



cascatbel

D10.7 Highlights of CASCATBEL's annual progress for public dissemination

Version 1.2

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1. SUMMARY

The present report contains highlights of annual progress of the CASCATBEL project for public dissemination in its 2nd year of activity, in concrete: project objectives, work progress, achievements, project management, dissemination and communication activities.

2. PROJECT OBJECTIVES, WORK PROGRESS, ACHIEVEMENTS AND PROJECT MANAGEMENT

2.1 Project description

CASCATBEL aims to design, optimize and scale-up a novel multi-step process for the production of second-generation liquid biofuels from lignocellulosic biomass in a cost-efficient way through the use of next-generation high surface area tailored nano-catalysts. On the one hand, the sequential coupling of catalytic steps is an essential factor for achieving a progressive and controlled biomass deoxygenation and reduce hydrogen consumption, avoiding the previously highlighted problems that hinder one/two-step bio-oil upgrading processes. On the other hand, the use of tailored nano-catalysts allows optimising reaction yields (increasing liquid yield and preventing bio-oil contamination) and facing limitations of current catalysts in terms of selectivity and deactivation rates. Finally, the scaling up of the process is important for fully exploring and understanding the catalytic and reaction dynamics, assessing catalysts life-cycles and demonstrating the viability of the CASCATBEL process in relevant environments, from both technical and economic perspectives.

The strategy proposed in CASCATBEL is leading to the preparation of advanced biofuels having composition and properties very similar to petroleum-derived fuels. This is a very relevant advantage regarding the commercial implementation of this technology, as it would not require any significant changes in the already existing infrastructures and engines.

CASCATBEL activities are structured in eleven work packages (WP) which are tightly linked to each other as shown in the figure below:

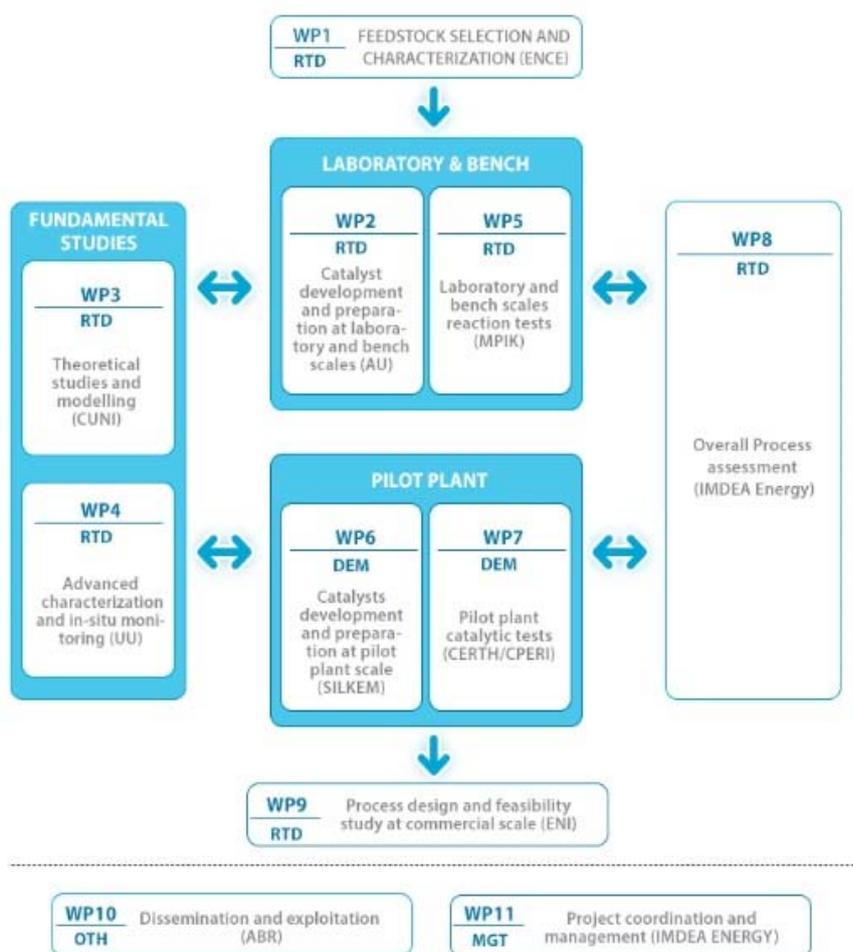


Figure 1 Work programme structure of CASCATBEL project

2.2 Project objectives for the second year of the project

During the second year of execution, CASCATBEL aimed at the following objectives:

Table 1 Objectives of the CASCATBEL project during the 2nd year

OBJECTIVE	DESCRIPTION
O1	To lay the foundations for project results exploitation by facilitating its protection, analysis and transfer.
O2	Synthesis and basic characterization of the catalyst samples to be tested in the different chemical reactions considered in the cascade process.
O3	Understanding at molecular level of the behaviour of representative catalytic systems.

O4 Application of advanced characterization and in-situ techniques to gain a profound insight into the different phenomena taking place during the catalytic reactions and about the nature and environment of the active sites.

O5 Optimization of the thermal pyrolysis of selected biomass samples in order to optimize both the bio-oil production and energy yield.

Assessment of the performance of the catalysts prepared in WP2 in the different reactions considered in the cascade scheme, using laboratory scale reaction systems and mainly model substrates.

O6 To perform process assessment as a transversal activity to aid in the decisions to be taken regarding the different milestones to be achieved in this period.

The assessment will be carried out taking into consideration a variety of criteria: technical, economic, environmental and toxicological criteria.

Along of the reporting period the following milestones were achieved:

Table 2 Milestones of the CASCATBEL project during the 2nd year

MILESTONE	NAME	ACHIEVEMENTS
MS3	Bio-oil stabilization	Optimum method for the stabilization of bio-oils defined. Related deliverables: 1.2, D5.1, D5.2, D8.10.
MS4	Best catalysts for bench scale	Catalysts to be investigated in bench scale reaction tests selected (six catalysts per chemical step). Related deliverables: D2.1, D3.1, D4.1, D5.3, D8.3.
MS5	Viability of creating new standards	Convenience and viability of creating new standards related to the project topics agreed. Related deliverables: D10.6.

2.3 Work progress and achievements

Seven out of the eleven WPs continue their activities in the second year of the project. One WP was completed in the first year of the project (WP1-Feedstock selection and characterization in month 8) and a second WP was completed in the second year (WP2-Catalyst development and preparation at laboratory and bench scales in month 24). The progress and achievements of each of those WPs is summarized as follows:

WP1- Feedstock selection and characterization

WP1 was successfully concluded in month 8 as planned in Annex I. This WP was devoted to the analysis of the European context of biomass availability and the selection and characterization of the optimum raw materials for bio-oil production.

WP2- Catalyst development and preparation at laboratory and bench scales

The objective of WP2 defined for second year of the project was the synthesis and basic characterization at laboratory scale of the catalyst samples to be tested in the different chemical reactions considered in the cascade process. The catalyst samples have been subjected to a basic characterization procedure to check that the syntheses have been successful and that they show the expected physicochemical properties. WP2 was successfully completed in month 24.

WP3- Theoretical studies and modelling

The main objectives in WP3 for this period were the development of theoretical studies and modelling for understanding at molecular level the behaviour of representative catalytic systems.

Zeolites, metal oxides and carbon-based catalysts containing transition metal nanoparticles were investigated theoretically at the density functional theory level. The role of deposition of metal nanoclusters on the regular and defective surfaces of metal oxides has been investigated with the aim to elucidate the role of chemical reduction of the catalysts in the enhancement of its activity.

WP4- Advanced characterization and in-situ monitoring

The main objective for this period was the application of advanced characterization and in-situ techniques to gain a more profound insight into the different phenomena taking place during the catalytic reactions. The results obtained in this WP are highly valuable for the optimization of the catalytic materials and reaction conditions.

WP5- Laboratory and bench scales reaction tests

The performance of the catalysts prepared in WP2 was assessed in the different reactions considered in the cascade scheme: catalytic pyrolysis and bio-oil intermediate deoxygenation (ketonization, aldol condensation and esterification) taking into account the nature of the active sites needed in each case. In addition, non-catalytic biomass pyrolysis tests were also carried out to study the effect of the biomass pre-treatment and bio-oil stabilization. Most experiments in WP5 during this period were performed in laboratory scale reaction systems.

WP8- Overall process assessment

Assessment consists in integrating the results reported in different work packages, taking into account a series of indicators specifically defined for each activity according to the following criteria: process-related parameters, economic factors, environmental impacts,

nanosafety and toxicological issues.

WP10- Dissemination and exploitation

The dissemination and communication activities carried out within this period are detailed in Section 3.

In order to evaluate the exploitability of the results and the normative applicable to the process, a deep study on existing related standards and regulation gaps has been developed and presented as deliverable of the project.

WP11- Financial and administrative management.

Main management activities were oriented:

- To create an effective project management structure.
- To ensure efficient communication mechanisms within the consortium partners.
- To organize the information of the project.
- To synchronize the efforts of the WPs with the project time schedule, and to supervise the overall activities and ensure the proper level of coordination and cooperation within the consortium.
- To compile technical deliverables.
- To develop and sustain quality control procedures for the delivered documentation.

During this period the following meetings took place:

Table 3 Meetings of the CASCATBEL project during the 2nd year

PROJECT MEETING	DATE	VENUE
Governing Board Meeting	28 th April 2015	Brussels, Belgium
First Review Meeting	29 th April 2015	Brussels, Belgium
Technical Committee Meeting	21-22 th October 2015	Bled, Slovenia

2.4 Deliverables and Milestones

The following table shows the Deliverables and Milestones that have come out from CASCATBEL activities during this second year of implementation.

Table 4 Deliverables submitted during the second year of the project

DELIVERABLE	TITLE	DELIVERY DATE
D2.1	Catalyst samples for laboratory scale tests: preparation and basic characterization.	31/01/2015
D3.1	Report on the molecular and nanostructural properties of representative catalysts employed in laboratory scale experiments.	30/04/2015
D4.1	Report on the advanced characterization and catalytic properties under working conditions of representative catalysts employed at laboratory scale.	30/04/2015
D5.2	Report on the bio-oil stabilization methods.	30/04/2015
D5.3	Report on the catalytic tests at laboratory scale.	30/04/2015
D8.10	Assessment of the results obtained at laboratory scale in biomass pyrolysis to aid in the selection of the bio-oil stabilization methods.	30/04/2015
D5.4	Bio-oil samples from bench-scale biomass pyrolysis.	31/05/2015
D8.3	Assessment of the results obtained in the catalytic tests at laboratory scale to aid in the selection of catalysts for bench scale tests.	31/05/2015
10.6	Report on the convenience and interest of creating new standards.	31/05/2015
D2.2	Catalyst samples for bench scale tests: preparation and basic characterization.	31/10/2015
D5.5	Report on the biomass pyrolysis tests at bench scale.	31/10/2015

3. DISSEMINATION AND COMMUNICATION ACTIVITIES

3.1 Scientific publications

A number of scientific publications of project's results have been performed in scientific articles in international journals related to the research topics of the project (renewable energy, biomass, biofuels, bio-oils, thermochemical transformations, nano-porous materials and catalysis). In the first year of the project five scientific publications were prepared and published. In the second year this amount increased with a total of thirteen publications:

- Keller, T.C.; Isabettini, S.; Verboekend, D.; Rodrigues, E. G. and Pérez-Ramírez, J.*. *Hierarchical high-silica zeolites as superior base catalysts*. Chemical Science, **2014**, 5, 677-684.
- Keller, T. C.; Rodrigues, E. G. and Pérez-Ramírez, J.*. *Generation of Basic Centers in High-Silica Zeolites and their Application in Gas-Phase Upgrading of Bio-Oil*, ChemSusChem, **2014**, 7, 1729 – 1738.
- Pacchioni, G.*. *First Principles Calculations on Oxide-Based Heterogeneous Catalysts and Photocatalysts: Problems and Advances*. Springer Science+Business Media News **2014**.
- Chen, H. T.; Tosoni, S. and Pacchioni, G.*. *Adsorption of Ruthenium atoms and clusters on anatase TiO₂ and tetragonal ZrO₂ (101) surfaces: A Comparative DFT study*. The Journal of Physical Chemistry, **2014**.
- Ciddor, C.; Bennett, J.; Hunns, J.; Wilson, K. and Lee, A. F. *. *Catalytic upgrading of bio-oils by esterification*. Journal of Chemical Technology and Biothechnology, **2015**.
- Chen, H. T.; Tosoni, S. and Pacchioni, G.*. *Hydrogen Adsorption, Dissociation, and Spillover on Ru₁₀ Clusters Supported on Anatase TiO₂ and Tetragonal ZrO₂ (101) Surfaces*. ACS Catalysis, **2015**, 5, 5486–5495
- Osatiashtiani, A.; Lee, A. F.; Granollers, M.; Brown, R.; Olivi, L.; Morales, G.; Melero, J. A. and Wilson, K.*. *Hydrothermally Stable, Conformal, Sulfated Zirconia Monolayer Catalysts for Glucose Conversion to 5-HMF*. ACS Catalysis, **2015**, 5 (7), 4345-4352.
- Keller, T. C.; Desai, K. D.; Mitchell, S.; and Pérez-Ramírez, J.*. *Design of Base Zeolite Catalysts by Alkali-Metal Grafting in Alcoholic Media*. ACS Catalysis, **2015**, 5 (9), 5388–5396.
- Tosoni, S.; Chen, H. T. and Pacchioni, G.*. *A DFT study of Ni clusters deposition on titania and zirconia (101) surfaces*. Surface Science, **2015** (Published on line).

- Chen, H. T.; Livraghi, S.; Giamelo, E.; and Pacchioni, G.*. *Mechanism of the Cyclo-Oligomerisation of C₂H₂ on Anatase TiO₂ (101) and (001) Surfaces and their Reduction: An Electron Paramagnetic Resonance and Density Functional Theory Study*. ChemplusChem, **2015** (Published on line).
- Chen, H. T.; Pacchioni, G. and Tosoni, S.*. *A DFT Study of the Reactivity of Anatase TiO₂ and Tetragonal ZrO₂ Stepped Surfaces compared to the Regular Terraces*. ChemPhysChem, **2015** (Published on line).
- Maanyil, J.; Inocêncio, V. C.; Lee, A. F.; and Wilson, K.*. *Mesoporous sulfonic acid silicas for pyrolysis bio-oil upgrading via acetic acid esterification*. Green Chem, **2015** (Published on line).
- Stefanidis, S.; Heracleous, E.; Kalogiannis, K. and Lappas, A. A.*. *Optimization of bio-oil yield by demineralization of low quality biomass*. Biomass & Bioenergy Journal. **2015** (Publication on line).

3.2 Participation in National and International meetings and events

The partners of the project have participated in a variety of national and international meetings and events related to renewable energy, biomass and catalysis, presenting the CASCATBEL project and/or its results. In the first year of the project the partners participated in two events and during the second year this participation increased with their participation in twenty nine events, as summarized below:

- 46. Symposium on Catalysis, Prague (Czech Republic), organization of the scientific event and oral presentations, 3-5th November 2014.
- BIOTECH, Madrid (Spain), project presentation, 24th November 2014.
- Workshop des FSP “Integrierte Biotechnologie und Prozesstechnik“, Hamburg (Germany), oral presentation, 15th December 2014.
- 2nd Euro-Asia Zeolite Conference, Nice (France), oral presentation, 25-28th January 2015.
- GENERA-Energy Fair, Madrid (Spain), project presentation, 25th February 2015.
- Computational Catalysis Symposium, Beijing (China), oral presentation, 31st May-2nd June 2015.
- 10th Panhellenic Chemical Engineering Conference, Patra (Greece), oral presentation, 4-6th June 2015.
- Humboldt-Universität Berlin, Berlin (Germany), lecture, 11th June 2015.

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- 6th Czech –Italian-Spanish Conference on Molecular Sieves and Catalysis, Amantea (Italy), oral presentations, 14-17th June 2015.
 - International symposium on Zeolite and Microporous Crystals ZMPC2015, Sapporo (Japan), oral presentation, 28th June-2nd July 2015.
 - Summer School: “Catalysis for the production of energy and protection of the environment”, San Sebastian (Spain), lecture, 6-8th July 2015.
 - RAL Open Day-Science up close, Oxford (United Kingdom), Stand/Display on Bioenergy and Biofuels production from waste and the role of Catalytic processes, 11th July 2015.
 - SECAT’15 Meeting of the Spanish Catalysis Society, Barcelona (Spain), oral presentation and poster, 13-15th July 2015.
 - University College London, London (United Kingdom), oral presentation, 17th July 2015.
 - University of Bath, Bath (United Kingdom), oral presentation, 27th July 2015.
 - MPG-Forum, Frankfurt (Germany), lecture, 13rd August 2015.
 - ACS Symposium, Boston (USA), plenary lectures, 18-19th August 2015.
 - International Congress and Expo on Biofuels & Bionenergy, Valencia (Spain), oral presentations, lectures, keynote lecture and posters, 25-27th August 2015.
 - LCM 2015-Mainstreaming Life Cycle Management for sustainable value creation, Bordeaux (France), poster, 30th August-2nd September 2015.
 - 16th DFT International conference on Density Functional Theory and its applications, Debrecen (Hungary), poster, 31st August-4th September 2015.
 - SCS Fall Meeting, Laussane, oral presentation, 4th September 2015.
 - Università Milano Bicocca, Milano (Italy), oral presentation, 7th September 2015.
 - ISFR 2015-8th International Symposium on Feedstock Recycling of Polymeric Materials, Leoben (Austria), keynote lecture, 7-10th September 2015.
 - 17th International Symposia for Advancing the Chemical Sciences (ISACS17)- Challenges in Chemical Renewable Energy, Rio de Janeiro (Brazil), plenary lecture, 8-11th September 2015.
 - Catalysis for Energy UK-Swiss Meeting, Oxford (United Kingdom), lecture, 8-11th September 2015.
 - International Porous & Powder Materials Symposium, Izmir, lecture 15-18th September 2015.
 - Workshop on Layered Materials 2015, Trest (Czech Republic), oral presentation and

posters, 15-19th September 2015.

- MIMENIMA Symposium 'Porous Structures -Where Science meets Application', Grömitz (Germany), lecture, 17th September 2015.
- Biocluster of Madrid Network event, Madrid (Spain), project dissemination with leaflets, 13-15th October 2015.
- University Duisburg, Essen (Germany), lecture, 28th October 2015.

3.3 Networking activities

With the aim of promoting synergies with different groups working on thematic areas related to CASCATBEL, the project has joined the following clusters:

- **Nanosafety cluster.** The goal of this cluster is to maximise the synergies between the existing FP6 and FP7 projects addressing all aspects of nanosafety including toxicology, ecotoxicology, exposure assessment, mechanisms of interaction, risk assessment and standardisation.

- **European cluster on catalysis.** The main aim of this initiative is to better integrate fragmented activities in Europe, create synergies between European projects and provide input on potential future catalysis-related research to the European Commission.

- **Engineering and upscaling cluster.** This cluster intends to: identify common interests (scientific, technical and commercial) in on-going research and innovation activities; support policy making; identify methods to support and strengthen dissemination activities of the projects of the cluster and help projects to support their individual and common innovation and exploitation activities.

- **SPIRE PPP-Sustainable Process Industry through Resource and Energy Efficiency-Public Private Partnership.** This event has been launched as part of the Horizon2020 framework programme. The mission of SPIRE is to ensure the development of enabling technologies and best practices along all the stages of large scale existing value chain productions that will contribute to a resource efficient process industry.

- **KETs for regional growth: Synergies between Horizon 2020 and ESIF.** The main aim of the present workshop is to raise awareness on KETs (advanced materials, nanotechnology, micro- and nano-electronics, industrial biotechnology, photonics, and advanced manufacturing systems) as drivers for industrial competitiveness in regions.

- **The Business Booster (TBB) by KIC Innoenergy.** The concept of this initiative is dedicated to promote innovation, entrepreneurship and education in sustainable energy, by bringing together academics, business and research institutes.

3.4 Newsletters

Three issues of CASCATBEL's electronic newsletter have been distributed among more than 250 stakeholders. Besides, the newsletters have been made available for download from the project's website.

3.5 General Public Communications

CASCATBEL has appeared in various publications and events oriented to the dissemination of scientific activities to the general public:

- EERA Newsletter, 4th December 2014.
- Article in Yearbook 2014 Research Center Integrated Biotechnology and Process Engineering, 15th December 2014.
- COPE Radio, project dissemination, Madrid, 5th March 2015.

4. CONCLUSIONS

During the second year of duration, CASCATBEL has achieved its set objectives within the designed time frame and no significant deviation has been detected. The mechanisms established for management, communication and quality control have proved to be effective.

In general, sound planning and high quality and proactive consortium members have been the keys for a successful implementation of the project.