

Presentation of the funded projects in 2010 for the "Sustainable Chemistry – Industry – Innovation" Programme

ACRONYM and project title	Page
BIOBLEND : Bio-compatibilizers for blending cellulose with synthetic polymers	3
BIOCOS : Innovative access to biomass-based chitooligosaccharides and their derivatives for agrochemical applications	5
CATASURF : Catalytic surfactants for the design of oxidizing polyphasic microdispersed reaction media. application to microreactors.	7
FATCLEAVALD : Synthesis and functionalization of aldehydes from unsaturated fatty acids or esters cleavage	9
FISSCARDEN : Sorption – controlled flocculation for selective sequestration of radionuclide cations in view of nuclear effluent decontamination	10
GALAC : From glycerol to acrylic acid via lactic acid.....	12
ISOSORB-CO : Hydroesterification of olefins : synthesis of new isosorbide based plasticizers	14
NATURADYRE : Efficient bio-oxidations for the synthesis of natural or enantiopur compounds	15
PANACEE : Command of hospital aqueous waste (oncological): toxicity analysis and eco-combination of treatment processes; in situ validation	16
POLYTERP : Polyterpens by enzymatic conversion of isoprene.....	18

POMEWISO : Polymeric membranes made without organic solvent	20
PREDIMOL : Molecular modelling prediction of physico-chemical properties of products.....	21
PROCIP : Project chart for process intensification development	23
SANBACT : Conception of new surfaces with antibacterial properties by a multidisciplinary and a multiscale approach	25
SUCROL : Lignocellulosic biorefinery for the production of cellulose and pentoses for the production of green surface active agents.....	27

CD2I programme

YEAR 2010

Project title

BIOBLEND : BIO-compatibilizers for BLENDing cellulose with synthetic polymers

Abstract

The use of natural polymers from renewable resources as an alternative to petroleum-based polymers faces one major issue: the lack of efficient analytical tools required to accurately describe their complex structure. This currently represents a major difficulty in the development of tailored, accurately controlled grafting procedures aimed at modifying natural polymers, such as cellulose, to improve their macroscopic properties. Similar issues are encountered in the alternative strategy consisting of blending natural polymers with synthetic materials of well-established industrial applications. As a result, compatibilizers consisting of cellulose grafted with synthetic chains are developed from cellulose in a semi-empirical manner. To tackle this problematic, we propose a different approach that focuses on the development of both grafting procedures and analytical methodologies on less complex - though relevant - polysaccharides of well-defined smaller size, to produce compatibilizers to be used to stabilize cellulose/polystyrene blends. Overall, the present research project aims at developing analytical methodologies, combining nuclear magnetic resonance and mass spectrometry, to characterize the structure of copolymers consisting of polysaccharidic chains grafted with polystyrene blocks. A systematic analytical control will be performed to assess i) the structure and purity of starting polysaccharides, ii) the coupling yield with reactive group modifiers, iii) the size of the grafted synthetic polymers and iv) the density and uniformity of the grafted blocks. To prepare grafted polystyrene-polysaccharide copolymers, we propose to implement innovative and convenient strategies based on NMP process using the so-called SG1 (phosphorylated N-(2-methylpropyl)-N-(1-diethylphosphono-2,2-dimethyl propyl)-N-oxyl) as the controlling agent to allow styrene polymerization at quite low temperature, a mandatory condition with regard to the thermal stability of natural polymers. The efficiency of the so-produced copolymers to act as compatibilizers to blend cellulose with PS will be determined, allowing the copolymer synthesis to be optimized in a rational manner and their structure/property relationships to be investigated. Research efforts will be done in

both polymerization chemistry and structural spectrometry to design and synthesize these macromolecules, in order to introduce increasing amounts of cellulose into blends with polystyrene. This would inherently increase the final material biodegradability while limiting the use of non-renewable resources.

Partners LCP UMR 6264
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MMC UMR 7167

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ANR funding 610 480 €

Starting date and duration January 2011 – 36 months

Reference ANR-10-CDII-009

Cluster label AXELERA

Project title**BioCOS : Innovative Access to Biomass-Based Chitooligosaccharides and their Derivatives for Agrochemical Applications****Abstract**

In a world engaged in vital transformations, it is essential that we invent new development strategies. The expected conjugated growth of global population and of the median development level of this population in the next decades will lead to an increase in demand (food, energy, raw materials), which will inevitably increase pressure on the environment (pollution by byproducts, waste, greenhouse gases, fertilizers, ...). Reduction of this impact, together with the desire of decreasing society's dependence on fossil carbon sources, has directed researchers' attention towards the use of biomass as a renewable resource. Further, reduction of the use of fertilizers and pesticides, via their replacement by new, bio-inspired, growth promoters, might prove an efficient way to limit soil, water, and atmosphere pollution, while maintaining sufficient crop supply in a global economy. Our project targets the use of chitin, which is one of the most abundant naturally occurring polymer, and also a major byproduct of the shrimp and crab industry, as a starting material for the elaboration of high added-value biologically active and well-defined chitooligosaccharides (COS), via environmentally-friendly processes. These compounds or their derivatives can have numerous biological activities. This includes the fascinating activity of nodulation factors, LipoChitoOligosaccharides (LCOs) exhibiting growth promoting properties on various types of crops, at a concentration which reduces their potential environmental impact to almost zero. The biological activity of our products, as well as their potential technology transfer, will be evaluated by the industrial partner of the consortium: Bayer CropScience. An easy and much improved access to LCOs will be developed. Presently, availability of LCOs and their chitooligosaccharidic precursors (ChitoOligoSaccharides, COS) is the critical issue worldwide, and chemical or biochemical means have only enabled access to limited quantities of such compounds so far. Furthermore, it is difficult to get these compounds, which are also produced by Nature as mixtures, in pure form. Our project intends to transform chitin, and chitin-derived chitosan, by using recent advances in synthetic and enzymatic chemistry. Accessing scaffolds controlled both in size and substitution pattern is the core of the project. The major goal is to study and provide routes to these compounds in gram quantities, which will be a very significant achievement in comparison with the state of the art in this domain. This would allow treating fields in the range of one million hectares. The objective is to decrease the use of fertilizers by at least 10% while maintaining the same culture yield. We will also evaluate the impact on the reduction of plant

protection compounds, although it is more difficult to estimate with the scarce knowledge currently available. Our focus will initially concentrate on crops of major interest, such as corn, wheat, and soybean whereby seeds could be treated with such compounds. It is expected from this project that an easy access to compounds able to stimulate plant growth will be discovered. These molecules could represent very useful "green chemicals" for agricultural use.

Partners ICMMO UMR 8182
IMP UMR 5223
CERMAV UPR 5301
Bayer Cropscience SAS

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ANR funding 602 326 €

Starting date and duration November 2011 – 36 months

Reference ANR-10-CDII-008

Cluster label AXELERA

Project title

CATASURF : Catalytic surfactants for the design of oxidizing polyphasic microdispersed reaction media. Application to microreactors.

Abstract

Nowadays, "Green Chemistry" is a central issue in both academia and industry with regard to chemical synthesis. Chemical producers are facing increased requirements of both regulatory and economic nature that have to be met with in order to remain a competitive and sustainable player. Academic researchers have to take into account this changing in their research programs. Among the diversity of transformations required for the manufacture of fine chemicals, pharmaceuticals, agrochemicals, synthetic fibres, plastics..., oxidation holds a prominent place as a core technology for producing chemicals of a higher oxidation state. However, traditional oxidation methods based on metal or organic stoichiometric oxidants are unacceptable for practical synthesis because of their high cost, their high waste or their toxic reagents and dangerous processing. Hence, there is a need for the invention of clean and safe oxidation procedures. Catalytic oxidation methods are attractive from an economic, environmental and safety viewpoint. Among the various oxidants used in catalytic oxidation reactions, hydrogen peroxide is still receiving much attention because of its relevance to sustainable chemistry. Within this context, the basic research CATASURF project aims at developing new "green" catalytic processes for fine-chemicals manufacture with a low environmental impact involving H₂O₂ as the oxidant. The project mainly comprises two approaches driven both by the respect of the molecular and energy economy principles and by the development of an environmentally friendly and safe process: 1) Elaboration of efficient oxidizing microdispersed reaction media, i.e. three-liquid-phase microemulsion systems or triphasic emulsions based on catalytic surfactants and environmentally friendly solvents, ensuring an easy recovery of both products and catalyst in two different phases. 2) Transfer of the systems from the batch reactor technology to the microreactor technology. The problem solving requires a multi-disciplinary approach involving highly complementary research groups specialized in synthetic organic oxidation chemistry, polyoxometalates, surfactants, (micro)emulsions, colloidal chemistry and microfluidic. Thus, the CATASURF project associates four partners: the Group EA "Chimie Moléculaire et Formulation" at the University of Lille, the Group Polyoxometalates of the "Institut Parisien de Chimie Moléculaire", the Group UMR 5257 of the "Institut de Chimie Séparative de Marcoule" and the DSM Innovative Synthesis Company at Geleen in The Netherlands. DSM is recognized as a global technology leader with respect to application of

microreactor technology for the manufacture of chemicals. Its microreactor facilities are applied for the production of chemical intermediates that are impossible to prepare otherwise on a commercial of several hundreds of tons per year. The industrial collaboration with a chemical producer such as DSM, as well as its expertise in microreactor technology, will be highly beneficial to the academic partners and will ensure optimum process conditions and proper translation of academic findings into a future possible industrial application. On the other hand, the elaboration of microstructured reaction media based on catalytic surfactants is conditioned by a deep understanding of the physicochemical properties (surface activity, self-aggregation, microstructure characterization...) to which the Group of Marcoule will bring its solid expertise.

Partners

EA CMF 4478
IPCM UMR 7201
ICSM UMR 5257
DSM Innovation Synthesis BV

Coordinator

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ANR funding

812 006 €

Starting date and duration

November 2010 – 48 months

Reference

ANR-10-CDII-001

Project title	FatCleavAld : Synthesis and functionalization of aldehydes from unsaturated fatty acids or esters cleavage
Abstract	<p>This proposal is a collaborative project between ARKEMA, SCR (Rennes) and LACCO (Poitiers). It deals with some fundamental aspects of the transformation of unsaturated molecules derived from vegetable oils and fats with the expectancy of a near future industrial application by ARKEMA. The aim of the project is the cleavage of unsaturated fatty acids or esters to form aldehyde – acid/ester molecules. This “platform molecule” (PM) will then be transformed into amino – acid/ester (reductive amination) or alcohol – acid/ester (selective reduction). Once purified, these products will be used as monomers for the synthesis of polyamides and polyesters, (Polymerization is not part of the proposal). The main goal of this project is the elaboration and development of a new sustainable route for the synthesis of these monomers/polymers fully arising from renewable resources. During the first step of the project, the cleavage of the unsaturated fatty compounds will be studied by cross methathesis with acrolein or by oxidative cleavage (H₂O₂, O₃ or N₂O); reductive ozonolysis being a secure way to obtain the target PM. From the aldehyde formed, reductive amination and selective reduction will be performed comparing homogeneous and heterogeneous catalysis on the economic viability and sustainability aspects. Finally, a study on the purification processes of the obtained monomers will be performed.</p>
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ANR funding	448 535 €
Starting date and duration	November 2011 – 36 months
Reference	ANR-10-CDII-003

Project title**FISSCARDEN** : Sorption – controlled flocculation for selective sequestration of radionuclide cations in view of nuclear effluent decontamination**Abstract**

The FISSCARDEN proposal is an application-oriented R&D project with the ambition to develop an innovative decontamination process that will offer a realistic and cost-efficient solution for the removal of some radionuclide cations from multi-component effluents related to low- and intermediate level radioactivity, leading to small amounts of ultimate (solid) waste thus generated and simultaneously meeting the requirements for more energy-saving and environmentally friendly waste conditioning. Aqueous effluents of interest to the industrial partners involved in this project contain three major groups of ionic species: (i) monovalent and polyvalent radionuclide cations (Cs, Co, Sr, and Ni) (ii) non-radioactive alkaline cations (Na, K), (iii) nitrate and borate anions, with the overall salt content being up to 150 g/L. During the project duration, it will be necessary to optimize the separation process at the laboratory scale and demonstrate its viability through the construction of a laboratory pilot system used to simulate certain features of industrial-scale units. Novel separation-dedicated materials will be designed, developed and tested in simulated waste solutions. This industrial-type research, done by a partnership combining the expertise of academic and industrial partners, will implement the principles of eco-design in both the process development and the materials conception. The Consortium comprises 3 research organisations (AIME and IAM in the ICGM UMR CNRS 5253, GPEB UMR CIRAD 016) and 2 industrial partners (ONET Technologies and COATEX). The project will be co-ordinated by Jerzy ZAJAC (ICGM-AIME). The work plan includes 4 scientific and technical work-packages, and a fifth work package devoted to project management, dissemination and valorisation activities. The Consortium will exploit the results obtained in the project lifetime in accordance with the interests of France, taking into account the international competitiveness of French industry.

Partners

ICGM-AIME UMR 5253
ICGM-IAM UMR 5253
IEM-GPM UMR 16
Onet Technologies R&D
Coatex

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ANR funding	668 691 €
Starting date and duration	January 2011 – 36 months
Reference	ANR-10-CDII-015
Cluster label	TRIMATEC

Project title**GALAC : From Glycerol to Acrylic acid via LACtic acid****Abstract**

Due to the predictable rarefaction of petroleum, it is essential to develop new approaches for the synthesis of intermediate products such as acrylic acid. This C3 platform molecule is produced now at 4Mt/year from propene. One alternative route is the synthesis of acrylic acid in two steps from glycerol with acrolein as intermediate. But this strategy leads to expensive supercritical and acid conditions or to rapid catalyst deactivation. Hence, no industrial transfer is expected for the moment using this chemical route. In this project, we propose to prepare acrylic acid from glycerol but via lactic acid intermediate. This project is in adequation with the Axis 1 of the proposal. To our knowledge, this parallel route has not been studied and covered two important successive steps: the first one yields to the formation of lactic acid which is also an important molecule platform (precursor of polylactic acid, pyruvic acid) and for which very few studies has been carried out. The second step, the dehydration of lactic acid to acrylic acid, is very sensitive due to the high reactivity of the product and the large problems of deactivation of the catalyst. While the dehydration reaction is well known for a large range of substrates, very few reports concern their application to lactic acid dehydration. We wish to study carefully these two steps considering the added-value of both products (lactic acid and acrylic acid). The development of heterogeneous catalysts will be studied to achieve high yields in both steps. Then the lactic acid formed in the first step will be used in the second step without drastic purification. We will develop the synthesis and the characterization of the catalysts for each step (supported metallic catalyst for the first step and solid acid for the second step) and we will adapt the reaction conditions to reach the highest yields. The support of theoretical teams will help in understanding the reactivity of the highly functionalized glycerol substrate and lactic acid over different model catalysts and to design the best catalytic systems. The combination of these different contributions will help to establish the viability of the system. Futhermore, a constant exchange with the industrial partner involved in this project will be a guidance for experimental conditions optimisation to transfer as quickly as possible the processes to industry. This project gathers 5 academic research teams and an industrial partner to take benefit from all competences: theoretical studies of heterogeneous catalysis, experimental skills in developing new metallic or solid acid catalysts, industrial transfert.

Partners

IRCELYON UMR 5256
UCCS UMR 8181
LC-ENS UMR 5182
NOVANCE

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ANR funding	912 300 €
Starting date and duration	42 months
Reference	ANR-10-CDII-011
Cluster label	AXELERA

Project title	Isosorb-CO : Hydroesterification of olefins : Synthesis of new isosorbide based plasticizers
Abstract	<p>From an industrial point of view, the synthesis of new relevant products is a key issue to insure future economic growing. The context of sustainable development opens new commercial opportunities as substitutes to more traditional, well established, but sometimes toxic chemicals. Agro-based substitutes are particularly attractive as they are obtained from renewable feedstocks and potentially less toxic than their synthetic counterparts. In this context, the market of plasticizers is attracting an important attention. Several commercial phthalate esters, produced on a very large scale, are commonly used as plasticizers but are also often pointed out for their inherent toxicity. As a consequence, the search for their replacement by new safer compounds is stimulated as their replacement is often required by consumers. In answer to this problematic, the introduction of agro-based compounds appears as a valuable approach. Two laboratories from the Unité de Catalyse et Chimie du Solide (UCCS, UMR 8181) located in Lille and Lens have been associated with Roquettes Frères to develop a new catalytic and highly atom economic synthetic pathway for the synthesis of agro-based plasticizers. The field of the project includes the evaluation of their plasticizing properties under flexible PVC application. In addition, the separation and recycling of the catalyst from the reaction mixture by mean of immobilization in a separate liquid or solid phase will be investigated.</p>
Partners	<p>UCCS – Lille UMR 8181 UCCS-Artois UMR 8181 ROQUETTE FRERES</p>
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ANR funding	482 723 €
Starting date and duration	November 2010 – 36 months
Reference	ANR-10-CDII-006
Cluster label	MAUD

Project title	NaturaDyRe : Efficient Bio-Oxidations for the synthesis of natural or enantiopur compounds
Abstract	<p>This project is aimed to providing a new tool to chemists in laboratory or industrial production: a highly efficient regio- and / or enantioselective biocatalysed Baeyer-Villiger oxidation in high concentration. In a first step, a set of new enzymes displaying complementary activities will be proposed to face up to the weakness of the current offer of Baeyer-Villigerases (a dozen available enzymes in laboratory and only one commercialised). The genes of putative BVases will be identified in genomic data banks by comparison of sequences then introduced into host microorganism via a high throughput cloning. High and medium throughput screenings intended to report respectively the activity and enantioselectivity profiles of these enzymes will be set up and carried out in order to develop a tool for making easier and faster the choice of the catalyst. On the other hand, productivity often reaches limits because of inhibition (or toxicity) phenomena. To move closer to industrial benchmarks, a process based on adsorbent resins will be implemented to increase concentrations. Besides their "green" and sustainable aspect, Baeyer-Villiger biooxidations present an enzymatic version more efficient in terms of enantioselectivity than the chemical version. In order to harness these features, Dynamic Kinetic Resolution (DKR) process associating in situ substrate racemisation simultaneously with microbiological Baeyer-Villiger oxidation (to overcome the maximal 50 % of yield inherent to classic resolutions) will be developed. Various chemical and enzymatic racemisation conditions will be investigated. DKR and resin-based process will be finally brought together in a Dynamic Kinetic Resolution process at High Concentration, which should lead to a significant increase in productivity. The approach proposed in this project will be validated by the industrial scale production of molecules of interest in the field of flavours or synthesis intermediates.</p>
Partners	iSm2 UMR 6263, CEA GEN, DSIMB UMR 665, Naturamole
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ANR funding	891 202 €
Starting date and duration	December 2010 – 48 months
Reference	ANR-10-CDII-014
Cluster label	PASS

Project title	PANACEE : Command of hospital aqueous waste (oncological): toxicity analysis and eco-combination of treatment processes; in situ validation
Abstract	<p>In the hospitals and pharmaceutical industry effluents, as well as in wastewater-treatment plants and more generally in wastewaters, diverse pollutants were able to be identified, genotoxics (hydrocarbons), endocrine disruptors (personal care products) or plastics (Bisphenol A)) The anticancerous molecules, although in lesser quantity represent an increasing danger. Anticancerous substances administered to the patients in great quantities are rejected trough urines, and are only partially degraded and eliminated by wastewater treatment plants. Considerable contents of these metabolites can be found in rivers and possibly in irrigation water, even in drinking water. The known consequences of their occurrence in the environment go from allergy to cancer by way of fertility losses even teratogenics effects. Within the project "Toxeaubam" (2005, ANR "blanc") we demonstrated the feasibility of a laboratory scale membrane bioreactor, we have also adapted ecotoxicity tests on a model molecule (the cyclophosphamide) and its main metabolites, added in a domestic wastewater. The effect of these molecules on the biodegradation and the filterability of biological sludge is also quantified, leading to propositions of operating conditions The aims of this project, PANACEE, bring an opening to the previous one. They are split into 3 interdependent objectives: 1) the evaluation of the occurrence of molecules, used in the treatments of cancers, in the effluents of the corresponding services (and associated molecules within the therapies, typically disinfection ones); 2) The measure and quantification of the toxic effects, (geno / cytotoxic and endocrine disruptors) of these effluents and the contribution of the molecules and their metabolites, as well as products of disinfection in these effects; 3) the development of an hybrid process constituted by a combination of biological and physical-chemical treatments (coupling of a membrane bioreactor with adsorption / oxidation processes or nanofiltration). The efficiency of the treatment will be quantified within the framework of a technical-economic balance assessment by the evaluation of the disappearance of the global toxic effects (finalized in task 2)), the analysis of the life cycle of molecules and the energy performances of the process. This project with vocation of industrial research, and anticipation on the eco-responsible needs of decontamination bound to discharges legislations under elaboration.</p>

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ANR funding	928 439 €
Starting date and duration	January 2011 – 48 months
Reference	ANR-10-CDII-004
Cluster label	Cancer-Bio-Santé Risques

Project title**POLYTERP : Polyterpens by enzymatic conversion of isoprene****Abstract**

Among the four main families of natural compounds produced by plants and animals, terpene derivatives constitute the largest and most diverse group of functional hydrocarbon-based derivatives including molecules from C5 hemiterpenes to very high molar mass polyisoprenes such as Natural Rubber (NR). They are synthesized in vivo in presence of specific enzymes from a common C5 elementary precursor, isopentenyl pyrophosphate (IPP). Although in vitro biosynthesis of many terpenoids is described, this strategy of synthesis remains restricted to laboratory studies because of the low availability and stability of IPP. We have recently discovered that isoprene (IP) can be recognized by enzymes and used as initial substrate in place of IPP to produce isoprenoids. In particular, it was found that addition of IP to fresh *Hevea brasiliensis* latex containing active cis-prenyltransferase yields to an over production of very high molar mass 1,4-cis polyisoprene with a structure close to NR. In this project we plan to develop this approach for the production of various terpenoids. The elementary mechanisms leading to the formation of new NR from IP will be first investigated. Besides the possibility to significantly improve the NR biosynthesis, this strategy will be extended to the preparation of other terpenoid of economical interest. To that aim complementary experiments using labeled IP will be conducted on fresh rubber particles and on specific enzymes involved in terpenoid synthesis (IPP/DMAPP isomerase, prenyl transferase,...). Enzymatic systems will be obtained from plant extracts and through cloning protocols. It is anticipated that the use of IP, a substrate readily available from oil and the biomass and easy to handle, in place of IPP will open extremely interesting perspectives for the production and valorization of terpenoids and of related compounds. This new synthesis pathway should permit enhancing the productivity of NR producing plants as well as an industrial scale-up of the production of terpenoids of interest using microbial platform technology.

Partners

LCPO UMR 5629
US2B UMR 5103
Biologie du fruit UMR 619
Dérivés Résiniques et Terpéniques
MICHELIN

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ANR funding	645 547 €
Starting date and duration	January 2011 – 36 months
Reference	ANR-10-CDII-010
Cluster label	Xylofutur

Project title	POMEWISO : Polymeric membranes made without organic solvent
Abstract	<p>We propose to implement new processes of membrane manufacturing by using lower critical solution temperature (LCST) polymers and their demixion in water. Three classes of polymer including poly(amic acids) and modified cellulose and chitosan will be studied. After determining the phase diagrams, the mechanism of phase separations will be characterized and the growth laws with time established. This will provide roadmaps for the membrane manufacturing. A range of process parameters (temperature, air flow rate and relative humidity) in which porous structures are obtained will then be assessed. Relationship process parameters-membrane morphology will be investigated through a quantification of the mass and heat transfers. Modelling of transfers and numerical simulation of composition paths will be examined to find relationship phase separation mechanism-processing-morphology. Consolidation of the film structure can be carried out by either thermally or radiation induced cross-linking. Finally, the functional performance properties including permeability and rejection will be determine for liquid permeation.</p>
Partners	<p>IEM GPM UMR 5635 IEM IMB UMR 5635 CEA DSM SISMM CEMAGREF ITAP</p>
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ANR funding	647 550 k€
Starting date and duration	March 2011 - 36 months
Reference	ANR-10-CDII-012

Project title**PREDIMOL : Molecular modelling prediction of physico-chemical properties of products****Abstract**

The new EU regulation REACH (for "Registration, Evaluation, Authorization and Restriction of Chemicals") has entered in its product-registration phase after December 2008. It requires the evaluation of the physico-chemical, toxicological and ecotoxicological properties of more than 143,000 substances which have been pre-registered by 65,000 companies in order to allow their use before 2018. More precisely, the reduction of the environmental and economic impact of the chemical products used in industry is based on a systematic and reliable knowledge of their physico-chemical properties. Considering the huge number of chemical compounds used nowadays in industry, their modifications and the introduction of new products on the one hand, and the reduced number of laboratories (properly equipped and certified) for the determination of the physico-chemical properties on the other hand, a lack of knowledge of these properties is foreseeable. It is of great urgency that private and public research develops fast and reliable methods for property-screening, which would benefit from the transfer of methods from the private sector (automation and production of large volumes of data). Moreover, all new substances will require an early examination to identify possible hazards. It is necessary to anticipate the risks and to recognize the dangerous substances as soon as possible in their development. In this economic, social and regulatory context, it is necessary to find reliable solutions to this problem. Taking into account the number of properties, the number of substances, the timing, the economic costs, the feasibility at the R&D level, the ethics (tests on animals), the risks for the manipulator, in particular for the characterization of the dangerous physico-chemical properties (explosibility, flammability), the experimental measurement of all the data is not realistic. Thus, the development of alternative predictive methods for the evaluation of the properties of chemical substances is recommended in the framework of REACH and the associated system of classification, the CLP (for "Classification, Labelling and Packaging of chemical substances and mixtures"). Molecular Modelling can play a critical role in this context. Indeed, for several decades, modelling and molecular simulation in all forms (in particular quantum chemistry, molecular dynamics and Monte Carlo methods with empirical force-fields, and empirical correlations) have progressed enormously. In fact, this development is fuelled by the revolution in the power and availability of computers. During the last 25 years, compute power in all its dimensions has enormously increased by several orders of magnitude: speed of operations, random access memory, disc storage capacity, connectivity, parallelism, and power consumption. Similarly, the

price for the same functionality decreased from several million Euros to a few hundred Euros, therefore by a factor of 10,000! It is imperative to seize this opportunity in the context of the systematic, effective, and reliable prediction of the physico-chemical properties of chemical compounds. This is the context and scope of the PREDIMOL project, where molecular modelling represents an interesting way of development, which is not concurrent but complementary to the experimental characterization, in order to predict in a reliable and fast manner, the whole range of physico-chemical properties of substances required by EU-REACH's regulation (annexes VII and IX). Thus, PREDIMOL project is an industrial research project aiming at answering the research effort and innovation related to the implementation of REACH.

Partners

INERIS
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LCP UMR 8000
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Coordinator

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ANR funding

952 386 €

Starting date and duration

November 2010 – 36 months

Reference

ANR-10-CDII-007

Cluster label

AXELERA

Project title**PROCIP : Project Chart for Process Intensification Development****Abstract**

The scope of the collaborative project is to develop a technical project management methodology to be able to speed up the decision through the process intensification. For the industrials, process intensification has to allow decreasing the time to market for a product by designing the most optimum process in term of energy consumption, safety, environment considerations, investment cost... The main objective of the project "PROCIP" is therefore the development of a general process intensification methodology which includes a software implementation as well as validation and support via efficient experimental techniques. To reach the objectives fixed by this project, multidisciplinary skills are necessary (skills in process, in modelling, in PI technologies, in project development, in industrial investment). So, we gathered these skills around the consortium: - Of industrials: BlueStar Silicones France and Rhodia; - Of SME: Processium, - And of complementary laboratories in Chemical engineering: Nancy-LRGP, Toulouse-LGC, Lyon-LGPC

The association of the skills of these participants appeared as an evidence by their domains of research concerning the process intensification and their objectives to develop industrial demonstrations. The project is organized in 3 main technical parts: - Tools and methodologies to measure the basic data of the chemistry or process involved, - Characterization of equipments, in the field of process intensification : develop standardized methods to compare equipments performances as heat exchange capacity, mixing efficiency, mass transfer coefficient... - Software for Best Available Technology orientation. The objective fits with the recommendations of the call as it will bring a methodology to help the process engineer to think process innovation differently and to share the BAT sooner in the project development phase with the chemists. On an industrial plan, this work will permit to improve greatly the design of new processes thanks to a powerful software tool to look for the opportunity to implement intensified technologies. The survey of industrial cases will be done during the project in order to improve the relevance of the results. The industrial applicability will be therefore very fast. The large panel of studied technologies will facilitate portability on a large domain in chemical and pharmaceutical industries From the network of the partners and following meetings with Axelera Steering committee on "Factory of the Future", others industrials are interested to test the software developed in the Procip Project. It is a part of the dissemination but the evaluations will be used to improve and tackle the pitfalls and weaknesses of the software. On a commercial plan, after the end of the project, Processium will continue the tool

improvement in order to make a decision aiding tool usable for new reactive process developments and possibly to spread its application fields while integrating a systemic process vision (separation, environment, chemistry,...). This tool will accompany efforts already hired by Processium in separation process synthesis.

Partners BLUESTAR Silicones France
RHODIA OPERATIONS
LGPC UMR 2214
LGC UMR 5503
PROCESSIUM
LRGP UPR 3349

Coordinator Richard Vivier – BLUESTAR Silicones France
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ANR funding 1 123 234 €

Starting date and duration February 2011 – 48 months

Reference ANR-10-CDII-013

Cluster label AXELERA

Project title**SANBACT** : Conception of new surfaces with antibacterial properties by a multidisciplinary and a multiscale approach**Abstract**

The proposed program falls within the field of health safety and materials hygiene. It's focused on the prevention and the battle against the pathogenic bacterial adhesion and the hazardous biofilms formation using methods which enable the eco-preservation of the environment. The program particularly features on the surface modification of industrial materials (plastics, metals) used in very diverse domains (medical, pharmaceutical, food, etc.) in the aim of providing them one or several antibacterial functionalities: anti-bioadhesive (based on physical and physico-chemical effects) combined or not combined with bactericidal properties, bacteriostatical properties or a "slow down growth" effect. All these properties and combined effects can be summarized as antibiofilm effects (biological effect). Thus, these new surfaces should be able to reduce the consumption of biocides and water now needed to ensure a hygienic status to the contaminated materials during the cleaning/disinfection procedures generating a significant amount of effluent. Consequently, this project exhibits a threefold interest: economical, environmental and of public health. New surfaces will be developed through an integrative and multiscale approach of the bioadhesive phenomena . In this new approach, the size, the morphology, the presence or absence of exocellular structures as well as the physicochemical and physiological characteristics of the targeted bacteria will be necessarily taken into account. These surfaces are obtained either by grafting or by deposition of bioactive substances (i.e. "natural" substances acting on the "development cycle" of the bacteria) or molecules with defined specificities (hydrophobic to hydrophilic) and that, in order to be able to answer to a variety of applicative situations. In all cases, only raw materials compliant with the environmental legislation (REACH, Biocides) will be implemented. Their realization will lead to original structures and to specific physico-chemical properties tightly controlled via multi scale analysis (nanometric to macroscopic). These new anti-bacterial surfaces will have to be validated for conventional materials used in different technological fields of application. Due to their specificities, sampling and analysis methodologies adapted to the measurement of low levels of biocontamination will necessarily have to be developed. That's why, in parallel with the "surface engineering" part of the project, methods for the sampling and the recovery of contaminating flora and techniques for biocontamination evaluation with detection limits below 10 cells / mm² will be developed and / or improved. Through a multidisciplinary and multi-scale approach the project will lead to significant advances in the scientific knowledge of: - Bacteria / new surfaces

interactions and especially the role of each component of the cell envelope (pili, flagella, capsules ...) in these interactions. - Reactivity of bacterial cells after contact with these native or modified abiotic surfaces (physiological changes which can result in morphological modification and growth modification or in a variation in their genetic expression and in their virulence expression...). This set of knowledge is now essential in a process of rational and effective control of surface biocontamination. Result of a federative multidisciplinary approach linking complementary skills, the project combines actors from institutional research laboratories (INRA, AgroParisTech, CNRS, Universities), from technical centers (CTTM and ISHA) and from industrial (Eudica) who already worked together.

Partners

INRA-AgroParisTech
PCI-CNRS UMR 6120
CMOM EA 3155
Centre de Transfert de Technologie du Mans
LCOM/G2M/ICMMO UMR8182
ISHA-Anadiag
EUDICA

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ANR funding

950 353 €

**Starting date
and duration**

November 2011 – 48 months

Reference

ANR-10-CDII-002

Project title	SUCROL : Lignocellulosic biorefinery for the production of cellulose and pentoses for the production of green surface active agents
Abstract	<p>Summary The French pulp industry is competing against South American (Brazilian) and Asian (Indonesian) companies which are capable of producing wood pulp at a much lower price, thanks to the availability of a cheaper raw material (eucalyptus, acacia). The definition of a new economical model is the only way to stay alive in this competition. The model which seems the most appropriate today is the paper biorefinery in which all the main wood chemical components are extracted and used in a most valuable manner. This project aims at defining an extraction process for the hemicelluloses present in hardwoods, which will take place before kraft cooking and which will give a flow of pentoses in an appropriate form for chemical purposes, without affecting the quality of the kraft cellulose. The use of pentoses has been investigated to a much lesser extent than that of hexoses. This is due to the fact that the latter are dominant in the agro-materials used today as sugar sources. However the situation is different in hardwood trees and most of the agricultural residues (straw...) in which they may represent more than 30% in weight. The surface active agents industry has recently developed new families of biomass based products (like the alkylpolyglycosides -APG). Their potential is very high but their development is slowed by their relatively high cost. The availability of new sources of xylose at a cheaper price will represent a real breakthrough for the development of new applications for the APG. The synthesis and properties of the xylose-based APG will be investigated.</p>
Partners	Grenoble INP UMR 5518 Fibre Excellence R&D Kraft Seppic
Coordinator	Christine Chirat – Grenoble INP Christine.chirat@pagora.grenoble-inp.fr
ANR funding	268 922 €
Starting date and duration	December 2010 – 36 months
Reference	ANR-10-CDII-004
Cluster label	AXELERA