DEMCAMER
Catalytic Membrane Reactors

# Design and Manufacturing of Catalytic Membrane Reactors by Developing New Nano-architectured Catalytic and Selective Membrane Materials

This project is supported by the European Community's Seventh Framework Programme Grant Agreement N° NMP3-LA-2011-262840

Duration: 4 years. Starting date: 01-July-2011
Contact: joseluis.viviente@tecnalia.com






DEMCAMER
Catalytic Membrane Reactors

## Summary

The **aim** of DEMCAMER is to **develop innovative multifunctional Catalytic Membrane Reactors** (CMR) **based on new nano-architectured catalysts and selective membranes** materials to **improve their performance, durability**, **cost effectiveness** and **sustainability** (lower environmental impact and use of new raw materials) over four selected **chemical processes:**

- Autothermal Reforming (ATR),
- Fischer-Tropsch Synthesis (FTS),
- Water Gas Shift (WGS),
- Oxidative Coupling of Methane (OCM))

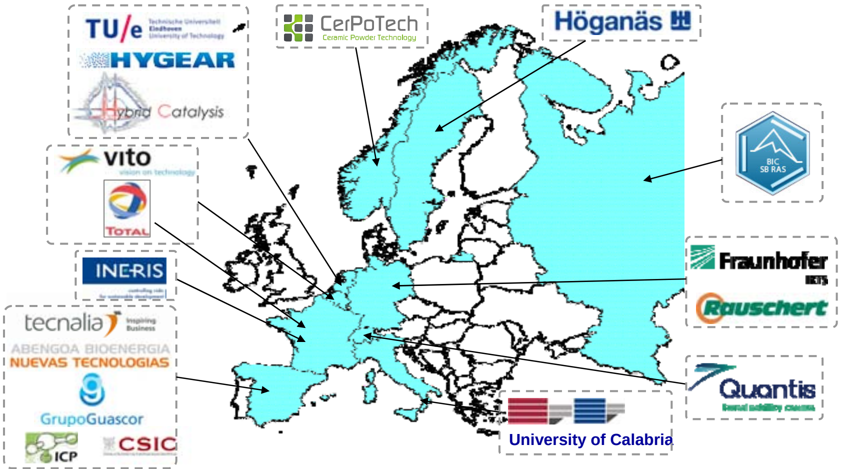
**for pure hydrogen, liquid hydrocarbons and ethylene production.**

Moreover DEMCAMER will bring the proof of concept of these novel CMRs by the set-up and validation of pilot prototypes relevant for each process.

DEMCAMER Catalytic Membrane Reactors

# Partnership

This research is carried out by a multidisciplinary and complementary team consisting of 17 top level European organisations from 10 countries: 8 Research Institutes and Universities working together with representative top industries in different sectors (from raw materials suppliers to chemical end-users).







DEMCAMER Catalytic Membrane Reactors

# Consortium Composition

1 TECNALIA, Spain
2 VITO, Belgium
3 UNICAL, Italy
4 TU/e, Netherlands
5 ICP-CSIC, Spain
6 FhG-IKTS, Germany
7 BIC, Russian Federation
8 INERIS, France
9 RKV, Germany
10 CERPOTECH, Norway
11 HYBRID, Netherlands
12 HYGEAR, Netherlands
13 ABNT, Spain
14 GUASCOR, Spain
15 QUANTIS, Switzerland
16 HÖGANÄS, Sweden
17 TOTAL PB, Belgium
18 TOTAL PF, France

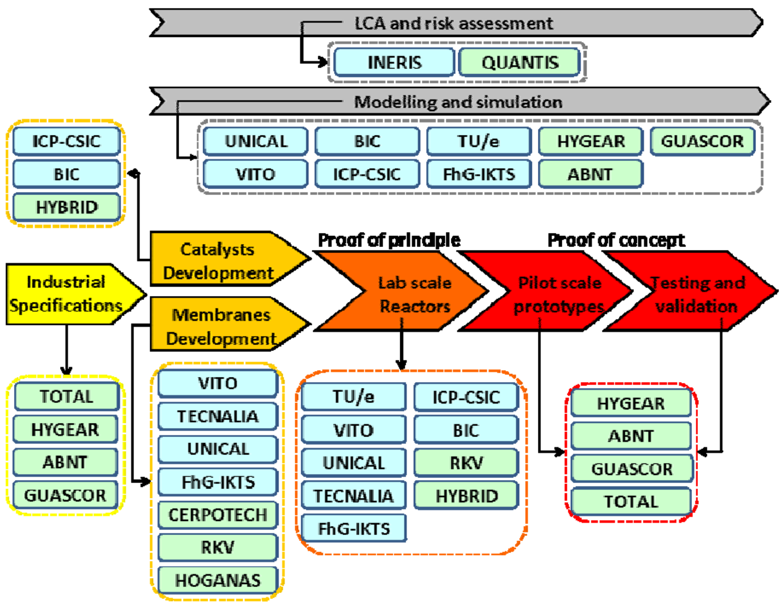
# Project Structure

- Development of novel catalyst materials
- Development of innovative membranes
- Novel catalytic membrane reactors will be designed on the basis of catalysts and membranes previously developed and using new reactor configurations supported by simulation
- Modelling and simulation at different levels: materials (membranes and catalysts), reactor prototypes and control system
- Lab scale and prototype reactors testing and validation
- Life Cycle Analysis, industrial risk assessment study



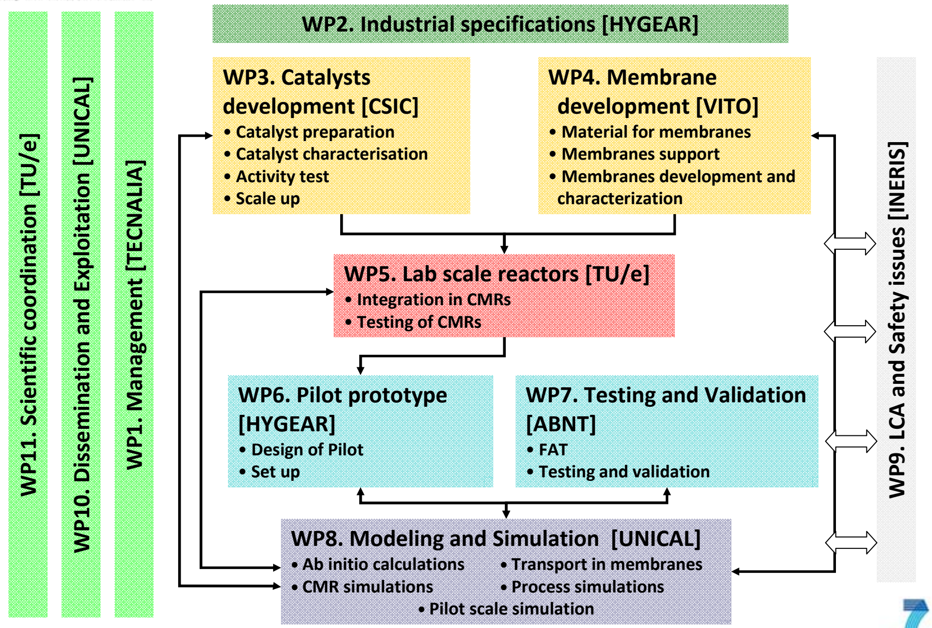



# Partnership Synergies



DEMCAMER Catalytic Membrane Reactors

## Overview of the Work Structure








DEMCAMER Catalytic Membrane Reactors

## Scientific and Technical Objectives (I)

- New membrane materials with improved separation properties, long durability and reduced cost
- New nano-architectured catalysts with better performance and at reduced cost
- Understanding the fundamental physicochemical mechanisms and the relationship between structure/property/performance and manufacturing process in membranes and catalysts, in order to achieve radical improvements in membrane reactors
- Design, model and build up of novel more efficient membrane reactor configurations based on the new membranes and catalysts

DEMCAMER
Catalytic Membrane Reactors

## Scientific and Technical Objectives (II)

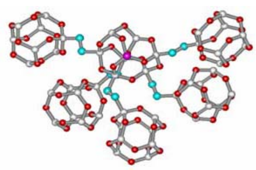
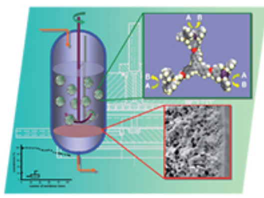
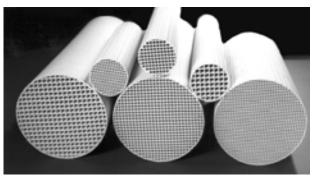
- Validating the new membrane reactor configurations, at semi-industrial prototype level, in four selected chemical process (ATR, WGS, OCM, FTS) for pure hydrogen, liquid hydrocarbons and ethylene production
- Improving the cost efficiency of membrane reactors by increasing their performance, decreasing the raw materials consumption and the associated energy losses
- Use of new raw materials (i.e. convert non-reactive raw materials)
- Assessment of the health, safety and environmental impact of the four CMR developed processes, a complete LCA of the developed technologies will be performed




DEMCAMER
Catalytic Membrane Reactors

## Catalytic Materials

- Development of ATR - WGS - OCM - FTS catalysts
- Physicochemical characterisation of ATR - WGS - OCM - FTS catalysts
- Activity tests in the ATR - WGS - OCM - FTS reactions
- ATR – WGS – OCM - FTS catalysts scale-up and conformation

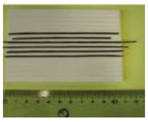
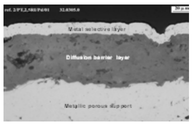






(Disclosure or reproduction without prior permission of DEMCAMER is prohibited).

DEMCAMER
Catalytic Membrane Reactors

# Membranes Development (I)

- Development of materials for MIEC, zeolite and metallic membranes preparation
- Development of ceramic and metallic membrane supports and interdiffusion layers
- Development and optimisation of MIEC membranes for $O_2$ and $H_2$ separation
- Development and optimisation of metallic membranes for $H_2$ separation
- Development and optimisation of zeolite membranes for $H_2$ and water separation

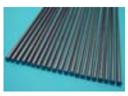
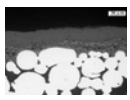
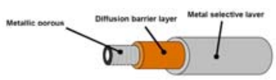
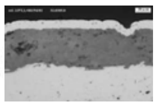
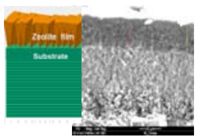




DEMCAMER
Catalytic Membrane Reactors

# Membranes Development (II)

Novel materials and membranes for application in catalytic reactors:

| | | |
|---|---|---|
| MIEC membranes | Hollow fibres ($H_2$ and $O_2$ permeation) |    |
| | Coatings ($O_2$ permeation) |   |
| Metal membranes ($H_2$ permeation) | |    |
| Zeolites ($H_2$ permeation and water removal) | |     |


(Disclosure or reproduction without prior permission of DEMCAMER is prohibited).

DEMCAMER
Catalytic Membrane Reactors

# Development of Lab Scale CMR

- Selection of Catalytic Membranes Reactors components: catalysts, membranes materials, supports and sealings
- Integration of these elements in lab scale reactors specifically designed for ATR, WGS, OCM and FTS
- Validation of the lab scale reactors performances and identification of best designs for pilot prototypes

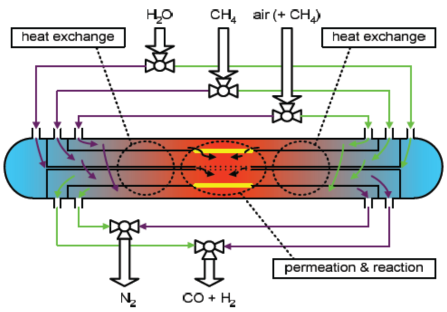



DEMCAMER
Catalytic Membrane Reactors

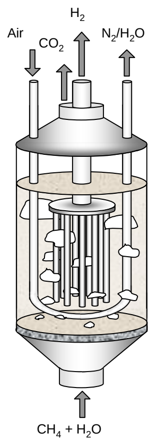
# Reactor Configurations (I)

## Autothermal Reforming (ATR)

reverse flow membrane reactor



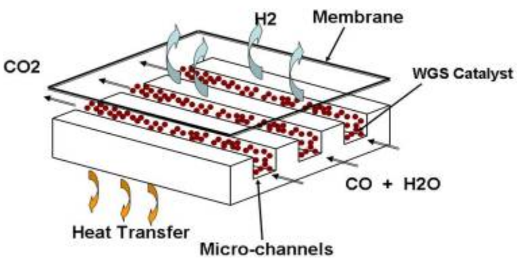

fluidised bed membrane reactor



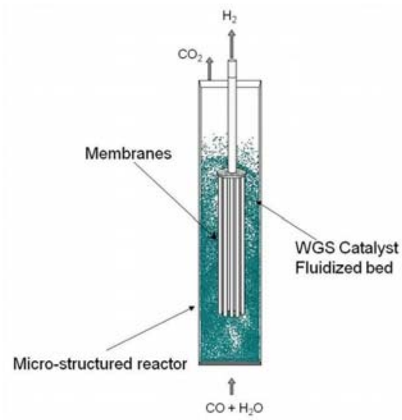
# Reactor Configurations (II)

## Water Gas Shift (WGS)

Packed bed micro reactor




Fluidised bed micro reactor

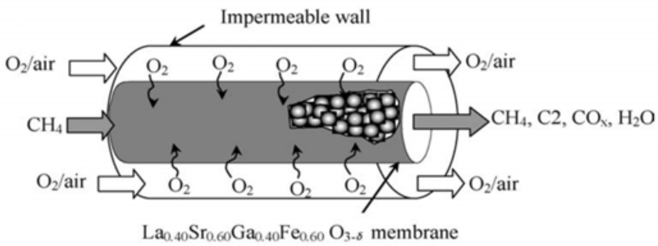






# Reactor Configurations (III)

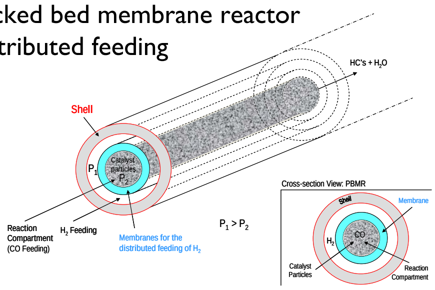
## Oxidative Coupling of Methane (OCM)



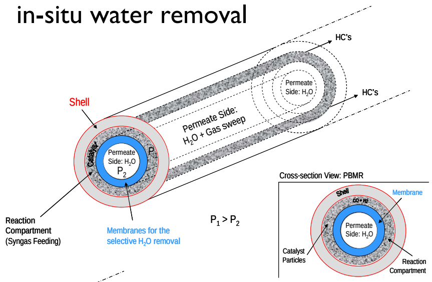
# Reactor Configurations (IV)

## Fischer-Tropsch Synthesis (FTS)

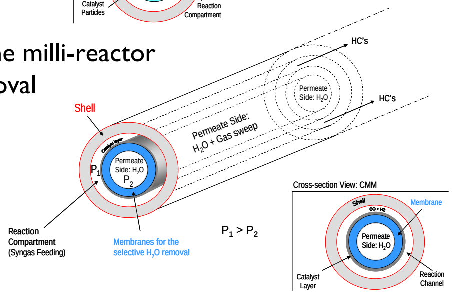
packed bed membrane reactor
distributed feeding




in-situ water removal




catalytic membrane milli-reactor
in-situ water removal









# Modelling and Simulation (I)

### For membranes:

- Study of zeolite membranes properties by means of molecular modelling and quantum chemical calculations will allow:
  - Identification of structure-function relationships at molecular level
  - Identification of the optimal procedure for evaluating the selectivity
  - Identification selectivity of gases
- Comparative analysis between the fundamental transport properties of Pd and Pd-based alloys and the corresponding properties of new (non-Pd) alloys formed from different metals

### For catalysts:

- Search for the optimal catalyst's structure for ATR, WGS, OCM, FTS by correlation between their morphological and structural properties and their catalytic performance

DEMCAMER
Catalytic Membrane Reactors

## Modelling and Simulation (II)

For ATR:
- Develop a reliable dynamic model in a reverse flow membrane reactor

For WGS:
- Develop a phenomenological model for fluidised bed membrane micro-reactors
  - o Develop a reliable 2D model for membrane micro-reactors
  - o Compare fluidised bed and packed bed membrane micro-reactors
  - o Analyse 1D or 2D dimensionless models for fixed bed membrane reactor

For OCM:
- Develop a reliable 1D detailed model for the study of hollow fibre MIEC membranes reactors with packed bed configuration

For FTS:
- 2D simulations of a fixed bed catalytic membrane reactor




DEMCAMER
Catalytic Membrane Reactors

## Modelling and Simulation (III)

Evaluation of the membrane separation properties:
- Mathematical models describing the permeation in metal and zeolite membranes
- Identification of elementary steps affecting the permeation through the membrane and their influence on mass transport properties

Processes:
- Design of new processes integrated with catalytic membrane reactors
- Analysis of the performance of the integrated processes as function of the operating conditions assuring the best performance of the whole integrated process

Pilot scale:
- Modelling of the pilot scale reactors for ATR, WGS, OCM and FTS
- Definition and modelling of control strategies and control routines for the pilot scale reactors

## Pilot Scale Prototypes

- Design and setup of the pilot scale catalytic membrane reactors
- Pilot reactors for ATR, WGS, OCM and FTS processes
- Depending on the working pressure all reactors will be designed and manufactured according the “Pressure Equipment Directive” of the EC (97/23/EEC)
- Overall system controls for the different reactor types will be designed and constructed to ensure automatic operation of the systems. The design of the system control will consider safety aspects and control strategies developed according to Pilot scale modelling
- All system components will be mounted into an enclosure and will undergo a Factory Acceptance Test (FAT) before being set into operation (testing) in WP7 - Validation and Testing.





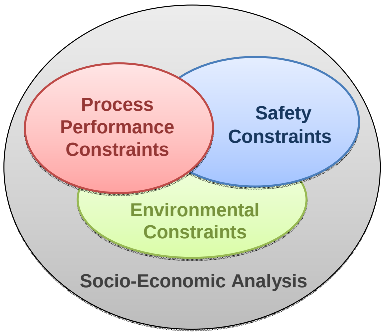

## Pilot Prototypes Testing and Validation

- Testing and validation of the pilot scale prototype reactors
- For testing and validating of the pilots, corresponding test plans and protocols will be defined including parameters and/or values that have to be derived from the tests, such as system efficiency, etc.
- Results will be compared to the requirements and specifications
- Test results will be used in Modelling and Simulation to validate and improve the pilot scale models and the system control strategies, as well as for the LCA and the accidental industrial risk assessment

# Life Cycle Assessment and Safety Issues

Assessment of socio-economic sustainability of the proposed technologies from an environmental and safety perspective.

- Environmental Life Cycle Assessment analysis of the CMR process
- Identification and evaluation of key safety parameters and risk analysis
- Proposal of recommendations for the safe operation of the CMR technology
- Socio-economic analysis to evaluate the sustainability and feasibility of the CMR technology (process performance, environmental and safety constraints) compared to currently available technologies









## Thank you for your attention