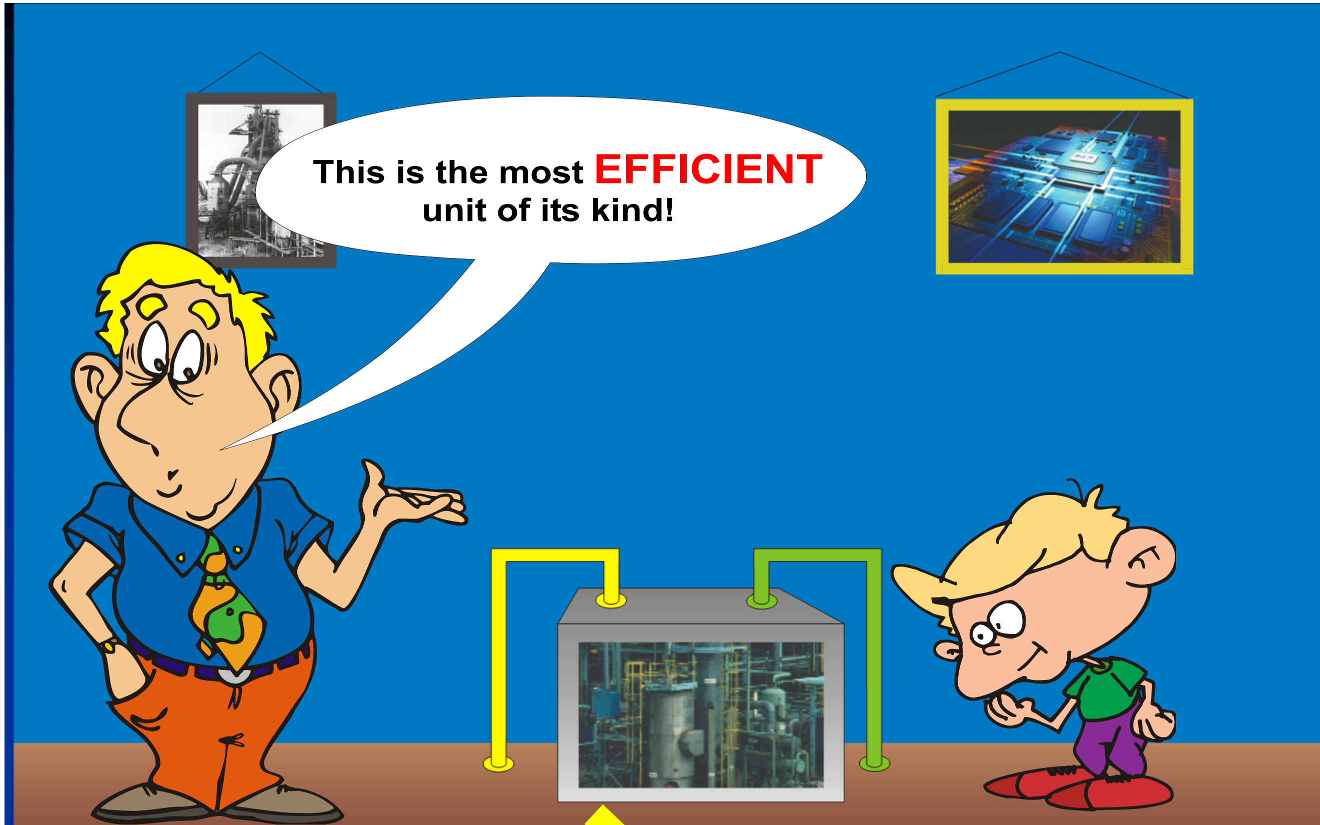
"Container Village" ChemPark

Lab – Pilot – Production in the same Professional Environment

The approach: "in one box" from process idea to a plant

Lab work, evaluation plant and small production in the same environment

Volker Hessel - The first NEXTLAB2014 Conference, IFPEnergies nouvelles 2-4 February 2014, Rueil-Malmaison (F)



Process Intensification: towards a Plant in a Shoe Box or in Banana container?

WHY and HOW Process Intensification
and Process Intensification Reactors?

The necessary Evolution DSM 2005
of Chemical and Process Engineering
with a time and length multiscale appro

In conclusion

MOLECULES INTO MONEY
shortening time to market thanks to **INNOVATION**

due TO PROCESS INTENSIFICATION,

- that offers strategic competitive advantage in SPEED-TO-MARKET, COST, PRODUCT INNOVATION and ENVIRONMENTAL PROTECTION with
- CLEAN TECHNOLOGIES, INNOVATION PROCESS DESIGN, NEW REACTION MEDIA, GREEN SOLVENTS IN CHEMICAL PROCESSES…..

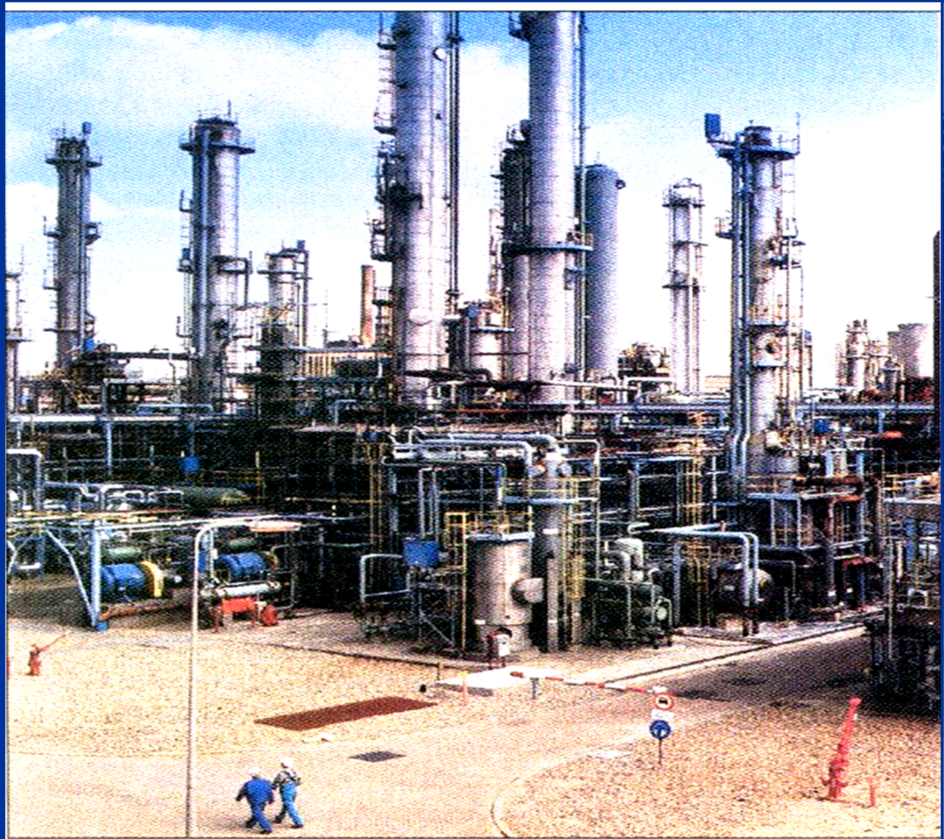
so citing the French Révolutionnaire Danton

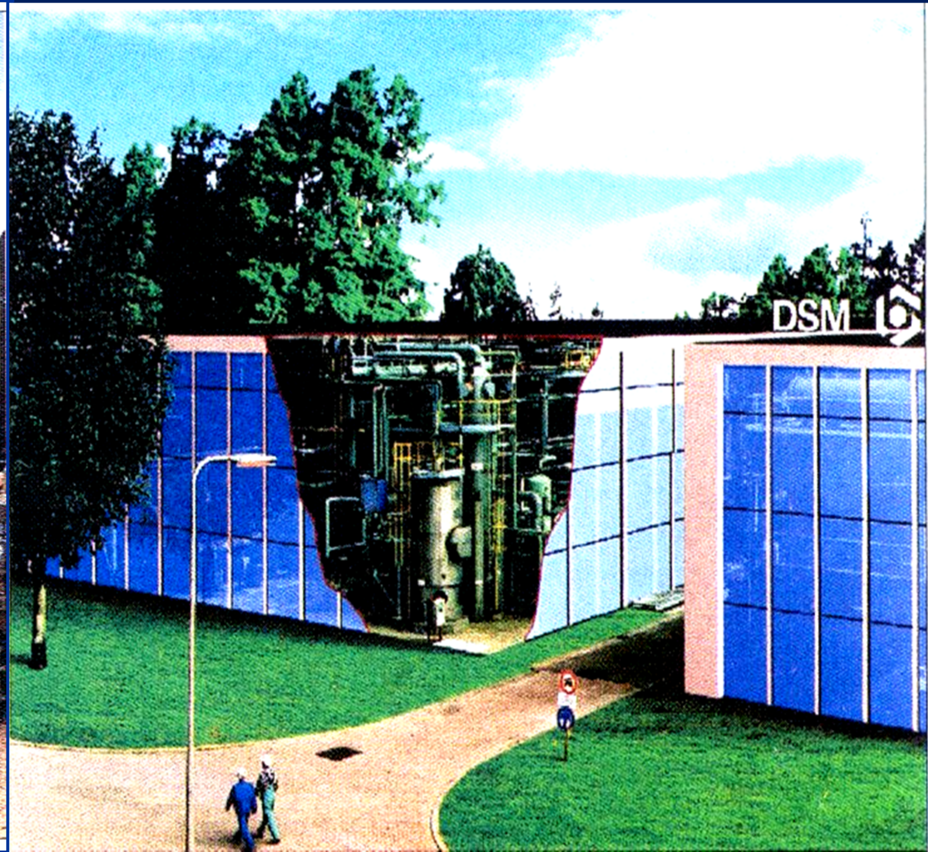
DE L'AUDACE
TOUJOURS DE L'AUDACE
ENCORE DE L'AUDACE

For the best of our Science as a KEY TECHNOLOGY SERVING MANKIND
in the context
Market demands versus Innovation with
Green Sustainable Technology Development and Processes

combining both market pull and technology push aiming the factory of the future.

Une vision de l'usine du futur mettant en oeuvre le Génie des Procédés Moderne Durable "Vert" avec l'Intensification des Procédés (à droite), à comparer avec une usine conventionnelle (à gauche). (Rendering courtesy of DSM)

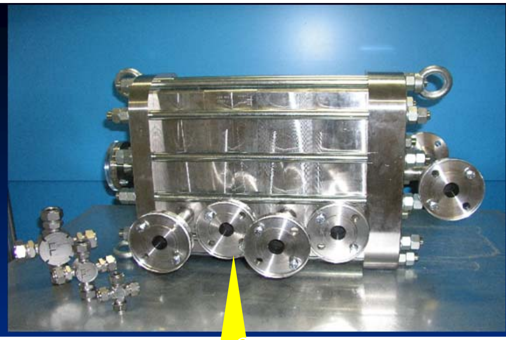




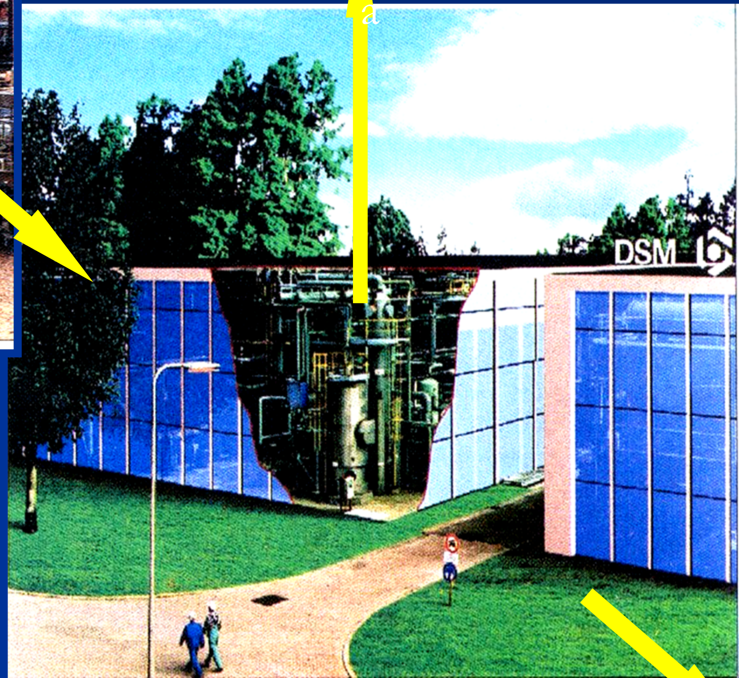
Opérant avec des PROCEDES NON POLLUANT, TRES EFFICACES mettant en oeuvre l'Intensification des procédés pour la production de produits verts (ciblés)

- ECONOMIES de 30 % (MATIERES PREMIERES + ENERGIE + COÛTS OPERATOIRES)

Mais de moins en moins un rêve!...C'etait l'objet de cette conférence



Modern Chemical Engineering involving process intensification for the Plant of Future



Sustainable Développement
A plant in a
- Shoe box or
- Banana Container

These 21st century demands concern the required tracks for the future of chemical and process engineering

A great number of these topics are listed in the European and North American **« roadmaps »** published in the last decade which have pointed out a planetary global anxiety and concern where chemical engineering shall play a crucial role:

- **sustainability, health, safety and environment, energy, water, food and drinks,**
- **biosystems engineering, solar energy, nuclear fusion, etc.**

So the existing processes and the future processes will be progressively adapted to the **principles of the « green chemistry ».**

And **«roadmaps»** proposed to respond to the changing needs of the chemical and related industries in order both to meet the previous today's economy demands and to remain competitive in global trade,

- **militate for the evolution of chemical engineering** *in favour of a modern process engineering voluntarily concerned by* **sustainability (the green process engineering)**

- that **will face new challenges** bearing on complex systems **at the molecular scale, at the product scale and at the process scale.**

SO ORGANIZING AT DIFFERENT SCALES THE COMPLEXITY OF THE CONCUBINAGE BETWEEN THE PHYSICS AND MOLECULAR PROCESSES

IS TODAY NECESSARY

TO UNDERSTAND AND DESCRIBE THE RELATIONSHIPS BETWEEN THE PHENOMENA AT THE NANO AND MICRO SCALES TO BETTER CONVERT THE MOLECULES INTO PRODUCTS WITH A REQUIRED END-USE PROPERTY AT THE PROCESS SCALE

This is the modern green chemical engineering approach (Multiscale Approach)

aiming PROCESS INTENSIFICATION

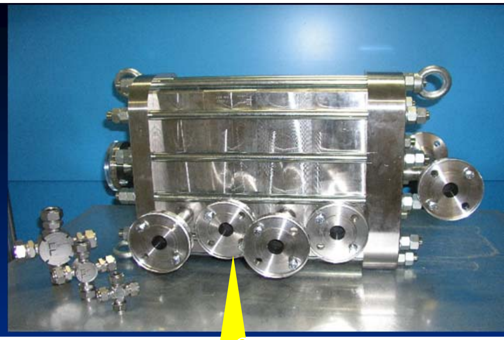
to obtain sustainable products (green) with sustainable processes (green)

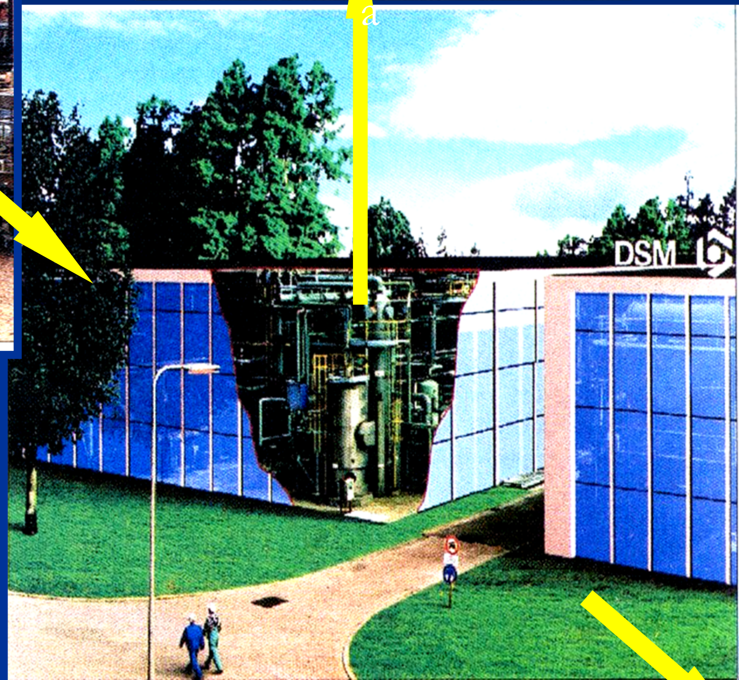
« Le couple Produits verts/ Procédés verts »

Process Intensification for Eco-design/ Eco-product/Eco-technologies)

Charpentier J.C., Chem Eng Res Des., 2010, 88 , 248-254

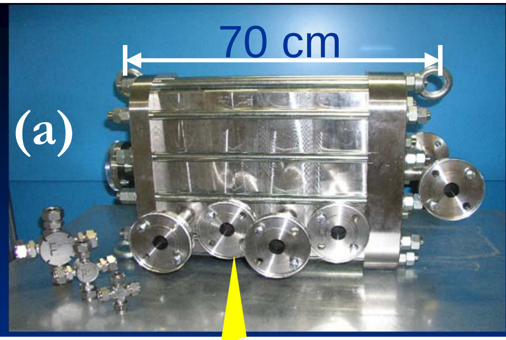
Charpentier, J.C., Techniques de l'Ingénieur, J500, 9, 2013



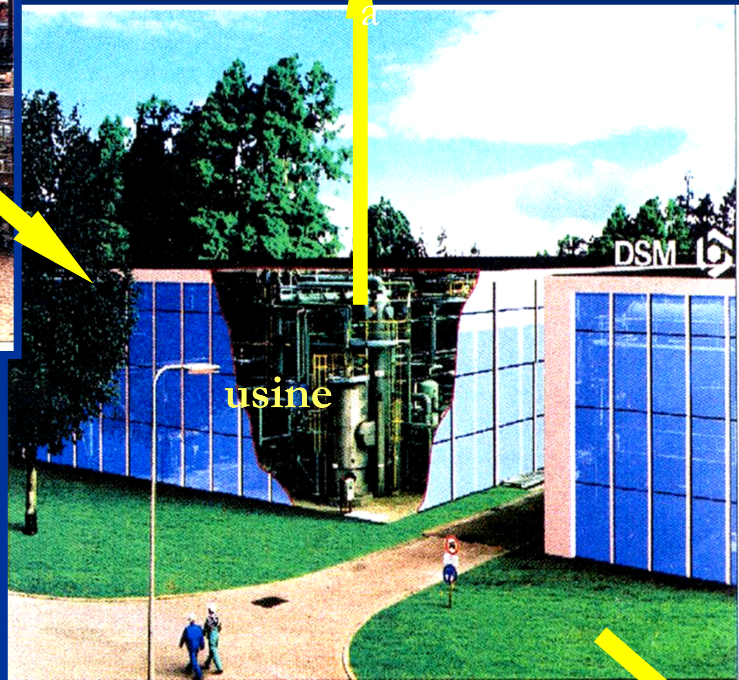


Modern Chemical Engineering involving process intensification for the Plant of Future

Sustainable Dévelopment
A plant in a
- Shoe box or
- Banana Container



Le Génie des Procédé
pour l'usine du futur

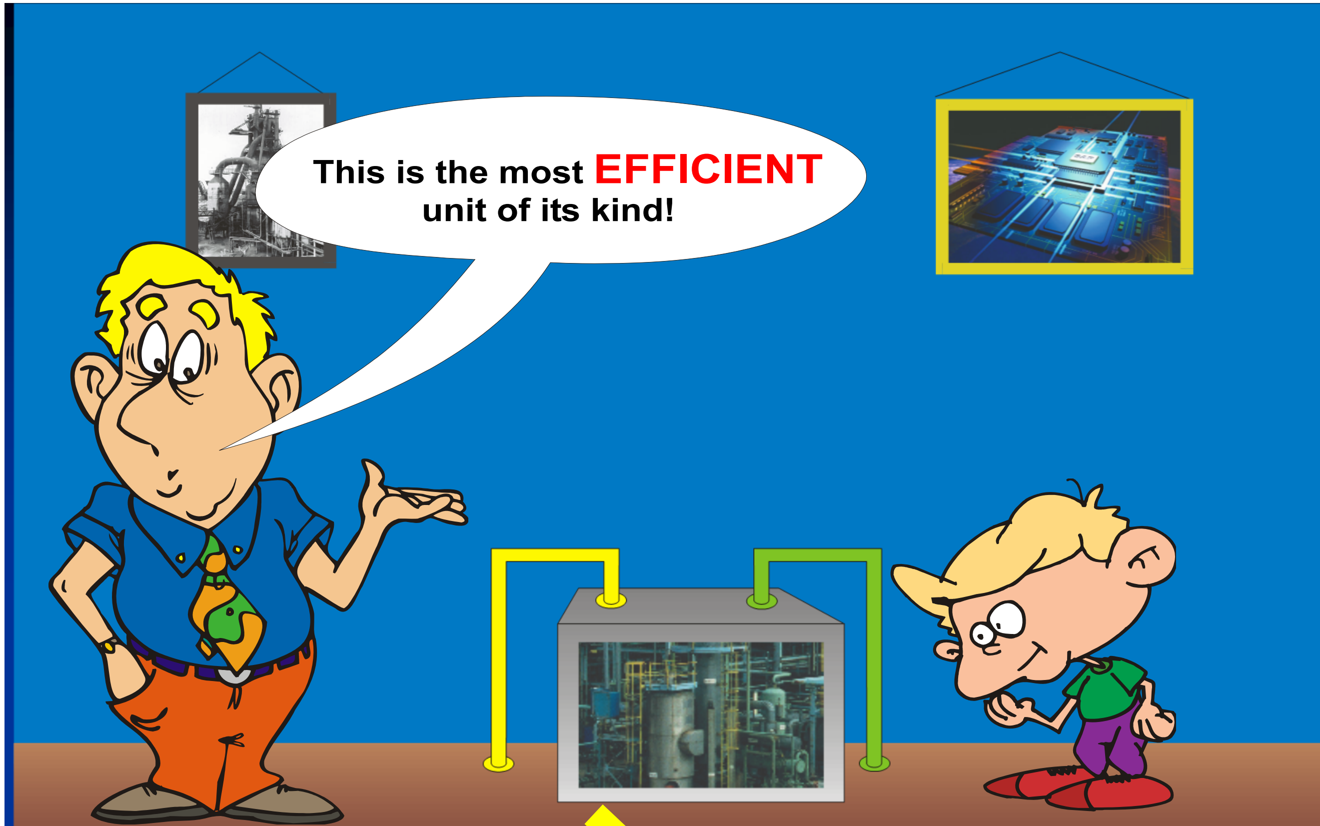


Développement Durable:
Une usine dans une boite

- Shoe box
- Banana Container

Four Solaire, Odeillo

Centrale
Solaire
Themis
Targassonne



Process
Intensification:
towards a
Plant
in a Shoe Box or
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WHY and HOW Process Intensification
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of Chemical and Process Engineering
with a time and length multiscale appro

Les temps changent…..mais…

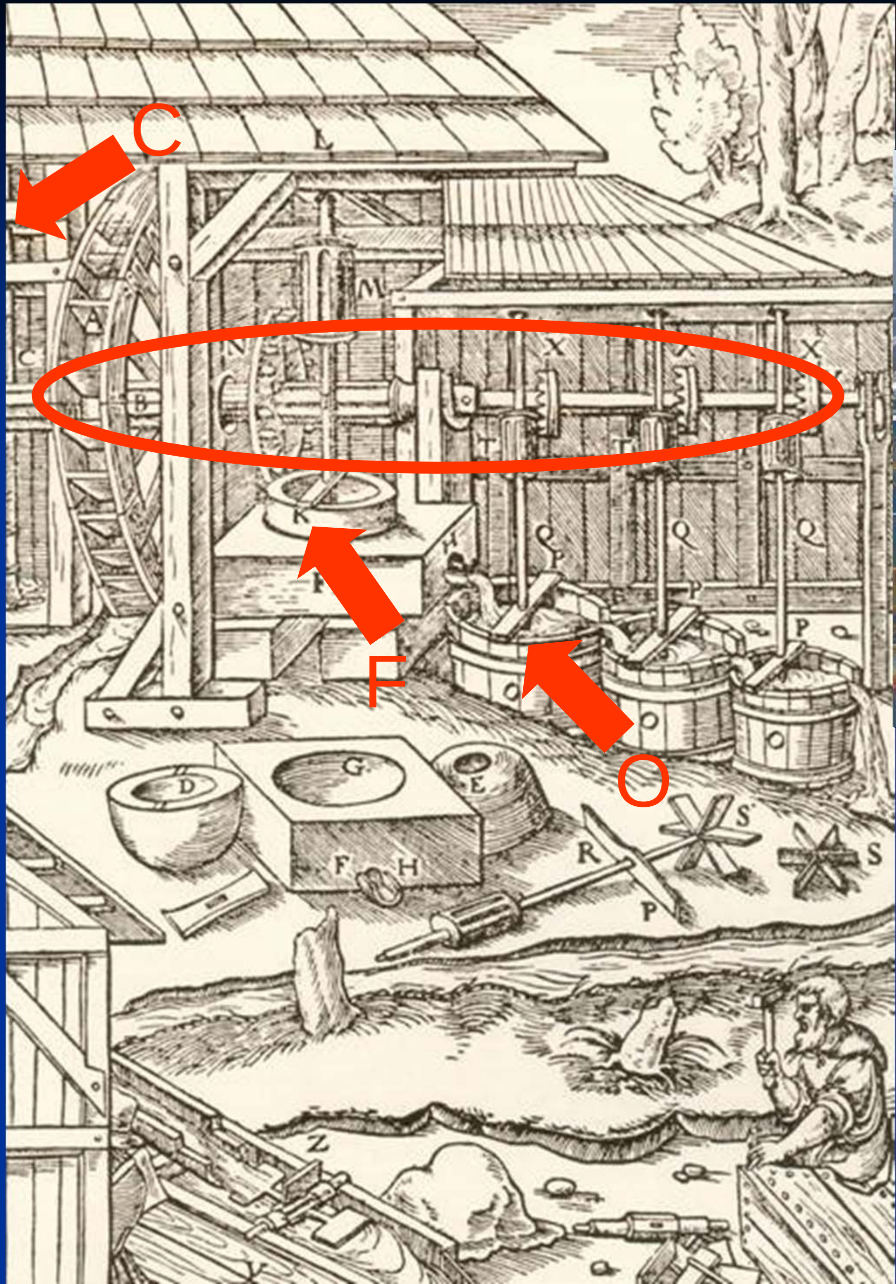
LE MONDE DES INDUSTRIES CHIMIQUES ET CONNEXES EST AU COEUR D'UN GRAND NOMBRE de DEFIS SCIENTIFIQUES ET TECHNOLOGIQUES

dus

- au comportement non durable de l'humanité (question d'énergies et de matières premières)

- à la croissance rapide des connaissances en chimie et biochimie

- et aux demandes du 21ème siècle clairement focalisées sur des exigences sociétales



G. Agricola, *De Re Metallica* **1556**

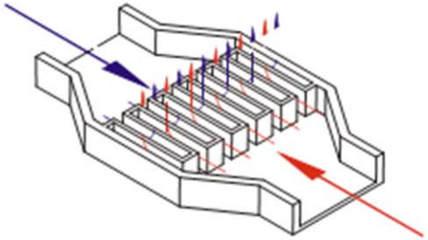
Industrie de production chimique, 2006

UN VRAI BESOIN D' INNOVATION…

Stankiewicz et al. Comput and Chem Eng 2008, 32, 3

MIXING PRINCIPLES AND CORRESPONDING IMM MICROMIXERS

Lamination for hydro-dynamic or shear decay



Interdigital Micromixers

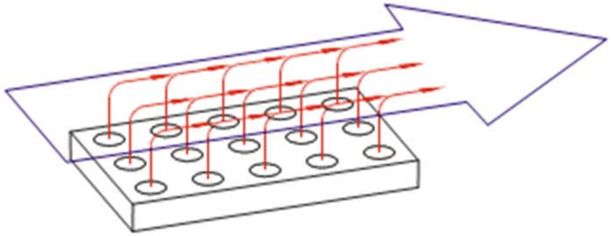
SIMM-V2
SSIMM
...

Bas-relief induced recirculation flow

Caterpillar Micromixers

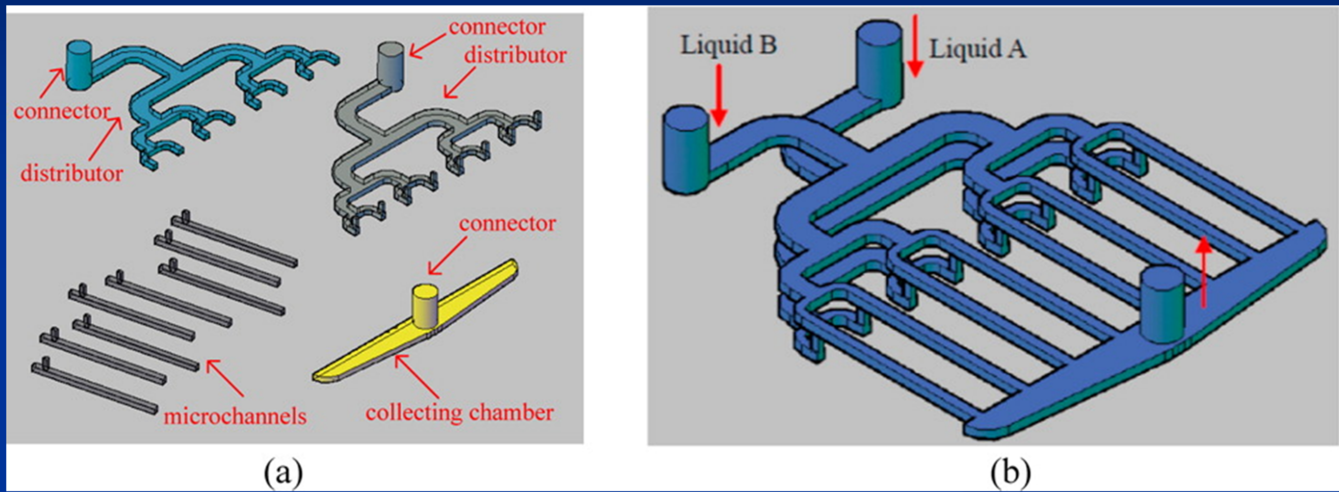
CPMM-R300-V1.2, CPMM-R600-V1.2
CPMM-R1200-V1.2, CPMM-R2400-V1.2
...

Injection in turbulent flow



Star Laminator Micromixers

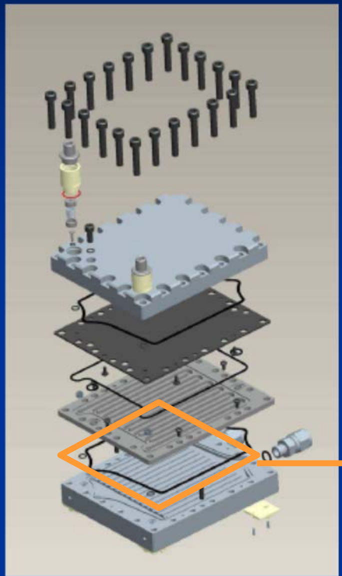
StarLam 15
...

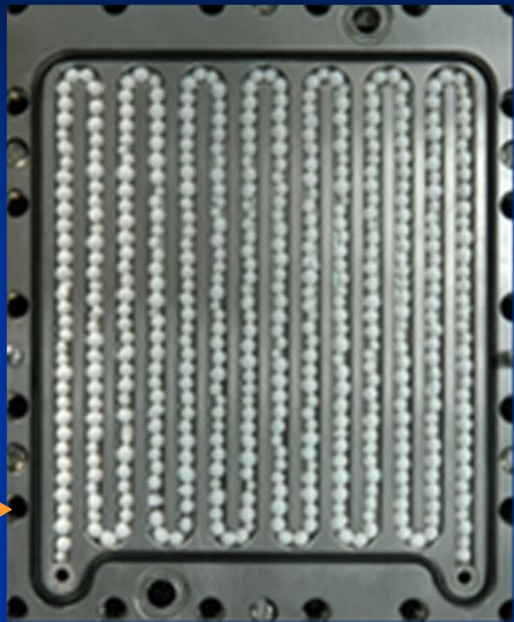


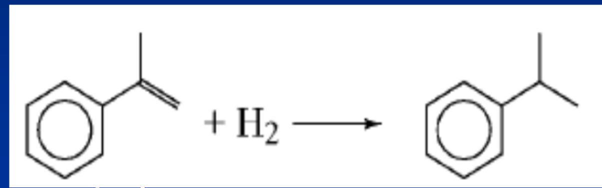
Multichannel micromixer design: components (a), assembly (b).

Published in: Yuanhai Su; Anna Lautenschleger; Guangwen Chen; Eugeny Y. Kenig; *Ind. Eng. Chem. Res.* **2014,** 53, 390-401.
Copyright © 2013 American Chemical Society

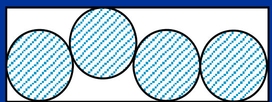
Le Réacteur Filaire: Gaz-liquide-solide (pour tests de catalyseurs)



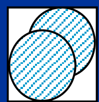




α-methyl styrene cumene



Side view



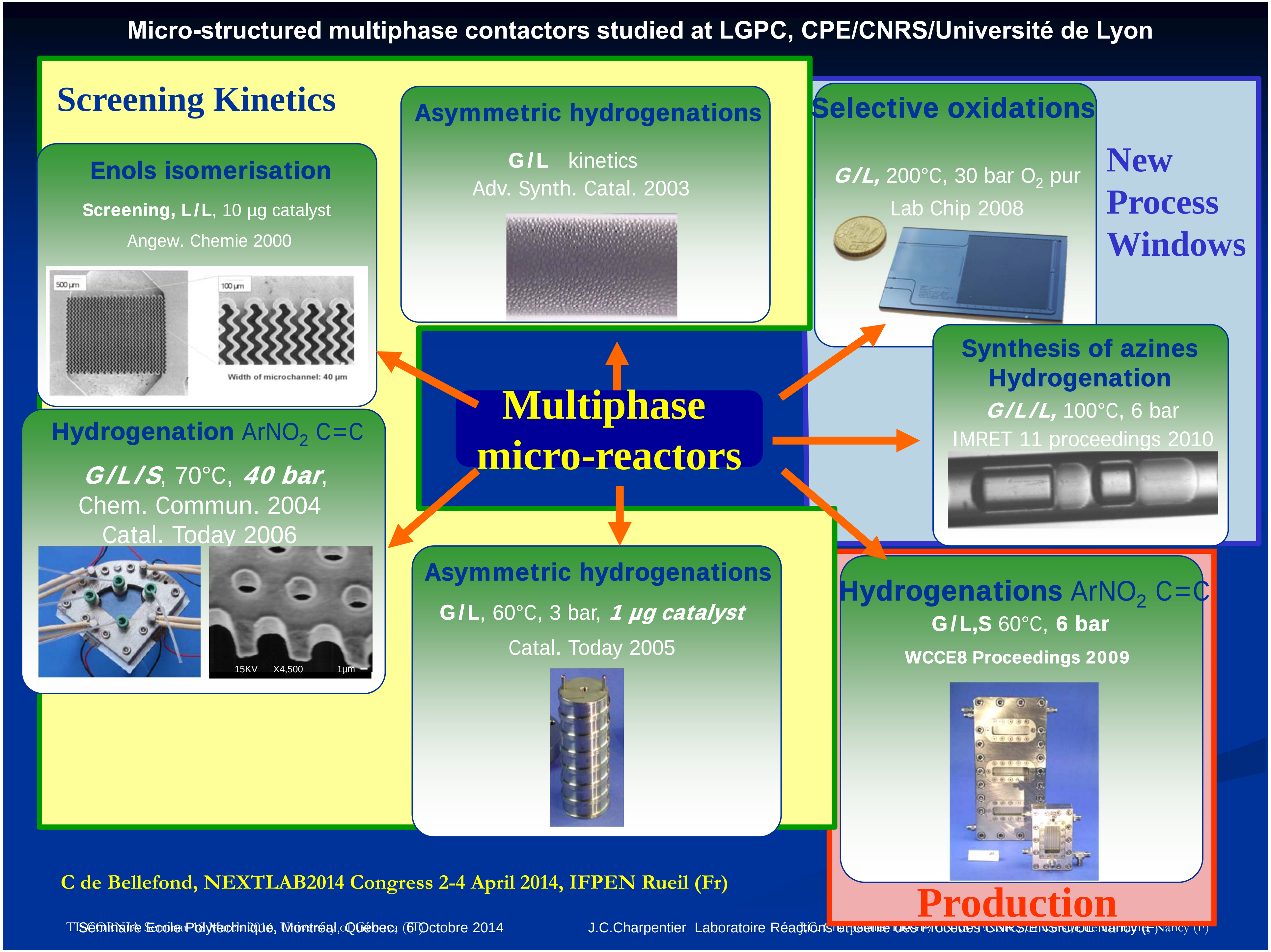
CrossSection

Chanel 4x4 mm, d_P = 3 mm, u_{LS}/u_{GS} = 20

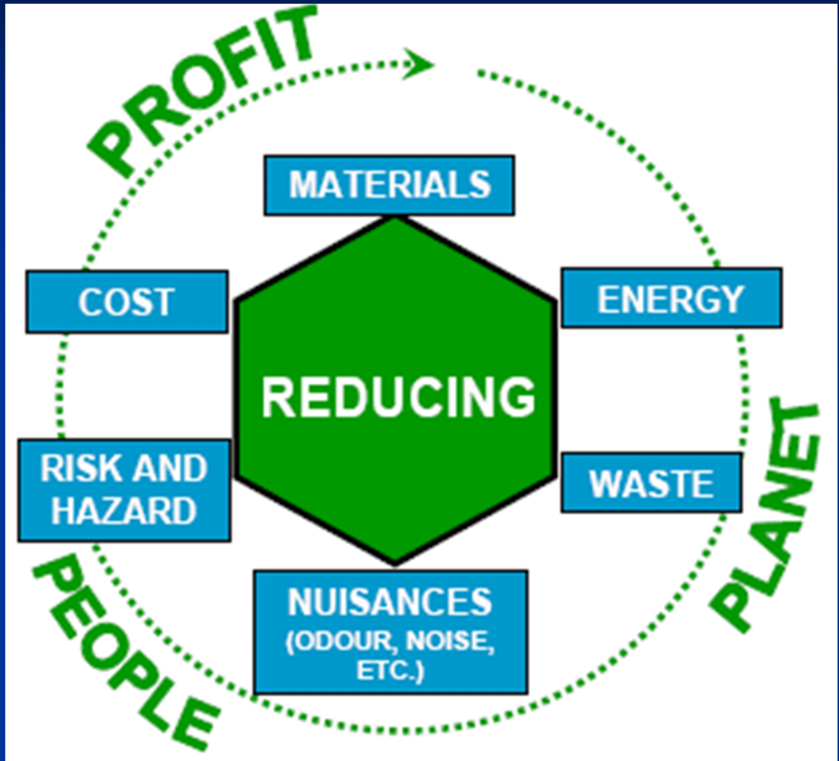
(Side view)

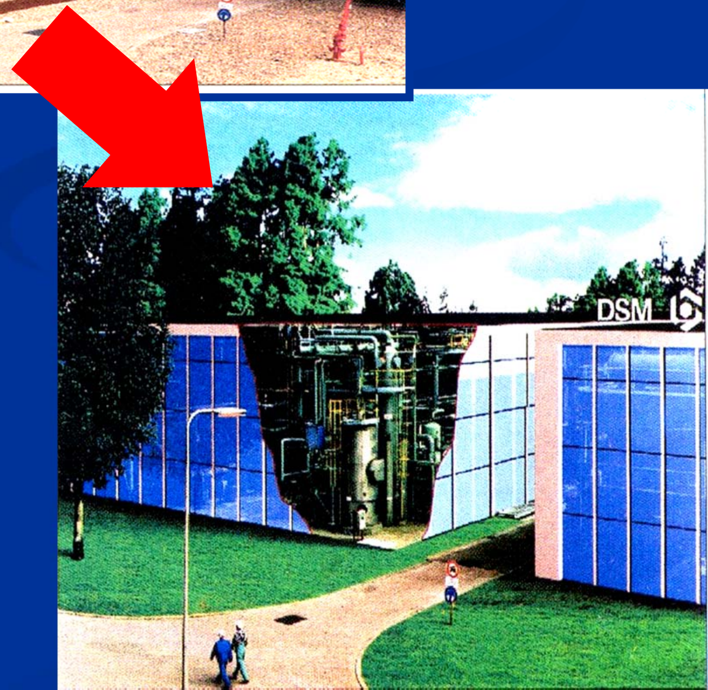
Alternative to basket type reactors
Shaped catalysts (dp 1-3 mm)
U_{LS} same as in industrial fixed-bed reactors
Good mass transfer performances
Commercially available (Erfeld Microtechnik)

Thèse Ana Hipolito 2010 CNRS/CPE/Université de Lyon


Micro-structured multiphase contactors studied at LGPC, CPE/CNRS/Université de Lyon
Screening Kinetics
Enols isomerisation
Screening, L/L, 10 µg catalyst
Angew. Chemie 2000
500 µm
100 µm
Width of microchannel: 40 µm
Asymmetric hydrogenations
G/L kinetics
Adv. Synth. Catal. 2003
Selective oxidations
G/L, 200°C, 30 bar O2 pur
Lab Chip 2008
New Process Windows
Multiphase micro-reactors
Synthesis of azines
Hydrogenation
G/L/L, 100°C, 6 bar
IMRET 11 proceedings 2010
Hydrogenation ArNO2 C=C
G/L/S, 70°C, 40 bar,
Chem. Commun. 2004
Catal. Today 2006
15KV X4,500 1µm
Asymmetric hydrogenations
G/L, 60°C, 3 bar, 1 µg catalyst
Catal. Today 2005
Hydrogenations ArNO2 C=C
G/L,S 60°C, 6 bar
WCCE8 Proceedings 2009
Production
C de Bellefond, NEXTLAB2014 Congress 2-4 April 2014, IFPEN Rueil (Fr)
Séminaire Ecole Polytechnique, Montréal, Québec, 6 Octobre 2014
J.C.Charpentier Laboratoire Réactions et Génie des Procédés CNRS/ENSIC Nancy (F)

PROCESS INTENSIFICATION

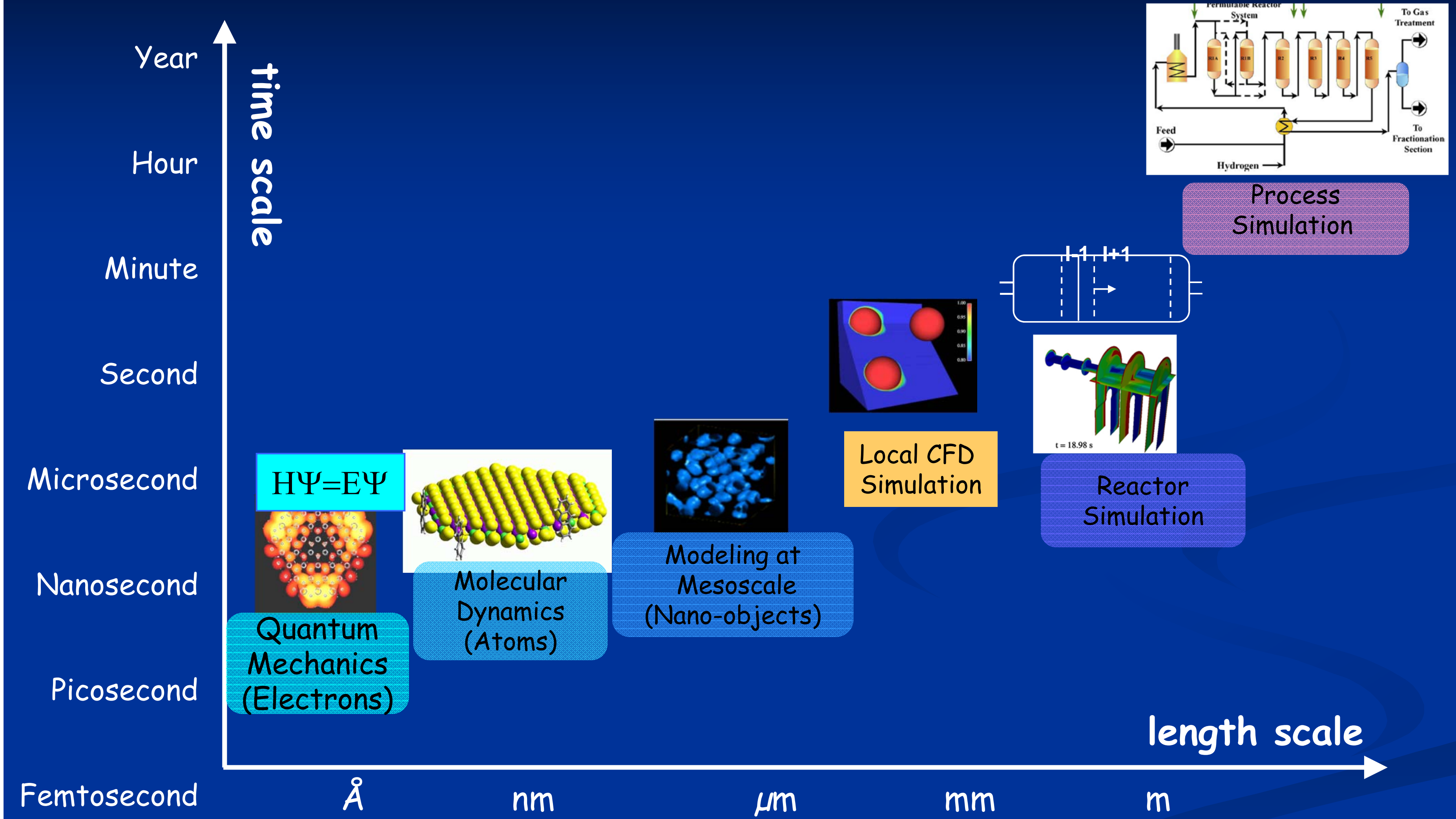




- Sustainable and Clean Technologies
- New Reaction Media and Green Solvents
- Environment Safety and Risk Management
- Biocatalytic Processes, Biorefinery..

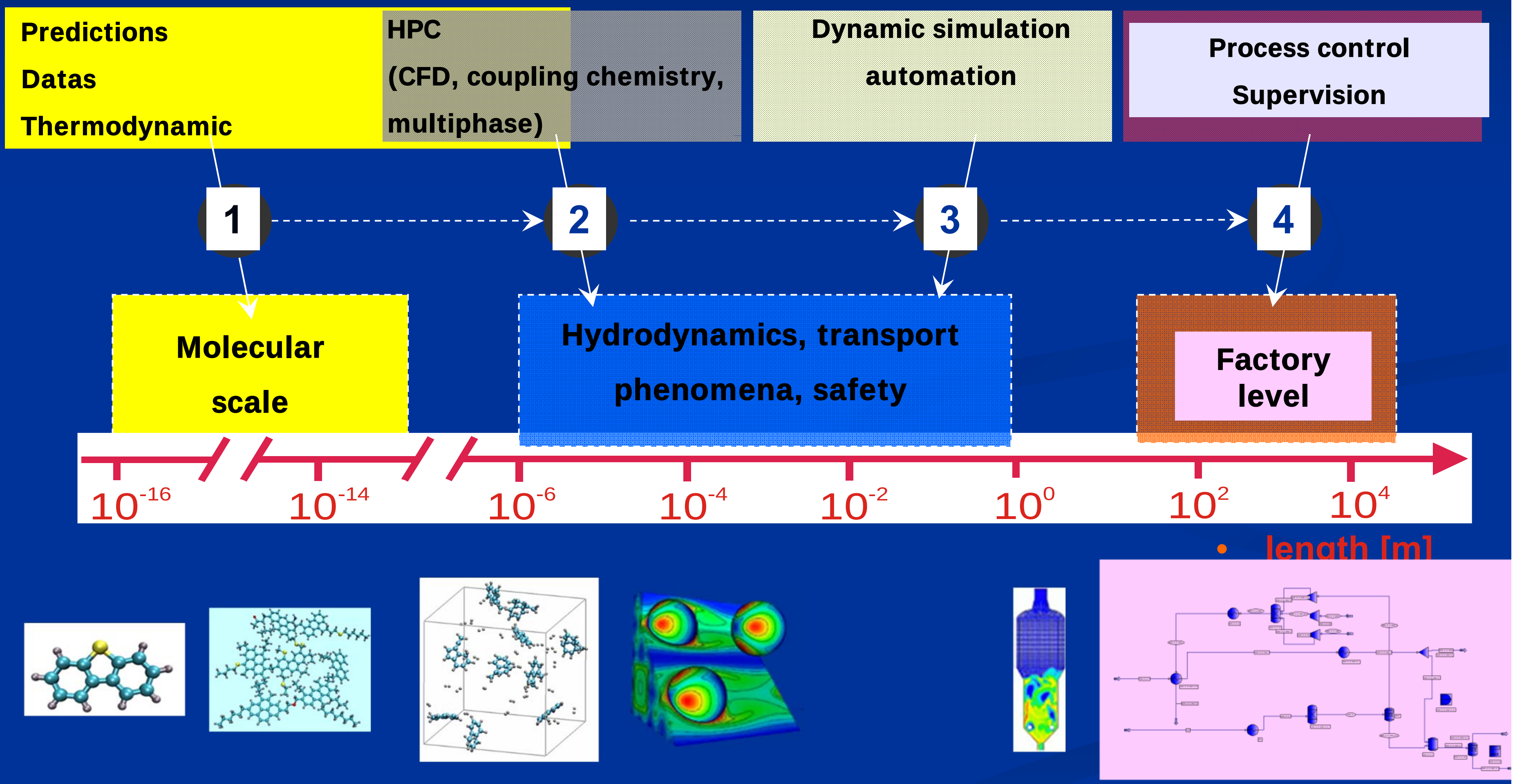
Challenges for modeling in chemical engineering

The multiscale approach for the couple green product/process



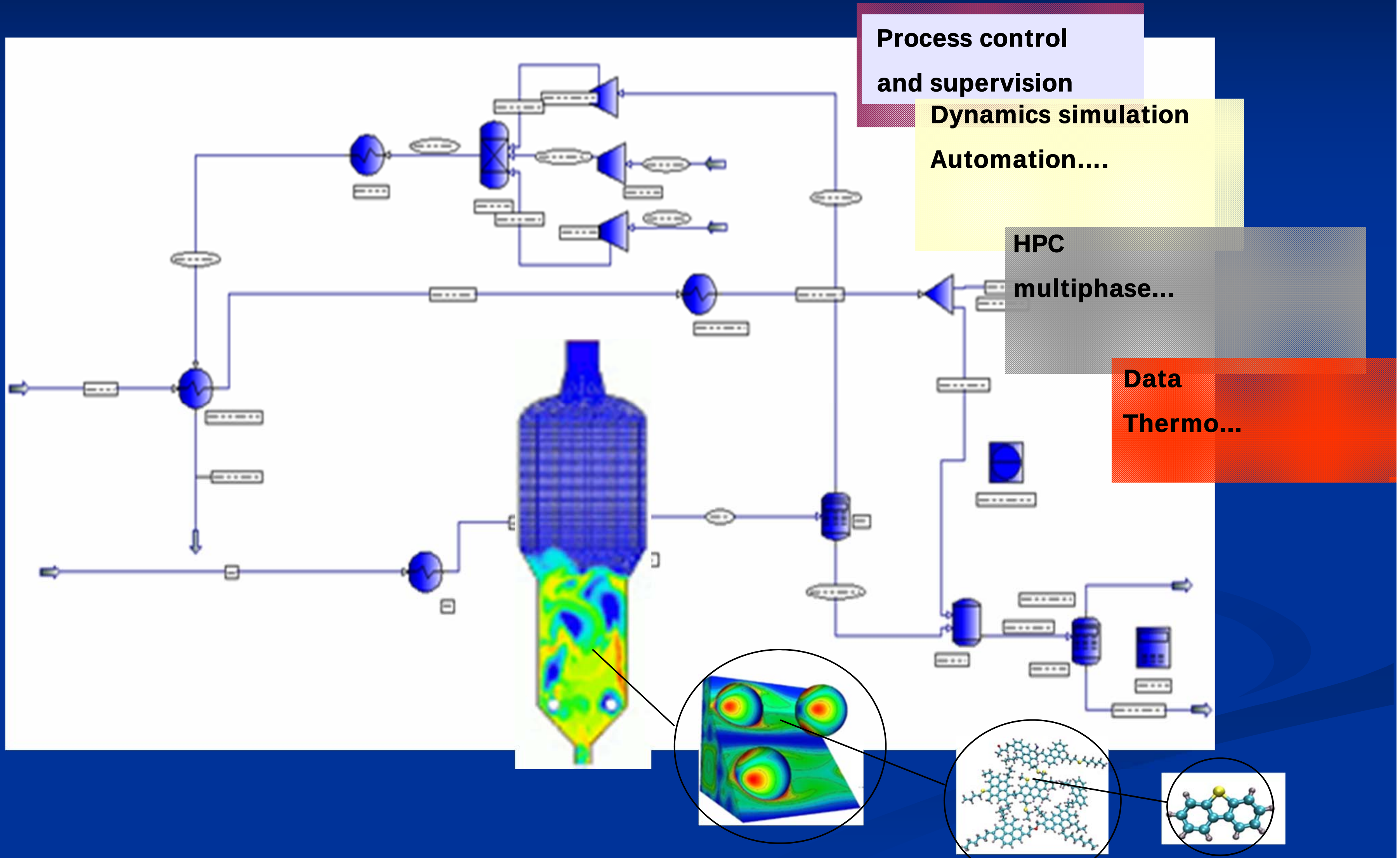
The integrated multiscale system approach involves to understand how phenomena at a smaller length scale relate to properties and behaviour at a longer length scale of the chemical supply chain.

Step by step multiscale approach of Green Process Engineering

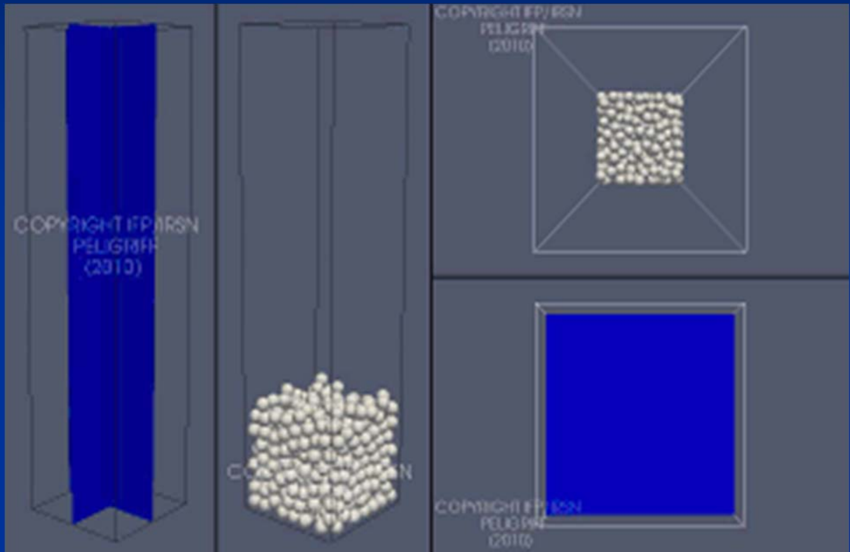


J.C. Charpentier LRGP/CNRS/ENSIC/Université de Lorraine, Nancy (F)

Integrated multiscale approach for Green Process Engineeering



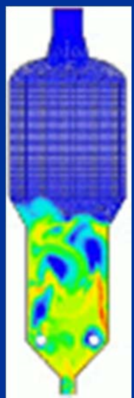
International Conference on
Multiscale Approaches for Process Innovation

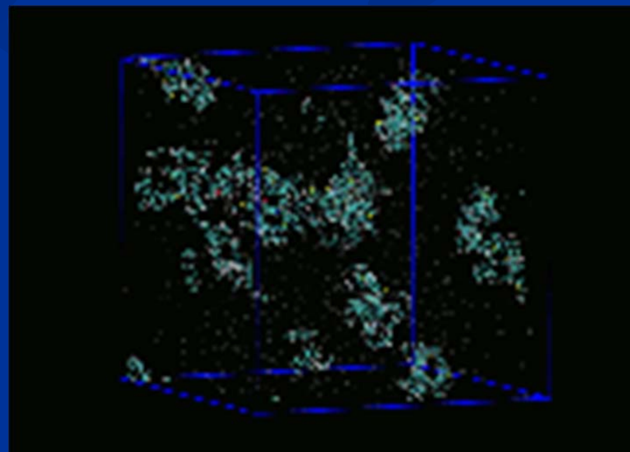


MAPI

Lyon, France

25 – 27 January 2012

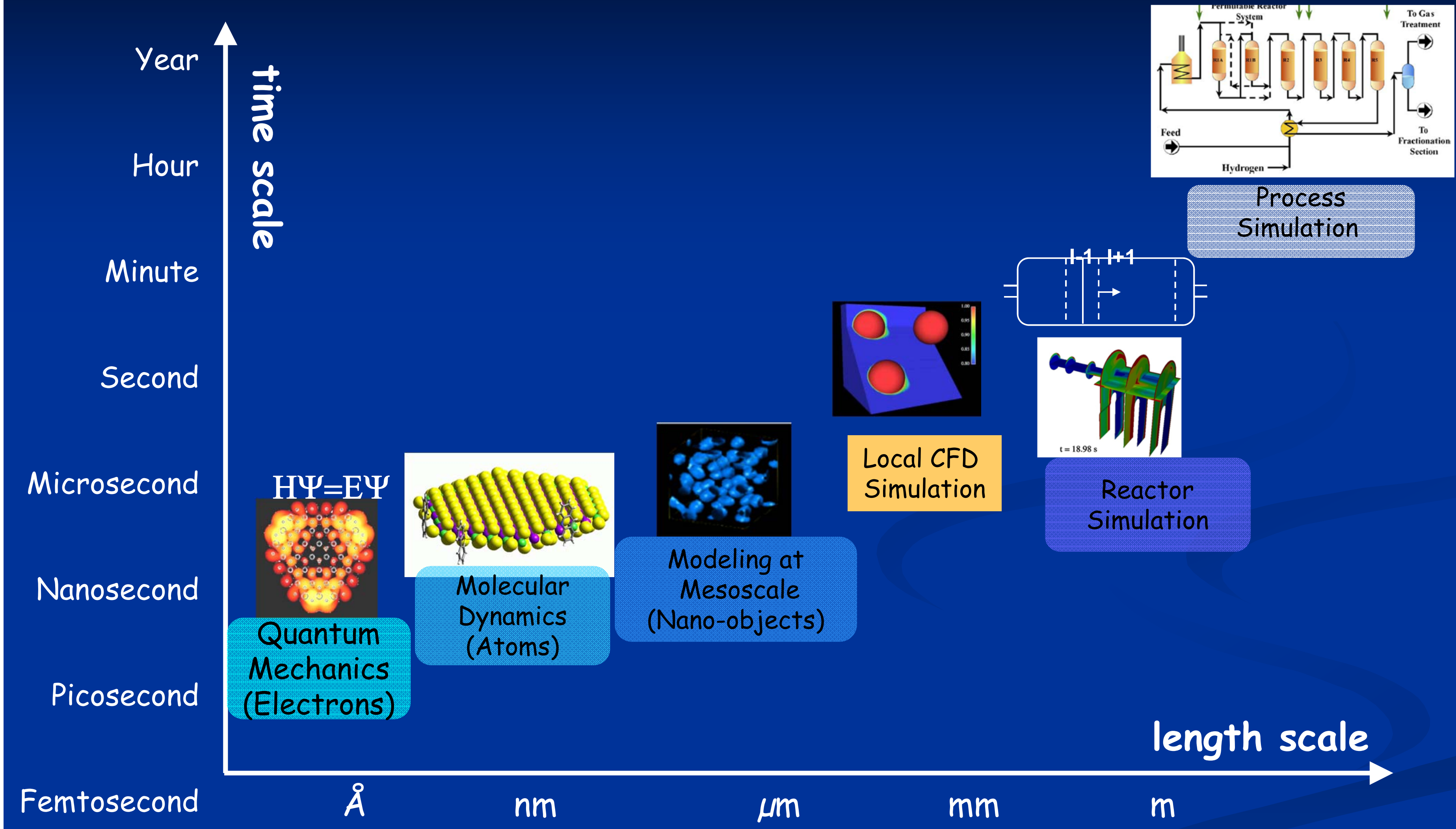




J.C. Charpentier LRGP/CNRS/ENSIC/Université de Lorraine, Nancy (F)

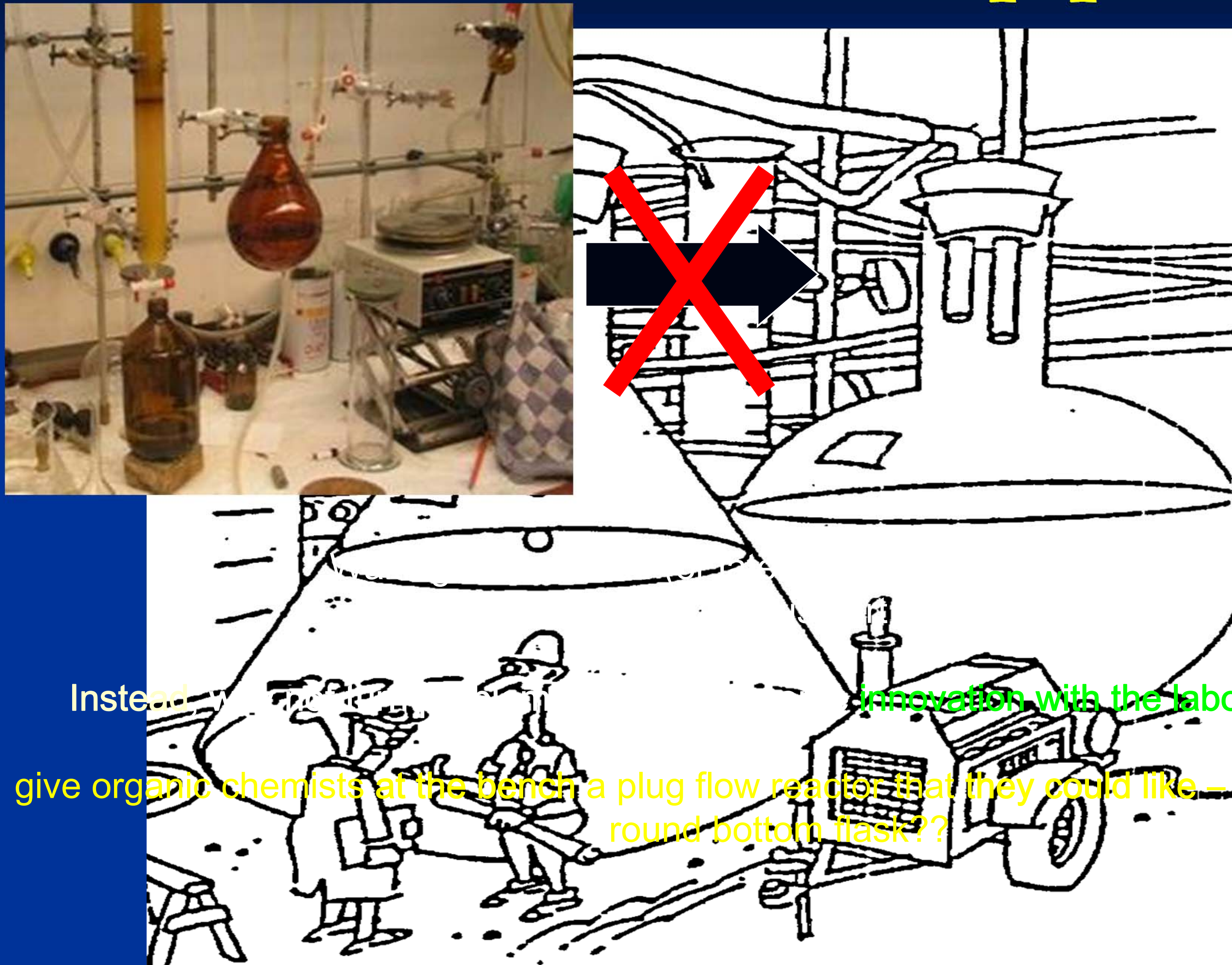
Challenges for modeling in chemical engineering

The multiscale approach for the couple green product/process



The integrated multiscale system approach involves to understand how phenomena at a smaller length scale relate to properties and behaviour at a longer length scale of the chemical supply chain.

That same old scale-up problem



Inste… innovation with the laboratory of future:

give organic chemists at the bench a plug flow reactor that they could like – or, even prefer to a round bottom flask??

but Innovation….

outline

- The world of chemistry and related industries at the heart of a great number of scientific and technological challenges due to the non-sustainable mankind

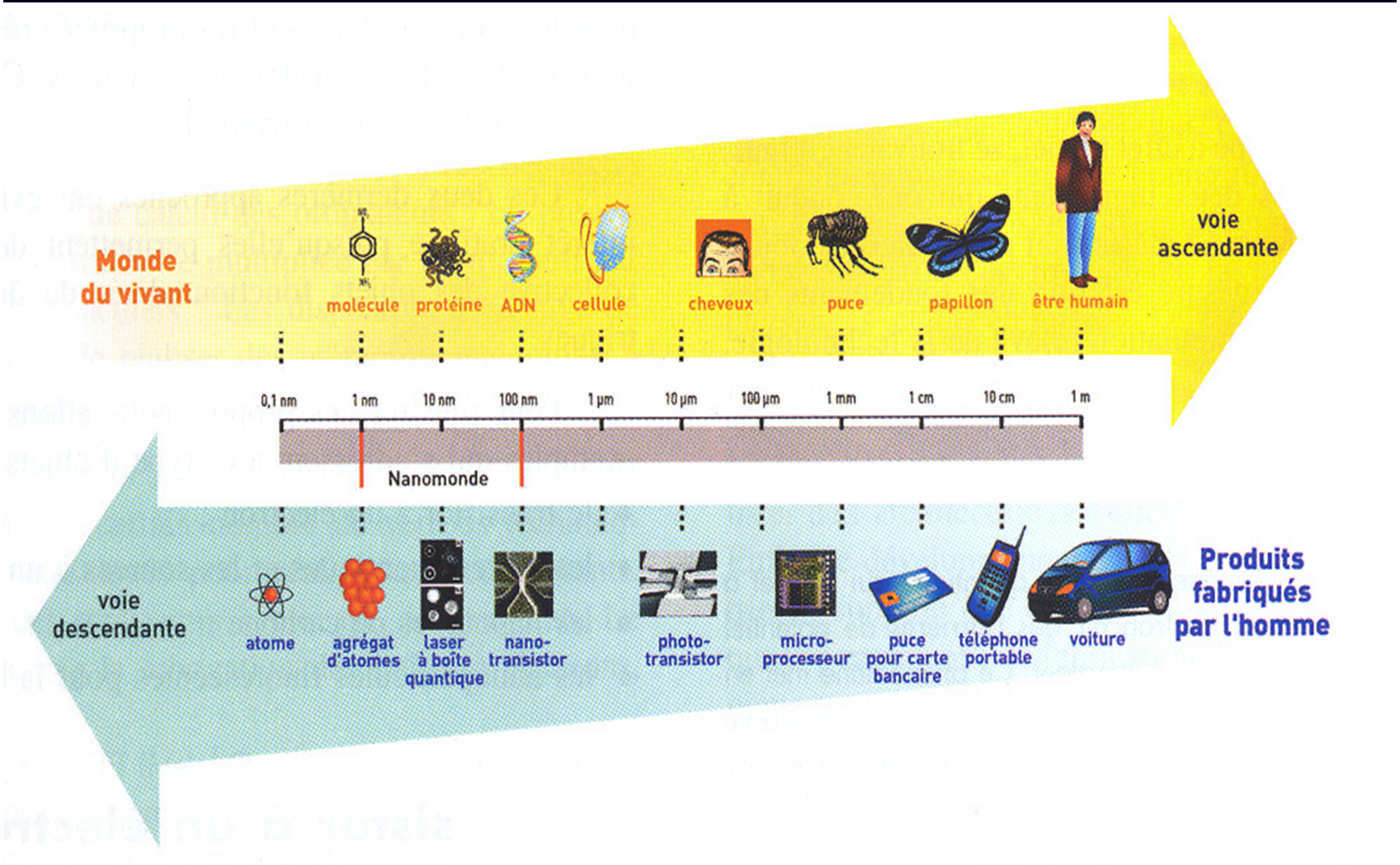
- What are we waiting from chemical and process engineering and WHY?
  (product with required end-use properties first on the market, sustainable clean product and process design,…)

- The today chemical and process engineering approach: Did you say "The triplet molecular Process-Product-Processes Engineering (3PE)"

- Chemical Engineering: QUO VAMUS ?
  The multidisciplinary and multiscale integrated approach for a necessary key-technology serving a great number of mankind needs,

i.e. (towards a green process engineering but how?)

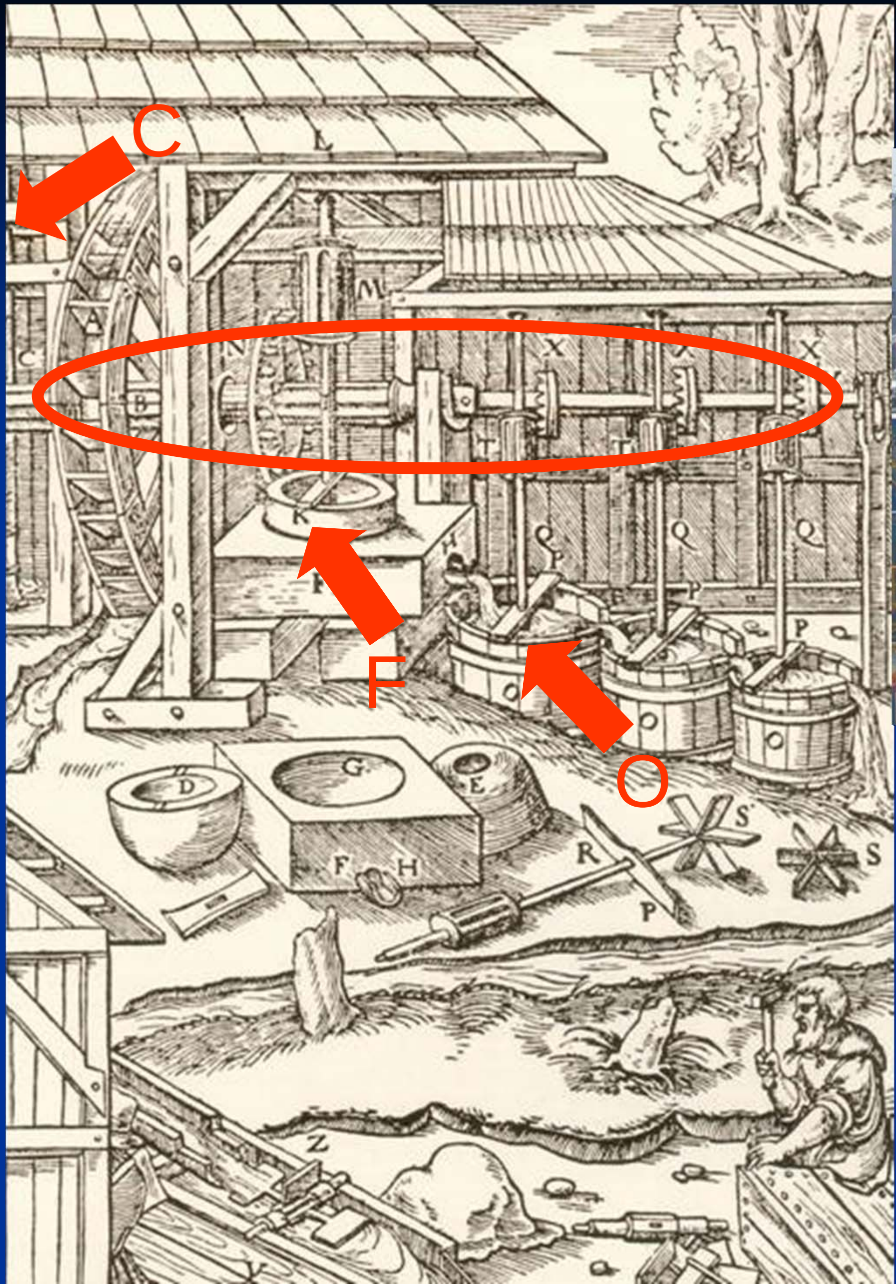
4 proposed tracks


Monde
du vivant
molécule
protéine
ADN
cellule
cheveux
puce
papillon
être humain
voie
ascendante
0,1 nm
1 nm
10 nm
100 nm
1 µm
10 µm
100 µm
1 mm
1 cm
10 cm
1 m
Nanomonde
voie
descendante
atome
agrégat
d'atomes
laser
à boîte
quantique
nano-
transistor
photo-
transistor
micro-
processeur
puce
pour carte
bancaire
téléphone
portable
voiture
Produits
fabriqués
par l'homme

PRODUCTION-TYPE (3200 l/h; 0.7 bar) STARLAM MICRO MIXER

Microstructured mixer part of a production plant at industrial site in Germany and operated at about 3000l/h successfully since some weeks

B. Werner, V. Hessel, P. Löb, *Chem. Ing. Tech.* **76**, 5 (2004) 567-574
Chem. Eng. Tech. **78**, 4 (2005) 401-407



G. Agricola, *De Re Metallica* 1556

Chemical Process Industry, 2006

A CLEAR NEED FOR INNOVATION…

A Stankiewicz (2006)

3 - MANUFACTURING END-USE PROPERTIES
Product Design and Engineering

Growing market place demand for sophisticated and controlled and structures products combining several functions and properties

- "translation" of molecular-scale processus into phenomenological macroscopic scale laws

- understanding of these operations which control end-use properties and quality features

Taste, feel, smell, colour, handling properties, biocompatibility…

EMPHASING THE CHEMICAL SUPPLY CHAIN

- Product quality is determined at the nano and microscales and

- Product with a desired property must be investigated for both structure and function

The key of success ? It is

-To obtain the desired end-use properties and then to control product quality by controlling the microstructure formation

- So a thorough understanding of the structure/property relationship at both
  Molecular scale (e.g., surface physics and chemistry)
  Microscopic scale (e.g., coupling reaction mechanisms and fluid mechanics)
is of primary importance to be able to design production processes

This understanding helps to make the leap from the nanoscale to the meso and macro scales of the production processes that ensure the customer product quality requirements

(INTEGRATED MULTISCALE COMPLEX SYSTEM APPROACH)

But!!! though tempting, don't hide some limits of hybrid technologies….

The use of multifunctional reactors is limited by the resulting problems with control and simulation i.e., the interaction between simultaneous reaction and distillation introduce more complex behaviour, involving multiple steady-states and output multiplicities and so different conversion and selectivity…

This leads to challenging problems in dynamic modelling, design, operation, and strong non-linear control (Computer-aided Process Engineering - CAPE)

Too much integration can exert a negative influence, requiring detailed modelling of the underlying processes and a careful selection of the chemical and physical systems properties and operation conditions(CAPE)

Their control requires sophisticated model predictive control, robust control, and adaptative control, where mathematical predictive control may be required to run 100 to 1000 times faster than real time!(CAPE)

BUT !!!

The bottleneck of good models of multiphase and complex systems is the understanding of the physics, chemistry and biology of the interaction rather than **the refinement of numerical codes**

What is needed in models is less anatomy and more physiology

for models, EINSTEIN'S citation :
« Keep things as simple as possible, but not simpler »

also FUZZY LOGIC is of great help in the CONTROL and AUTOMATION of processes as well as

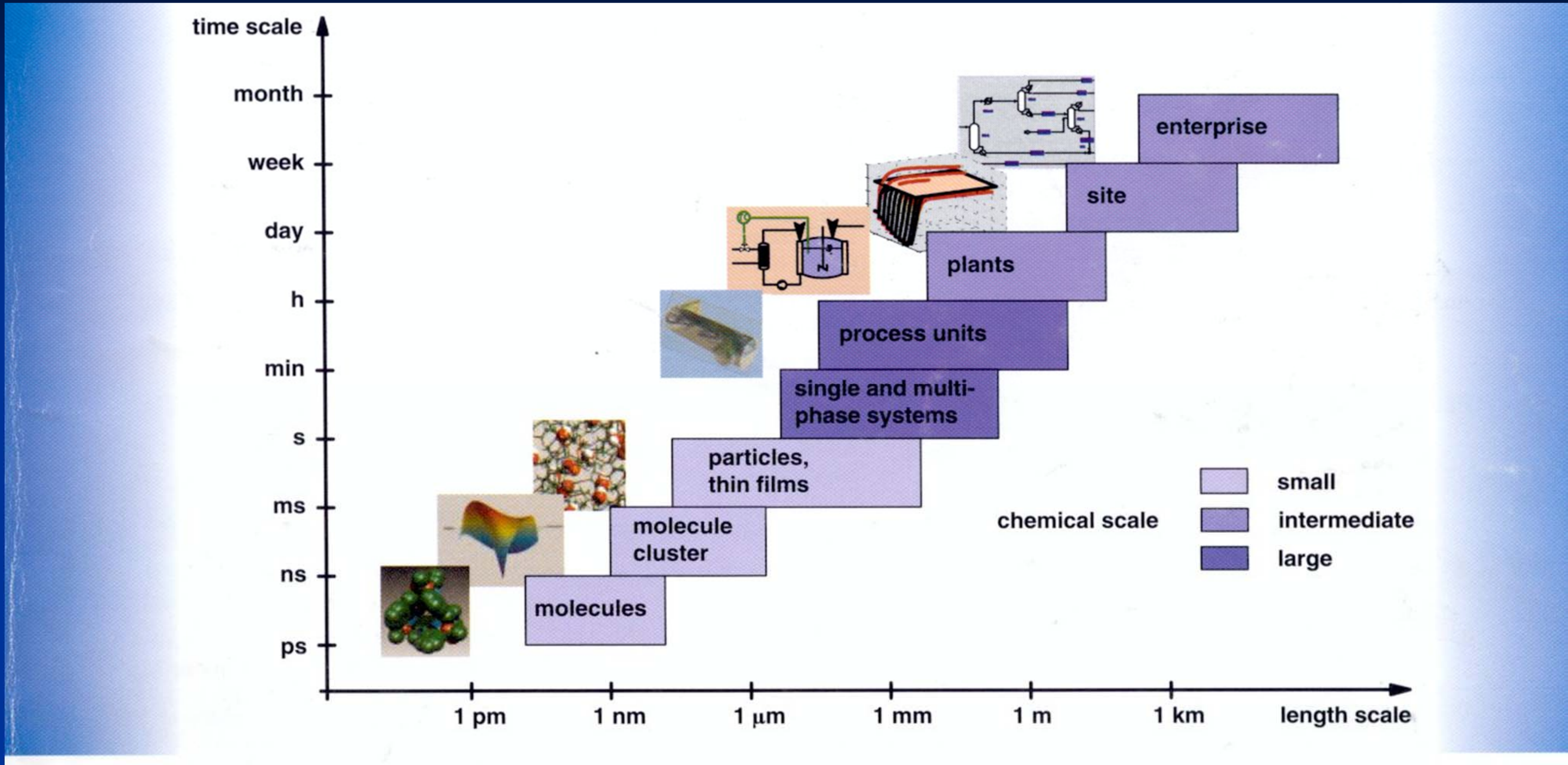
NEURAL NETWORKS

- **for diagnosing on-line defects**
- **for the design and the analysis of new processes**
- **for analysing trends**

(e.g, hydrodynamics and mass transfer parameters in trickle beds, in bubble columns and in sparging reactors)

Remember!!! that AUTOMATION in world scale plants provides high work force productivity, whereas in high-margin multipurpose plants, it provides the capability to reach quality specification and required troughputs quickly when restarting the process……BUT!!!

THE CHEMICAL SUPPLY CHAIN



Chemical and Process Engineering is now concerned with the understanding and development of systematic procedures for the design and operation of chemical process systems, ranging :

FROM nano and microsystems-scales where chemicals have to be synthesize and characterize at the molecular-level

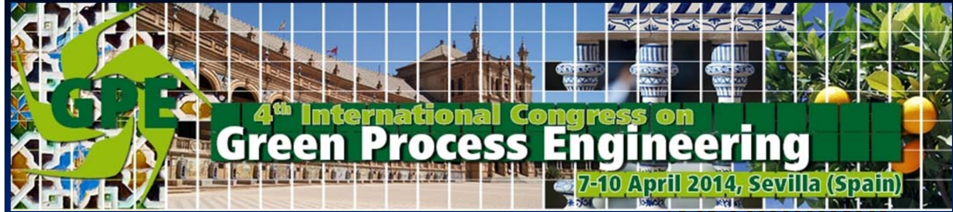
TO industrial-scale continuous and batch processes

Too many chemist and chemical engineering congresses in the past decade have focused on weakness and threats. Instead this congress tries to focus on strenght and opportunities:

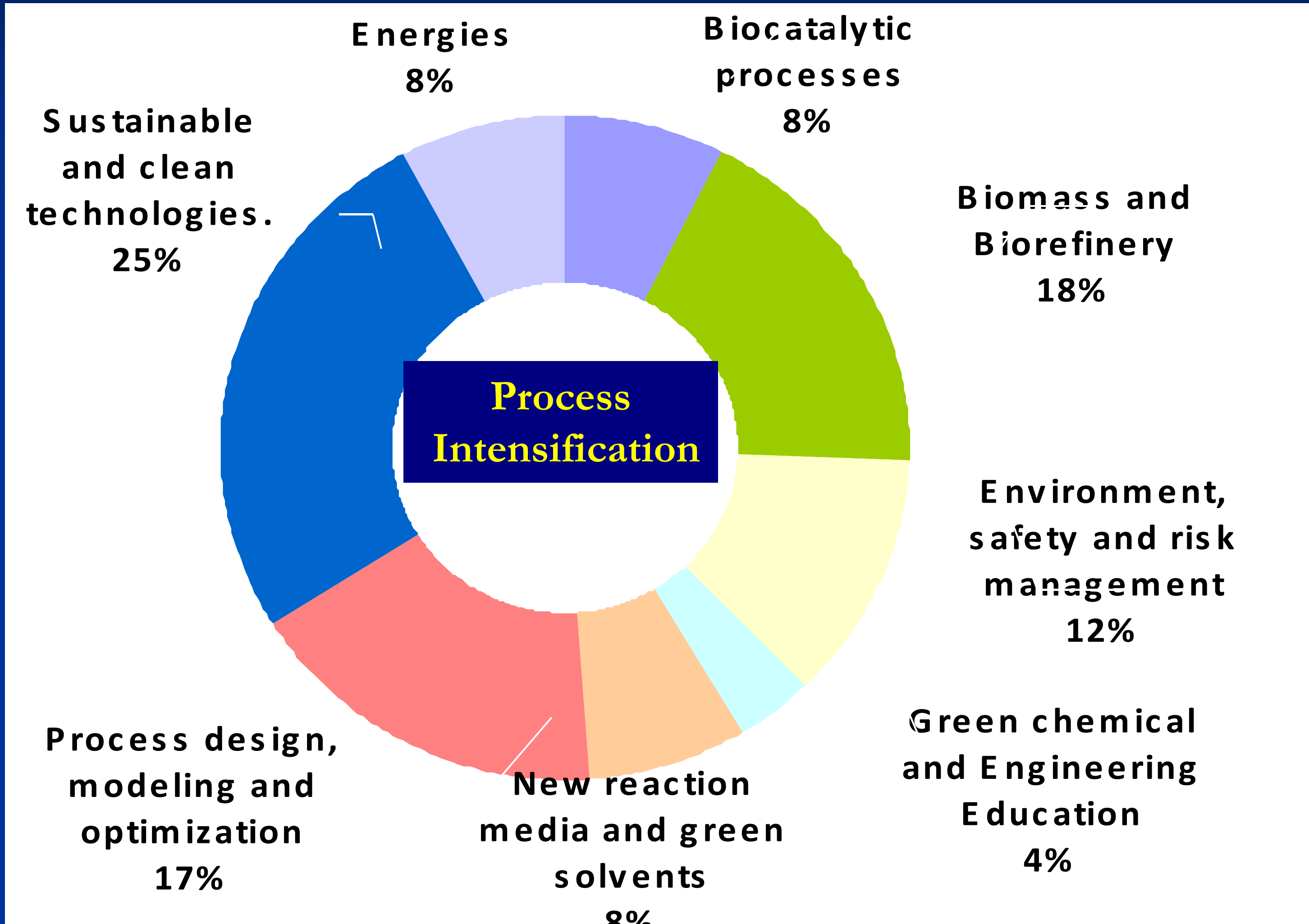
WE MUST BE CONFIDENT!!!!!

By cutting Chemical Engineering CAKE in a different way, especially with the strength involved in GREEN PROCESS ENGINEERING with notions of Process Intensification and Product Design and Engineering I try to convince the CAKE to be both richer and larger as GPE has a key contribution to SUSTAINABLE DEVELOPMENT and quality of life

So….. bravo for the organizers of the
1st International Congress
on **Green Process Engineering**



GPE 4: TOPICS



UNIVERSITAT JAUME·I SusChem INPACT EFCE UNIVERSIDAD DE MURCIA J.C. Cha Red Española de Química Sostenible Green Chemistry Network of Spain Flucomp

4 Simultaneous tracks for the future of Green Process Engineering with a multiscale approach for the design of the factory of future

1-To increase productivity and selectivity through intelligent operations and multiscale control of processes: i.e. Molecular information engineering
Micro and-Nano and Micro tailoring of porous and cristalline Materials (nanotechnology) ← Green Process Engineering with multiscale approach

2- Design of novel equipment based on scientific principles and new modes of production: process intensification with multifunctional reactors or microstructured reactors (microfluidic) ← Green Process Engineering with multiscale approach

3- Manufacturing end-use properties: development of a multidisciplinary product-oriented engineering i.e. product design and engineering with special emphasis on solids technology and complex fluid processing ← Green Process Engineering with multiscale approach

4- Implement multiscale and multidisciplinary computational chemical engineering modeling and simulation to real-life situations: from the molecule scale up to the overall complex production scale.
Automation, control and safety , LCA ← Green Process Engineering with multiscale approach

Charpentier J. C., Oil & Gas Science and Technologies, 2013, 68, 952-964

outline

- Some reminds on chemical engineering, its evolution and on process intensification

- The world of chemistry and related industries at the heart of a great number of scientific and technological challenges due to
    - the Rapid increase of knowledge in chemistry and biochemistry
    - the 21th century demands clearly focalized on societal exigencies
    - the non-sustainable mankind

- What are we waiting from chemical and process engineering and WHY?
(product with required end-use properties first on the market, sustainable clean product and process design,…)

The answer:

- The today chemical and process engineering approach:
    Did you say "The triplet molecular Process-Product-Processes Engineering (3PE)"

- Chemical Engineering: QUO VAMUS ?
    The multidisciplinary and multiscale integrated approach for a necessary key-technology serving a great number of mankind needs,

i.e. (towards a green process engineering thanks to process intensification for the factory of future)

but how?

4 proposed tracks

PROCESS INTENSIFICATION
SUSTAINABLE RELATED DIMENSION
with
Producing much more and better with much less

This means

- To produce more targetted products and better in smaller volumes, with a better efficiency and selectivity, in using less raw materials and energy, less solvents, with reduced transport costs,

- More sustainable production with innovative technologies leading to a better use of raw materials and energies

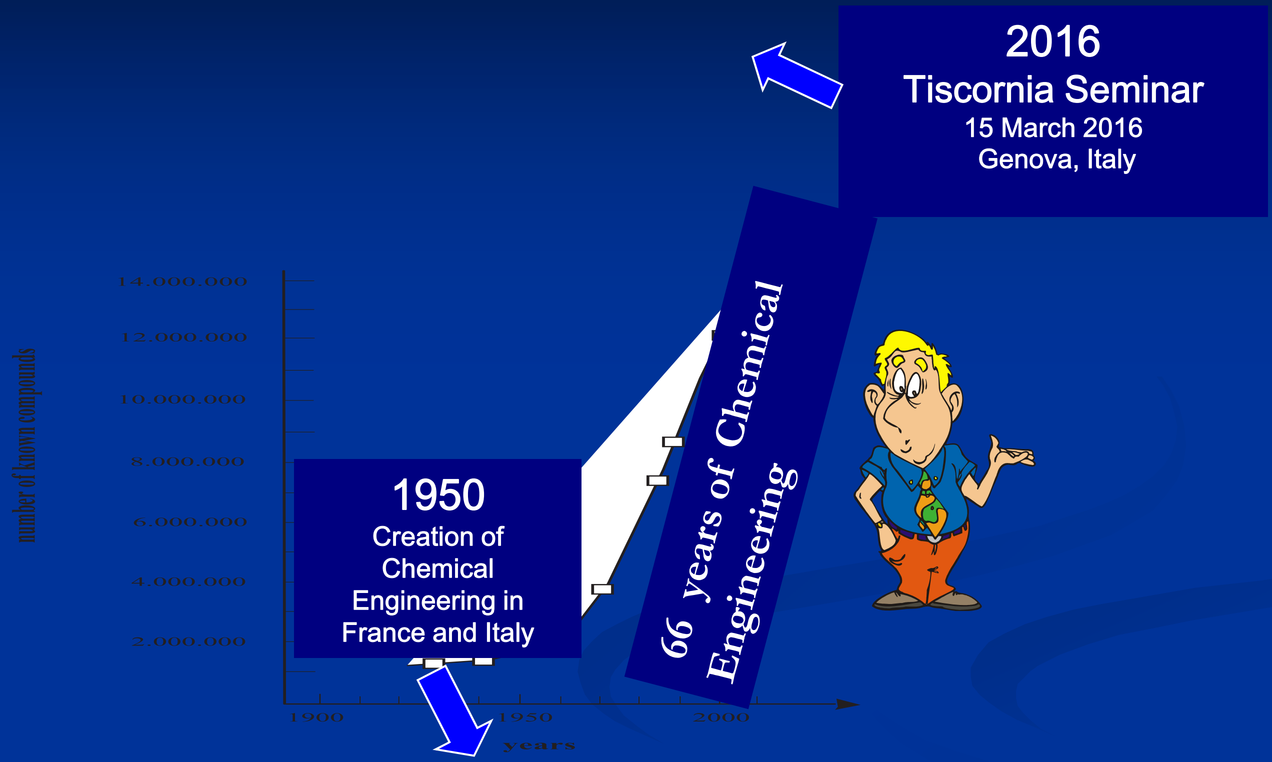
Thus this requires for chemical engineering

- Design of clean and efficient processes with innovative technologies and new process intensification reactors

Evolution of chemical engineering towards th design of the plant of future….

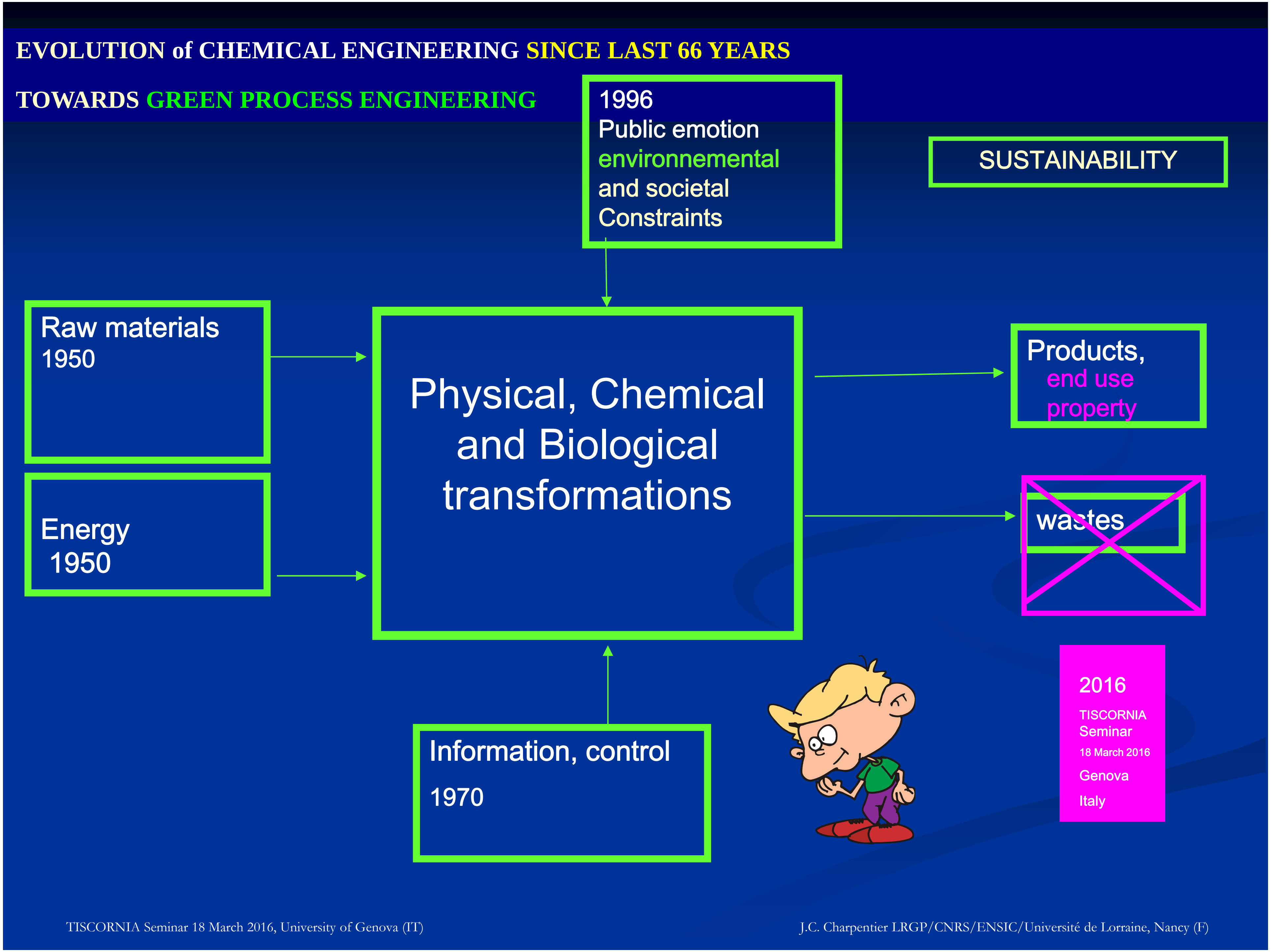
WHY and HOW Process Intensification and Process Intensification Reactors?

due to The necessary Evolution of Chemical and Process Engineering



Rapid knowledge in chemistry and biochemistry

- more than 14 million molecular compounds have been synthesized in 2015
- **only a small number of them is found in nature**
- **others are and will be conceived and manufactured by scientists and engineers to meet the needs of man and to satisfy his quest for knowledge (i.e., post-genomic era)**


EVOLUTION of CHEMICAL ENGINEERING SINCE LAST 66 YEARS
TOWARDS GREEN PROCESS ENGINEERING
1996
Public emotion
environnemental
and societal
Constraints
SUSTAINABILITY
Raw materials
1950
Energy
1950
Physical, Chemical and Biological transformations
Products,
end use
property
wastes
Information, control
1970
2016
TISCORNIA
Seminar
18 March 2016
Genova
Italy
TISCORNIA Seminar 18 March 2016, University of Genova (IT)
J.C. Charpentier LRGP/CNRS/ENSIC/Université de Lorraine, Nancy (F)

Historical paradigms of Chemical Engineering

1st Paradigm: Unit Operations

initiated by Arthur D. Little – ca. 1907 book: "Principles of Chemical Engineering" by Walker, Lewis and McAdams (1923) focus on equipments, construction and performances

2nd Paradigm: Transport Phenomena

appeared in 1960' book: "Transport Phenomena" by Bird, Stewart and Lightfoot (1960) focus on momentum, heat and mass transfer modeling

3rd Paradigm: INTEGRATED SYSTEM TIME and LENGTH MULTISCALE Approach (G3P)

for a modern green sustainable Chemical Engineering

(**involving Process Intensification** for the élaboration of the required end use properties of the green product, etc…)

(vers l'Usine du Futur) (Factory of the Future)

(Charpentier J.C., Chem Eng Res Des, 2010, 88, 248)