The SMARTCATs COST Action

CHEMISTRY OF SMART ENERGY CARRIERS AND TECHNOLOGIES: A EUROPEAN COST NETWORK

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The Energy Trilemma

Equity

The accessibility and affordability of energy supply across the population

Sustainability

Efficient and from renewable, low-carbon sources

Security

Reliability of management of primary energy supply
The Combustion Trilemma

- A new energy production and distribution system based on smart grid concepts and utilizing Smart Energy Carriers (SEC).
- SECs are conventional and novel energetic molecules from conventional or alternative (re)sources selected on the basis of their best-available production and/or utilization technologies.
- SECs are strong candidates as possible solutions for energy storage, transfer and transformation from renewable (local) sources (wind, solar, biomass, waste).
The SMARTCATs COST Action aims to set-up a Europe-wide network of leading academic and research institutions and key industries to promote the use of smart energy carriers on a large scale in order to increase fuel flexibility and carbon efficiency of energy production and to support distributed energy generation strategies.

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
- H₂ enriched gas turbines

SECs features:
- exploiting many and diverse sources
- providing the most suitable energy mix for the end-use technology energetically and CO₂ efficient on the basis of used technologies
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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

standardized validation experiments
advanced diagnostic tools
predictive models
micro meso macro

INNOVATIVE COMBUSTION TECHNOLOGIES
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A total of 75 organizations from 25 participating countries (EU and Associated States) plus the US, China and Brazil. Strong industrial participation.
The Working Groups

WG1
Smart energy carriers gas phase chemistry: from experiments to kinetic models

WG2
Chemistry for control of by-products in smart energy carrier conversion

WG3
Chemical and optical advanced diagnostics for smart energy carriers conversion monitoring

WG4
Standard definition for data collection and mining toward a virtual chemistry of smart carriers

WG5
Integration of fundamental knowledge towards technology application for SECs exploitation
The Working Groups – WG1

AIM: Improve knowledge on detailed chemistry and thermochemistry for pyrolysis, 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

New kinetic models AND improved effectiveness of existing models

Natural gas mixtures (compressed or liquefied natural gas, syngas, bio-natural gas containing also large amount of CO₂ and H₂O)

Simple molecules present in 1st and 2nd generation biofuels (large normal and iso-paraffins, alcohols, esters, saturated and unsaturated cyclic ethers (e.g. derivative 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)
The Working Groups – WG1

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)
• Uncertainty analysis (critical for the use of such models within the engineering design process)

Experiments

from microscale to macroscale

Laminar flat flame burner at low pressure
Shock tube
Rapid compression machine
The Working Groups – WG2

**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)

- Development of more accurate chemical models for pollutants – fundamental experiments
- Development of inventory of noxious emissions from combustion devices (conventional vs alternative fuels)
The Working Groups – WG2

Approaches and tools

- Experiments: gaseous, liquid and solid pollutants

- Modeling: gaseous pollutants and particle formation and growth

- Solid characterization
The Working Groups – WG3

**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**

- Advanced sampling and chemical analysis coupled with laser-based and mass-spectrometric diagnostics
- Simple combustion devices and chemical kinetics experiments
- Time and species resolved analysis of combustion processes
- Elementary chemical reactions
- Fluid-dynamics/chemical-kinetics interaction

- **Time Resolved Mass Spectrometry**
  - Technische Universität Freiberg (Germany)

- **Photo-Electron Photo-Ion Coincidence spectroscopy**
  - University Duisburg-Essen (Germany)

- **Laser Induced Fluorescence for radical detection in flame**
  - PSI-Villingen (Switzerland)

- **University of Lille (France)**

2nd ECATS Conference, 7-9 November 2016, Athens, Greece
The Working Groups – WG3

Identification of suitable markers of combustion progress and efficiency

Evaluation of diagnostic tools in "harsh" conditions

Perspective

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
The Working Groups – WG4

**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.
The Working Groups – WG4

- 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.
Heat release markers for the combustion of alternative aviation fuels in gas turbines (Skevis et al., 2nd ECATS Conference)
The Working Groups – WG5

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

![Diagram showing connections between WG1, WG2, WG3, and WG4 to WG5.](image-url)

bridge the research-innovation gap
The Working Groups – WG5

- 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
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NETWORKING TOOLS

• Workshops, meetings, conferences

Meetings are organised in any COST country participating in the network. They can be of different types, such as Management Committee meetings, Working Group Meetings, Workshops and Conferences. They are open to the whole scientific community and provide visibility opportunities for the COST Action. COST contributes to the travel and subsistence costs of participating scientists, and to the organisation costs of the meeting (1st SMARTCATs General Meeting, Thessaloniki, Greece, 8/2015, Workshop on Smart Energy Carriers for Power, Industry and Engines, Thessaloniki, Greece, 8/2015, 2nd General Meeting, Lisbon Portugal, 11/2016, Workshop on Smart Energy Carriers in SMEs, 11/2016)

• Training schools

Training Schools provide intensive training in emerging research topics within the laboratories and organisations involved in the COST Action. Participants are mainly, but not exclusively, young researchers involved in COST Actions. (Workshop on Data Collection and Mining toward Virtual Chemistry of Smart Energy Carriers, Napoli, Italy, 4/2016, Training school on uncertainty analysis of SECs kinetic mechanisms, Budapest, Hungary, 6/2015).

• Short Terms Scientific Missions

Short-term scientific missions (STSM) are exchange visits between researchers involved in a COST Action, allowing scientists to visit an institution or laboratory in another COST country. They are aimed at fostering collaboration, sharing new techniques and infrastructure that may not be available in other participants' institutions or laboratories. STSM are intended especially for young researchers.
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