



cascatbel

D10.9 Highlights of CASCATBEL's annual progress for public dissemination

28/10/2016

Project Acronym	CASCATBEL
Project Title	CAScade deoxygenation process using tailored nanoCATalysts for the production of BiofuELs from lignocellulosic biomass
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	Nr.	Name
Deliverable	10.9	Highlights of CASCATBEL's annual progress for public dissemination.
Work Package	10	Dissemination and exploitation.
Task	10.1	Dissemination and cooperation with other initiatives.

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1. SUMMARY

The present report contains highlights of progress of the CASCATBEL project for public dissemination in its 3rd year of activity, in particular about project objectives, work progress, achievements, 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 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 catalyst 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:

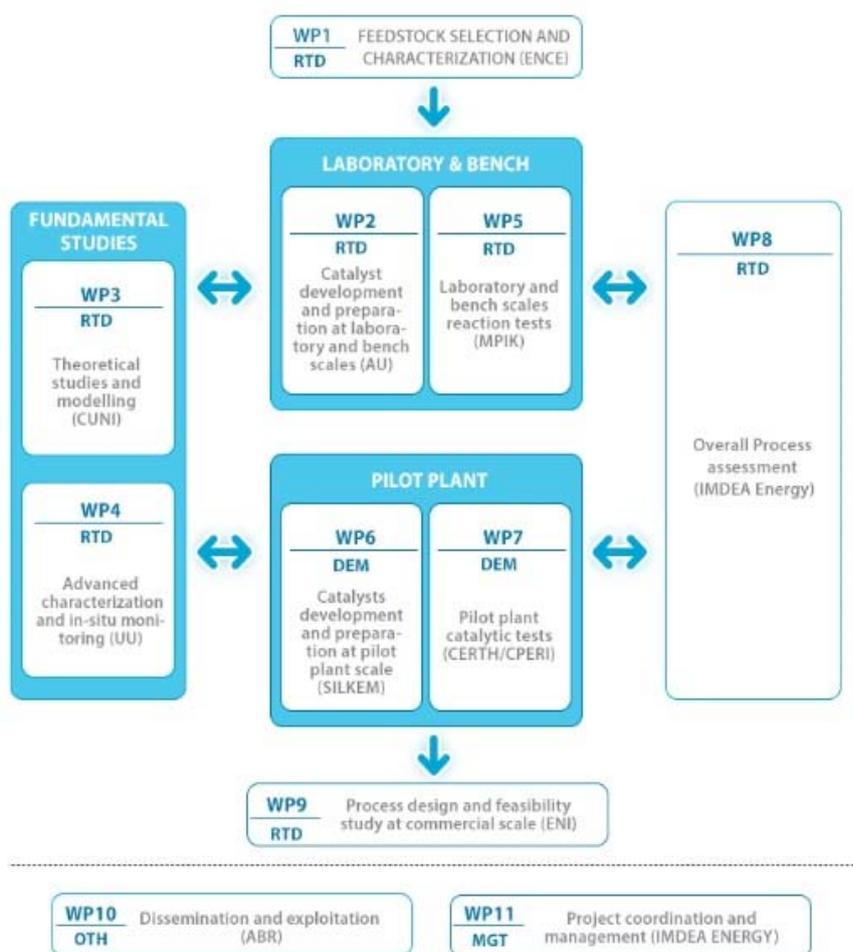


Figure 1 Work programme structure of CASCATBEL project.

2.2 Project objectives for the third year of the project

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

Table 1 Objectives of the CASCATBEL project during the 3rd year.

OBJECTIVE	DESCRIPTION
01	Modelling of the reactant/products adsorption and interaction with the active sites; modelling of the catalyst deactivation phenomena and modelling of the reaction kinetics and catalyst deactivation rates.
02	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.
03	Optimization of the thermal pyrolysis of selected biomass samples in order to optimize both the bio-oil production and energy yield.

04	Preparation at pilot plant scale of selected catalyst for: a) catalytic pyrolysis, b) intermediate bio-oil deoxygenation and c) bio-oil hydrodeoxygenation.
05	Pilot plant scale tests of: a) biomass catalytic pyrolysis; b) intermediate bio-oil deoxygenation and c) bio-oil hydrodeoxygenation.
06	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 is carried out taking into consideration a variety of criteria: technical, economic, environmental, safety and toxicological criteria.
07	Dissemination of the project results to scientific and general public as well as to foster relations with stakeholders.
08	To lay the foundations for project results exploitation by facilitating its protection, analysis and transfer.

Along the reporting period the following milestones were achieved:

Table 2 Milestones of the CASCATBEL project during the 3rd year.

MILESTONE	NAME	ACHIEVEMENTS
MS6	Catalysts for pilot plant catalytic pyrolysis.	The best catalysts for the catalytic pyrolysis have been selected.
MS7	Intermediate bio-oil deoxygenation: best treatment and catalysts for pilot plant scale.	The best catalysts for the intermediate deoxygenation step have been selected-
MS8	Catalysts for pilot plant bio-oil HDO	The best catalysts for the hydrodeoxygenation step have been selected.

2.3 Work progress and achievements

Eight out of the eleven WPs have been active along the third year of the project. The progress and achievements of each of those WPs is summarized as follows:

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.

WP4- Advanced characterization and in-situ monitoring

The main objective for this period in WP4 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.

WP5- Laboratory and bench scales reaction tests

In this WP the performance of the catalysts prepared in WP2 was assessed in the different reactions considered in the cascade scheme taking into account the nature of the active sites needed in each case.

WP6-Catalysts development and preparation at pilot plant scale

Preparation of the selected catalyst have been accomplished in a quantity sufficient for the pilot plant experiments.

WP7-Pilot plant catalytic tests

Testing the performance of the catalysts prepared in WP6 at pilot plant scale have been already started in the third year of the project.

WP8- Overall process assessment

The assessment of the different alternatives has been performed integrating the results reported in different work packages and 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.

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 3rd year.

PROJECT MEETING	DATE	VENUE
Governing Board Meeting	16 th February 2016	Milan, Italy
Governing Board Meeting	16-17 th May 2016	Thessaloniki, Greece
Governing Board Meeting	24-25 th August 2016	Stockholm, Sweden
Technical Committee, Innovation Committee and Governing Board Meeting	17 th October 2016	Brussels, Belgium
Second Review Meeting	18 th October 2016	Brussels, Belgium

2.4 Deliverables

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

Table 4 Deliverables submitted during the third year of the project.

DELIVERABLE	TITLE	DELIVERY DATE
D3.2	Report on the reactant-active site interactions of representative catalysts employed in bench scale experiments.	29/01/2016
D4.2	Report on the advanced characterization and catalytic properties under working conditions of catalysts employed at bench scale.	29/01/2016
D5.6	Report on the biomass catalytic pyrolysis tests at bench scale.	29/01/2016

D5.7	Bio-oil samples from bench-scale biomass catalytic pyrolysis.	29/01/2016
D8.4	Assessment of the results obtained at bench scale in biomass catalytic pyrolysis to aid in the selection of catalysts for pilot plant tests.	29/02/2016
D5.8	Report on the bio-oil intermediate deoxygenation catalytic tests at bench scale.	29/04/2016
D5.9	Bio-oil samples from bench-scale intermediate deoxygenation.	29/04/2016
D8.5	Assessment of the intermediate deoxygenation step to aid in the selection of the most convenient one and of catalyst for pilot plant tests.	31/05/2016
10.8	Workshop on thermochemical lignocellulose conversion technologies.	31/05/2016
D5.10	Report on the bio-oil catalytic HDO tests at bench scale.	29/07/2016
D8.6	Assessment of the results obtained at bench scale in bio-oil HDO to aid in the selection of catalysts for pilot plant tests.	31/08/2016
D6.1	Report on the adaptation of the catalyst synthesis procedures to be applied at pilot plant scale.	30/09/2016

3. DISSEMINATION AND COMMUNICATION ACTIVITIES

3.1 Scientific publications

A total of 22 scientific articles were prepared based on the results of the project and published in indexed journals along the third year:

- 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 16, **2015**, 3642-3651.
- Stefanidis, S.; Heracleous, E.; Kalogiannis, K. and Lappas, A. A.*. *Optimization of bio-oil yields by demineralization of low quality biomass*. Biomass and Bioenergy 83, **2015**, 105-115.

- Tosoni, S.; Chen, H. T. and Pacchioni, G.*. *A DFT study of Ni clusters deposition on titania and zirconia (101) surfaces*. Surface Science 646, **2016**, 230–238.
- Chen, H. T.^a; Livraghi, S.^b; Giamello, E.^b and Pacchioni, G.*^a. *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 81, **2016**, 64-72.
- Manyil, J. C.; Inocêncio, C. V. M.; Lee, A. F. and Wilson, K.*. *Mesoporous sulfonic acid silicas for pyrolysis bio-oil upgrading via acetic acid esterification*. Green Chem 18, **2016**, 1387-1394.
- Keller, T. C.; Polozij, M.; Puértolas, B.; Thang, H. V.; Nachtigall, P. and Pérez-Ramírez, J.*. *Understanding the structure of cationic sites in alkali metal-grafted USY zeolites*. J. Phys. Chem. C. 120, **2016**, 4954-4960.
- Puigdollers, A. R.; Illas, F. and Pacchioni, G.*. *Structure and properties of zirconia nanoparticles from density functional theory calculations*. J. Phys. Chem. C. 120, **2016**, 4392-4402.
- Puértolas, B.; Keller, T. C.; Mitchell, S. and Pérez-Ramírez, J.*. *Deoxygenation of bio-oil over solid base catalysts: From model to realistic feeds*. Applied Catalysis B: Environmental 184, **2016**, 77–86.
- Rubes, M.; He, J.; Nachtigall, P. and Bludsky, O.*. *Palladium clusters on graphene support: An ab initio study*. Chemical Physics Letters 646, **2016**, 56-63.
- Hernando, H.^a; Jiménez-Sánchez, S.^a; Feroso, J.^a; Pizarro, P.^{ab}; Coronado, J. M.^a and Serrano, D. P.*^{ab}. *Assessing biomass catalytic pyrolysis in terms of deoxygenation pathways and energy yields for the efficient production of advanced biofuels*. Catal. Sci. Technol. 6, **2016**, 2829-2843.
- Hunns, J. A.^a; Arroyo, M.^b; Lee, A. F.^a; Escola, J. M.^b; Serrano, D.*^{bc} and Wilson, K.*^a. *Hierarchical mesoporous Pd/ZSM-5 for the selective catalytic hydrodeoxygenation of m-cresol to methylcyclohexane†*. Catal. Sci. Technol. 6, **2016**, 2560-2564.
- Berenguer, A.; Sankaranarayanan, T. M.; Gómez, G.; Moreno, I.; Coronado, J.M.; Pizarro, P. and Serrano, D. P.* *Evaluation of transition metal phosphides supported on ordered mesoporous materials as catalysts for phenol hydrodeoxygenation*. Green Chem. 18, **2016**, 1938-1951.
- Chen, H. T.; Tosoni, S. * and Pacchioni, G. *A DFT study of the acid–base properties of anatase TiO₂ and tetragonal ZrO₂ by adsorption of CO and CO₂ probe molecules*. Surface Science 652, **2016**, 163–171.
- Puigdollers, A. R.; Tosoni, S. and Pacchioni, G.*. *Turning a Nonreducible into a Reducible Oxide via Nanostructuring: Opposite Behavior of Bulk ZrO₂ and ZrO₂*

Nanoparticles Toward H₂ Adsorption. The Journal of Physical Chemistry 120, **2016**, 15329–15337.

- Chen, H. T.; Tosoni, S. and Pacchioni, G.*. *Role of Oxide Reducibility in the Deoxygenation of Phenol on Ruthenium Clusters Supported on the Anatase Titania (101) Surface*. ChemCatChem 8, **2016**, 2492-2499.
- Rubeš, M.^a; He^b, J.; Nachtigall^a, P. and Bludský, O. ^{a,b,*}. *Direct hydrodeoxygenation of phenol over carbon-supported Rucatalysts: A computational study*. Journal of Molecular Catalysis A 423, **2016**, 300-307.
- Ruiz Puigdollers, A.; Illas, F. and Pacchioni, G. *Effect of nanostructuring on the reactivity of zirconia: a DFT+U study of Au atom adsorption*. J. of Physical Chemistry C, 120, **2016**, 17604-17612.
- Feroso, J.^a; Hernando, H.^a; Jana, P.^a; Moreno, I.^{a,b}; Prech, J.^c; Ochoa-Hernández, C.^c; Pizarro, P.^{a,b}; Coronado, J.M.^a; Cejka, J.^{c,**} and Serrano, D. P.^{a,b,*}. *Lamellar and pillared ZSM-5 zeolites modified with MgO and ZnO for catalytic fast-pyrolysis of eucalyptus woodchips*. Catalysis Today 277(1), **2016**, Pages 171–181.
- Morales-García, A.*; Rubeš, M. and Nachtigall, P. *The interaction of Pd clusters with the bulk and layered two-dimensional Silicalite-1 supports*. Catalysis Today 277, **2016**, 108-117.
- He, J.; Morales-García, A.; Bludský, O. and Nachtigall, P.*. *The surface stability and equilibrium crystal morphology of Ni₂P nanoparticles and nanowires from an ab initio atomistic thermodynamic approach†*. CrystEngComm. 18, **2016**, 3808-3818.
- Thang, H. V.^a; Frolich, K.^b; Shamzhy, M.^c; Pavla Eliášová, P.^c; Rubeš, M.^a; Čejka, J.^c; Bulánek, R.^b and Nachtigall, P.^{*a}. *The effect of the zeolite pore size on the Lewis acid strength of extra-framework cations†*. Phys. Chem. Chem. Phys. 18, **2016**, 18063-18073.
- Osatiashtiani, A.; Durndell, L. D.; Manayil, J. C.; Adam F. Lee, A. F. and Wilson, K.*. *Influence of alkyl chain length on sulfated zirconia catalysed batch and continuous esterification of carboxylic acids by light alcohols†‡*. Green Chem. 18, **2016**, 5529–5535.

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 CASCABEL project and/or its results. Along the third year of the project the partners participated in 38 events, as summarized below:

- German Chemical Society-University of Bayreuth Workshop, Bayreuth (Germany), oral presentation, 29th October 2015.

- Tcbiomass 2015-The International Conference on Thermochemical (TC) Biomass Conversion Science, Chicago (USA), oral presentation, 2-5th November 2015.
- 47. Symposium on Catalysis, Prague (Czech Republic), oral presentations and posters, 2-4th November 2015.
- Symposium on catalysis, Prague (Czech Republic), Poster, 7-9th November 2015.
- 2nd UK Catalysis Conference, Loughborough (United Kingdom), oral presentation, 6-8th January 2016.
- International Workshop on Oxide Surfaces (IWOX-X), Dalian/ Liaoyang (China), oral presentation, 15th January 2016.
- Infoday Joint Call ERA-NET Cofund BESTF 3 (BIOENERGY SUSTAINING THE FUTURE 3), Madrid (Spain), oral presentation, 18th January 2016.
- Joint workshop of ENMIX, FASTCARD, CASCABEL, BIOGO: Nanoporous materials and sustainable production of biofuels and biochemical, Stuttgart (Germany), plenary lecture and oral presentations, 20-21st January 2016.
- AEC Meeting, Madrid (Spain), oral presentation, 9th February 2016.
- NCCC-Netherlands' Catalysis and Chemistry Conference XVII, Noordwijkerhout, (Netherlands), poster, 7-9th March 2016.
- XLVIII Polish annual conference on catalysis, Krakow (Poland), plenary lecture and oral presentation, 16th March 2016.
- 49 Jahrestreffen Deutscher Katalytiker Congress, Weymar (Germany), oral presentations, 16th March 2016.
- School on layered materials, Prague (Czech Republic), oral presentations, 21th March 2016.
- British Zeolite Association Meeting 2016, Bath (United Kingdom), Oral presentations, 21-23rd March 2016.
- Designing New Heterogeneous Catalyst: Faraday Discussion, London (United Kingdom), posters, 4-6th April 2016
- Departmental Seminar at Shanghai Jiao Tong University, Shanghai (China), oral presentation, 5th May 2016.
- Workshop on thermochemical lignocellulose conversion technologies, Porto Carras-Chalkidiki (Greece), invited lectures, presentations and posters, 18-20th May 2016.

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- Workshop Biomass Resources for Renewable Energy Production, IMDEA Energy Institute, Móstoles, Madrid (Spain), oral presentations, 2-3rd June 2016.
 - NorthWestern, Chicago, (USA), lecture, 3rd June 2016.
 - 16th International Congress on Catalysis, Beijing (China), oral presentation and posters, 6th June 2016.
 - ITAC-16- 16th International Conference on Theoretical Aspects of Catalysis, Zakopane (Poland), invited lecture, 19-23rd June 2016.
 - 18th International zeolite conference: Zeolites for a sustainable world, Rio de Janeiro (Brazil) oral presentations, 19-24th June 2016.
 - 4th TMFB International Conference, Aachen (Germany), posters, 21-23th June 2016.
 - SECAT's Meeting of the Spanish Catalysis Society, Ciudad Real (Spain), posters, 27-29th June 2016.
 - Spectrocat 2016-Summer School on Vibrational Spectroscopy Applied to Catalysis, Caen (France), poster, 27th June-2nd July 2016.
 - Smart Biorefinery: Outlook and Prospects, University of Warwick, Warwick (United Kindon), oral presentation, 7th July 2016.
 - MSE Kolloquium, TUM, Munich (Germany), lecture, 7th July 2016.
 - Fritz-Haber Institut der Max Planck Gesellschaft, Berlin (Germany), oral presentation, 12th July 2016.
 - The 2016 CAMD Summer School on Electronic Structure Theory and Materials Design, Lyngby (Denmark), posters, 14-19th August 2016.
 - Workshop on catalysis for waste valorization, Aston University, Birmingham (United Kingdom), keynote, 1st September 2016.
 - Workshop on layered materials, Prague (Czech Republic), poster, 5-9th September 2016.
 - 3rd International Symposium on Catalysis for Clean Energy and Sustanaible Chemistry, Madrid (Spain), oral presentation, 7-9th September 2016.
 - EuCheMS, Seville (Spain), lecture, 12th September 2016.

- Oxide 2016, VI International workshop on oxide-based materials, Napoli (Italy), 21-24th September 2016.
- HIMAT2016, Erlangen (Germany), invited lecture, 27-29th September 2016.
- European Biomass to Power, Seville (Spain), oral presentation, 5th October 2016.
- HEIKA Symposium, University of Heidelberg, Heidelberg (Germany), lecture, 13th October 2016.
- 14th Panhellenic Catalysis Symposium, Patra (Greece), lecture, 13-15th October 2016.

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 and events:

- **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 on catalysis 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. CASCATBEL project was presented in the 2nd *Workshop on Impact of the Sustainable Process Industry (SPIRE) PPP*, Brussels, 21-22nd April 2016.

- **Joint workshop of ENMIX, FASTCARD, CASCATBEL, BIOGO.** In this Joint workshop the participants (from ENMIX, FASTCARD, CASCATBEL and BIOGO projects) presented their projects and lectures about the obtained research results. Along the event, held on 19-21st January 2016, in Stuttgart (Germany), the project partner's participants discussed from different points of view about their projects, its development, possible synergies and future collaborations.

- **Sustainable Energy Week.** The Networking Village has held on 13-17th June 2016, in Brussels (Belgium), aimed to explore policies and projects with EU institution and stakeholder representatives.

3.4 Newsletters

Four 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:

- Issue 6-April 2016
- Issue 7-June 2016
- Issue 8-August 2016
- Issue 9-October 2016

3.5 General public communications

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

- Magazine Parliament. Joint publication of FASTCARD, CASCATBEL and BIOGO projects, May 2015.
- The Science Week, Madrid (Spain), CASCATBEL leaflet, 2-15th November 2016.
- 7th European Researchers' Night, organized in IMDEA Energy Institute, Madrid (Spain), CASCATBEL leaflet, 30th September 2016.

3.6 Workshop

A three-day workshop, linked to and organized by CASCATBEL, was held on 18-20th May, 2016, at the Porto Carras hotel in Chalkidiki, Greece. The main goal of the workshop was to present the most up-to-date technological and research advances in the field of lignocellulosic biomass valorization via thermochemical process routes: gasification, pyrolysis and liquefaction. Prominent scientists and experts from both academia and industry working on these topics were selected and invited to share their knowledge and expertise. The invited speakers were from inside and outside the CASCATBEL project. Special attention was paid in having a balance mix of speakers from academia and industry, in order to also have the views of the industrial sector about the advances required in the field of thermochemical biomass conversion. The program consisted of 23 invited lectures and 23 posters.

✓ Workshop website

The workshop website was hosted in cper1.certh.gr, which gave information about all aspects of the workshop: venue, dates, speakers, program, abstract submission, on-line registration, and information on how to reach the venue etc. <http://cascatbel.cper1.certh.gr>.

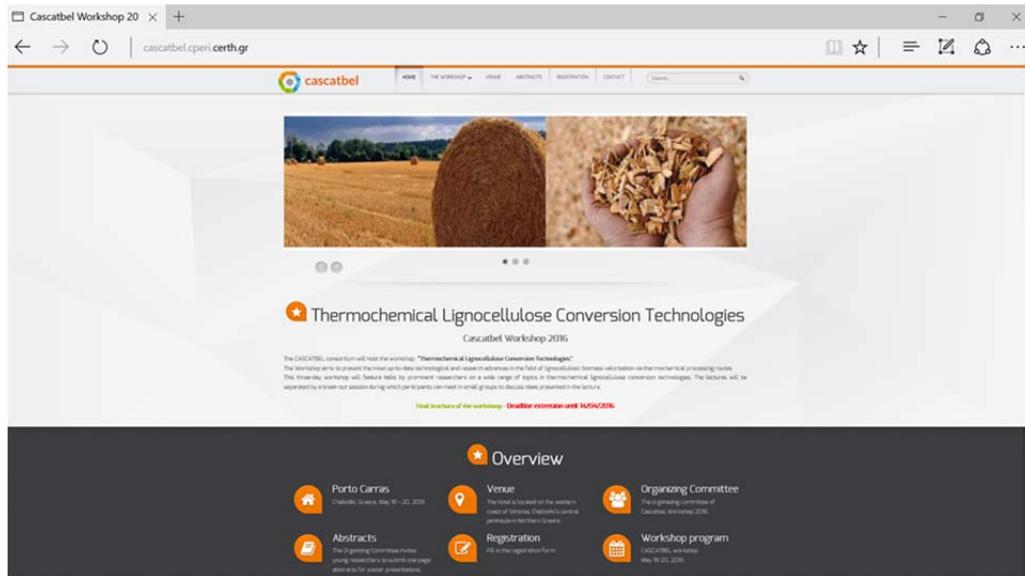


Figure 2 Workshop website.

✓ **Flyer**

An informative flyer was prepared and was distributed both in electronic and printed form.

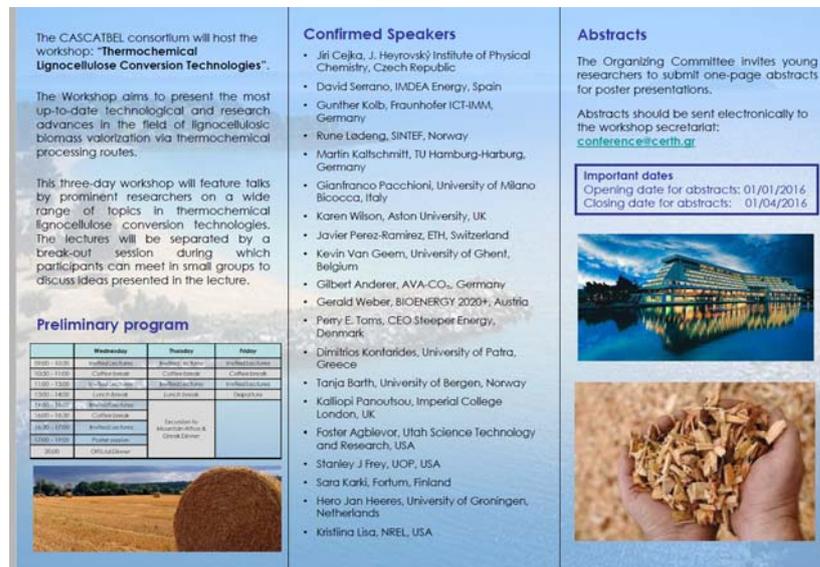


Figure 3 Workshop flyer.

✓ **Mailing**

Mails were sent to more than 800 recipients to relevant universities, research organizations, companies etc, using available mailing lists from CERTH, the CASCATBEL coordinator and lists of other partners.

In terms of impact, the workshop was very successful, with 71 participants, coming from 15 countries and representing important academic and industrial institutions. The workshop served as a means to disseminate important results and advances that were realized in the

frame of the CASCATBEL project. It was also very successful in terms of networking and fostered interesting discussions between the participants from industry and academia for future collaborations and the outlook for the biomass thermochemical conversion technologies.

4. CONCLUSIONS

During the third year of duration, CASCATBEL has achieved the planned objectives according to the designed time frame and no significant deviation has been produced. The mechanisms established for management, communication and quality control have proved to be effective.

Regarding the research activities in this period, bench scale tasks were finished whereas pilot plant testing of the most promising catalytic systems was started. Assessment of the results obtained at bench scale has been performed according to technical, economical, environmental, safety and toxicological criteria. Most of the experimental tasks performed in this period has been carried out in more practical conditions compared to the laboratory stages, using real biomass and bio-oil samples and addressing the issues related to the catalyst agglomeration and shaping in technical forms, the effect of transport phenomena and the extension of catalyst deactivation. The best catalysts identified at bench scale present a good performance for promoting a progressive deoxygenation while keeping a high bio-oil yield in both mass and energy terms.

An intense dissemination activity of the project and the results so far achieved has been developed, which is reflected in the 22 scientific articles published in indexed journals and the 30 communications presented in scientific events.

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