505654-1

PROFORM

TRANSFORMING NANO-PARTICLES INTO SUSTAINABLE CONSUMER PRODUCTS THROUGH ADVANCED PRODUCTS AND PROCESS FORMULATION

STREP

3-NMP [New Production Processes and Devices]

D30-2: Publishable Final Activity Report

Period covered: from 1 July 2004 to 31 December 2007
Date of preparation: January 2008

Start date of project: 1 July 2004 Duration: 3.5 years

Project co-ordinator name: Dr Gűl Őzcan-Taşkin
Project co-ordinator organisation name: BHR Group Ltd, UK

TABLE OF CONTENTS

1. Project Execution

1.1 Motivations

There has been an increasing need for the European chemical process industries to advance and integrate the knowledge and expertise from different disciplines, to be able to produce new products, and develop new process technologies. Such capabilities bring market opportunities and economic sustainability, whilst maintaining safe and energy efficient operations, with minimal waste production. Flexibility is another important driver for these industries as they require the ability to respond rapidly and proactively to changing customer needs, without compromising on safety, health or the environment. One prominent example is the formulation and manufacture of products that contain dispersions of fine particles. The practical application of nanotechnology in the process sector relies heavily on the ability to incorporate nano-particles into products in a fully dispersed and stable state, which when used for its intended purpose, allows the material to fully express its functionality. Due to limitations of the knowledge in the field, the design of these processes based on fundamental understanding has not been possible. Therefore, a trial and error type of approach has been taken for design and scale up. In addition to the waste associated with the preliminary trial work, the actual manufacturing processes, which are not optimised, result in excessive waste production from off-specification materials. These are typically due to, for example, the re-agglomeration of particles requiring major investment in downstream “clean up” of equipment, along with the costs and energy requirements of recycling off-specification products. There has been a clear need to develop design guidelines based on a fundamental understanding to ensure safe, reliable and optimal operation of these processes.

Little has been known about the relative importance or predominance of the different dispersion mechanisms present in different process equipment used to disperse nano-particles in liquids. Thus, the design of such processes has been based on empirical methods. The work proposed within PROFORM was intended to replace at least part of this empiricism by more targeted and quantifiable methods, which build on a fundamental understanding of the mechanisms involved and of their relative importance under given operating conditions. Substantial achievements have been made in the area through this project as a result of combined efforts from experimental and theoretical studies carried out as described in the following sections.

1.2 Project Objectives

The success of the processes mentioned above (in terms of achieving the desired product quality, energy efficiency, safety and cleanliness) requires multi-disciplinary knowledge and skills. Therefore, this project has aimed to mobilise and bring together the expertise that has typically been confined to a specific area and develop an integrated approach for new processes and products that involve particle processing at the micro and nano scales.

The main objective of PROFORM has therefore been to develop the next generation of process tools and methodologies for the design and manufacture of products containing nano-particles in a highly dispersed, functional and stable state. This has required the development of fundamental understanding of the phenomena related to the processing of nano-particles, specifically the dispersion of nano-particles in liquids. Consequently, the physical properties of dispersed nano-particle products can be improved and waste can be reduced to achieve economic and environmental savings.

The overall objective of the project has been met with the preparation of Design Guides and the initial design of a software based formulation adviser. These have been produced as a result of efforts from different parts of the project. There are plenty of opportunities to develop and enhance these design procedures with additional features addressing other specific relevant phenomena and processes in future projects. The project has also allowed the identification of topics in which further work in the field is required either in terms of technique development or process and equipment design.

1.3 Contractors Involved

The consortium consisted of 10 partners from 4 European Sates with complementary expertise, comprising academic institutions, SMEs and large companies.

List of Participants

Partic. no.	Participant name	Country
1	BHR Group Limited	UK
2	Karlsruhe University, Institute of Food Process Engineering	DE
3	Bayer Technology Services GmbH	DE
4	Loughborough University, Department of Chemical Engineering	UK
5	Unilever UK Central Resources Ltd	UK
6	Birmingham University, School of Engineering	UK
7	Warsaw University of Technology, Department of Chemical and Process Engineering, Division of Mechanical Engineering and Process Dynamics	PL
8	Poznan University, Faculty of Chemical Technology, Institute of Chemical Technology and Engineering	PL
9	Rockfield Software Ltd	UK
10	Centre for Computational Continuum Mechanics	SL

1.4 Methodologies and approaches employed

The project was organised in several workpackages and the overall approach is schematically shown below.

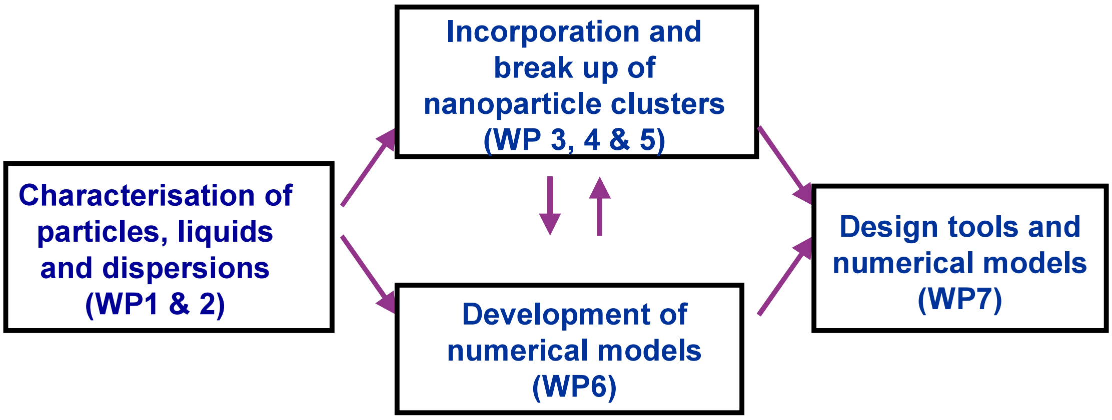


Figure 1. Overall approach taken

All workpackages required the involvement of different partners. Appropriate techniques were adapted to carry out the experimental programme. In order to ensure that results obtained by different partners using different devices and operating under different conditions are comparable, ring tests were organised.

Parallel to physical experiments, numerical modelling studies were carried out using population balance modelling. Development of models describing the rheology of nano-particle suspensions, break up of nanoparticle clusters (schematically shown in Figure 2) were undertaken maintaining close links with experimental workpackages to ensure a two-way interaction.

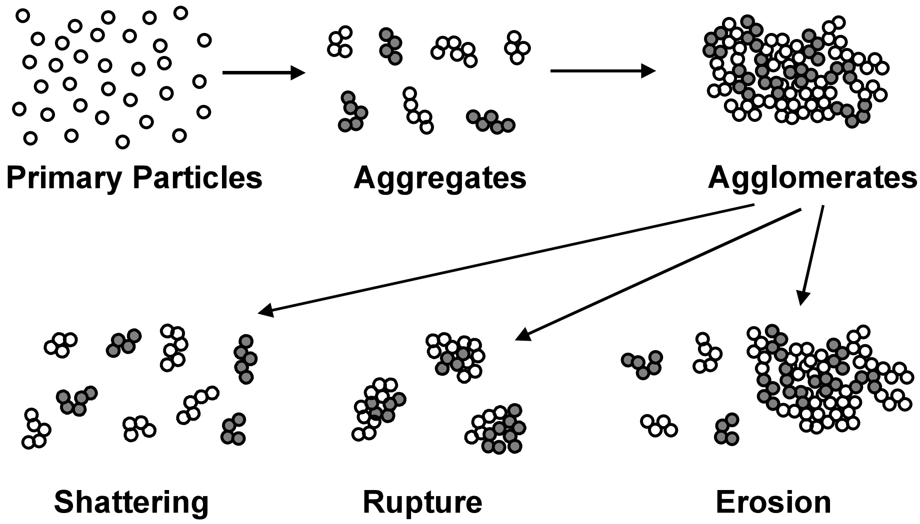


Figure 2. Schematic representation of particle clusters and their breakage through different mechanisms

The third strand of the project was the preparation of Design Guides. Again, the related activities were carried out maintaining strong links with other workpackages to ensure both the inclusion of all the major findings from the project in the Design Guides and also relevant research activities are undertaken working towards these Design Guides.

Methods employed can be summarised as follows:

- Particle size: laser diffraction or light scattering (example results are shown in Figure 6)
- Morphology: microscopy, electron microscopy (example results are shown in Figure 7)
- Rheology: vane-and-basket geometry
- Wettability: immersion test or cone method
- Stability: zetapotential (example results are shown in Figure 4)
- Incorporation: visual observations
- Torque: strain gauges or calorimetry
- Aggregate strength: micromanipulation technique or calculations
- Surface free energy: iGC
- Solubility: iGC
- Flow characteristics: visual observations, Laser Doppler Anemometer (LDA), Particle Image Velocimetry (PIV), chemical tracer technique, Computational Fluid Dynamics (CFD)
- Numerical modelling: population balance equations
- Initial design of software based advisor: in-house developed software programmes, one based on inverse analysis

1.5 Work performed

Experimental and numerical studies have been carried out for different particles and process devices. Different steps of the process and equipment typically used are shown in Figure 4.

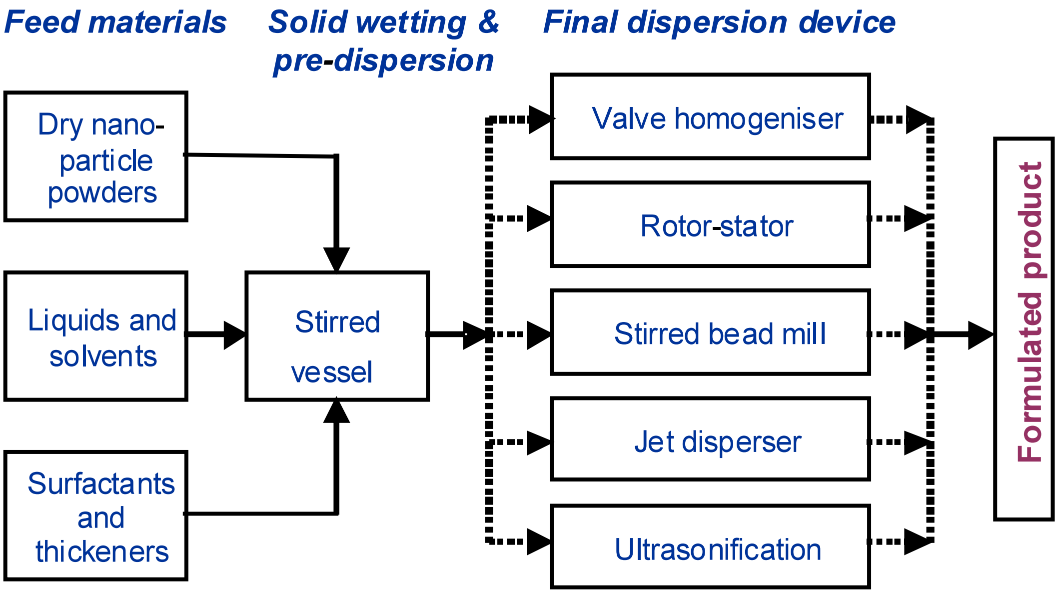


Figure 3. Incorporation and dispersion of nano-particle clusters and different process devices used

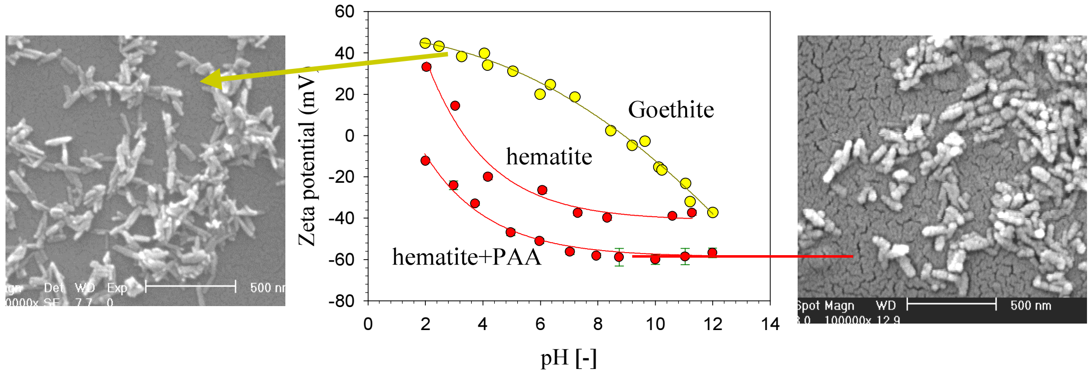
The scope of work undertaken in the workpackages shown in Figure 1 can be summarised as follows:

- identification of relevant characterisation methods (for particles, liquids and dispersions) and characterisation of these;
- investigation of the incorporation and dispersion of nanoparticles in liquids;
- identification of criteria to determine equipment performance and assessment of the comparative performance of different process equipment;
- investigation of the importance of liquid composition in conjunction with processing conditions;
- identification of appropriate computational methods for the integration of inter-related phenomena operating over a range of length- and time-scales;
- development of numerical models describing the rheological properties of nano-particle suspensions and the dispersion process in relation to processing conditions;
- development of Design Guides.

1.6 End results

End results can be summarised as follows:

- standard methods and protocols for characterising nano-particles and their interactions with the fluids (Figure 4 shows example results on the stability of iron oxide aggregates);
- a database containing the relevant physical properties of nano-particles used within the consortium;
- experimental results on the effects of processing conditions on the incorporation and break up of nano-particle clusters in liquids;



Goethite: stable at pH=3, ZP = 45mV,
not stable at pH = 4 - 12 (ZP = 40 ~ - 40mV).

Hematite: unstable in pH range of 3-12 (ZP = 35 - -35mV)
PAA necessary for stabilization at pH ~9, (ZP = - 55mV),

Figure 4. Stability of iron oxide nanoparticles

- results on the combined effects of the chemical composition of suspensions and processing conditions (Figure 5 shows example results);
- assessment of the comparative performance of a range of process equipment;
- numerical models describing the dispersion of nano-particles in liquids;
- numerical models for rheological properties of nano-particle suspensions;
- validated simulation tools for the break up of nano-particle clusters using the process devices investigated throughout the project;
- Design Guides including the initial design of a software based advisor.

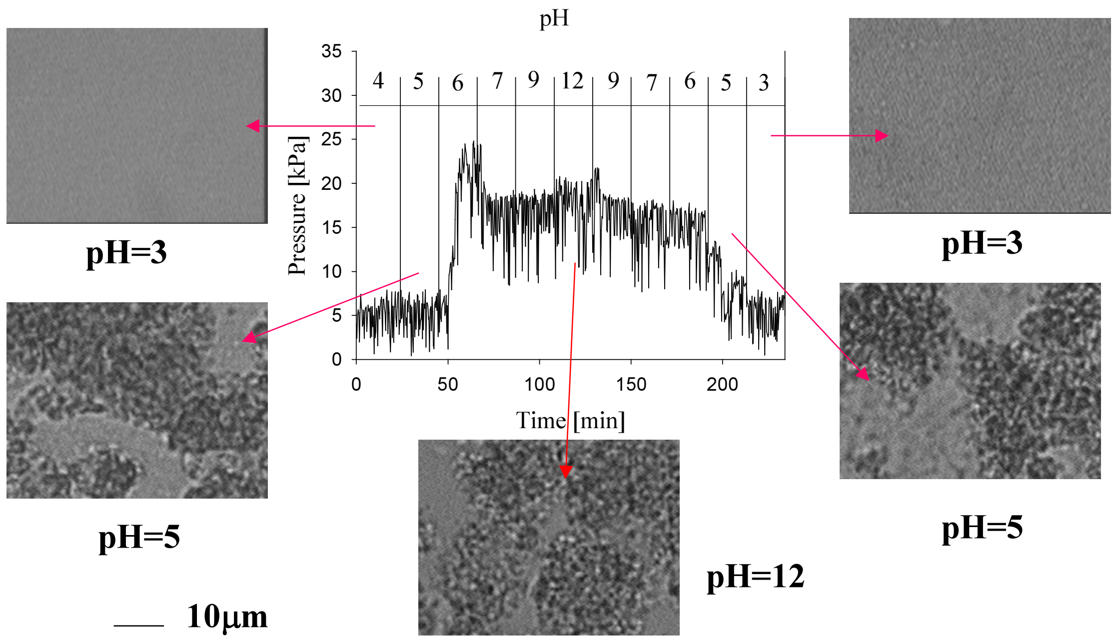


Figure 5. Morphology of Goethite suspension at different pH and pressure difference

A list of deliverables containing the project results is provided in the Appendix.

1.7 Overall Evaluation of the Project and Major Achievements

Overall, the project has been hugely successful. Excellent progress has been made in all the workpackages as a result of contributions from partners of complementary expertise, which could not have been brought together without funding from the EC. The delays in the initial stages of the project due to the late arrival of the contract and payment could be compensated with the 6 months project extension. As a result, all of the Tasks and project deliverables were successfully completed.

There has been a good level of interaction between the different aspects of the research programme throughout the whole life time of the project. It has thus been possible to relate and bring together the findings and results from different partners and workpackages. This allowed the development of

- an equipment review, a Design Guide and the initial design of a software based formulation adviser which encapsulated the major findings of PROFORM

which is a major achievement in terms of meeting the overall project objectives.

The achievements from the different parts of the projects that have allowed this are listed below; further details are given under each workpackage.

- Measurements made on the physical properties of particles and dispersions could be related to the results obtained from different process devices (Figures 6 and 7). These include the particle size data, suspension rheology, comparative wettability of the particles, morphology, surface free energy, solubility and stability of dispersions. Mathematical models representing the rheology of these dispersions were also identified.

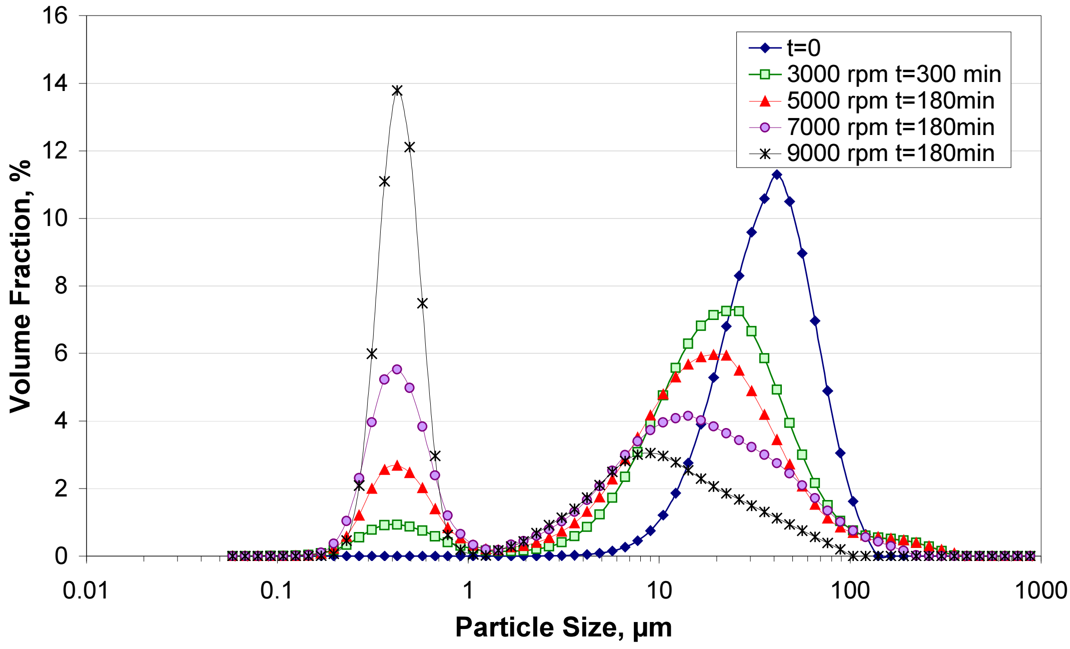
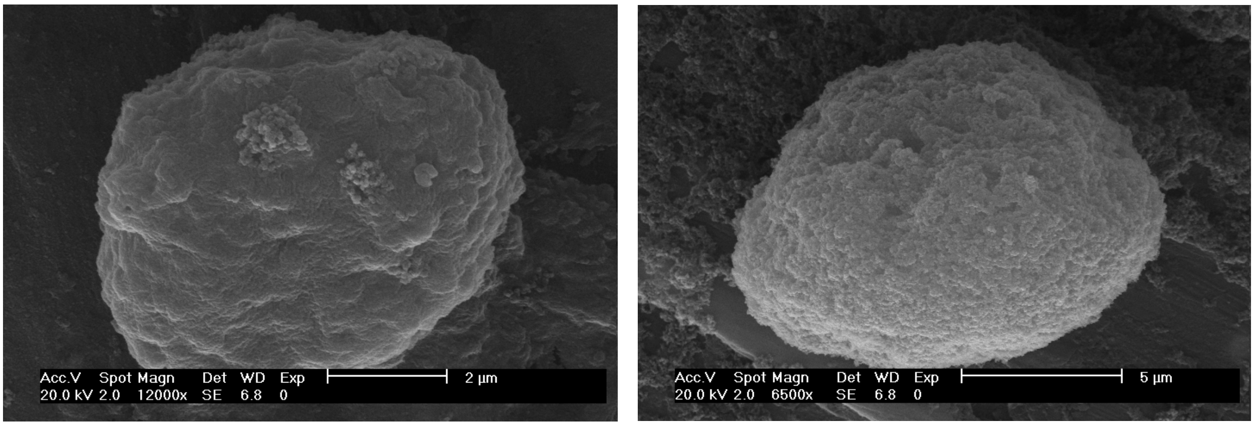


Figure 6. Evolution of PSD in time: bi-modal distribution obtained with the peak for coarse material shifting to the left and the one for fines increasing in volume suggests breakage through erosion.



(a) t= 1 min **(b) t= 180 min**

Figure 7. Large agglomerates at the start of the experiment have a smooth surface as shown in (a). At the end of the experiment their rough surface suggests that small aggregates are eroded over time as shown in (b)

- Two software programmes were developed to calculate the Flury-Higgins interaction parameter, solubility parameter, corrected solubility parameter and its components corresponding to dispersive, polar and hydrogen bonding interactions using the iGC method.

- A two phase model for the prediction of solubility was developed .

- Combined effects of changing the chemical composition (pH, addition of surfactants), processing conditions (power input, processing time or residence time, temperature), particle and liquid phase properties (concentration, primary particle size, hydrophobicity, aggregate strength) have been demonstrated for several test systems. Some examples are shown in Figures 3 and 4.

- Based on the studies with several different particles and devices over a range of operating conditions:

  - Criteria could be identified for assessing the performance of different process devices for the incorporation and break up of nano-particle clusters in liquids. Some of the practical limitations associated with different devices were also noted.

  - Several industrially relevant recommendations could be drawn for the design and operation of processes that require the incorporation and break up of nano-particle clusters in liquids.

  - Experimental protocols to identify the mechanism of break up have been developed. Figures 6 and 7 show example results for the case of erosive breakage.

  - Numerical models have been developed describing dispersion of nano-particles and aggregates in a liquid medium for different mechanisms of break up.

- Flow within several different types of devices were studied using different techniques such as the LDA, PIV or CFD- some of these devices had not been investigated previously.

- A general model was constructed that includes:
  - CFD to model suspension flow in systems of complex geometry;
  - Population balance equations to model the evolution of particle populations;
  - rheological models for simulating the effects due to suspension structure (including the effects of PSD, dispersed phase concentration, agglomerate or aggregate structure and local

shear distribution);
- models for agglomerate structure;
- models describing the kinetics of breakage (through different mechanisms), aggregation and re-structuring of agglomerates;
- models for the tensile structure of aggregates;
- models for stresses acting on agglomerates;
- models for coupling the flow, population and rheology.

Figures 8 and 9 show example results from these numerical modelling studies for the high pressure jet and ultrasonic devices respectively.

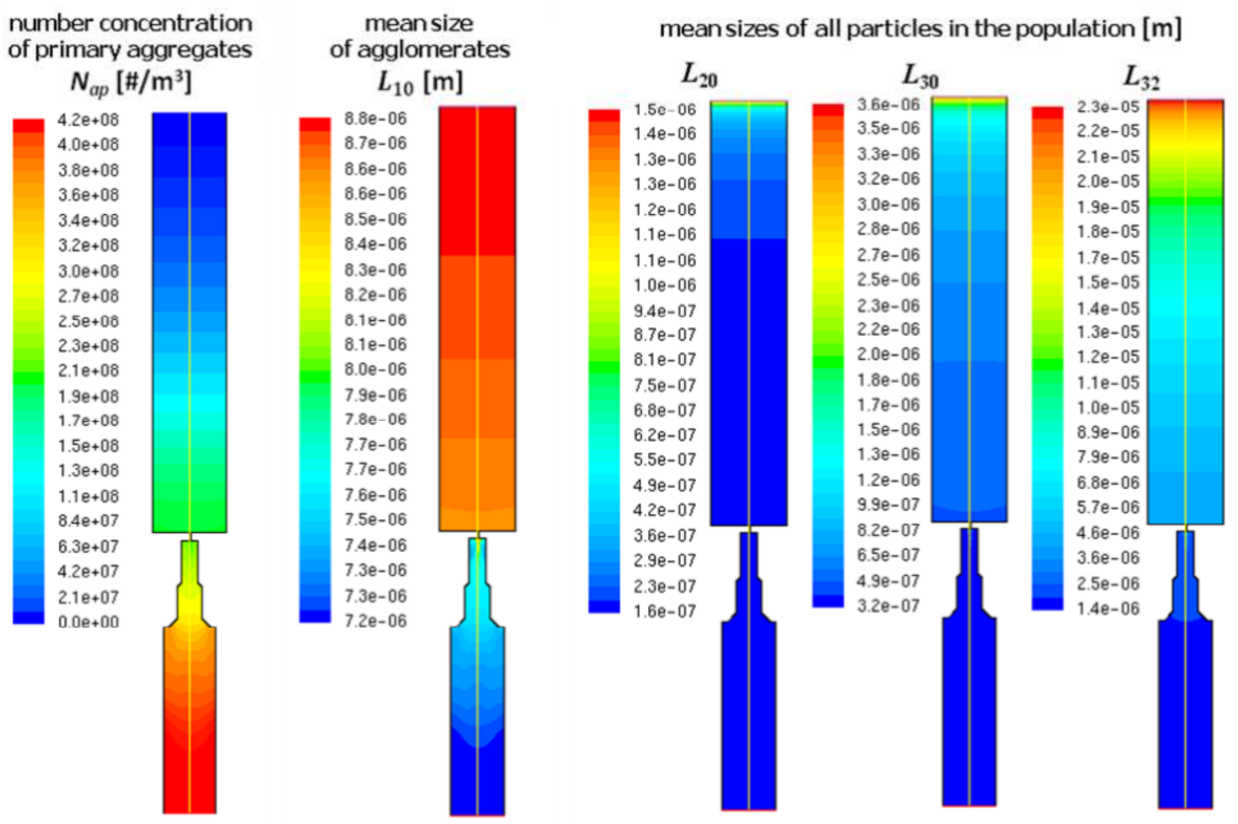


Figure 8. Particle size distribution and number concentrations for a nozzle diameter of 80 μm and inlet pressure of 2400 bar

1.8 Impact of the project

The experimental and numerical methods employed, adapted or developed during this project and the major findings of the programme are enabling capabilities for industrial applications that require the design and operation of processes for the incorporation and break up of nano-particle clusters in liquids.

Industrial partners have already started to implement the relevant aspects of the project in their businesses. The way in which each partner uses the knowledge generated during the project is different in line with the type of business of different partners. The project has allowed academic partners to widen the scope of their teaching material to educate more engineers and scientists to strengthen the European industry and undertake further research. Many undergraduate, doctoral and post-doctoral researchers trained whilst working on this project are continuing their career in the field in both academia and industry.

Some of the findings of the project have also been disseminated to share the overall trends with other professionals in the field. Section 2 describes in more detail the dissemination and use of the knowledge as a result of which the European industry will benefit.

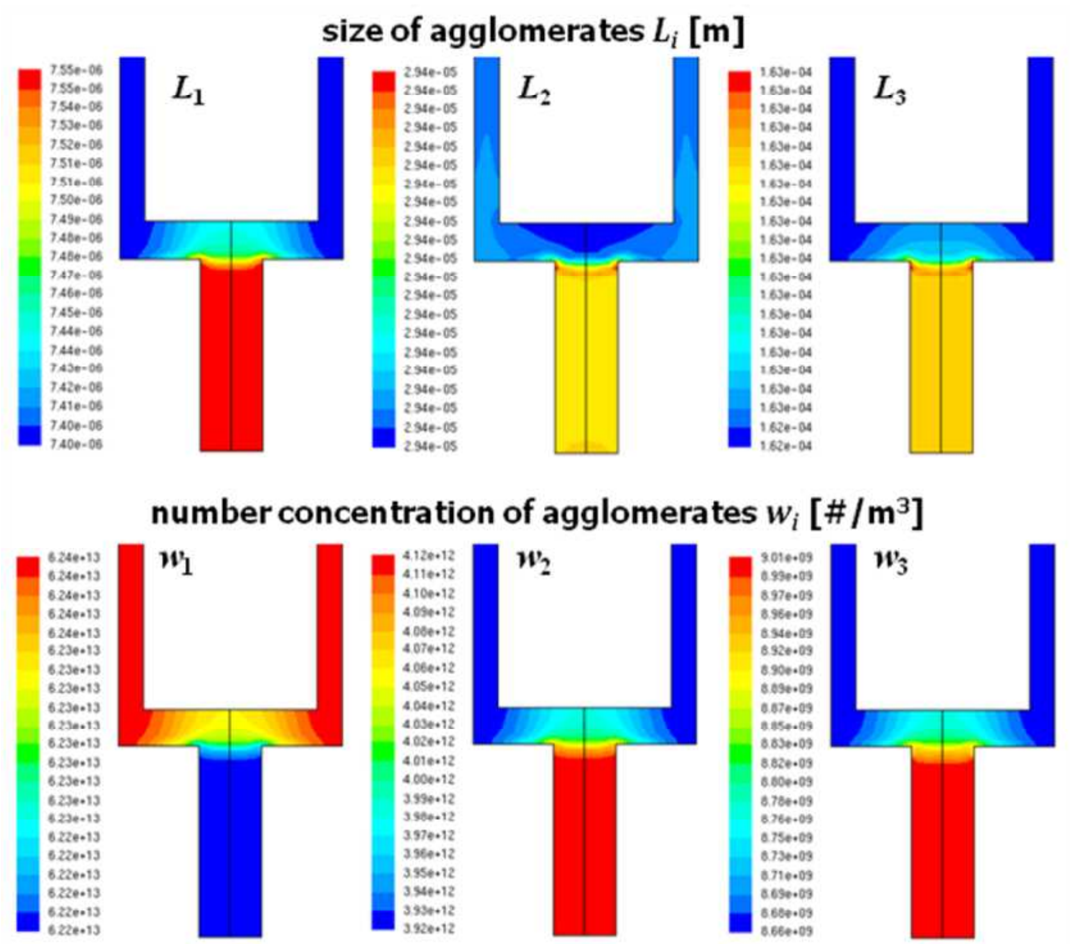


Figure 9. Axial distributions of agglomerates size and number concentration for 3 classes of agglomerates for Aerosil concentration 5 wt.%, power input 58 W, flow rate 10 ml/min

2. Dissemination and use of knowledge

PROFORM partners have actively disseminated some of the findings from this project and have already started exploiting the knowledge generated. As the size and line of business of different partners are different, the way in which each organisation will exploit the knowledge is also different. These are outlined in the paragraphs below.

a) Publishable results

Exploitable results the project should achieve fall into the following broad categories:

- Procedures for experimental and numerical research on the dispersion of nanoparticle clusters in liquids
- Experimental data
- Numerical models describing the rheology of nanoparticle suspensions
- Numerical models describing the break up of nanoparticle clusters in liquids
- CFD codes that incorporate the above models
- Surfactant selection tools
- Expertise on optimising the operation and design of some of the process equipment for the incorporation and dispersion of nanoparticle clusters in liquids
- Finite element software product, ELFEN developed by Rockfield Software, that incorporates models for agglomeration and deagglomeration of nanoparticle clusters at nano\micro-, meso- and macro scales
- Numerical approaches to sensitivity analyses, inverse modelling and optimisation of break up processes developed by C3M with special emphasis on stirred media milling applications
- Software programmes for iGC developed by PUT team enabling the calculation of surface characteristics for solid materials, solubility parameters and interaction parameters
- Comparative equipment performance
- Design Guides
- Prototype software based formulation process adviser

Practical Applications

The practical applications that the outcome of this project can be used are:

- Process design in chemicals and related industries (personal and health care, fine chemicals, agrochemicals, food, coatings and paints) where the dispersion of nanoparticles in liquids is required

- Design of new equipment by equipment manufacturers

How the results might be exploited or how they might be used in further research

PROFORM is a STREP, which has aimed to investigate the process of dispersing nanoparticles in liquids- a common step during the manufacture of several final products in the form of nanoparticle dispersions- and based on this investigation produce industrially relevant Design Guides. The research has from the very start been planned to be a generic one to study the principles of the process and did not aim at developing a specific chemical product or hardware. There are, however, several aspects project findings, which can be implemented for product development. The results of the project, which include software programmes as listed above, will be exploited in different ways and used in further research by different partners as explained in the paragraphs below and in Sections (b) and (c).

Need for further development work

The results obtained within PROFORM have great potential for further investigations. In addition to the in-house company specific research that will be undertaken by BTS and Unilever to implement the findings of this project to specific products and processes, PROFORM partners have identified several areas in which further research, process\ product development or demonstration work needs to be undertaken. These are:

- study of the stability and re-agglomeration in laminar and turbulent flows;
- novel equipment design and scale up for the production of fine nanoparticle dispersions;
- manufacturing and characterisation of nano-fluids for enhanced heat transfer;
- novel and improved characterisation methods of nanodispersions (including on-line measurement and control);
- further improvements in multi-scale, multi-field, multi-phase and multi-objective aspects of wet deagglomeration processes which will also respond to the needs of SMEs;
- process design on the manufacture of nanoemulsions;
- design of nano-dispersion formulation for specific applications: improvement of the bio-availability of poor soluble actives, much faster take up of drugs (immediate release), formulation of intravenous drug formulations, improved optical properties, stable suspensions for new food and consumer care products.

Need for further collaboration

The above topics require further collaboration due to the multi-disciplinary nature of the area. Some of the activities will require new partners, such as equipment manufacturers, partners from other industrial sectors or with other complementary expertise. Proposals for grant applications in relation to FP7 and National Calls for Proposals are in preparation for both fundamental research and application projects.

Contact details

1. Dr N. Gűl Őzcan-Taşkin: BHR Group Ltd Cranfield Bedforshire MK43 0AJ UK
2. Prof. Heike P. Schuchmann: University of Karlsruhe Institute of Food Process Engineering, Keiserstrasse 12 Karlsruhe D- 76128 Germany
3. Dr Olaf Behrend: Bayer Technology Services GmbH, Process Technology-RPT-HVMR / Bldg. E41, D-51368 Leverkusen, Germany
4. Prof. Chris D. Rielly: Loughborough University, Department of Chemical Engineering, Loughborough, Leicestershire LE11 3RB UK
5. Prof Adam Kowalski: Unilever Port Sunlight Laboratory 2216, Quarry Road East Bebbington Wirral CH63 3JB UK
6. Prof Andrzej Pacek: University of Birmingham School of Engineering, Edgbaston Birmingham B15 2TT, UK
7. Prof. Jerzy Baldyga: Politechnika Warszawska, Faculty of Chemical and Process Engineering, ul. Warynskiego 1, Warszawa, 00-645 Poland
8. Prof. Adam Voelkel: Politechnika Poznańska, Institute of Chemical Technology and Engineering, pl.M.Sklodowskiej-Curie 2, 60-965 Poznań, Poland
9. Dr William Ferguson: Rockfield Software Ltd., Technium Kings Road, Prince of Wales Dock, Swansea, SA1 8PH, UK
10. Dr Tomaz Rodic: C3M d.o.o., Vandotova 55, p.p. 431, Ljubljana 1102,Slovenia

b) Exploitation and use potential

Results generated (short description)	**Owner(s)** (name of the legal entity)	Sector(s) of Application	Exploitation / use potential measures	Timetable for use or exploitation
Experimental techniques and analysis of data on the characterisation of particles and dispersions	BHR Group, BTS, Unilever, Universities of Karlsruhe, Loughborough, Birmingham, Poznan	Chemicals and related industries (health and personal care, food, paints, fine chemicals, coatings)	In future R&D projects and consultancy services	from 2007 onwards
Experimental data	The partner who obtained the data	Chemicals and related ind. (food, health & personal care, paints, fine chemicals, coatings)	In future R&D projects	The partner who owns the data- from 2007 onwards
Validation of the suitability of an experimental technique for determining the rheology of suspensions as a measure of nanoparticle dispersions	Unilever	Chemicals and related industries (health and personal care, food, paints, fine chemicals, coatings)	Product formulation	from 2007 onwards
Validation of models describing the rheological behaviour of nanoparticle suspensions	Unilever	Chemicals and related industries (health and personal care, food, paints, fine chemicals, coatings)	Product formulation and in future R&D and consultancy projects, undergraduate and postgraduate courses	from 2007 onwards
Numerical models of deagglomeration	Warsaw University of Technology	Chemicals and related industries (health and personal care, food, paints, fine chemicals, coatings)	Product formulation, design of new equipment, future R&D and consultancy projects	from 2007 onwards
Validated CFD code incorporating breakage models	Warsaw University of Technology (validation data from BHR Group and Karlsruhe University)	Chemicals and related industries (health and personal care, food, paints, fine chemicals, coatings)	Product formulation and in future R&D and consultancy projects	from 2007 onwards
Models describing the rheological behaviour of nanoparticle suspensions based on population balance modelling	Warsaw University of Technology	Chemicals and related industries (health and personal care, food, paints, fine chemicals, coatings)	Product formulation and in future R&D and consultancy projects.	from 2007 onwards
Experimental method and numerical procedure to investigate the local phenomena over a range of Re in the turbulent regime (application of test	Warsaw University of Technology	Chemicals and related industries (pharmaceuticals, pigments, fine chemicals)	Product formulation and in future R&D and consultancy projects	from 2007 onwards

Results generated (short description)	**Owner(s)** (name of the legal entity)	Sector(s) of Application	Exploitation / use potential measures	Timetable for use or exploitation
parallel reactions)				
Fundamental knowledge required for the development of new specific apparatuses (high pressure jet nozzles, ultrasonics and parallel disc mills) suitable for breaking up nanoparticle clusters	Karlsruhe University (based on the work carried out at Karlsruhe University during PROFORM)	Chemicals and related industries (health and personal care, food, paints, fine chemicals, coatings), equipment manufacturers	Future development projects	2007 onwards
Validation of the suitability of a parallel disc type mill for breaking up nanoparticle agglomerates	Karlsruhe University	Chemicals and related industries (health and personal care, food, paints, fine chemicals, coatings), equipment manufacturers	Product formulation	2007 onwards
Optimised nozzle geometry for high pressure dispersion (HPPF configuration)	Karlsruhe University	Chemicals and related industries (health and personal care, food, paints, fine chemicals, coatings), equipment manufacturers	New equipment design for product formulation	2007 onwards
Expertise on the performance of in-line rotor-stators for deagglomeration of nanoparticle clusters (pre-existing expertise extended during PROFORM)	BHR Group (based on exp.work carried out during PROFORM)	Chemicals and related industries (health and personal care, food, paints, fine chemicals, coatings)	Further research and consultancy projects	2007 onwards
Expertise on the performance of in-line rotor-stators for deagglomeration of nanoparticle clusters (pre-existing expertise extended during PROFORM)	Unilever (based on the experimental work carried out during PROFORM)	Chemicals and related industries	Development of new process strategies & equipment. These may feature in product application patents or be maintained as confidential know-how.	2007 onwards
Expertise on the performance of stirred tanks for incorporation and deagglomeration of nanoparticle clusters in liquids (pre-existing expertise extended during PROFORM)	BHR Group and Loughborough University	Chemicals and related industries (health and personal care, food, paints, fine chemicals, coatings)	Further research and consultancy projects	2007 onwards
Strategy for optimising stirred media mill processes: effect of	BTS	Chemicals and related industries (health and	Further in-house research for applications in	2007 onwards

Results generated (short description)	**Owner(s)** (name of the legal entity)	Sector(s) of Application	Exploitation / use potential measures	Timetable for use or exploitation
process parameters and use of excipients		personal care, food, paints, fine chemicals, coatings), equipment manufacturers	specific products	
Expertise for the potential use of high pressure jet dispersing	BTS (based on the work carried out at BTS during PROFORM)	Chemicals and related industries (health and personal care, food, paints, fine chemicals, coatings), equipment manufacturers	Further in-house research for applications in specific products	2007 onwards
Surfactant selection tools for nanodispersions	BTS and Poznan University of Technology	Chemicals and related industries (health and personal care, food, paints, fine chemicals, coatings)	Product formulation and in future R&D and internal and external consultancy projects	2007 onwards
Validation of a method for determining solubility parameters to characterise surfactants	BTS	Chemicals and related industries (health and personal care, food, paints, fine chemicals, coatings)	Proprietery use for contract R&D and marketing to accelerate formulation development	2007 onwards
Validation of a method (method initially developed prior to PROFORM) for determining solubility parameters by partition coefficient method	BTS	Chemicals and related industries (health and personal care, food, paints, fine chemicals, coatings)	Proprietery use for contract R&D and marketing to accelerate formulation development	2007 onwards
Determination of solubility parameters by suspension method	Poznan University of Technology	Chemicals and related industries (health and personal care, food, paints, fine chemicals, coatings)	Future R&D projects	2007 onwards
Enhanced tool (initially developed prior to PROFORM) in visual basic and Excel for surfactant selection	BTS	Chemicals and related industries (health and personal care, food, paints, fine chemicals, coatings)	Proprietery use for contract R&D and marketing to accelerate formulation development	2007 onwards
Software for calculating parameters used in the characterisation of surface properties of nanoparticles by mean of iGC	Poznan University of Technology	Polymers, coatings, fillers, minerals and pharmaceuticals industries	Free licence to use given to all PROFORM partners, other marketing opportunities under consideration	2005 onwards
Two software	Poznan	Polymers,	Free licence to use	2005 onwards

Results generated (short description)	**Owner(s)** (name of the legal entity)	Sector(s) of Application	Exploitation / use potential measures	Timetable for use or exploitation
programmes to calculate Flory-Huggins interaction, solubility, corrected solubility parameters and its components corresponding to dispersive, polar and hydrogen bonding interactions using the iGC	University of Technology	coatings, fillers, minerals and pharmaceuticals industries	given to all PROFORM partners	
Models for agglomeration & deagglomeration of agglomerate on nano/micro-, meso-, macro-scales incorporated in finite element software product-ELFEN	The software product ELFEN has been enhanced by Rockfield Software (with validation data from PUT for the development of DVLO contact law and BTS for bead milling experiments)	1. Producers of nano-materials 2. Producers of mill equipment	Copyright	By Rockfield Software- Start 2008
Equipment Review	BHR Group	Chemicals and related industries (health and personal care, food, paints, fine chemicals, coatings), equipment manufacturers	Copyright. Free licence upon written request to use only for internal purposes: BTS, Karlsruhe, Loughborough, Unilever, Birmingham, Warsaw (partners that contributed data)	2007 onwards
Design Guides	BHR Group	Chemicals and related industries (health and personal care, food, paints, fine chemicals, coatings), equipment manufacturers	Copyright. Free licence upon written request to use only for internal purposes: BTS, Karlsruhe, Unilever, Loughborough, Birmingham, Warsaw, Poznan (partners that contributed data)	2007 onwards
Numerical framework for sensitivity analyses, inverse modelling and optimisation of stirred media milling technology	C3M (validation data from BTS) in cooperation with RSL	Chemical, health and consumer care, food agro, pigments, paint, lacquer, plastics, ceramics and electronics	Analysis services Customised software packages	from 2007 from 2009
Initial design of software based formulation process adviser	C3M and Warsaw based on the Design Guide	Chemicals and related industries (health and personal care, food, paints, fine chemicals, coatings), equipment	Future R&D projects for further development (Note: Any subsequent exploitable software will be licenced as per 4.3.3 of the Collaboration	From 2008 onwards

Results generated (short description)	**Owner(s)** (name of the legal entity)	Sector(s) of Application	Exploitation / use potential measures	Timetable for use or exploitation
		manufacturers	Agreement of PROFORM)	

c) Innovation-related activities

c.1 BHR Group Ltd

BHR Group is an independent SME specialising in research, development and consultancy. R&D projects undertaken at BHR Group are either with partial funding (for example PROFORM) or industrial clubs, which rely entirely on industrial funding. Consultancy projects are typically carried out for a single client. All of these projects are confidential unless a special agreement is reached with the members or partners to disseminate all or part of the findings.

BHR Group envisages exploiting some of the project outcome in future R&D and consultancy projects in this field in line with its current activities. These are likely to be with test systems different to those used in PROFORM. Therefore, it is anticipated that the overall approach taken in running physical and numerical experiments and analysis of results that will be relevant to new projects.

With this effect BHR Group will make further applications for projects within FP7 in the areas identified during PROFORM and listed in Section (a) of this document. BHR Group is also in the process of launching an industrial club, DOMINO, which is an R& D project with no external funding other than the yearly subscription fees of member companies. The kick off meeting of this project was held on 18 October 2007 with representatives from 6 industrial companies. These comprise mainly companies that manufacture chemicals with one equipment manufacturer. Some of the PROFORM partners have been invited to join. There will be close collaboration with academia and research organisations, which may well include some of the academic partners of PROFORM.

c.2 Karlsruhe University Institute of Food Process Engineering

Karlsruhe University has incorporated several aspects of the project in the application of new research projects financed by state (AIF, DFG) and chemical and food industry. Within these projects, the incorporation of functional nanoparticles in emulsion type products will be investigated.

Experimental work carried out at Karlsruhe University at lab-scale has shown HPPF (High Pressure Post Feeding) configuration to be very promising. An industrial equipment manufacturer has been contacted to build a larger prototype. Patenting of this device was considered and extensive discussions were held with the in-house patent department. The recommendation from the patent department was to patent this device for a specific chemical product, i.e. patent the manufacturing process for a chemical product rather than the equipment design. This meant working with an industrial partner. The generic findings from PROFORM were tested with the specific products of several industrial companies during projects undertaken outside PROFORM. One of these has already led to a patent application, details of which are as follows:

Title: Verfahren zum Herstellen von nanopartikelbeladenen Polymerpartikeln

Number: 200700222 (priority) date: 23.03.2007

The HPPF- nozzle consists of a modified process control flow. This construction allows the feeding of the pre-dispersion straight after the outlet of the nozzle. Hence, no abrasive particles are passing the nozzle leading to a prolonged service life of the high pressure system.

The development of the HPPF-nozzle is a spin-off of the work carried out within the project PROFORM. The University of Karlsruhe restricts the number of patent applications. Therefore, the University decided to collaborate with an equipment manufacturer based on the HPPF idea. The patent application is therefore made by this company in relation to processes that involve reactive products.

Several researchers at undergraduate, postgraduate and postdoctoral level have been trained and gained further knowledge in the field of dispersing nanoparticles during the project PROFORM.

c.3 Bayer Technology Services GmbH (BTS)

Bayer is an integrated chemical and pharmaceuticals company with production, research and development facilities for polymers, base and fine chemicals, pharmaceuticals and agrochemicals. Bayer Technology Services is Bayer's central technology department providing engineering, product and process development services to all business units of the company as well as third parties.

Bayer Technology Services will undertake further in-house research to implement the generic recommendations and principles obtained from this project to the formulation, scale up and manufacture of their specific products in their health care, fine chemicals and agrochemicals businesses. The results related to the determination of solubility parameters in addition to those from break up studies carried out in conjunction with other partners have enhanced the knowledge base of BTS. These particularly relate to the evaluation and adaptation of simulation methods for practical purposes, taking a structured approach for technology-specific use of additives, improved understanding of deagglomeration, experimental protocols for efficiency comparison of different technologies and limits and potentials of different particle size characterisation methods for assessing deagglomeration success. It is anticipated that the tools developed within PROFORM will accelerate the formulation development of new products, facilitate knowledge transfer, form the basis for future expert system and will aid the targeted selection of suitable technology for future applications.

c.4 Loughborough University Department of Chemical Engineering

Loughborough University have incorporated some aspects of the findings from this project in the taught modules as listed in Section (d) below. Several researchers at undergraduate, postgraduate and postdoctoral level have been trained or gained further experience in the field who are anticipated to take up employment in Europe. Loughborough University expects to take part in other related research projects in the field.

c.5 Unilever UK Central Resources Ltd

Unilever, an Anglo-Dutch company, is one of the largest consumer goods companies in the world. Unilever UK Central Resources at Port Sunlight has vast experience in developing processes requiring intensive dispersion for home and personal care products.

Unilever will undertake further in-house research to implement the generic recommendations and principles obtained from this project to the formulation, scale up and manufacture of their specific products in their consumer care businesses. Unilever designs processes on the basis of mechanistic models supported by heuristics. The quality and performance of a product can be greatly enhanced by the design of process strategies and equipment, which assemble ingredients so as to provide the optimal functional and aesthetic profile. Chemical products are increasingly characterised by complex multiphase, non-Newtonian flows and a reliance on controlling the detail of intermediate structures and physical processes. The success of existing strategies can be seen directly in either the poor quality or sub optimal performance of the product or an uneconomic or poor sustainability profile of the manufacturing process. From this, it will be understood that the design of a manufacturing process must be concurrent with the design of the product. An important distinction between formulated products and ingredients is that whilst for the ingredient, the consequence of an inefficient process can be overcome by additional purification stages (albeit at some cost), for formulated products the product must be scrapped and disposed off.

Mechanistic models based on a fundamental understanding of how the interaction of process and material properties affect product performance can greatly enhance value and also the rate at which it is achieved. Firstly, they ensure much more effective use of ingredients by ensuring that they are in the optimal form within the product and secondly they ensure that these products can be brought to market quickly and without the usual long ramp up in production. In the first case, this capability is exploited through either improved product functionality which ensures our products are market leaders with improved performance and aesthetics which appeals to consumers or alternatively we maintain performance though using less material and obtain a benefit through reduced costs. In the second case, the challenge is to maintain performance of the product during scale-up, which necessarily requires work at several scales. The extent of this work and the range of testing scales can be drastically reduced where we are confident that we understand how the materials and process interact.

Dispersion of powders is increasingly important for product performance and new materials are constantly being launched. As a consequence, exploitation of the results of PROFORM will be directed to these new test systems. The challenges of scaling up products to full manufacturing scale are well known and need no further discussion here. However, it is worth mentioning here the challenges faced in the very early stages of product development. During the early stages there are several candidate materials and the challenge is to quickly narrow down to a lead candidate. Even at this early stage, evaluation can involve testing with consumers - an expensive and time consuming activity - and the products must be manufactured at a scale representative of manufacturing. The challenge is therefore to ensure that the product manufactured at this scale is consistent with that formulated at the bench scale, where selection is based on in-vitro tests. Failure to obtain the optimum dispersion at this scale can result in promising candidates performing poorly and so being rejected. The rigorous experimental protocols developed within this project are subtly different from that of other systems (e.g. emulsions) and are already being incorporated into existing innovation projects.

On a longer timescale the modelling capabilities developed within PROFORM will be exploited in the design of new processes and their scale up and in the design of improved process equipment and strategies. Of particular interest to Unilever are the full 3D simulations of rotor-stator devices where we see a synergy with the experimental protocol and models developed outside of project PROFORM - discussion with WUT have started along these lines and also with one of our equipment suppliers.

c.6 Birmingham University, School of Chemical Engineering

Birmingham University has incorporated some aspects of the findings from this project in the undergraduate taught modules partially as lectures and partially as labs. The experimental rigs and procedures developed in this project were used to carry out 4th year research projects in the area of particle technology and emulsification.

This project has also led to further collaboration with the group investigating the effect of magnetic field on nano-fluids. Birmingham University expects to take part in other related research projects in the field.

c.7 Warsaw University of Technology, Department of Chemical and Process Engineering

Warsaw University of Technology has incorporated several aspects of the findings from this project in the taught modules at undergraduate and postgraduate level (lectures, practicals, training of PhD students and young postdoctoral researchers). Students and researchers are trained to take up employment in Poland and other European countries. Warsaw University of Technology is ready to participate in new projects in the field. These include two national projects, two new FP7 proposals and consultancy.

c.8 Poznan University of Technology, Faculty of Chemical Technology

The group at Poznan University of Technology lead by Prof Adam Voelkel is involved in the application of chromatographic and non-chromatographic methods for characterising of surface layers and description of surface phenomena.

The acquired knowledge of this research group will be further used in the scientific activity in two or three FP7 projects (at proposal stage) as well as consultancy for individual clients. Several researchers at undergraduate, postgraduate and postdoctoral level have been trained or gained further experience in the field during the course of PROFORM.

c.9 Rockfield Software Ltd

Based on the developments undertaken within the PROFORM project, Rockfield Software Ltd is planning the following commercial activities: -

- Software licensing - It is anticipated that the enhancement of the capabilities of Rockfield's commercial software, ELFEN, in the areas of modelling of complex behaviour of particles on the nano, meso, and macro levels will reinforce its leading position within the Finite/Discrete Element software market.

- Consultancy services - The enhanced knowledge base, developed by Rockfield within this project, in the areas of algorithmic development, modelling and simulation of nano-particle interaction and agglomeration will be used widely to initiate and undertake future projects. Models validated in co-operation with industrial partners provide a solid base for future commercial consultancy projects for relevant industries. These will be initially short duration consultancy projects, which will apply the expertise gained to specific problems.

c.10 C3M

The numerical framework developed by C3M will be first offered as an analysis service and then extended to customised software packages. In these activities collaboration with RSL, WUT and other PROFORM partners is envisaged.

The numerical approaches developed by C3M can be applied for decision support in designing the following parameters of stirred media milling technology: mill type, geometry, grinding media size, density, elasticity and filling ratio. These parameters must be carefully harmonised to achieve multiplicative synergetic effects that can lead to the successful production of nanoparticle dispersions. The technical and economic potential for use and exploitation has been identified in many areas of chemical, pharmaceutical, cosmetics, food\agro, pigments, paint, lacquer, plastics, ceramics and electronics where several nano product properties can be improved by optimisation of stirred media milling technology. C3M is in the process of informing these market segments about the new possibilities generated by PROFORM project. A presentation was given to the potential industrial end-users (manufacturers of process equipment, measuring devices, grinding beads and nanoproducts) during the "Symposium on Grinding and Dispersing in Stirred Media Mills" which was held in Braunschweig, Germany in October 2007. Next presentation to industrial audience will be made during the event titled "Nano-Engineered Inks and Pigments 2008 Vienna, Austria. Individual discussions with interested Slovenian companies are scheduled for March 2008.

In addition to the industrial exploitation of knowledge and software developed in the PROFORM project C3M is investigating possibilities to perform further research in this area in the scope of 7th Framework programme, Eureka or other programmes on European level.

d) Report on engaging with the public

- It has mainly been the Project Co-ordinator's responsibility to publicise this project. A number of oral and poster presentations have been made and articles published in professional magazines and a dedicated web site has been created. These are listed below.

In addition several partners have included information about PROFORM on their web sites and displayed posters.

PROFORM- Publicity Record

1. BHR Group e-news, December 2004, sent to 6000 people on BHR Group's database.
2. Information on BHR Group web page.
3. Poster at Karlsruhe University Department of Food Process Engineering. December 2004 onwards
4. Information on Karlsruhe University Department of Food Process Engineering web page.
5. Information on the web page of the Technical University of Poznan.
6. Information on the web page of the Technical University of Warsaw.
7. Press release sent to 94 addresses (mostly magazines, 8 e-news, 2 news agencies), 2005.
8. PROFORM website created, 2005, www. proform-fp6.com
9. News appeared at the web site of The Chemical Engineer (Institution of Chemical Engineer's publication) and in the March issue of The Chemical Engineer, 2005.
10. News appeared in the March 2005 issue of Chemical Engineering USA
11. E-news appeared in South Pacific, 2005
12. E-news on Nanotechnology Now, 2005.
13. E-news on Cordis Wire, 2005.
14. E-news on Nano Tsunami, 2005.
15. E-news on Azonano.com, 2005.
16. Meeting held with Dr David Parker of Faraday Partnership to explore future collaboration possibilities. Dr David Parker gave a presentation to PROFORM partners during the 6th Project Partners' Meeting at Loughborough November 2006.
17. Presentations were given to FMP (Fluid Mixing Processes consortium run by BHR Group) members based on published work. FMP is an industrial consortium that consists of companies from chemicals and related (pharmaceuticals, personal care) industries, equipment manufacturers and software houses.
18. Project Co-ordinator, Dr Gűl Özcan-Taşkin, gave an invited lecture during an event organised by the Institute of Nanotechnology "Nano-particles for European Industry- Manufacture, Scale-up Stabilization, Characterization and Toxicology" 2-3 May 2006, London, UK
19. The Project Co-ordinator prepared an article titled "Transforming Nanoscience into Products" which was published in the May\June 2007 issue of the professional magazine, Process Engineering.
20. C3M organised a lecture for Slovenian researchers and industrial process designers, Ljubljana, December 14, 2007. This was given by Prof. Jerzy Bałdyga on "Numerical simulation of deagglomeration of nano-particle clusters in high shear devices".

- Most partners of PROFORM have published some aspects of their research either in the form of papers in recognised journals or poster and oral presentations during conferences, some of which were accompanied by a published paper, in accordance with 6.2 in DoW. As some of these have authors from more than one partner organisation, a list of publications for the whole consortium is provided below rather than one per contractor to avoid duplication. Several other publications are envisaged in the future in addition to business-to-business marketing activities.

Publications from PROFORM

Voelkel, A. (2005) "Inverse gas chromatography- a useful tool in the examination of surface and bulk properties" by. 19th ECIS Conference, Norway, September 2005.

Adamska, K.; A. Voelkel (2005) "Hansen solubility parameters for polyethylene glycols by inverse gas chromatography" 19th ECIS Conference, Norway, September 2005.

Őzcan-Taşkin, N.G.; Eagles, W.P.; Clements, P.J.; Xie, L.; and Rielly, C.D. (2006) "Suspension of nanoparticle agglomerates in a liquid" 12th European Conference on Mixing, 2006, Bologna Italy

Xie, L.; Rielly, C.D.; Eagles, W.P.; Őzcan-Taşkin, N.G. (2006) “De-agglomeration of pre-wetted nano-particles using mixed flow and high shear impellers”. 12th European Conference on Mixing, June 2006, Bologna Italy

Sauter, C.; Pohl M. and Schuchmann, H.P. (2006) “Ultrasound for dispersing nano-particles” 12th European Conference on Mixing, June 2006, Bologna Italy

Baldyga, J.; Krasiński, A. and Orchiuch, W. (2006) “Rheological effects in concentrated aggregated suspensions- application of population balance modelling”. 12th European Conference on Mixing, June 2006, Bologna Italy

Sauter, C.; Pohl M. and Schuchmann, H. P. “Preparation of stable nano-dispersions” 5th World Congress on Particle Technology 23 -27 April 2006, Orlando (USA)

Sauter, C.; Pohl M. and Schuchmann, H. P. “Herstellung nanoskalliger dispersionen” 3rd Symposium “Produktgestaltung in der Partikeltechnologie” 22/23 Juni 2006, Pfinztal (Germany)

Baldyga, J.; Krasiński, A. and Orchiuch, W. (2006) “Reologia stężonych, zagregowanych zawiesin nanoczastek- wykorzystanie bilansu populacki” IV Polish Conference on Mechanical Operations in Process Engineering. Poland, June 2006.

Baldyga, J.; Krasiński, A. and Orchiuch, W. (2006) “Reologia stężonych, zagregowanych zawiesin nanoczastek- wykorzystanie bilansu populacki” Inzynieria I Aparatura Chemiczna, 4s/2006, 8-10.

Olejnik-Szymańska K. and Voelkel A. (2006) “Stability of modified nanoparticles of fumed silica dispersed in water and organic solvents” 1st European Chemistry Congress, 27-31 August 2006, Budapest, Hungary.

Adamska, K. and Voelkel, A. (2006) “Methods of Characterization of Pigments – Three Dimensional Solubility Parameter” PHOPOC, Third European Students Conference on Physical, Organic and Polymer Chemistry; 18- 20 September, Wien, Austria.

Batko, K. and Voelkel, A. (2006) “Determination of the Hamaker Constant for the Iron Oxides” PHOPOC, Third European Students Conference on Physical, Organic and Polymer Chemistry, 18-20 September, Wien, Austria.

Olejnik-Szymańska, K. and Voelkel A. (2006) “The influence of different surfactants and their different concentration on stability of nanomaterials water dispersions” PHOPOC, Third European Students Conference on Physical, Organic and Polymer Chemistry, 18- 20 September, Wien, Austria.

Padron, G. A.; Eagles, W.P.; Őzcan-Taşkin, N.G.; Orciuch, W.; Makowski, L.; Baldyga, J. (2006) “Break up of nanoparticle clusters using an in-line rotor-stator- Experimental results” AIChE Annual Meeting, November 2006, San Francisco, USA

Orciuch, W.; Krasinski, A.; Baldyga, J.; Eagles, W.E. and Őzcan-Taşkin, N.G. (2006) “Break up of nanoparticle clusters using an in-line rotor-stator- Validated CFD results” AIChE Annual Meeting, November 2006, San Francisco, USA

Ding, P. and Pacek, A. (2006) “Aggregate size/structure and rheological properties of nano-sized goethite aqueous suspensions” AIChE Annual Meeting, November 2006, San Francisco, USA.

K. Adamska, A. Voelkel, (2006) "Hansen solubility parameter for polyethylene glycols by inverse gas chromatography", J. Chromatogr. A, 1132, p: 260-267.

Sauter C.; Pohl M.; Schuchmann H.P. (2006); “Herstellung Nanoskaliger Dispersionen” Symposium “produktgestaltung in der partikeltechnologie” Jun 2006

Pacek, A. W.; Ding P.; Utomo, A.T. (2007) “Effect of energy density, pH and temperature on deaggregation in nano-particles-water suspensions in high shear mixer” Powder Technology, 173; p: 203- 210.

Ding P.; Pacek, A. W. (2007) “Deagglomeration of goethite nano-particles using ultrasonic communition device" Powder Technology, in press.

Xie, L.; Rielly, C.D.; Eagles, W.P.; Őzcan-Taşkin, N.G. (2007) “Dispersion of nanoparticle clusters using mixed flow and high shear impellers in stirred tanks” Trans. IchemE, Part A, Chemical Engineering Research and design, 85 (A5), p: 676-684.

Padron, G. A.; Eagles, W.P.; Őzcan-Taşkin, N.G.; McLeod, G. and Xie, L. (2007) “Effect of particle properties on the break up of nanoparticle clusters using an in-line rotor-stator” 1st International Conference on Industrial Processes for Nano and Micro Products, 3-4 April 2007, London, UK.

Padron, G. A.; Eagles, W.P.; Őzcan-Taşkin, N.G.; McLeod, G. and Xie, L. (2008) “Effect of particle properties on the break up of nanoparticle clusters using an in-line rotor-stator”. Accepted for publication in the Journal of Dispersion Science and Technology.

Baldyga, J.; Orciuch, W.; Makowski, L.; Krasiński, A.; Malski-Brodzicki, M. and Malik, K. (2007) “Shear flow of aggregated nano-suspensions- fundamentals and model formulation” 1st International Conference on Industrial Processes for Nano and Micro Products, 3-4 April 2007, London, UK.

Baldyga, J.; Orciuch, W.; Makowski, L.; Krasiński, A.; Malski-Brodzicki, M. and Malik, K. (2008) “Shear flow of aggregated nano-suspensions- fundamentals and model formulation” Accepted for publication in the Journal of Dispersion Science and Technology

Ding, P. and Pacek, A. (2007) “De-agglomeration of silica nano-particles in presence of surfactants” 1st International Conference on Industrial Processes for Nano and Micro Products, 3-4 April 2007, London, UK.

Ding, P. and Pacek, A. (2007) “De-agglomeration of silica nano-particles in presence of surfactants” Accepted for publication in the Journal of Dispersion Science and Technology

Xie, L.; Rielly, C.D.; and Őzcan-Taşkin, N.G. (2007) “Break-up of nanoparticle agglomerates by hydrodynamically limited processes” 1st International Conference on Industrial Processes for Nano and Micro Products, 3-4 April 2007, London, UK.

Xie, L.; Rielly, C.D.; and Őzcan-Taşkin, N.G. (2007) “Break-up of nanoparticle agglomerates by hydrodynamically limited processes”, Accepted for publication in the Journal of Dispersion Science and Technology

Baldyga, J.; Orciuch, W.; Makowski, L.; Malski-Brodzicki, M. and Malik, K. (2007) “Break-up of nano-particle clusters- process modelling” 1st International Conference on Industrial Processes for Nano and Micro Products, 3-4 April 2007, London, UK.

Baldyga, J.; Orciuch, W.; Makowski, L.; Malski-Brodzicki, M. and Malik, K. (2007) “Break-up of nano-particle clusters- process modelling” Accepted for publication in the Journal of Dispersion Science and Technology

Adamska K.; Batko K.; Olejnik-Szymańska K.; Voelkel A. (2007) “Characterization of Surface Layer of modified Nanomaterials and Properties of their Dispersions” ” in “Surfactants and dispersed system in theory and practice – SURUZ”, Palmapress, 2007, pp. 243-246

Olejnik-Szymanska, K.; Voelkel, A. (2007) “Preselective Evaluation Of Nanomaterials Stability In Dispersions Systems” in “Surfactants and dispersed system in theory and practice - SURUZ”, Palmapress, 2007, pp. 469-472.

Őzcan-Taşkin, G. (2007) „Transforming nano science into products”, May/June 2007 issue of Process Engineering

Sauter C.; Schuchmann P. (2007) “Alternative Dispersing Systems: Influence of processing on the size distribution and stability of nano-particles”; Symposium "Grinding and Dispersing in stirred media mills" at Braunschweig October 2007

Sauter C.; Schuchmann P. (2007) “High pressure for dispersing and de-agglomerating nanoparticles in aqueous solutions Grinding and Dispersing in stirred media mills" at Braunschweig October 2007

Tomaž Rodič (2007) “3D Multi-body and Multi-scale Model of De-agglomeration in Stirred Media Mills; Symposium "Grinding and Dispersing in stirred media mills" at Braunschweig October 2007

Bałdyga J.; Orciuch W.; Makowski L.; Ozcan-Taskin G.; Eagles W.; Padron G. (2007) Break up of nano-particle agglomerates I a rotor-stator device” 18th Physical Metallurgy and Material science conference-Advanced &Technologies June 2007 Poland

Bałdyga J.; Orciuch W.; Makowski L.; Malski-Brodzicki M; Malik K. (2007) “Break up of Nano-Narticle clusters in high-shear devices”, 6th European Congress of Chemical Engineering, 16-21 September 2007, Copenhagen, Denmark.

Bałdyga J.; Orciuch W.; Makowski L.; Malski-Brodzicki M; Malik K. (2007) “Break up of nano-particle clusters in a high pressure device-process modelling”; 19th Polish Conference of Chemical and Process Engineering, September 2007

Bałdyga J.; Orciuch W.; Makowski L.; Malski-Brodzicki M; Malik K. (2007) “Geometry and break-up of cluster-fractal agglomerates”; 19th Polish conference of Chemical and Process Engineering, September 2007

Bałdyga J.; Orciuch W.; Makowski L.; Malski-Brodzicki M; Malik K. (2007) “Shear flow and formulation of aggregated nano-suspensions- model formulation and application to the rotor-stator system” 19th Polish conference of Chemical and Process Engineering, September 2007

Baldyga J.; Orciuch W.; Makowski L.; Ozcan-Taskin G.; Eagles W.; Padron G. (2007) “Break up of nanoparticle agglomerates in a rotor-stator device” Inzynieria Materialowa, 3-4/2007, p: 236- 241.

Baldyga J.; Orciuch W.; Makowski L.; Ozcan-Taskin G.; Eagles W.; Padron G. (2007) “Break up of nanoparticle agglomerates in a rotor-stator device” 18th Physical Metallurgy and Material Science conference- Advanced Materials and technologies, 18- 21 June 2007, Warsaw Poland.

Bałdyga J.; Orciuch W.; Makowski L.; Malski-Brodzicki M; Malik K. (2007) “Break-up of nano-particle clusters in a high pressure device- process modelling” Inżynieria Chemiczna i Procesowa, 28, 683-693.

Bałdyga J.; Orciuch W.; Makowski L.; Malski-Brodzicki M; Malik K. (2007) “Geometry and break-up of cluster-fractal agglomerates” accepted for publication in Inżynieria Chemiczna I Procesowa

Bałdyga J.; Orciuch W.; Makowski L.; Malski-Brodzicki M; Malik K. (2007) “Shear flow and formulation of aggregated nano-suspensions- model formulation and application to the rotor-stator system” accepted for publication in Inżynieria Chemiczna I Procesowa.

Bałdyga J.; Orciuch W.; Makowski L.; Malski-Brodzicki M; Malik K. (2007) "Break-up of nanoparticle clusters in high shear devices" *Chem. Eng. Process.*, 46, 851−861

Bałdyga J.; Orciuch W.; Makowski L.; Malski-Brodzicki M; Malik K. (2007) "Break-up of nanoparticle clusters in high shear devices" 6th European Congress of Chemical Engineering.

Bałdyga J., Orciuch W. and Makowski Ł. (2007) "Breakage and aggregation in nano-suspensions - modelling study", abstract in the proceedings of the 34th International Conference of SSCHE, 21 - 25 May 2007, Tatranské Matliare, Slovakia

Bałdyga J., Orciuch W., Makowski Ł, Henczka M., Malski-Brodzicki M. and Malik K. (2007) "CFD modelling of nano-particle clusters break-up in high-shear devices", presented on the NAMF Mixing XXI Conference, 17 - 22 June 2007, Park City, Utah, USA

K. Batko, A. Voelkel, (2007) "Inverse gas chromatography as a tool for investigation of nanomaterials", J. Colloid Interface Science, 315 (2007) 768-771

Ozcan-Taskin G.; Padron G.; Ding, P.; Pacek A.; Xie L.; Rielly C. (2008) "Processing of red and yellow iron oxide nanoparticles" Nano-engineered Inks and Pigments 2008 Vienna, Austria

Tomaž Rodič (2008) "M5 Numerical Modeling of Nano-milling Processes",Nano-engineered Inks and Pigments 2008 Vienna, Austria

Tomaž Rodič, Janez Langus and Martin Dutko, "M5 Multiscale aspects of stirred media milling technology for production of nanoparticles", ECCOMAS Thematic Conference on Multi-scale Computational Methods for Solids and Fluids, Ibrahimbegovic, F. Dias, H. Matthies, P. Wriggers (eds.), Cachan,France, November 28–30, 2007

Baldyga, J.; Orciuch, W.; Makowski, L.; Malik, K.; Őzcan-Taşkin, G.; Eagles, W.; Padron, G. (2008) "Dispersion of nanoparticles in a rotor-stator mixer" Accepted for publication in Nauman special issue of Industrial & Engineering Chemistry Research, scheduled for June 2008.

Ding, P.; Pacek A. (2008) "Effect of pH on de-agglomeration and rheology/morphology of aqueous suspensions of goethite nano-powder", Accepted for Journal of Colloids and Interface Science

- Several societal benefits related to this project can be stated:
  - ➢ The project has enabled the training of undergraduate and postgraduate students and postdoctoral researchers in the field who are expected to take up employment in the European industry.
    - 4 undergraduate, 3 postgraduate students and 1 postdoctoral researcher have been trained or gained further experience in the field at Loughborough University while working on PROFORM (half of these were female researchers)
    - 3 undergraduate students, 1 postgraduate student and a postdoctoral researcher gained additional experience in the field of wet processing of nano-powders at Birmingham University whilst working on PROFORM (two of these are female researchers).
    - 3 undergraduate, 4 postgraduate students and 1 postdoctoral researcher have been trained at Poznan University of Technology and gained scientific experience during realisation of PROFORM (all female researchers).
    - 5 undergraduate and 1 postgraduate students, (of whom two are female students), have been specifically trained on the dispersion techniques of nanoparticles and gained scientific experience at Karlsruhe University whilst working on PROFORM.
    - 3 undergraduate, 2 postgraduate students and 1 postdoctoral researcher have been trained at Warsaw University of Technology and gained scientific experience in numerical and experimental flow modelling\ measurements in relation to product formulation.

One of the postdoctoral researchers in this project (Dr L. Xie at Loughborough) has already been employed in another partner organisation, Unilever.

- Some aspects of published material from the project have been included in undergraduate, postgraduate and continuing education courses. The taught modules which have or will include information derived from the PROFORM project are:

  - Batch Mixing of Fluids and Particles- Loughborough University
  - Concepts of Chemical Product Design- Loughborough University
  - Soft-solid and Semi-solid Products-Loughborough University
  - Application of chromatographic techniques in chemical technology – Poznan University of Technology
  - Fluid Mechanics- undergraduate lecture at Warsaw University of Technology
  - Rheology of fluids of complex structure- postgraduate lecture at Warsaw University of Technology
  - Polymer processing- specialisation module at Warsaw University of Technology

APPENDIX I

Deliverables list

Del. no.	Deliverable name
D1	Experimental techniques and methodologies for particle characterisation
D2	Software architectural, functional and design specifications
D3	Brief report on the experimental plan and standardised experimental protocols
D4	1st annual report
D5	Data on physical properties of particles
D6	Key parameters that affect performance of stirred tanks, jet dispersers and ultrasound devices for (i) wetting / incorporation and (ii) de-agglomeration.
D7	Relationship between particle/aggregate size, strength and chemical composition of suspensions and process conditions
D8	Experimental techniques for determining rheology of suspensions
D9	Models for rheological properties of suspensions; laminar and turbulent flow conditions
D10	Mid term review report
D11	Identification of chemically limited systems
D12	2nd annual report
D13	Optimum operating conditions for different equipment for (i) wetting / incorporation and (ii) de-agglomeration.
D14	Surfactant selection tools for nano dispersions
D15	Data on rheological characterisation of suspensions
D16	Assessment of equipment characteristics
D17	Comparative data for reference suspensions in different devices
D18	Methods for determining solubility parameters
D19	Implementation of mechanistic models for all sub-processes
D20	Equipment review based on experimental characterisation for different systems
D21	Relationship between mixing conditions and the kinetics and effectiveness of different mixing procedures
D22	Models of particle-particle interaction
D23	Mechanistic models describing wetting, incorporation and dispersion of particles
D24	Mechanical effects on de-agglomeration
D25	Models of formation of primary aggregates
D26	Validation of simulations of flows and dispersion processes
D27	Design Guide for the incorporation and dispersion of nano particles
D28	Initial design of software based formulation process adviser
D29	Conference papers and articles
D30	Final report on findings, conclusions and recommendations with an executive analysis