CHEMISTRY OF SMART ENERGY CARRIERS AND TECHNOLOGIES

cost

Chemistry and Molecular Sciences and Technologies

1st Management Committee Meeting- Brussels, 6th March 2015

GRANT HOLDER CANDIDATE

Istituto di Ricerche sulla Combustione
Consiglio Nazionale delle Ricerche (102 Institutes)

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Istituto di Ricerche sulla Combustione

Consiglio Nazionale delle Ricerche (102 Institutes)

ITALY

- 54 permanent staff
- 30 researchers
- 17 technical staff
- 7 administrative staff
- + post-doctoral fellows, graduate & undergraduat

www.irc.cnr.it

GRANT HOLDER CANDIDATE

Istituto di Ricerche sulla Combustione
Consiglio Nazionale delle Ricerche (102 Institutes)

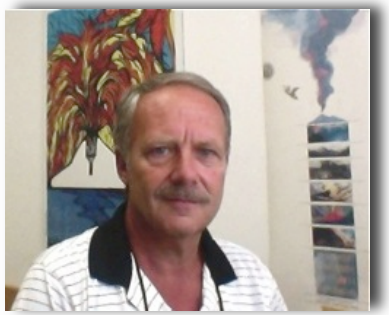
- Gained a longstanding experiences in coordination and participantion in:

  - European Framework Programs
  - Italian research programmes funded by the European Union (EU)
  - Italian research programmes

Administrative capacity

Financial stability

GRANT HOLDER CANDIDATE



Riccardo Chirone

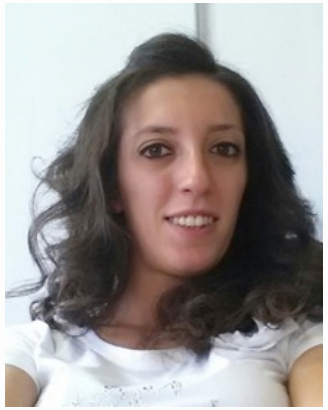
Director

Legal representative

Vincenzo Scognamiglio

Administrative Coworker

Financial representative



Antonella Napolitano

Administrative Coworker

Grant Manager

CHEMISTRY OF SMART ENERGY CARRIERS AND TECHNOLOGIES

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Chemistry and Molecular Sciences and Technologies

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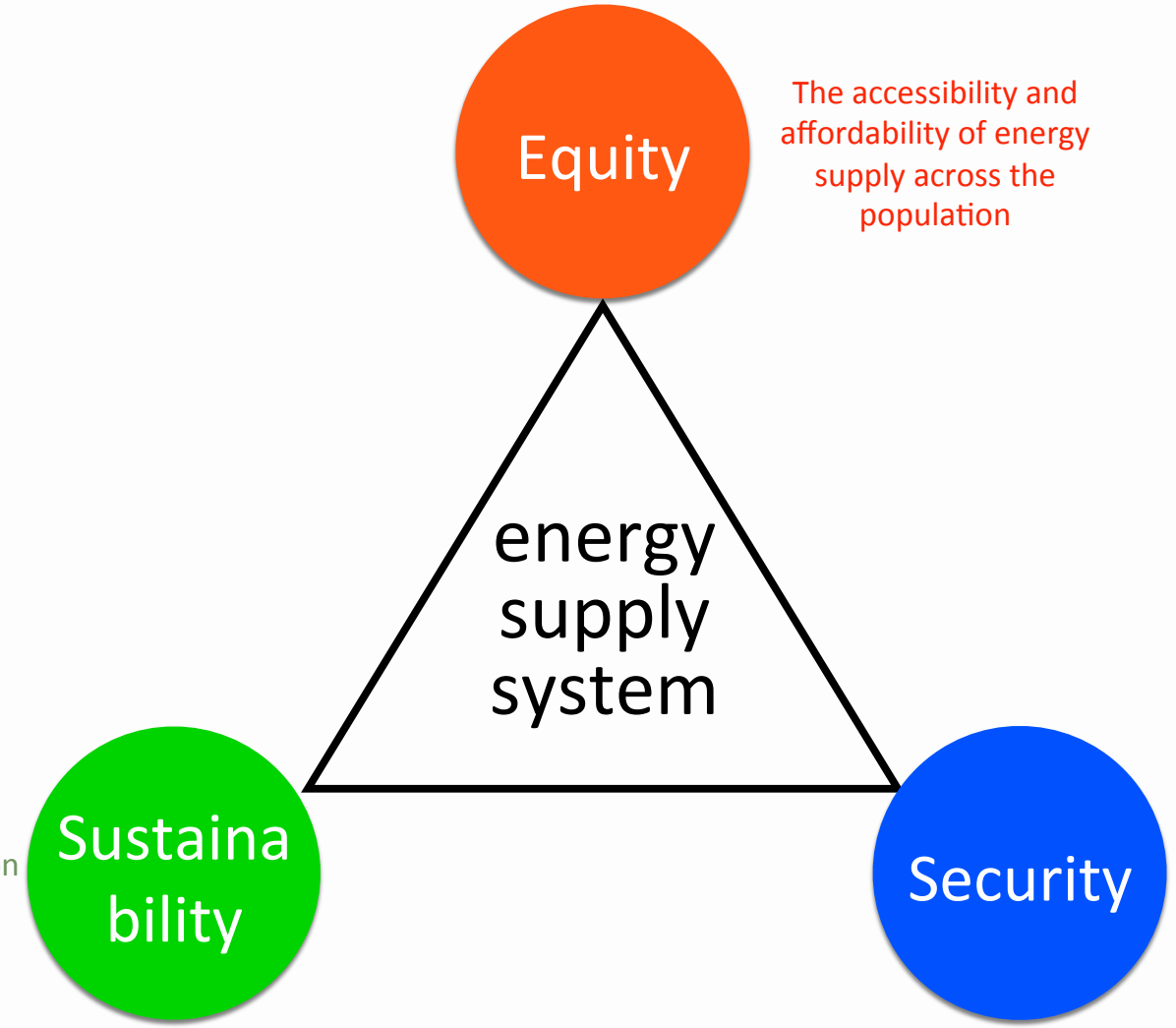
General background and motivation

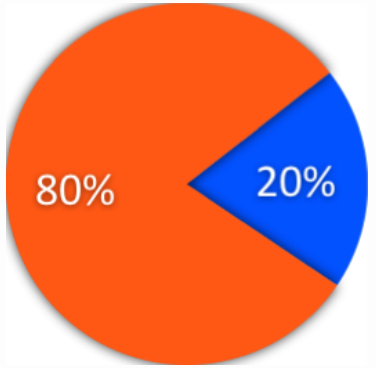
THE ENERGY TRILEMMA



General background and motivation

Total gross energy production in Europe

combustion
(conventional and alternative fuel)



others

General background and motivation

Drivers for Combustion processes/technologies development

equity and security

energy sources and fuels change (complex geo-political situation)

sustainabiliy

the long-term objective of low carbon society

energy, security, sustainability

smart energy distribution (more efficient production & distribution energy systems)

In this scenario..... toward

HORIZON 2020
THE FRAMEWORK PROGRAMME FOR RESEARCH AND INNOVATION

Greatest challenges of combustion-based energy systems:

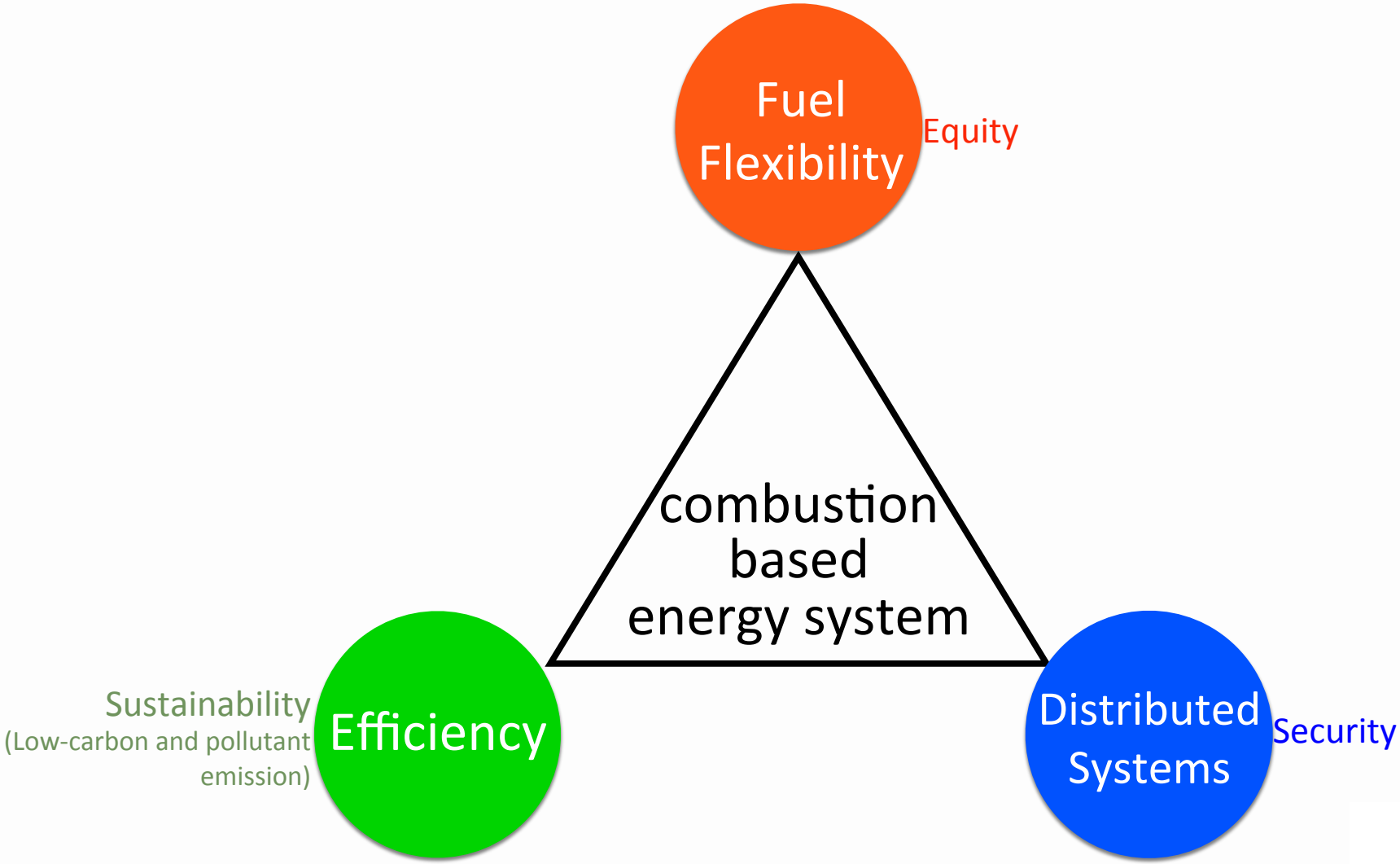
engines *furnaces* *gas turbines*

domestic burner *propulsion*

- maximum FUEL FLEXIBILITY
- minimization of GHG emission
- DISTRIBUTED energy

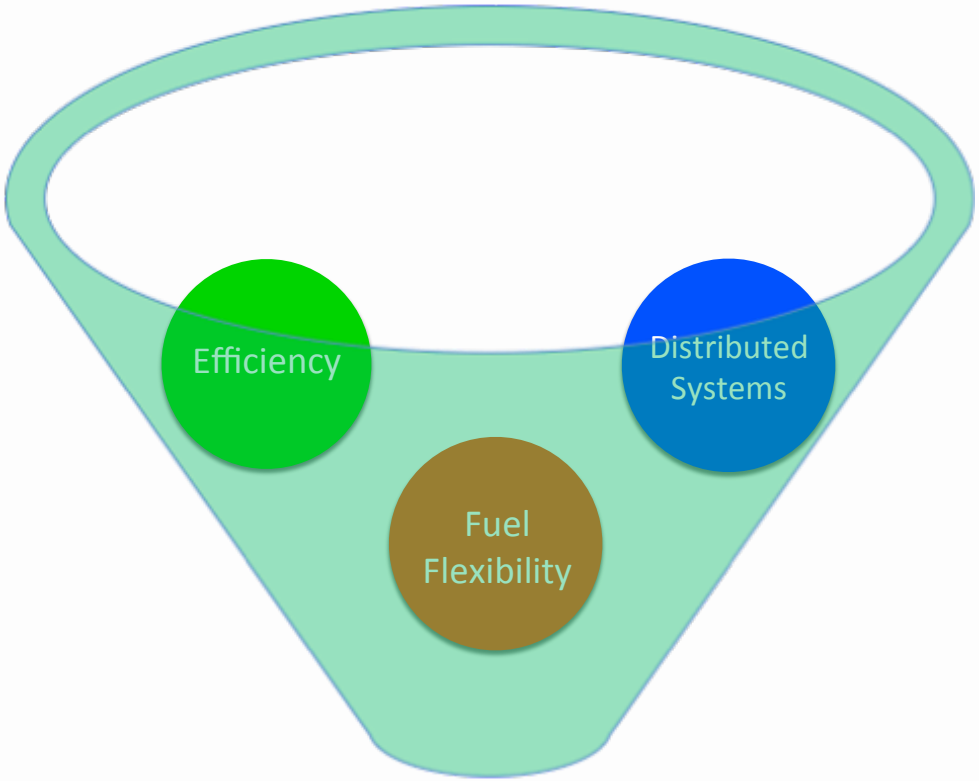
General background and motivation

THE COMBUSTION TRILEMMA



General background and motivation

THE COMBUSTION TRILEMMA

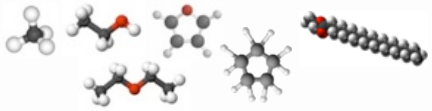


A more flexible use of energy carrier could allow for the design of a sustainable energy scenario

smart energy carriers

Smart Energy Carriers (SECs)

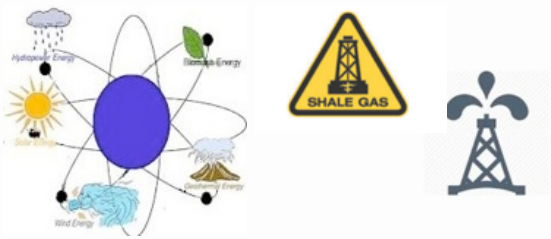
novel AND conventional energetic molecules

 and many others ....

increasing in number and typology

deriving from

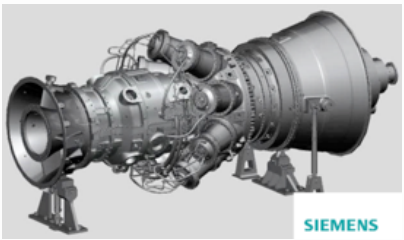
alternative or conventional (re)sources



increasing in number and typology

advanced processes and technologies

H_2 enriched gas turbines



SECs features:

exploiting many and diverse sources

providing the most suitable energy mix for the end-use technology

energetically and CO_2 efficient on the basis of used technologies

SMARTCATS ACTION AIM

Addressing the "grand challenge" of
matching the most promising SECs with the
advanced energy conversion technologies

In line with EU objectives & H2020

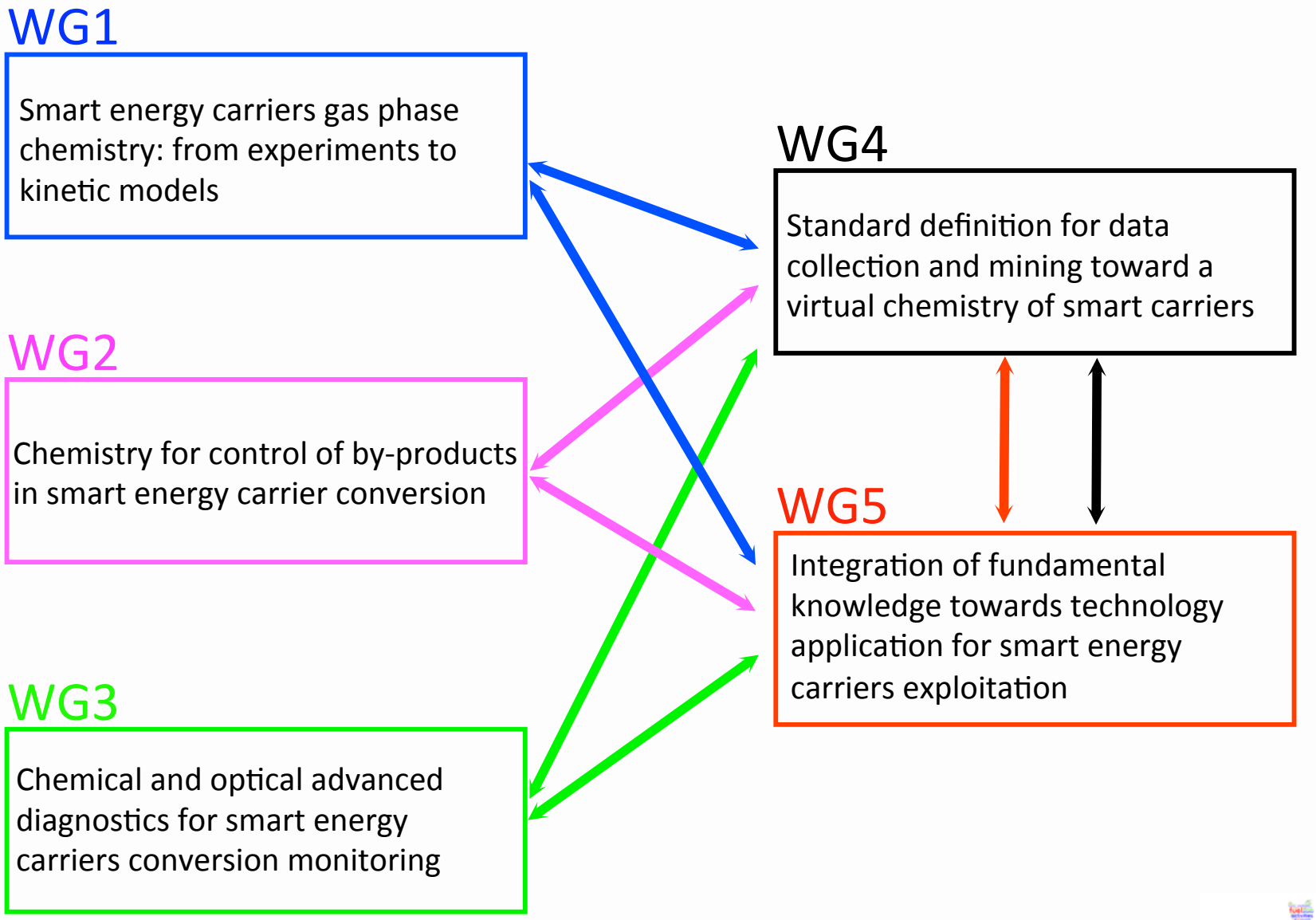
Synergies with Competitive low-carbon energy, Energy efficiency, Mobility for growth

In line with the challenged-based approach of H2020.

Strong and active industrial co-operation will help bridge the research and innovation divide

SMARTCATS STRATEGIC VISION

WORKING GROUPS



SMARTCATS

Workplan

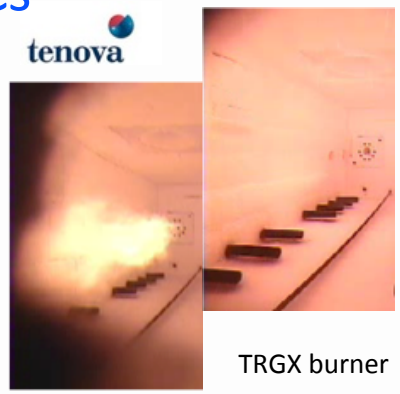
WG1

SECs gas phase chemistry: from experiments to kinetic models

AIM: Improve knowledge on detailed chemistry and thermochemistry for pyrolyis, oxidation and combustion of SECs

- New molecules
- Modified interaction
- New working conditions ranges (new technologies - higher pressures (>40-50 bar), low temperatures)

→ small changes can lead to huge differences →



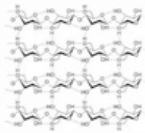
TRGX burner

New kinetic models AND improved effectiveness of existing models

Natural gas mixtures (compressed or liquefied natural gas, syngas, bio-natural gas containig also large amout of CO_2 and H_2O)

Simple molecules present in 1st and 2nd generation biofuels (large normal and iso-paraffins, alcohols, esters, saturated and unsaturated cyclic ethers (e.g derivate from furane))

Lignocellulosic biomasses components and molecules derived from their degradation (e.g gamma-valerolactone)



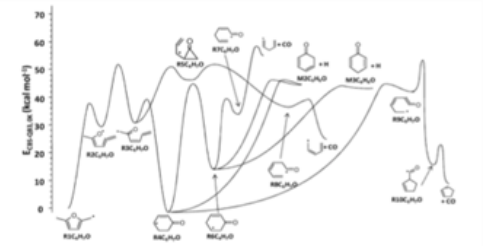
Complex mixtures found in 1st and 2nd generation biofuels (such as Fatty Acid Methyl Esters, Hydrogenated Vegetal Oil or in the proposed surrogates)

SECs gas phase chemistry: from experiments to kinetic models

Approaches and tools

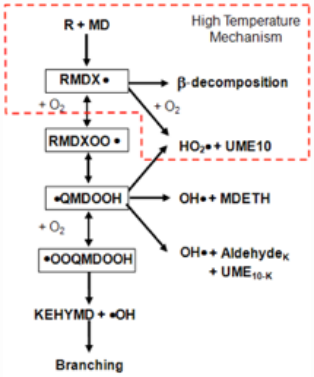
- Modeling
  - Automatic generated mechanisms (large molecules)
  - Simplification procedures (e.g. lumping)
  - Theoretical evaluation of
    - thermodynamic parameters
      - Modern quantum chemical methods (e.g. coupled cluster methods, density functional theory)
    - kinetic parameters
      - Statistical theories (RRKM theory, statistical adiabatic)
  - Uncertinty analysis (critical for the use of such models within the engineering design process)

Bielefeld University - CNRS



Dimethyl furan decomposition pathway

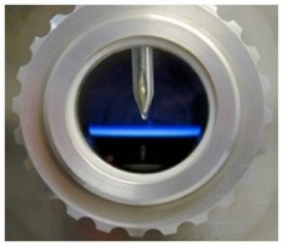
Politecnico di Milano



- Experiments

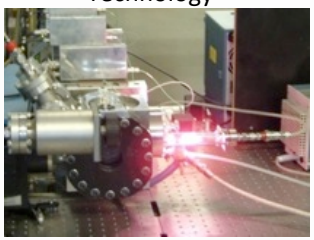
Temperature, pressure, composition

CNRS - DCPR



Laminar flat flame burner at low pressure

Karlsruhe Institute of Technology



Shock tube

National University of Ireland

Rapid compression machine

..... from microscale

to macroscale .....

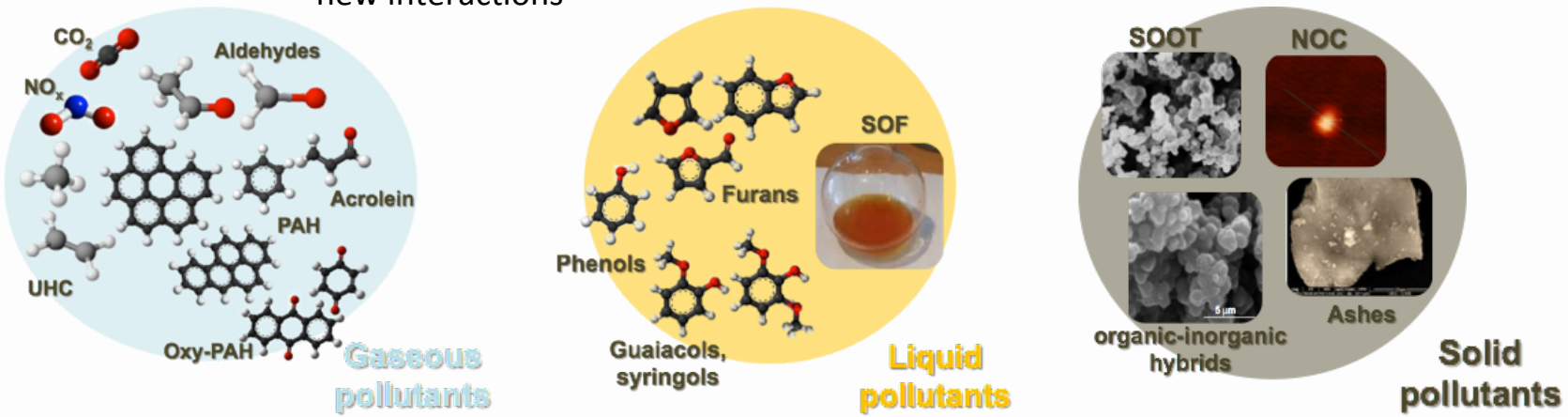
WG2

Chemistry for control of by-products in smart energy carrier conversion

AIM: increase the knowledge on the formation of organic and inorganic combustion by-products in order to improve the sustainability of SECs.

New "fuels" + New technologies = "New" pollutants (oxygenates, soot, etc)

new operative conditions
new interactions



- Development of more accurate chemical models for pollutants – fundamental experiments
- Inventory of noxious emissions from combustion devices (conventional vs alternative fuels)

Chemistry for control of by-products in smart energy carrier conversion

Approachs and tools

- Experiments: gaseous, liquid and solid pollutants

University of Zaragoza

Flow reactor

Istituto Superior Técnico

Drop tube

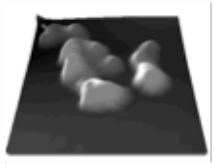
tenova

1-Digit Burner Prototype

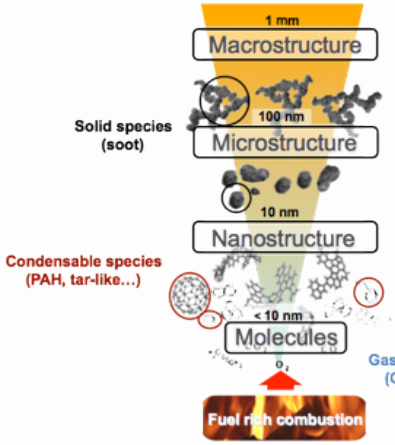
from microscale ..... to macroscale .....

- Modeling: gaseous pollutants and particle formation and growth

- Solid characterization



AFM of nanoparticles



Transmission Electronic Microscopy (TEM)

High resolution Transmission Electronic Microscopy (HR-TEM)

FT-IR Spectroscopy
UV-Spectroscopy
Raman spectroscopy

Chemical and optical advanced diagnostics for SECs conversion monitoring

AIM: provide a forum for the development and evaluation of diagnostic tools and procedures ranging from elementary reaction rate determination to real time measurements in practical devices.

FOCUS

Fundamental studies

Identification of intermediate stable and radical species for kinetic studies

➡Non intrusive optical techniques (LIF, Raman, Coherent Anti-Stokes Raman Spectroscopy,.....)

➡Intrusive techniques, e.g.GC, PhotoIonization Mass Spectrometry (PIMS) using vacuum-ultraviolet radiation from synchrotron source, Photoelectron-photoion coincidence spectroscopy (PEPICO)

➡.....

Application

➡Measurements and analysis of global "integral" combustion properties, e.g.: Ignition delay times, laminar burning velocity (heat flux burner, spherical bomb methods)

➡Emission measurements

in model flames and in complex systems

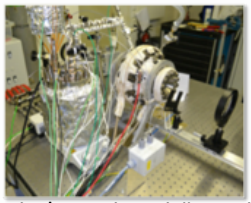
Time Resolved Mass Spectrometry

University Duisburg (Germany)

Laser Induced Fluorescence for radical detection in flame

University of Lille (France)

Heat flux burner



Technische Universität-Freiberg (Germany)

Chemical and optical advanced diagnostics for SECs conversion monitoring

PERSPECTIVE

Identification of suitable markers of combustion progress and efficiency

Evaluation of diagnostic tools in "harsh" conditions

→

Diagnostic capability transfer from fundamental to complex systems

→

Combustion and emission measurements in complex systems:Engines, Furnaces, Boilers, Household appliances ...

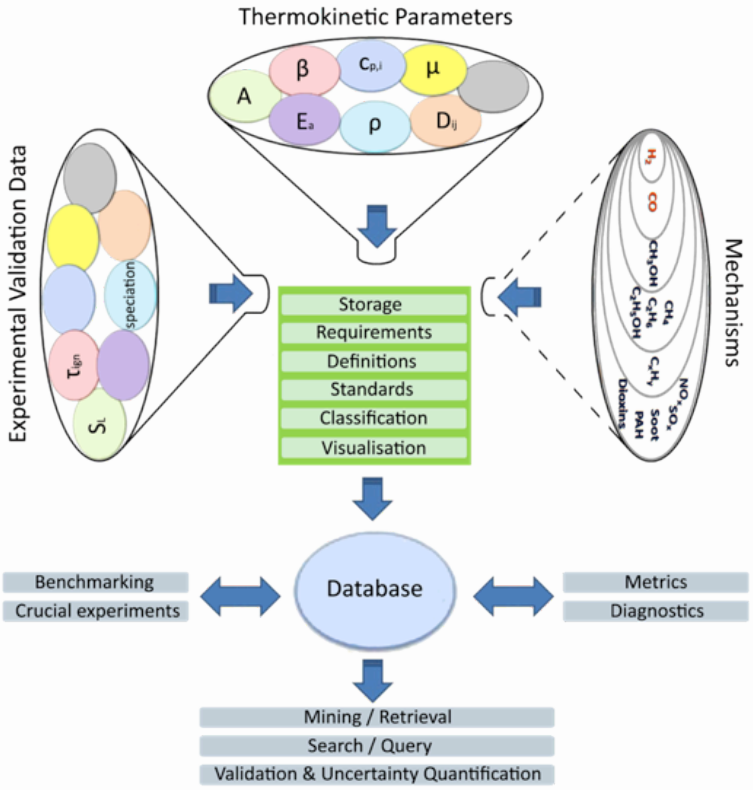
↓

Identification of possible markers and sensors for implementation of ICT monitoring and control systems

WG4

Standard definition for data collection and mining toward a virtual chemistry of SECs

AIM: identification of the main requirements and tools for the development of databases, software and mathematical tools for data collection and handling as well as chemistry optimization using data mining techniques.



Main Challenge:

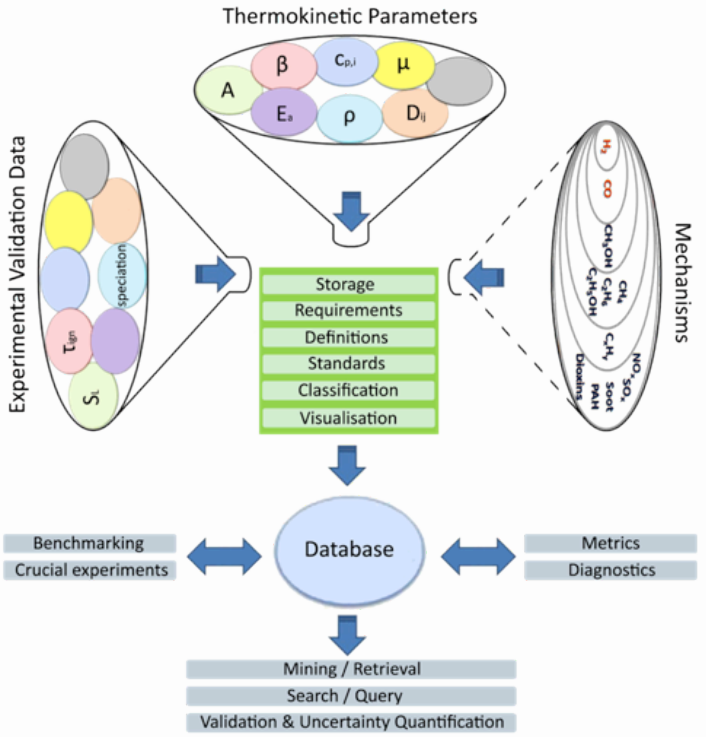
provide a forum for all experts in the combustion community to formulate a common set of requirements for a universal combustion database:

-capable of efficiently store the vast amount of raw data generated by experiments and modeling

-efficiently accessible for future use and maintenance.

Standard definition for data collection and mining toward a virtual chemistry of SECs

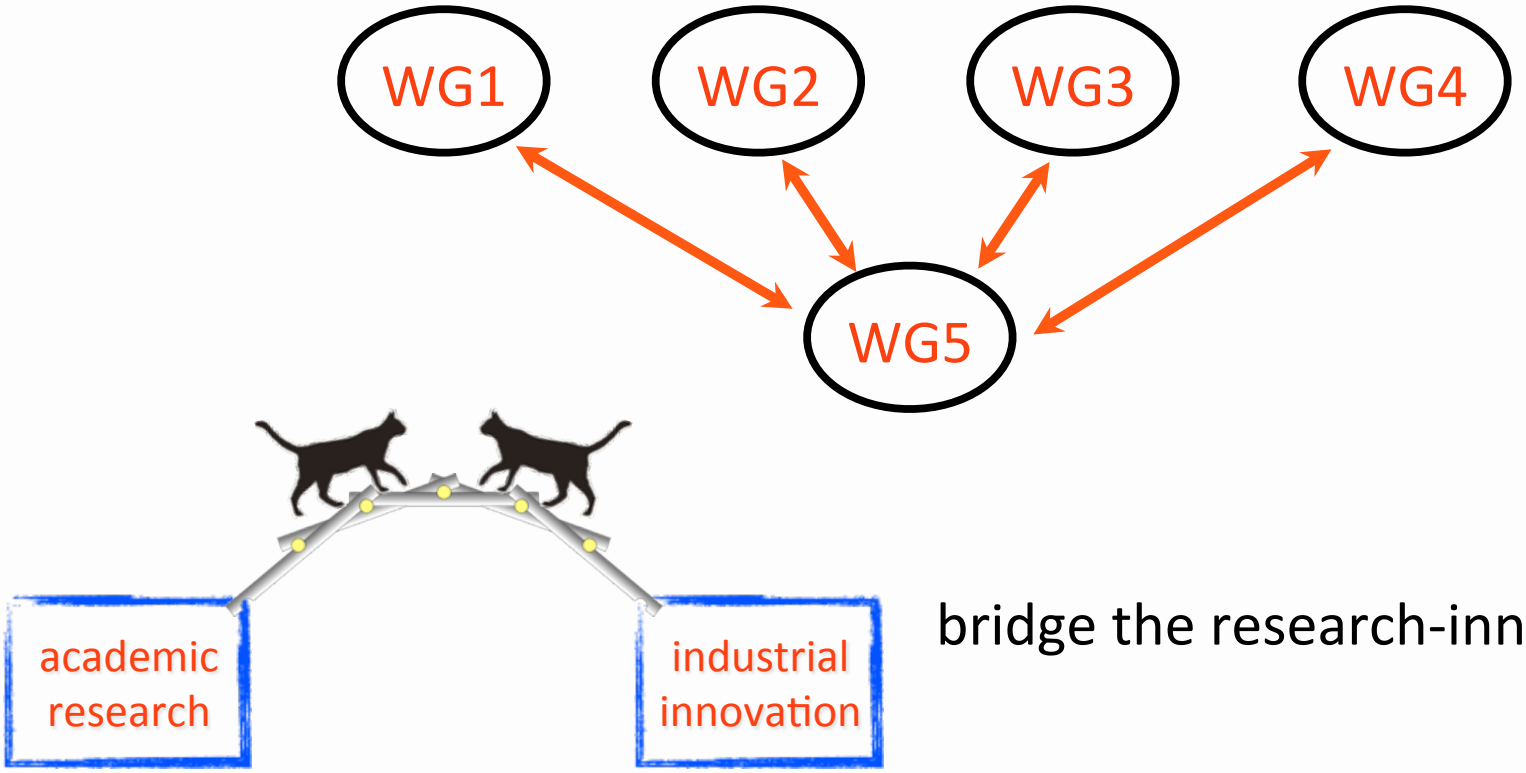
- Definition of specific sets of prerequisites and goals for the establishment of a combustion database that will allow efficient electronic communication of combustion-related data.
- Definition of critical raw, experimental and numerical data that needs to be made available for the evaluation and possible future re-evaluation of derived parameters and the format required for their efficient communication.
- Definition of crucial experiments needed to provide a consistent match between experimental evidence and model validation
- Active discussion and research involving the sensitivity and establishment of error bounds both in experimental data and modeling results.
- Development of methods, such as those from data mining, to analyze the vast quantities of already existing data in order to provide new insight into the combustion process.



WG5

Integration of fundamental knowledge towards technology application for SECs exploitation

AIM: provide optimized ready to use tools and techniques for an effective use of SECs on large scale.

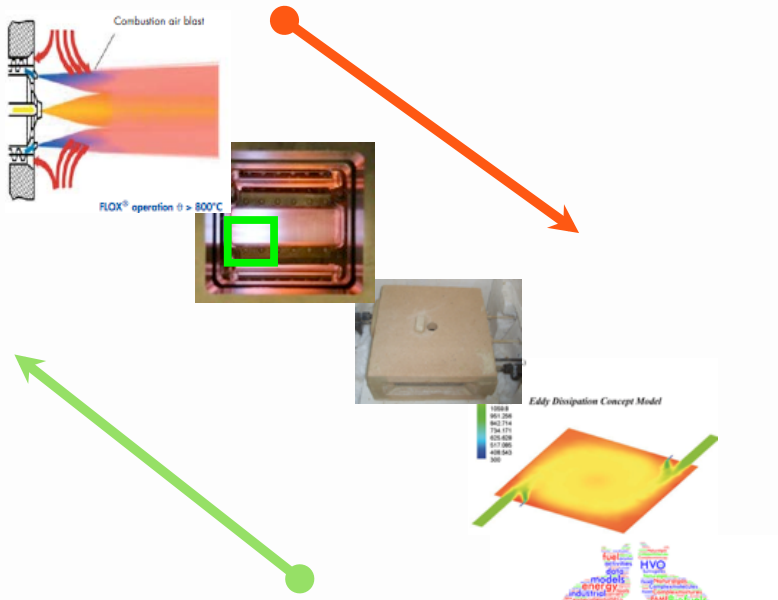


bridge the research-innovation gap

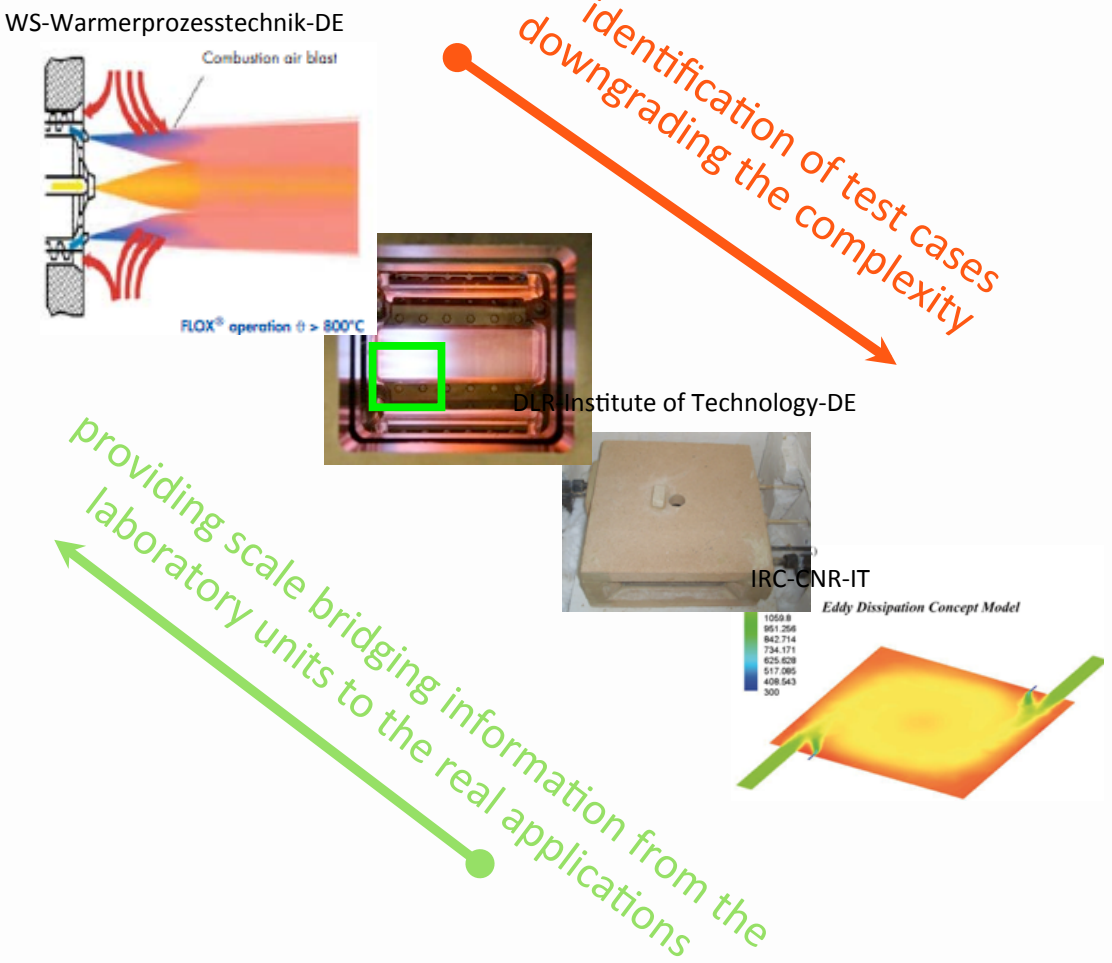
Integration of fundamental knowledge towards technology application for SECs exploitation

- Integration of detailed kinetic mechanisms in large scale numerical simulations
- Development/optimization of reliable, widely applicable and affordable turbulence/chemistry interaction models
- Assessment of the uncertainty related to numerical predictions for their use in new design and regulation

→ taking into account the typology of combustion regime and the features of target technology

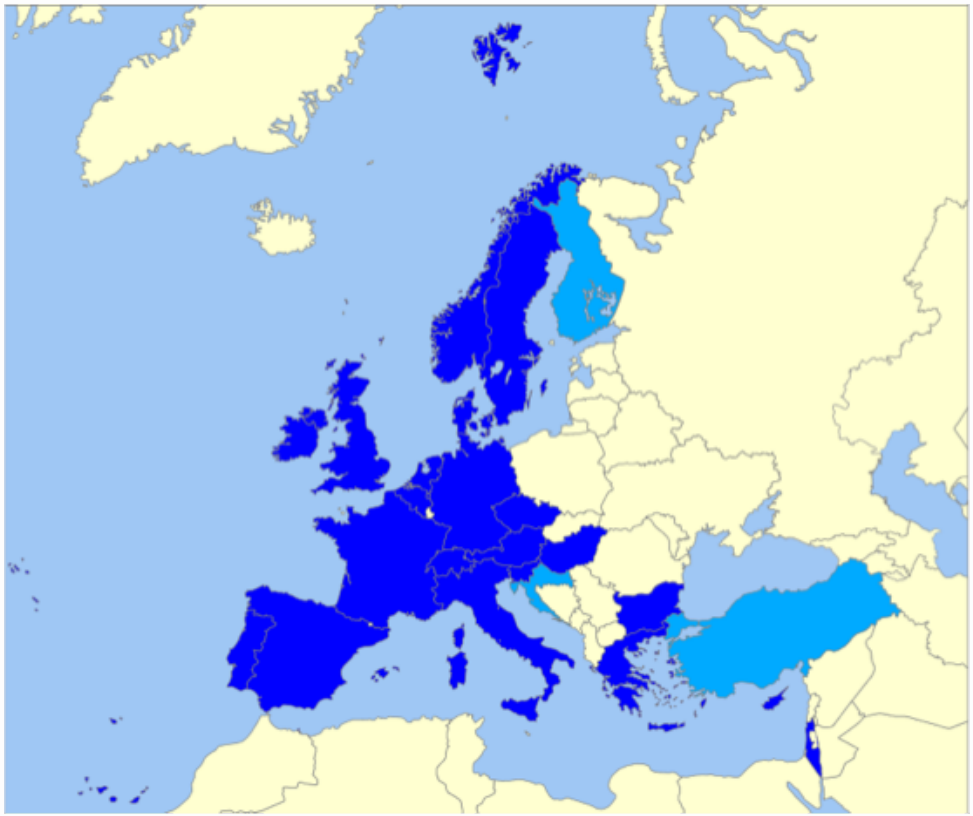


Integration of fundamental knowledge towards technology application for SECs exploitation



The SMARTCATs Action
Promotion of COST Policy

21 (+4)countries



15 companies

In the proposal:

2 non-cost countries

Promotion of COST Policy

- Inclusiveness of Target Countries:

Target Countries	MoU signed	ongoing
17	5	3
Bosnia and Herzegovina, Bulgaria, Cyprus, Czech Republic, Estonia, Croatia, Hungary, Lithuania, Latvia,Macedonia, Malta, Poland, Romania, Serbia, Slovenia, Slovakia, and Turkey	Bulgaria, Cyprus, Hungary, Slovenia, Czech Republic	Croatia, Turkey, Poland

within 1st year at least 50% of target countries

- Early Stage Researchers
- Gender Balance

→ Early Stage Researchers and Gender Balance Advisory Committee

SMARTCATs

Management Aspects

Distribution of Tasks

WG Leaders-Vice Leaders

Management Structure

WG1:

Smart energy carriers gas phase chemistry: from experiments to kinetic models

- Leader: Frédérique Battin-Leclerc

Laboratoire Réactions et Génie des Procédés, CNRS
Nancy, France

- Vice-leader: Olivier Herbinet

Université de Lorraine
Ecole Nationale Supérieure des Industries Chimiques
Lorraine, France

WG2:

Chemistry for control of by-products in smart energy carrier conversion

- Leader: Marìa Alzueta

Universidad de Zaragoza
Aragon Institute for Engineering Research
Zaragoza, Spain

- Vice-leader: Marìa Abian

Instituto de Carboquímica (ICB) –
Spanish National Research Council (CSIC)
Zaragoza, Spain

WG3:

Chemical and optical advanced diagnostics for smart energy carriers conversion monitoring

- Leader: Stefan Voss

Institute of Thermal Engineering
TU Bergakademie Freiberg
Germany

- Vice-leader: Oliver Welz

Institute of Combustion and Gas Dynamics –Reactive Fluids
Faculty of Engineering, University of Duisburg-Essen
Germany

WG4:

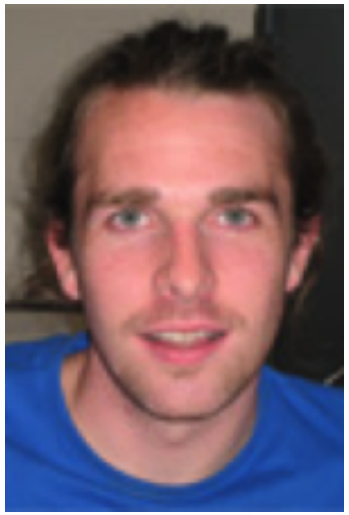
Standard definition for data collection and mining toward a virtual chemistry of smart carriers

- Leader: Edward Blurock

Malmö University
Sweden

- Vice-leader: Stephen Dooley

University of Limerick
Ireland



WG5:

Integration of fundamental knowledge towards technology application for SECs exploitation

- Leader: Alessandro Parente

Université Libre de Bruxelles
Belgium

- Vice-leader: Cathleen Perlman

LOGE
Sweden

Management Structure

Appointment of Horizontal roles

Short Term Scientific Mission Manager

Iliyana Naydenova
Technical University of Sofia
Bulgaria

Industrial Advisory Committee

Fabian Mauss

BTU Cottbus, Germany

Early Stage Researcher and Gender Balance Advisory Committee

Terese Løvas

Norwegian University of Science and Technology, Norway

Web Institution

GRANT HOLDER: IRC-CNR will host the website www.smartcats.eu

Web and Dissemination Manager

Raffaele Ragucci
IRC-CNR, Italy

Website Development

Zissis Malliotakis
NTUA, Greece

Core Committee tasks

- MC delegation of authority for the Core Committee:
  - for economic decision up to € 5000

- MC electronic vote:
  - time limit for e-COST invitations: 7 days
  - presumed consent

Timetable

YEAR	1				2				3				4			
Quarter	1	2	3	4	1	2	3	4	1	2	3	4	1	2	3	4
MC Meetings																
Workshops																
Conferences																
Training schools																
General Meetings																
STSM																
Dissemination																
Outreach																

Financial Scientific and Administrative Coordination (FSAC)

Allocated budget	**€ 129.000**
Total Expenditure	**€ 112.173,91**
FSAC (15% of total expenditure)	**€ 16.826,09**

- To cover:
  - ➡ general costs
  - ➡ local taxes

WORK & BUDGET PLAN- 1st GRANT PERIOD

The 1st GP will start on 1st June

WORK AND BUDGET PLAN SUMMARY	
COST NETWORKING TOOLS	EXPECTED COST
Meetings	€ 75.450,00
Training Schools	€ -00
STSMs	€ 32.000,00
Dissemination	€ 4.723,91
Other Expenses Related to Scientific Activities	€ -00
Total AScience Expenditure	€ 112.173,91
FSAC	€ 16.826,09
TOTAL Expenditure	€ 129.000,00

Workshop on Smart Energy Carriers
Thessaloniki (Greece) 3-4.9.2015 (2 days)

- The Workshop will bring together leading experts from industry and academia in the fields of energy and fuels to present:
- The latest developments in production, processing and utilization of smart energy carriers The needs and requirements of the industrial sector for the adoption of the smart energy carriers.
- OUTPUT:
  - A position paper on Smart Energy Carriers
  - A roadmap for SMARTCATS WG.

General Meeting- Naples 11-12 February 2016

STSM program

Allocated budget = € 32000

- It will start as soon as possible, after the 1st July.
- Promotion of STSM in companies

Dissemination/ Website

- Action webpage represents the accumulation point of the activities. First year objectives are:

1. A simple static page is already on line. MC members will have to register and provide some details to complete the Action info section.
2. Definition of website general architecture and acquisition of resources by the end of first trimester.
3. Interaction with WG4 members to identify requirements and best suited platform to be used for the design of a experimental/numerical data repository.
4. Set-up of a user interface and start of a broadcast service of SECS chemistry and technologies informative videos.

WEBSITE - Perspectives

- In the long run the Action webpage should collect all the public teaching, dissemination and reference materials produced in the Action development.
- News, blog and wiki sections will be implemented to stimulate discussion and disseminate information on the Action topics.
- The final aim is the creation of a reference portal in the field of innovative energy carriers.
- Additional economic/personnel resources will eventually be needed. (participation to EC calls, sponsorship, governmental).

Training/Dissemination tools
In the COST @ no cost

- Webinars
- Information on web page of other institutions, associations, platforms, associations (www.combustioninstitute.org, www.irc.cnr.it, possible information on EU platforms
- Flyers, posters, presentations during scientific meeting and conferences in the field.


TECHNOLOGY
RESEARCH
DEVELOP
DATA
ENERGY
SYSTEM
CHEMISTRY
ADVANCED
TOOL
FUEL
KINETIC
MODEL
NEW
INDUSTRY
COMBUSTION
CHEMICAL
AIM
USE
WG
ACTION
KNOWLEDGE
PROPOSAL
MECHANISM


HVO
BIOFUELS
FAME
HYDROTREATEDVEGETALOILS
SURROGATES
COMPLEXMIXTURES
NATURALGAS
COMPLEXMOLECULES

Thank you