	EUROPEAN COMMISSION RESEARCH AND INNOVATION DG	Final Report

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Project Acronym: COOPOL

Project Full Name: Control and Real-Time Optimisation of Intensive Polymerisation Processes

Final Report

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Final Report

PROJECT FINAL REPORT

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Final Report

4.1 Final publishable summary report

4.1.1 Executive Summary

The Coopol project was made up of an interdisciplinary consortium of 8 European organisations consisting of the Universities of Warwick (Warwick), Hamburg (UHAM), Aachen (RWTH), Cambridge (UCAM), the Institute of Chemical Technology Prague (VSCHT), Knowledge Transfer Network (KTN), Cybernetica AS, and BASF. The project's vision was to develop new methods and tools for modelling and control, based on real-time sensing to facilitate the development of a new paradigm of processes: intensive, low impact, sustainable chemical technologies. The project was carried out over a period of 36 months from 1 March 2012 to the 28 February 2015. The project was divided into 8 work packages, with a number of tasks under each.

WP2 – A smart-scale semi-batch reactor was built and a smart-scale continuous reactor improved with analytical methods established and validated. The project successfully demonstrated that continuous emulsion polymerisation can be stable when operated for a long period of time in a continuous smart-scale reactor. UHAM achieved a 62-hour long continuous emulsion polymerisation with 30 % solid content. Jointly, UHAM and RWTH successfully ran experiments for different reaction conditions in continuous and semi-batch mode. The model predicted closed-loop controller performed well for both types of processes.

Activities undertaken in **WP3** significantly advanced the use of novel sensing techniques, such as Raman spectroscopy, for monitoring emulsion polymerisation reactions. Considerable work was achieved in the development and implementation of software tools to analyse and extract useful information from measurement data. The observability analysis carried out for semi-batch processes reveals that, on the one hand there is a need for further development of sensors for online measurement of molecular property, and on the other hand, that there is a need to develop models that correlate polymer properties to existing measurement techniques.

WP4 focused on model-based predictive control and optimisation of polymerisation reactors in real time. A good performance of the employed mathematical models, i.e. their robustness, high speed and accuracy of predictions, was crucial for the successful implementation of control systems and the final demonstration of COOPOL's goals. To this end, WP4 played a central role in the project.

WP5 developed new technology for dynamic real-time optimisation and nonlinear model predictive control of polymerisation reactors has been developed. The technology has a short time to market. It is applicable for batch, semi-batch and continuous tubular reactors, but is most developed for the semi-batch case. The technology has been tested in simulations and demonstrated at pilot plant scale at a BASF plant in Ludwigshafen.

WP6 summarised the results of the COOPOL project by integrating and demonstrating the performance of the designed systems on a pilot plant. The demonstration was carried out at BASF facilities (Ludwigshafen), allowing a direct comparison between existing and developed control models. By implementing the closed loop model predictive control (MPC) system, which is built upon outcomes from WP2, WP3, WP4 and WP5. Judged by the above mentioned achievements, the COOPOL project is an excellent example of successful collaboration between European chemical industry and academia.

4.1.2 Summary description of project context and objectives

Transition of processing industries towards a more sustainable model of manufacturing is one of key priority topics for European Research Area. This transition requires adoption of novel reactor technologies, greener reactions and the increase in the use of intelligent systems in processing industries. The latter means improving processes through use of real-time information and ability to affect processes in real time. The long-term vision of COOPOL was to develop new methods and tools for modelling and control, based on real-time sensing, which will facilitate the development of a new paradigm of processes: intensive, low-impact, sustainable chemical technologies. The COOPOL consortium is focusing on one of the key areas of interest to European Chemical Industries, namely the polymer industry. Within the chemicals sector polymer production plays a significant role, with European market share of 25% and providing employment to 1.6 million people within EU27.

The key challenge for maintaining the competitiveness of European Chemical and Process Industries is sustainable production.[1] This has been highlighted by the European Technology Platform for Sustainable Chemistry, SusChem, and developed into specific calls for innovation in chemical production within European Commission's NMP programme. Within the challenge of sustainable production, the topic of Reaction and Process Design is one of the priority research areas of SusChem, within which *theoretical modelling of complex systems, data mining and optimum selection, integral analytics* and *process systems engineering* are highlighted as research priorities.[2]

These priority research topics have been addressed in COOPOL and are key *enabling technologies* for a wide sector of process industries, not only the Chemical Industry.

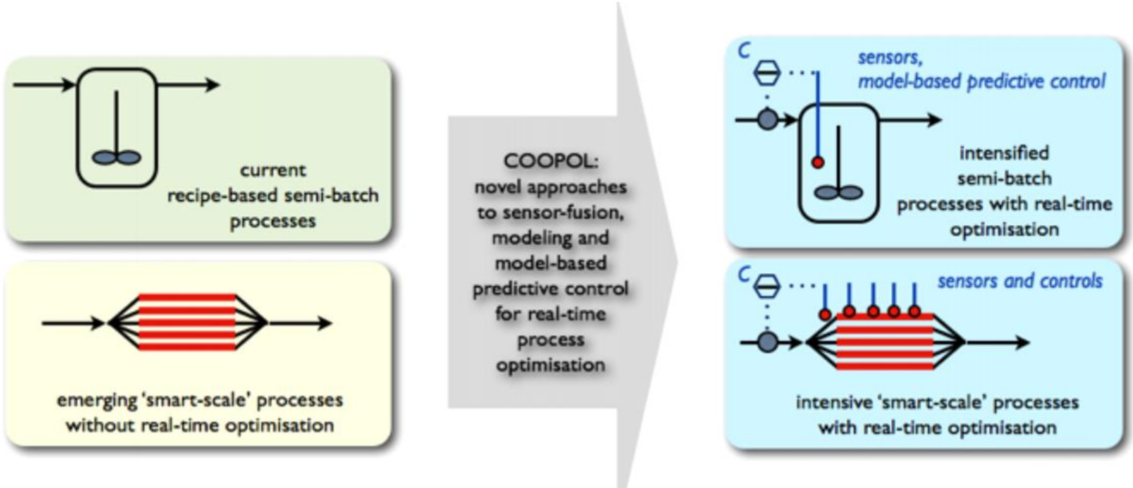
Many polymer products are manufactured using batch and semi-batch reactors. In most cases the process parameters, such as temperature profile, feeds, etc. follow a specific time schedule which has been fixed after an expensive period of product and process development. This tight recipe schedule is sensitive against disturbances e.g., unexpected variation in operating conditions, variation in feed purity etc., which inevitably leads to variations in polymer structure and to inter-batch variability and off-spec products. Furthermore, the use of empirically determined recipes with fixed-time controls does not allow intensification of the process which requires time-varying feeds and reactor temperature to run the reaction faster and hence closer to its limits, and also to switching from a semi-batch to other reactor or process types.

COOPOL aims to address the complex issues of real-time process control, based on advanced models and on-line sensors, and to develop a generic basis for widely applicable sustainable intensified processes. Ultimately, COOPOL's intention was to develop a new process control approach, linking molecular level information and understanding of the reaction chemistry with real-time sensing, rigorous modelling based on first principles, subsequent model reduction and non-linear model-predictive control (NMPC) with economic objectives, known as dynamic real-time optimisation

[1] A European Technology Platform for Sustainable Chemistry (2006), Technology Platform launch document. Downloaded from www.suschem.org.

[2] Innovating for a better future. SusChem Strategic Research Agenda 2005. www.suschem.org.

(DRTO). Our objective is to achieve, through robust real-time optimisation-based control and sensing methodologies and their application, the intensification of (i) the existing processes, and (ii) the development of novel intensive 'smart-scale' processes. The approach of COOPOL delivers significant advance in the state-of-the-art in model-based predictive control and at the same time produces tangible and exploitable benefits for the European industry in the short, medium and long-term.
This concept is shown in Figure 1.1.



Our specific science and technology objectives were:

- to develop intensive 'smart-scale' reactor technology with real-time feed-back control for emulsion polymerisation applications,
- to develop a novel sensor-fusion approach for off-line and on-line inference of process parameters and state information in the polymerisation processes,
- to develop advanced models of polymerisation processes, utilising new types of sensors and the model based experimental analysis methodology accounting for emulsion stability and rheology,
- to develop realistic optimisation models and economic objectives, and,
- to explicitly consider uncertainty in the optimisation problem formulation for increased robustness.

The scientific and technological progress of COOPOL led to the demonstration of the developed optimisation and control methodology in the intensification of industrial semi-batch polymerisation processes by the main end-user partner (BASF). The key enabling technologies of COOPOL, namely sensors, reactor technology, modelling and control were developed in close collaboration between academic and industrial partners. An integrated work programme, closely linking fundamental research with industrial focus and implementation, led to rapid transfer of research into innovation.

The new processes were benchmarked against current industrial processes, including technological, economic, risk and environmental factors. This formed the basis for evaluation of research, new tools and processes, and led to wider implementation of the COOPOL tools, facilitated by a comprehensive plan of implementation and dissemination activities. The availability of evaluation and benchmarking data was essential to the success of COOPOL dissemination and outreach programmes, promoting the wider use and adoption of advanced modelling and control tools to achieve better product quality and process efficiency, and to promote the role of advanced technologies and sustainable manufacturing in society among young scientists and the general public.

4.1.3 Description of main S & T results/foregrounds

The COOPOL collaborative research project involved 8 European partners organised around 8 work packages. Each work package was led by a specific partner with the involvement of other partners as required.

WP	WP NAME	Lead	Contributors
1	Coordination and Management	**WARWICK**	Warwick
2	Smart-scale and Intensified Semi-batch Polymerisation	**UHAM**	Warwick, CYB, BASF, UCAM
3	Observation: from sensor tip to state estimates	**RWTH**	Warwick, UHAM, RWTH, VSCHT, CYB, BASF
4	Modelling	**VSCHT**	Warwick, UHAM, RWTH, VSCHT, CYB, BASF
5	Operation, Control and Evaluation	**CYB**	Warwick, RWTH, VSCHT, CYB, BASF, UCAM
6	Implementation and Demonstration	**BASF**	CYB, BASF
7	Dissemination	**KTN/CIKTN**	ALL
8	Scientific Coordination	**WARWICK**	Warwick

4.1.3.1 Project coordination and Management

The management team, based at the University of Warwick, was responsible for supervising and monitoring the progress of the research activities (scientific and technical) and their correspondence with the DoW and finding resolutions to critical issues. A number of mechanisms were developed in the Implementation Section of DoW, which were added to during the life of the project to help maintain a coherent and efficient project management over the entire lifespan of COOPOL.

COOPOL project coordinator main responsibilities were

- Managing COOPOL's legal and contractual obligations
- Organising and following-up of major meetings among the partners
- Coordinating periodic and final reports delivered to the European Commission, which involved collating, proof-reading, and editing contributions from partners
- Scientific review of all project deliverables and periodic reports submitted
- Submitting and uploading reports to the European Commission Portal
- Reviewing and submitting costs statements prepared and duly certified by Contractors
- Establishing and managing communication procedures and tools for facilitating exchange among the partners
- Maintaining contact with partners and tracking official communications
- Developing and managing a secure collaborative web-site for the project to be used internally for communication and information/document exchange
- Supporting partners with various procedures requested by the European Commission

In order to assess the effectiveness of the management team and the methods of communication developed during this project, a short questionnaire was sent out to Coopol work package leaders.

The questions were formulated to gain feedback on the following themes: management approach, communication channels, administration, collaboration, knowledge exchange.

Overall WP leaders considered that the consortium was successful in accomplishing all its research goals. One partner mentioned that two goals still needed to be achieved, namely robust real-time optimisation and, online estimation methods of polymer product properties. The question was whether or not the management made a difference to the consortium achieving its goals, and partners believed that it was critical. One partner stated that "good management ensured that issues that arose during the project were dealt with before they became problems", and another partner that "[…] management throughout the project remained direct, focused to the point as well as assertive in order to achieve project goals (milestones) within deadlines".

Largely, partners were satisfied with the leadership. Having a robust and well-written project proposal was named as being the main foundation in establishing the consortium's positive working practices. Also, key individuals from the industry ensured the project remained orientated in producing excellent scientific results whilst also being relevant to industry, as the following comment illustrates: "the project also benefited from a strong industrial focus, represented by the active involvement of BASF's employees. Their clear vision on where the project was heading, both during the proposal and execution phases, made it easier to plan, manage and execute the scientific work". Cybernetica's expertise in implementation of on-line control and optimisation was regarded as essential and exceptional.

Also mentioned, was the important input received from KTN (part of Innovate UK an executive non-departmental public body, sponsored by the UK's Department for Business, Innovation & Skills) who led on dissemination with two major events, implementation on specific platforms, namely the project's website and online collaboration tool, as well as management of the exploitation strategy.
In terms of the communication tools used by the consortium, the critical timeline (excel document) was considered extremely useful, the only remark was that it would have been practical to have it posted on COOPOL's online collaboration platform.

By far, partners deemed that the most effective tool was face-to-face consortium meetings, as demonstrated by the following comments: "consortium meetings helped to check the progress of the project, provided feedback to young researchers. The discussion at these meetings was never just formal but always a heated but friendly debate about challenging problems of common interest"; "such physical meetings ensured that consortium partners understood each other's point of view clearly and addressed problems by brainstorming or experience"; "the consortium meetings provided a platform for researchers to present their contributions to the project […]"; "meetings were critical; without them the project could have not been successful". In hindsight, the frequency of these meetings could have been increased as well as the length, two-day consortium meetings were more productive than one day.

Opinions were divided on the WP leaders quarterly Adobe teleconferences, bandwidth issues made it difficult for some, whilst others, on the other hand, found these very useful. Telephone conversations and emails were seen as insufficient to discuss research concerns and explore solutions. A transfer of leadership during the project was seen as causing a bit of friction initially, but without any detrimental effect on the project, as this was dealt with rapidly.

The online collaboration platform was mostly seen as a repository; very valuable to access all of the project's documentation (minutes of meetings, deliverables and milestones submitted, partner's scientific dissemination outputs, etc.), but inflexible; there is no timeline or dependency feature and the structure is fixed. The EC participant portal, was viewed unfavourably by most partners; it is not user-friendly, difficult to upload information, text is hidden in non-expandable text boxes, etc. Timesheets were seen by many as a "controlling tool" time spent by partners on project "should be documented in the deliverables".

Communication with the coordinating partner was viewed by all as efficient and timely, having dedicated and competent project administrators was perceived as the main reason as one partner explains "highly skilled administrators has been a pleasure to work with, and an important factor in the successful execution of such a large and complicated project". The extensive amount of administrative and clerical work required on EC projects can be hindering. One of the questions asked was what could the administrators/coordinator have done differently to improve this? The answer was mainly nothing, as one partner mentions "[…] a lot of the administrative work was hidden and I am glad because of that".

On the whole the feedback received regarding management and communication, between partners, between working groups, and between the coordinator and partners and working groups, was very positive. In the spirit of the collaborative principles which guided the consortium throughout the project, and the value attributed to young researchers, the project leaders emphasised the importance of COOPOL's young researchers' contributions in achieving project objectives. They were seen as key players at the epicentre of all of COOPOL's research and development achievements, without whom a project of this breadth would have not been possible.

4.1.3.2 Smart-scale and Intensified Semi-batch Polymerisation

WP2 was divided into 3 main objectives:

- generation of experimental data for the model development and validation for WP3-5
- proof of long-term viability/stability of the \`smart-scale´ polymerisation process
- first experiments towards closed-loop control of \`smart scale´ polymerisation reactions run with RWTH in semi-batch and continuous reactor

The project wanted to demonstrate that continuous emulsion polymerisation can be stable operated for a longer time in a continuous smart-scale reactor. The results were presented at the COOPOL symposium in January 2015, it showed that the model could predict closed-loop control and that the demonstration could be successfully realised. For each type of process – batch, semi-batch and smart-scale – different polymer characteristics such as molecular mass (M_w and M_n), monomer conversion, pH and conductivity, etc. were analysed and compared. In the case of the semi-batch process, reaction educts, such as monomer and initiator, are added through the course of reaction, and the so called "starved" monomer conditions (i.e. a constant monomer concentration) are achieved over time.

Whereas, with the continuous and batch process all of the components are combined then added to the reactor at the start of reaction, with no further component added during reaction. Nevertheless, the products of all realised processes were comparable. The dependence of the product properties on specific process parameters associated with certain process was shown. The influence of different operational steps during the reaction have been investigated extensively and reported. Furthermore, polymer product from continuous process was analysed using different analytical methods. The results were implemented by RWTH in the model predicted closed loop controller.

At first the experimental setup was installed and tested. Then many experiments with a lot of sensor were carried out. The first step was to install and test the experimental setup, and carry out experiments with numerous sensors. The semi-batch experiments performed at the Universities of Hamburg and Cambridge including calorimetric, ionic conductivity, temperature [thermal balance] and Raman sensors. These measurements were performed with several styrene, butyl-acrylate, acrylic acid and acrylamide emulsion polymerisation recipes to demonstrate the ability to provide an increased system observability with the sensor-fusion approach, as compared to the current state-of-the art approach using the robust process sensors only. In addition to the sensors, mass-spectroscopy and acoustic levitation was used for data generation and recipe development.

Semi-batch experiments with full featured sensor equipment were carried out successfully mainly under the industrial relevant monomer-starved conditions. Coagulation and fouling on the reactor walls, as well as to control copolymer composition in the case of the lager differences in the monomer reactivity ratios were successfully realised. The experimental data was handed over to the COOPOL group. Furthermore several copolymers were produced in semi-batch emulsion polymerisation with styrene seeds as reaction template and fully characterised. On this seeds were polymerised the monomers styrene and butyl acrylate in monomer ratios of 20/80, 50/50 and 80/20 mol% (styrene/butyl acrylate). Thus complete analytical data are available especially with respect to WP 3-5. Seed recipes as well as semi-batch emulsion polymerisation recipes with different fouling levels were developed.

For each process type experiments, batch, semi-batch and smart-scale, different polymer characteristics such as molecular mass (M_w and M_n), monomer conversion, pH and conductivity, etc. were successfully analysed and compared to each other in order to validate and establish the similarities and differences between polymer properties of the three studied processes. The generated data was spread to the WP3/4 COOPOL partners as intended in the project proposal. It was shown, that a continuous emulsion polymerization can be stable operated for a prolonged time in a continuous smart-scale reactor. The successful realization was presented in deliverable 2.8. UHAM realized a continuous emulsion polymerization for 62 hours in an emulsion polymerization with 30 % solid content.

Together UHAM and RWTH successfully ran experiments for different reaction conditions in the continuous and semi-batch mode. The model predicted closed loop controller works well for both types of processes.

SMART SCALE REACTOR SETUP AND RECIPE DEVELOPMENT

Semi-batch experimental setup (UCAM)

For online monitoring of the polymerization reaction a Raman spectrometer, conductivity probe and temperature sensors were used. The Raman ball probe was purchased from Horiba, which is a spherical probe specially developed for dispersed mediums. The penetration depth is a few micrometers, which allows continuous data collection during the course of emulsion polymerization. A conductivity sensor was purchased from Mettler Toledo (4- electrode conductivity sensor) and used with a transducer which supported the software.

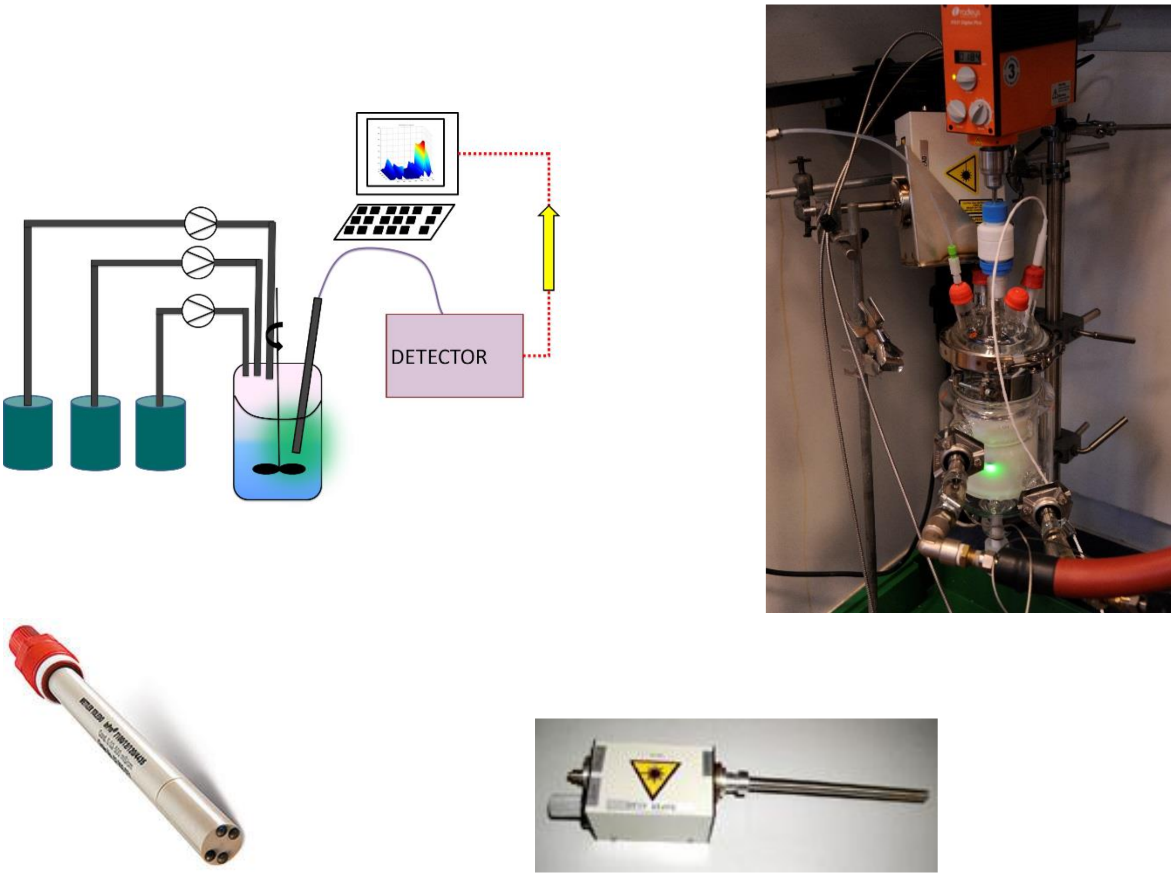


Figure 1: Experimental set-up and images of used Raman probe and conductivity sensor.

SEMI-BATCH EXPERIMENTAL SETUP (UHAM)

Figure 2 shows the experimental set up of the RC1 at UHAM, a reaction calorimeter by Mettler Toledo. The reaction vessel of the RC1 calorimeter is a stainless steel reactor from Büchi AG with a volume of 1.8 L. It has an upwardly promoting stirrer (6-leafed) with a diameter of 4 cm, the stirring blades had a slope of 45 ° with respect to the stirrer shaft.

The agitator had a length of 50 cm and a distance of 2 cm from the bottom of the reactor. The stainless steel reactor is connected to a computer-controlled thermostat, which maintained the reactor temperature at approximately constant values, whereby an isothermal operation is ensured. In addition, three pumps were used for dosage.

Raman probe (Kaiser Optical Systems – *RXN1*) and conductivity sensor (Mettler Toledo 4-electrode probe) were used to perform online measurements.

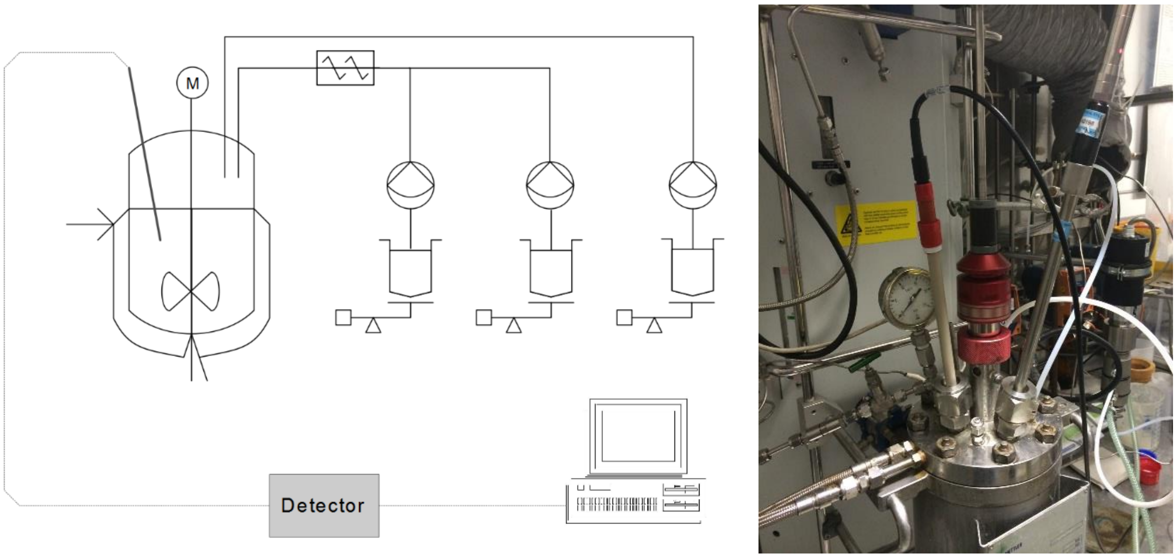


Figure 2: Semi batch set up UHAM

CONTINUOUS EXPERIMENTAL SETUP (UHAM)

Figure 3 shows the experimental set-up for the continuous smart scale reactor. The piping and instrumentation diagram of the continuous smart scale reactor is depicted in Figure 1. The reactor itself consists of a helically coiled PTFE tube (D = 22 cm, l = 10 m, d_i = 10 mm, V = 315 mL), equipped with static mixing elements in an interval of 12.5 cm. Monomers and emulsifier are pre-mixed in two CSTR reactors, heated up as needed by a heat exchanger and after addition of the initiator directed into the actual reactor. The flow rate normally is 1.1 g/s, resulting in a mean residence time of 12 min. In order to obtain information about the polymerization process the set up allows sampling at various residence times.

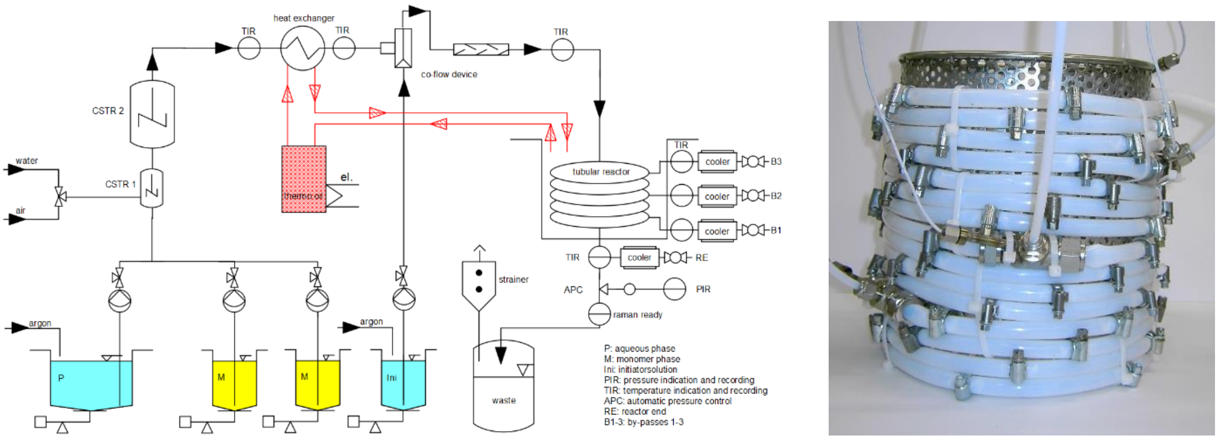


Figure 3: Piping and instrumentation diagram (PID) and reactor of the continuous smart scale reactor.

Seed Recipe Development

Aim was the development of monodisperse seed particles with small diameter and narrow particle size distributions. For this the emulsion polymerization of styrene was carried out with different emulsifier systems at different temperatures. The most important parameter in the experiments was the emulsifier system. On one hand the conventional emulsifiers SDBS and SDS and on the other hand less common emulsifier as mono- and diesters of the sulfosuccinates, as well as the sulfosuccinamates were used.

The development of the seed recipe was carried out in two semi-batch reactor, the stainless steel RC1 (Figure 2) and a second smaller glass calorimeter (RC1e) with a volume of 0.5 L shown in Figure 4.

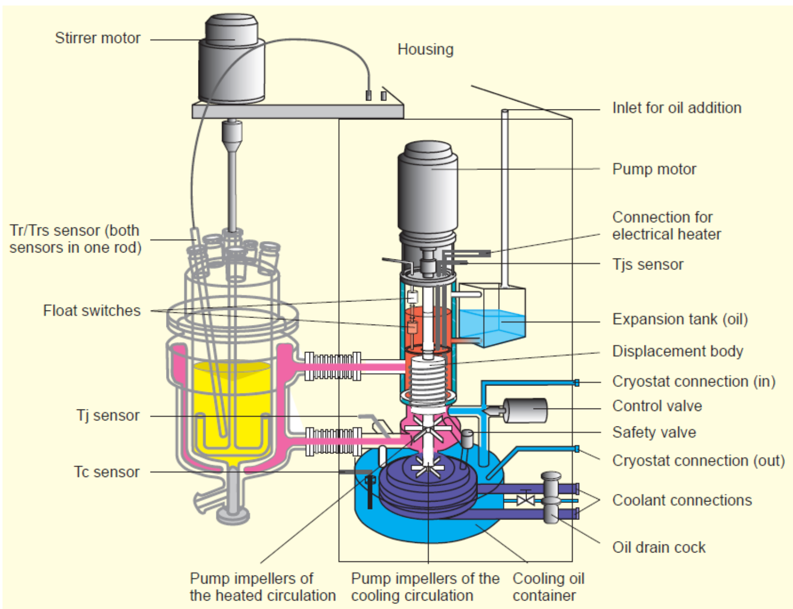


Figure 4: Drawing RC1 glass reactor at UHAM

The polymerization of styrene was carried out at 70 °C in the RC1e and at 95 °C in the RC1-calorimeter. The total reaction volumes were 1000 g and 400 g. The amount of styrene varied between 15 and 25 wt%, the emulsifier concentration between 12.00 and 34.28 wt% and the concentration of initiator and CTA between 1 and 2 wt%. An overview of the experiment parameters is shown in Tab. 2.

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The experiments with SDS as emulsifier generated very small particles between 30.43 and 32.53 nm with relatively small distributions independent of the initial monomer concentration. The addition of acrylic acid enabled the minimization of the particle size to 28.99/ 30.50 nm. In Tab.2 the experimental results for SDBS/SDS experiments at 95 °C are shown exemplary. It can be seen that EF1, the only experiment carried out with SDBS the particle sizes is a lot bigger than for the other samples. Furthermore the M_w and the PDI are higher than for the other samples.

Tab. 2: Analytical results for SDS/SDBS experiments at 95 °C

Experiment	$d_{Z\text{-}Ave}$ [nm] (DLS)	PDI (DLS)	M_w[g/mol] (GPC)	PDI (GPC)	Conv. [%] (GC)	Conv. [%] (Gravi)
EF1	57.98 ± 0.38	0.233 ± 0.011	468000	9.77	98.90	97.53
EF2	31.04 ± 0.26	0.120 ± 0.030	207000	5.08	99.56	98.07
EF9	30.51 ± 0.08	0.072 ± 0.009	209000	5.99	99.65	100.85
EF11	30.43 ± 0.10	0.082 ± 0.010	245000	3.57	99.57	99.54
EF15	32.53 ± 0.39	0.082 ± 0.018	187000	3.99	99.61	99.28
EF22	28.99 ± 0.29	0.101 ± 0.006	167000	4.95	99.33	101.28
EF28	30.50 ± 6.02	0.122 ± 0.034	111000	5.64	98.88	101.07

Figure 5 illustrates how particle size and PDI change for a reaction with 15 wt% solid content (12 wt% emulsifier, 1 wt% initiator, 95 °C) when replacing SDBS with SDS as emulsifier. While the particle size decreases from 57.98 nm to 31.04 nm, the PDI decreases from 0.233 to 0.120.

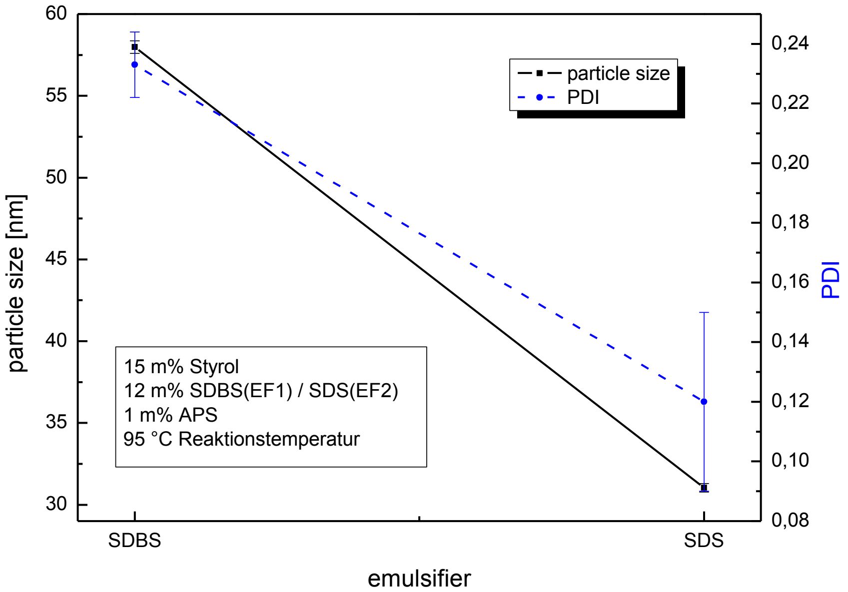

Figure 5: Particle size with varying emulsifier system.

For the less common emulsifier systems good results were achieved with AEROSOL® 22N (49.37 nm) and MA-80 % (48.26 nm). The particle size for AEROSOL® 22N recipes decreases with increasing emulsifier and initiator concentration to 43.58 nm. Overall particle size with this systems is larger compared to the conventional ones, but the PDI are much better. With the use of VA-044 as initiator comparable particle sizes could be realized as with SDS. The smallest particles had a diameter of 33.84 nm. The addition of CTA had no influence on particle size and PDI. As expected only the weight average molar mass was reduced.

EXPERIMENTAL DATA FOR MODEL DEVELOPMENT AND VALIDATION

Various experiments have been carried out in the continuous smart scale reactor with different monomer mass fractions (15 % to 50 %), different molar ratios of the two monomers styrene (S) and butyl acrylate (BA) of 80/20, 50/50 and 20/80 and two operation modes, i.e. isothermal and polytropic. In the case of isothermal conditions, the pre-emulsion was pre-heated to 90 °C and then fed into the reactor while the jacket temperature maintained at 90 °C. In experiments at polytropic process conditions, the pre-emulsion was fed into the reactor without preheating with jacket temperature maintained at 90 °C. Typical experimental data generated in the tubular reactor (see Figure) shows the trend of M_n and M_w after τ= 12 min for variations in monomer mass fraction, at a molar ratio of 80/20 (S/BA) at isothermal conditions (T = 90°C). Both M_n and M_w of the product decrease with increasing mass fraction of monomer. The effect is more pronounced for the weight average molar mass (M_w). This can be related to increase in reaction temperature for higher initial monomer contents.

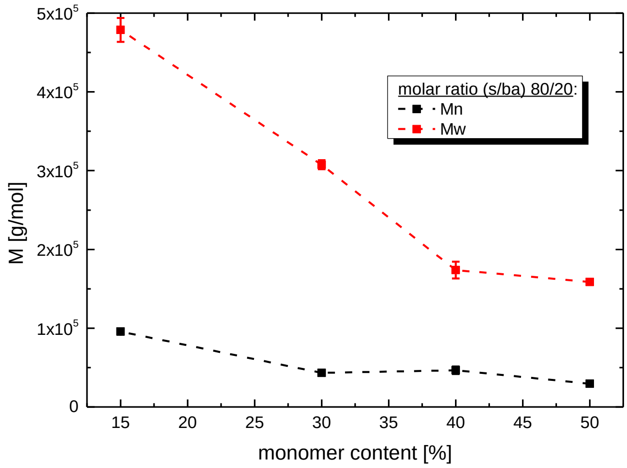

Figure 6: M_n and M_w for a molar ratio of 80/20 at different mass fractions monomer at isothermal conditions (τ = 12 min)

In Figure 7 a comparison of the particle size (left y-axis) of the product (τ = 12 min) for different mass and mole fractions of monomer (80/20, 50/50 and 20/80 (S/BA)) is shown. In the same figure, the right y-axis depicts the corresponding total conversions for different mole and mass fractions of monomers. Concentrating on the particle sizes, we observe that for monomer contents less than 30 wt%, an increase in the fractions of the monomer BA leads to decrease of particle size. However, for higher monomer contents (> 30%), the particle size increases strongly, which is accompanied by lower total conversions. The increase in particle size is not only attributed to higher solid contents but also to the swelling of the particles with unreacted monomer. This also explains why the recipes with higher fractions of monomer BA results in larger particle sizes (after τ = 12 min), as the monomer conversion in such experiments is much lower than those for higher styrene fractions. This explains why an increase of the particle size along the reactor length is observed for high mass fractions monomer and higher BA contents.

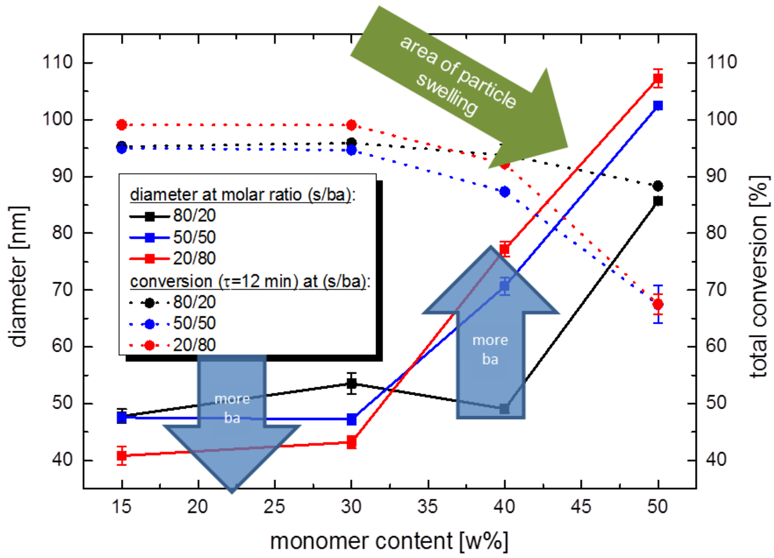

Figure 7: Particle size (left y-axis) and conversion (right y-axis) for different molar ratio of the monomers and at different mass fractions monomer

Besides generating data for model validation, the focus in the experiments was on productivity enhancement. Milestone 3 describes the applied strategies to achieve productivity enhancement and gives an overview of parameters influencing the product quality of the smart scale process. The milestone reports various strategies to increase the productivity of the continuous smart scale process. Experiments with high solid content up to **45 wt%** were conducted, thereby increasing the polymer production solid content by 50% from previous results with 30 wt% monomer. An increase in the inlet temperature, as well as in initiator concentration leads to faster and higher conversion rates, thereby resulting in nearly total monomer conversion after mean residence time of 6 minutes for a mass fraction of 30 %.

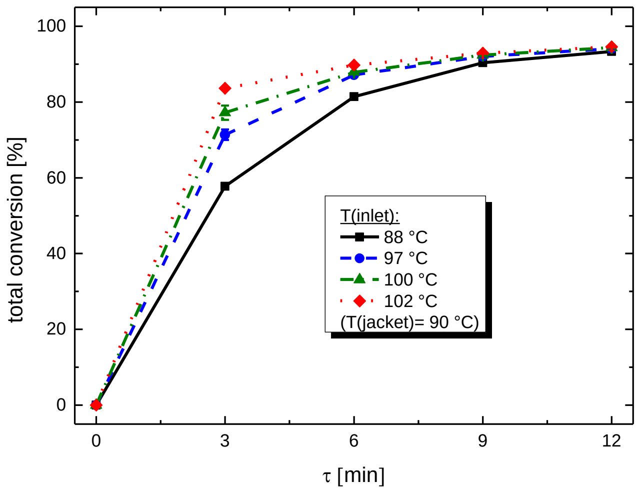

Figure 8: Conversion slopes for differents inlet temperatures (30 wt%, S/BA 50/50, T_{jacket}= 90 °C)

Increase in the inlet flow rate by factor two, increases the total productivity positively by factor two, without negative influence on heat transfer properties and conversion rates of the polymerisation reaction.

LONG-TERM STABILITY OF SMART-SCALE PROCESS

One essential point of the COOPOL project was to show, that a continuous emulsion polymerisation can be operated over an extended period of time in the smart-scale reactor. The successful realisation is presented in deliverable 2.8. In order to deal with the large amounts of reaction components and product an adoption of the existing reactor set-up was needed. This was realised with the installation of large reservoirs which were used to refill the original storage tanks (limited in weight). Additionally a second product tank was implemented.

Figure 9: Modified reactor set-up for long-term stability experiments.

The long-term stability of the reactor was investigated running 11 and 62 h experiments with 30 wt% monomer. While the shorter experiments ran stable in terms of all operation parameter for the 62 h experiment a slight decrease in conversion accompanied by pressure increase was observed starting after about 15 h run time.

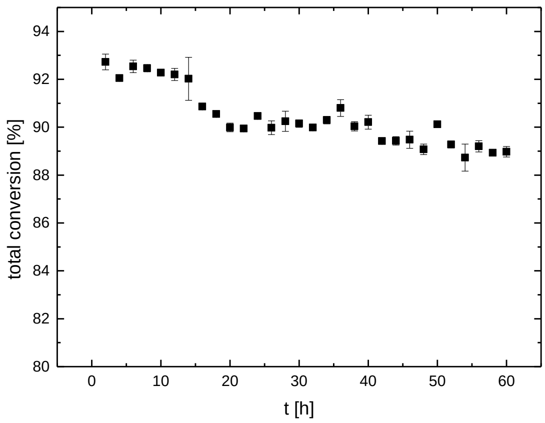

Figure 10: Total monomer conversion over an experiment run time of 62 h with 30 wt% monomer (S/BA 50/50).

This was due to clogging behind the static mixers in the second half of the reactor, i.e. at residence times of 6 to 12 min. As in this part of the reactor only about 7% of the total conversion is achieved, one could think about removing the static mixing elements in the second part of the reactor to avoid clogging induced through the high shear rate. Apart from that the process was stable in means of flow rates and temperature over a run time of 62 h. Furthermore both processes, i.e. the 11 h and 62 h run generated consistent products with only little deviations of about 3% in particle size and molecular weight.

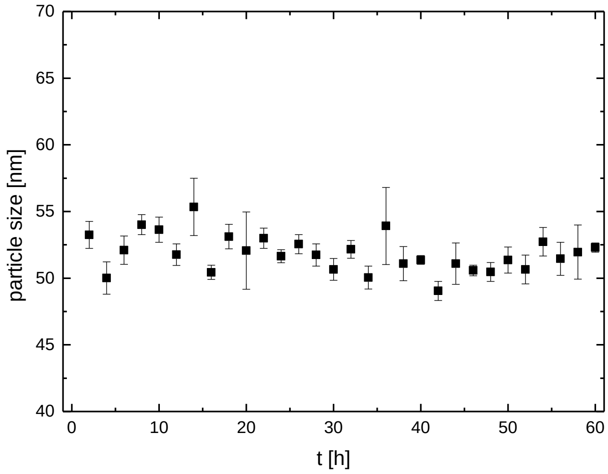

Figure 11: Particle size of the product for an experiment with 30 wt% monomer at a molar ratio of 50/50 (S/BA).

CONTROL EXPERIMENTS WITH RWTH

Control experiments were run in close cooperation with the RWTH Aachen as well in the semi-batch as in the continuous reactor. Via data hub connection RWTH Aachen was able to successfully run water as well as polymerisation experiments in the reactors located in UHAM. Stable dosing and temperature control was achieved as shown for the smart-scale reactor in Figure 12. The chart shows the feeds for an open-loop estimation experiment with 30 wt% monomer and a feed composition of 50/50 (S/BA).

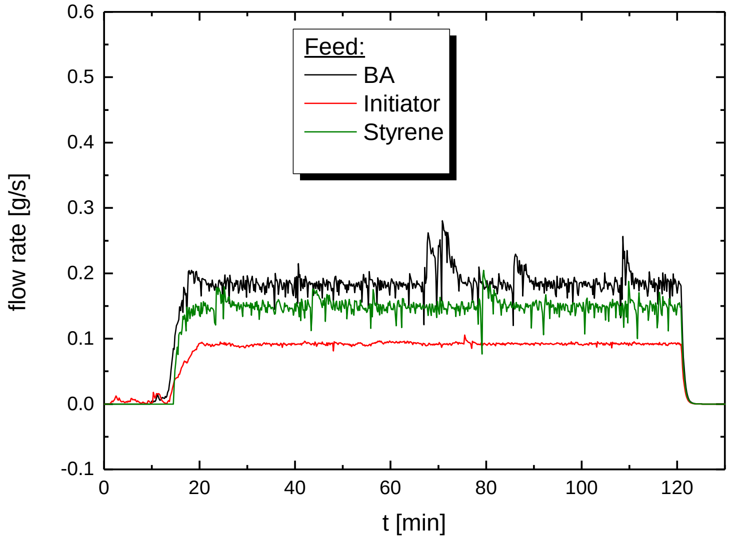

Figure 12: Flow rates of an experiment with 30 wt% monomer at a molar ratio of 50/50.

The temperature control is shown by an example from the semi-batch reactor (Figure). Shown in red is the jacket temperature, black is the reactor temperature. It can be nicely seen how the PID controller is keeping the reactor temperature at 75 °C by adjusting the jacket temperature, especially after the end of dosing when a lot of reaction heat is released. The jacket temperature reacts on the temperature increase by cooling.

The development of the particle size in a controlled semi-batch experiment is shown in Figure . It can be seen that the particle size increases nearly linear while dosing and flattens after end of dosing. The steady increase in particle size implies that stable dosing is achieved leading to constant particles growth.

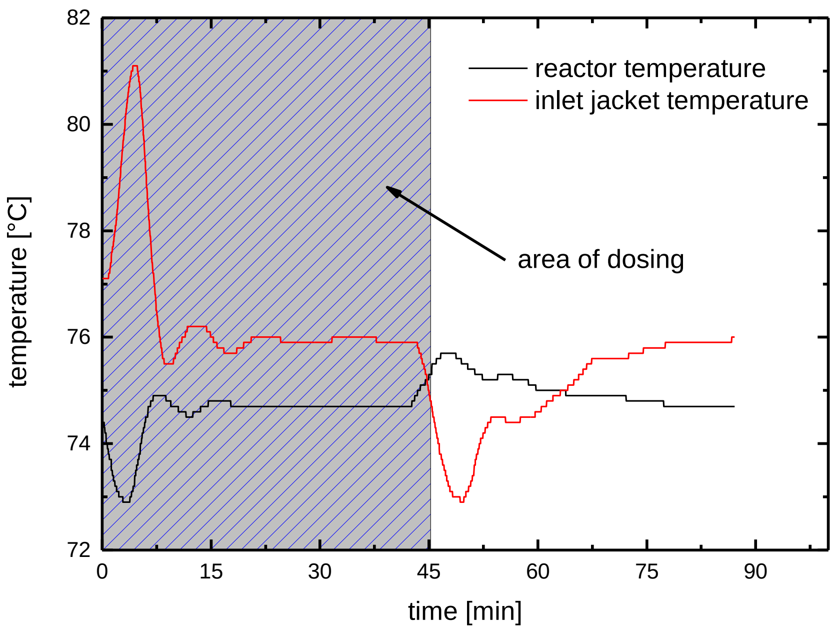

Figure 13: PID temperature control in the semi-batch reactor.

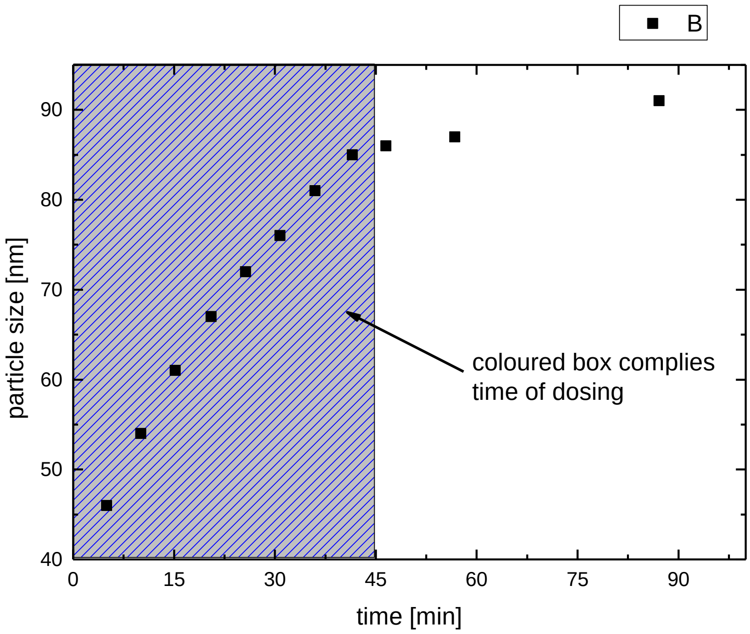

Figure 14: Particle size evolution for a controlled semi-batch experiment.

4.1.3.3 Observation: from sensor tip to state estimates

The objectives of WP3 were:

- To develop the sensor approach and analytical protocols to produce the necessary data for development of polymerisation reaction models and their validation.
- To develop approaches for on-line process monitoring for real-time model-predictive control in WP 5.

The experiments performed in WP2 involved a variety of sophisticated measurement technology suitable for in-line and off-line use, such as chromatography, spectroscopy, dynamic light scattering, electron microscopy etc. The data generated through experiments will be used to generate detailed physical and chemical models of the underlying polymerisation process, and to be potentially used in on-line processes. Along with a deeper understanding of the reaction mechanisms, this finally allows to derive reduced models in a systematic and theoretically justified way (WP 4) for on-line usage in estimation and control applications (WPs 3 and 5).

WP3 also dealt with the algorithms for the estimation of states and parameters from measurements in an online and offline setting. In complex systems like emulsion polymerisation it is necessary to establish if it is possible to estimate all states and parameters from the available measurements. Observability and identifiability analysis methods will be tested for the semi-batch emulsion polymerisation system to determine which states and parameters can be estimated reliably from the available data. The results of these studies would then be useful in WP5 where online state estimation will be coupled with the model predictive controller.

Activities and results from WP3

PEAXACT TRAINING FOR RESEARCHERS

PEAXACT is software which can be used for analysis of spectral data. Researchers in the COOPOL project were given training in the advanced use of PEAXACT. During this program the participants were given training on data driven analysis, model-based analysis and, calibration, validation and prediction using spectral data (Deliverable 3.3). The software PEAXACT is developed and maintained by S-PACT which is a spin-off from the chair of Process Systems Engineering at RWTH Aachen.

INITIAL CALIBRATION MODEL

An initial calibration model to predict product concentration was prepared for the two monomer (butyl acrylate, styrene) case using Raman Spectra (Deliverable 3.2). This activity was carried out by S-PACT.

SET UP OF INTERFACES TO INTEGRATE SENSOR DATA

LabVision and LabView are the frameworks for data processing that are being used in UHAM and UCAM. The Raman sensors in UHAM and UCAM which were not integrated with the common data processing framework have been integrated using an OPC (Open Platforms Communication) server. The OPC server is also used to integrate the hard sensors to the soft sensors and the process controller (Deliverable 3.1). Experiments have been done to test the soft sensors of the RWTH toolbox to predict unmeasured variables of the continuous emulsion polymerisation process. This activity was done in collaboration with S-PACT.

OBSERVABILITY ANALYSIS AND STATE ESTIMATION

Observability analysis studies were carried out for the semi-batch process to determine if all the states can be estimated with the existing set of sensors in industrial (few sensors)and laboratory reactors(more sensors). Observability analysis and simulation studies showed that unless online measurements of polymer property are available the polymer properties cannot be reliably estimated using soft sensor algorithms (Deliverables 3.4 and 3.5).

IDENTIFIABILITY ANALYSIS

Identifiability analysis was performed for the semi-batch emulsion polymerisation process for different sensor configurations. Identifiability analysis was performed for two sensor configurations: Case (I) – Reactor temperature, jacket inlet and outlet temperature. This case represents an industrial reactor. Case (II) – Reactor temperature, jacket inlet and outlet temperature, monomer conversions. This case represents a laboratory scale reactor, where it is assumed that online concentrations are available. The analysis showed that more parameters are identifiable for the case where online concentration measurements are assumed to be available.

<u>Soft sensors and sensor fusion:</u> The Extended Kalman Filter (EKF) was proposed as the soft sensor algorithm due to its simplicity, ease of implementation and computational efficiency. Observability analysis was carried out for different sensor configurations and it was shown for both the 4 monomer and 2 monomer semi-batch reactor that molecular properties are not observable with measurements

of only reactor temperature, jacket temperature and monomer conversions. Simulation studies showed that polymer properties can be estimated even if only few measurements of polymer property are included even when these are delayed.

Data processing framework to integrate sensor data with model predictive control: An OPC (Open Platforms Communications) based data processing framework has been set up at UHAM and UCAM to integrate the data from multiple sensors used for process monitoring with soft sensor algorithm and model-predictive control algorithms. The data processing framework was tested by connecting the OptoEcon toolbox for state estimation and control at RWTH Aachen to the smart scale process and semi-batch process at UHAM.

Identifiability analysis: The mechanistic models of emulsion polymerisation process have a large number of parameters, many of which are not precisely known. An identifiability analysis was performed to determine which parameters of the model can be estimated with different sets of sensors. Identifiability analysis was carried out for a scenario where reaction calorimetry is used to determine the reaction heat and a scenario where the individual monomer conversions are assumed to be available online using, for example, Raman spectroscopy. It was shown that in the case where online measurements of individual monomer concentration are available more parameters are identifiable than in the case with reaction calorimetry.

4.1.3.4 Modelling

SEMI-BATCH REACTOR MODELLING

Primary goal of this part of COOPOL was to develop and validate the model of semi-batch copolymerisation in monomer-starved regime involving two hydrophobic and two water-soluble monomers. This model represents the core element in the on-line control and optimisation of the latex production at BASF pilot plant.

The modelled process is extremely complex due to many reasons, such as complicated partitioning of monomers, pH dependency of polymerisation rate, different behaviour of dissociated and un-dissociated hydrophilic monomers, spontaneous formation of oligomers in the aqueous phase, or the distribution of hydrophilic/hydrophobic monomer units in polymer chains and its effect on the phase behaviour of copolymer. Moreover, copolymerisation of four monomers results in extremely large space of kinetic parameters. Conversely, it is anticipated that the developed control model shall provide the whole process trajectory in a few seconds along with the reasonable quality of predictions.

Utilising experimental data generated by project partners and found in previously published results, we simplified the system by assuming the simultaneous copolymerisation of hydrophobic monomers in polymer particles and the copolymerisation of hydrophilic monomers in the aqueous phase, respectively. Therefore we have developed fast and robust model providing predictions of monomers conversion, heat generated by the reaction, latex solid content and average molecular weights of the produced copolymer in a good agreement with experimental data from both laboratory and pilot-plant reactors. The model speed was further improved by the rational reduction of model equations and by the translation of model from MATLAB into C++ code, thus resulting in a simulation of several hours of real process time in approximately one second of *in-silico* simulation time.

To the best of our knowledge, model-based predictive control of latex quality implemented in such complex system at industrial scale has not been published yet. This work thus represents state-of-the-art in the field of emulsion copolymerisation real-time optimisation/control with immediate impact on the economic benefits and energy savings of the industrial processes.

Smart-scale Reactor Modelling

Utilising experimental data generated by project partners and found in previously published results,

The focus here was kept on developing a robust and rationally reduced model in order to simulate styrene/*n*-butyl acrylate emulsion copolymerisation in smart-scale continuous reactor in a short time, thus enabling its incorporation into model-based predictive control. This model is based on the dynamic model of an axially dispersed plug-flow reactor and uses the numerical method of lines to discretise the partial differential equations along the axial direction. It solves the balance equations for monomers, polymer, water, initiator, emulsifier, average number of radicals per particle, and six polymer moments (three for both living and dead chains).

The model provides good agreement with the measured laboratory data. Specifically, it allows the prediction of monomer conversion (see Fig. 1), copolymer composition, temperature profile and number-average molecular weight. Moreover, it allows estimating the number concentration of particles and particle size, if the temperature profile along the reactor is measured. To predict the slower reaction rate at the beginning of the reaction, the model incorporates the thermodynamic description of monomer partitioning based on Morton equations. As these equations are strongly nonlinear and considerably reduce the model robustness and speed, we developed and implemented a simple empirical function representing their solution (cf. Fig. 2).

The developed model was successfully tested for its performance, and it was incorporated in a framework of online state estimation and control – the OptoEcon toolbox. The tuning of the state estimator and controller was performed, and currently the open and closed loop tests using the state estimator and online controller are conducted.

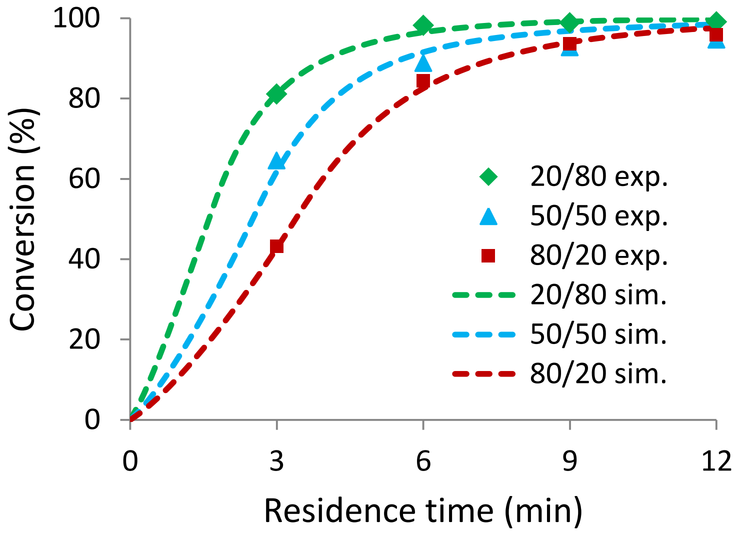

Figure 1: Comparison of experimentally measured and simulated styrene conversion along the smart-scale reactor for different Sty/BA ratios. The legend represents molar ratios of styrene and n-butyl acrylate fed to the reactor.

Only a handful of experimental and/or modelling studies were published in the open literature regarding the process intensification of emulsion copolymerisation in tubular reactors. Thus, the developed process model will be of interest for the broad polymer science and industry community.

Utilities for Monomer Partitioning, Emulsion Rheology and Dispersion Coagulation

The developed process models of emulsion copolymerisation should be not only robust, fast and accurate, but they shall also incorporate the up-to-date knowledge about the involved physical and chemical processes. As the rate of emulsion polymerisation is directly affected by the concentration of monomer species in polymer particles, one of WP4 objectives was to develop a rigorous approach for the prediction of **monomer partitioning** between water, droplet, and polymer particle phase. Therefore we developed an upgraded model, which is based on the thermodynamic description of monomer-polymer interactions derived from Flory-Huggins lattice theory of polymer solutions, first proposed by Morton *et al.* (1954). This thermodynamic approach allows for considering the effect of various process conditions and parameters on the sorption behaviour of monomers, e.g., temperature, average particle diameter, polymer cross-linking etc. To address the robustness and computational speed issues when nonlinear Morton equations are used, we developed and implemented an empirical function representing their solution (Fig. 2).

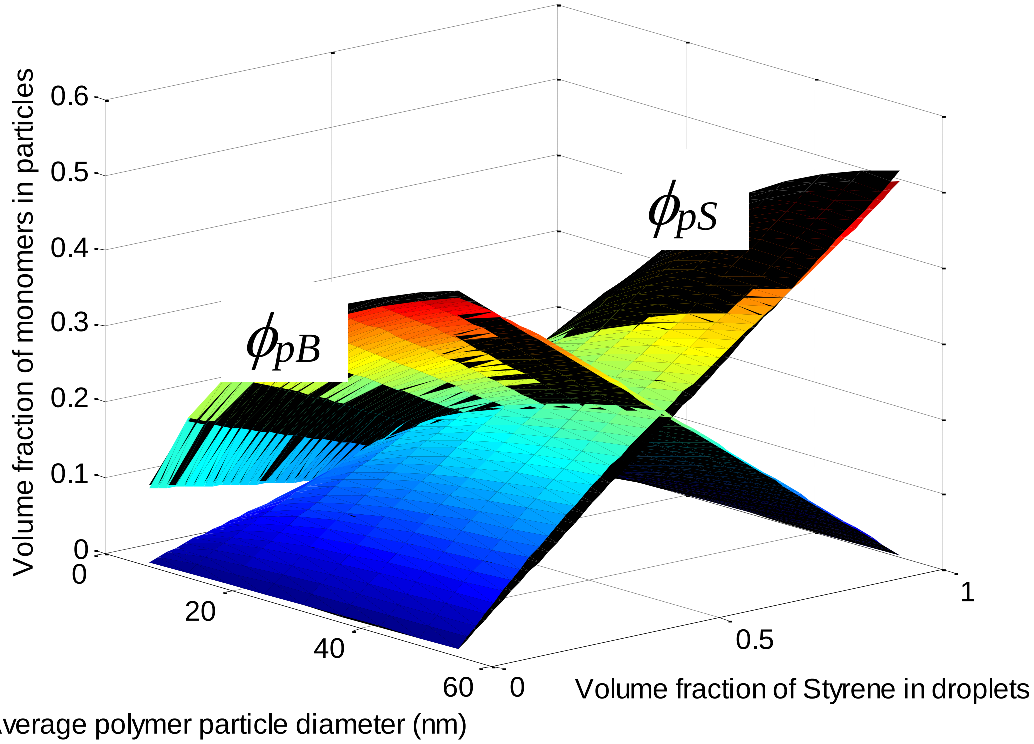

Figure 2: Comparison of volume fraction of monomers ϕ_{pS} (styrene) and ϕ_{pB} (*n*-butyl acrylate) in polymer particle phase calculated by Morton equations (coloured surfaces) and fit to data using empirical function (black surfaces). With increasing styrene fraction in droplets, volume fraction of styrene in particles ϕ_{pS} increases. Both ϕ_{pS} and ϕ_{pB} increase with increasing polymer particle diameter.

The most important result of the coagulation modelling based on the Discrete Element Method (DEM) was the prediction of the dispersion stability depending on shear rate, particle volume fraction and parameters of the electrostatic double layer. In agreement with available literature experimental data, the model predicts the characteristic coagulation time to be reduced for increasing shear rate, particle volume fraction and decreasing surface potential. Moreover, it was shown that in concentrated system the description of coagulation kinetics cannot rely on the commonly used doublet formation rate, since it seriously underestimates the actual rate of coagulation. The detailed modelling of coagulation and fouling is important not only for the purpose of the particular industrial process in this project, but it also helps to provide better insight into the behaviour of concentrated dispersions, an area which is still not completely understood

The rheological behaviour of dispersions is highly complicated; however, for the purpose of this project, the most important phenomenon is the dependence of viscosity on particle volume fraction. To model this effect, the semi-empirical correlation of Krieger-Dougherty was utilised, which made the evolution of the dispersion viscosity during reaction accessible for the process model.

4.1.3.5 Operation, Control and Evaluation

The main result of WP5 is exploitable with a short time to market: A new approach for dynamic real-time optimisation and nonlinear model predictive control of polymerisation reactors. The technology is applicable for batch, semi-batch and continuous tubular reactors, but is mostly developed for the semi-batch case.

Cybernetica provided Cybernetica CENIT as background technology to the project. CENIT is an industrially proven, state-of-the art technology for nonlinear model predictive control based on mechanistic models. CENIT is adaptable to different types of control applications, through the flexible software interface of the Cybernetica CENIT Model and Application Component.

In COOPOL WP5, an application for a four-monomer emulsion batch copolymerisation system was developed. The technology was demonstrated on a pilot plant at BASF in Ludwigshafen.

The foreground "Novel MPC" is an extension of prior art in that

- The technology is extended to emulsion polymerisation
- Combines continuous temperature, feed rate and reaction rate control with overall batch time minimisation and terminal specifications on product quality.
- Is applied and demonstrated at pilot plant for a four co-monomer batch application
- Is applied and demonstrated in simulations for a two co-monomer continuous polymerisation reactor ("smart-scale")

The "Novel MPC" shows great promise and is expected to fulfil the purpose set forth in the objective of the work package, and should in particular be applicable for the two main tasks:

1. Intensification of industrial scale semi-batch polymerisation reactors through optimisation and improved control
2. Model-based predictive control of continuous polymerisation in tubular lab-scale reactors.

In the development of the "Novel MPC", the following challenges were addressed and adequately solved:

1. Modelling: Make models of "balanced complexity" – fit for the purpose of on-line applications in general, and for Nonlinear Model Predictive Control (NMPC) in particular.
2. Estimation: Track model states on-line using soft sensing techniques using available sensors; a particular challenge is to find good estimates for the terminal product properties, as these states are not observable from state-of-the-art industrial sensors.
3. Control: The task at hand is model predictive control of (semi-)batch polymerisation with terminal constraints. That involves:
   - Minimisation of batch-time
   - Control of final product quality parameters
   - Continuous control polymerisation conditions
   - Impose safety and quality related constraints

The developed solutions are implemented and tested. A re-development of the models from WP4 was conducted in order to reduce complexity and facilitate efficient numerical solution of the models. Simulation case studies were carried out using Non-linear Model Predictive Control (NMPC) applied to the polymerisation reactors. Studies were made for four-monomer semi-batch seeded copolymerisation and for two-monomer copolymerisation in a continuous lab-scale reactor. This work is reported in deliverables D5.2 "Run-time environment for Model Predictive Control", D6.1 "Demonstration in simulation of on-line control of semi-batch polymerisation" and D6.2 "Demonstration in simulation of on-line control of a smart-scale polymerisation reactor".

The case studies related to the semi-batch reactor show that

- The developed model has satisfying agreement to plant measurements for the pilot reactor.
- Simulations and plant experiments using the "Novel MPC" indicate that:
    - Reactor temperature control is achieved with promising results. The NMPC, due to its predictive nature, is able to effectively counteract disturbances and keep the reactor temperature at the desired set point.
    - The feed rates for reactants are controlled (maximised) by the NMPC to reduce batch duration while safeguarding the limits of safety in the plant as well as the product quality specifications.
    - The product quality, represented by the molecular weight distribution, specifically the number-average molecular weight, is controlled to a desired terminal specification by the NMPC.
- The model-based approach is well suited for on-line optimisation and control of the semi-batch emulsion polymerisation process.

The case studies related to the smart-scale continuous reactor show that the reactor outlet temperature as well as the conversion of monomer can be controlled. To achieve this, a fairly numerically efficient model was developed for the controller calculations.

4.1.3.6 Implementation and Demonstration

WP 6 concentrates on the proof of concept and validation of the innovative methodologies for process observation through hard and soft sensors, novel control techniques for real-time optimisation and control of chemical processes and generic framework to implement model based methods for the process intensification of polymerisation processes within limited time-scale.

The objective of the WP can be divided into two parts and be outlined as

a) Implementation of model based closed-loop control and optimisation methods to continuous, smart-scale reactor as well as semi-batch polymerisation reactor and demonstrate process intensification results in simulations, and
b) Implementation of state-of-the art sensor technologies and developed novel control methods to pilot-scale semi-batch reactor at BASF and demonstrate process intensification of polymerization reaction in semi-batch reactor by closed loop control and optimization.

In order to meet the objectives of COOPOL (i.e., to achieve a considerable increase in product quality of polymerisation by employing novel process control approach for intensified semi-batch and 'smart-scale' continuous polymerisation processes) WP6 oversaw the development of

- smart-scale reactor technology for robust polymerisation process with reproducible product qualities over prolonged production period;
- novel sensor-fusion methods, model development of advanced polymerisation models incorporating product properties to be used in real-time optimisation tool box and realistic process constraints as well as economic objectives need to defined

4.1.3.7 Dissemination

The objective of the Dissemination work package was to maximise the impact of the project through wide dissemination of its results and achievements to audiences within the chemical industry and scientific community. The second objective of the dissemination WP was to help to increase the uptake of the technology, driving improvements in product quality, increased productivity and sustainability within the EU polymer industry. Where new IP has been generated careful assessment of its relative sensitivity and value to partners has been considered to avoid damaging premature disclosures hence this work package also includes IP control mechanisms.

Dissemination activities for the project were managed by CIKTN/KTN with inputs from all partners to ensure a consistent approach to information handling. A dedicated project website was created and maintained open to all whilst for internal project communication a secure website was installed. Approval protocols for result assessment prior to disclosure has been established and implemented with scientific presentations beginning to occur towards the end of the period.

EVENT MANAGEMENT

Two specific events were scheduled to disseminate project results and demonstrate technology advances to the wider chemical industry. The first of these events was at mid-term and was hosted by Hamburg University as a focussed scientific workshop with an invitation only delegate list. It involved a series of talks and a poster session in combination with the FP7 OPTICO project partners who were working in a similar area. The objective, to share non-confidential data between projects to identify common technology advances or barriers and more general potential exploitation opportunities, was achieved with a vibrant interaction throughout the event.

The second dissemination event was a larger workshop open to the scientific and industrial communities at large and hosted by Dechema in Frankfurt. This event involved significant effort to attract attendees through a variety of promotion events with a dedicated website set up along with online registration. The objective was to present the technology advances made during the COOPOL project and to advertise partner capabilities to generate maximum impact and was successful with around 100 delegates attending over the two days. The conference programme involved 6 talks from international experts and 6 from COOPOL partners to the broad polymerisation audience present. In addition 18 posters were presented in a poster session sponsored by a leading scientific journal publisher with over half the posters from COOPOL researchers. Many discussions were held and it was generally accepted that COOPOL results were of great interest to the community at large and that a high scientific standard had been reached for the event as a whole.

Gender Issues

The COOPOL partners and researchers formed a highly interactive team where gender was not considered in the performance of the scientific work. The balance of female to male researchers involved in the COOPOL project was 11% women in key project positions and a total of 25% women working on the project. These numbers are comparable with the wider science base and reflect the continuing problems attracting women into science.

WP objectives achieved

All of the objectives were achieved which consisted of:

- Development of project website – both public and private profiles
- Press release about COOPOL
- Brochure about COOPOL
- Develop exploitation strategy
- Mid-term dissemination event
- End of project dissemination event

Potential impact and main dissemination activities and exploitation results

4.1.4 Potential Impact

WP2

- Continuous emulsion polymerisation can be stable operated for a longer time
- Online process analytics by IR and Raman Spectroscopy for high solid contents of up to 50% were realised
- Online particle size determination

By implementing the results of the project in industry, natural resources can be saved by higher process efficiency.

WP3

The activities undertaken under WP3 were a significant step towards the use of novel sensing techniques such as Raman spectroscopy for monitoring of emulsion polymerisation reactions. Significant work has been done in the development and implementation of software tools to analyse and extract useful information from measurement data. The observability analysis that was carried out for the semi-batch processes has shown that, on the one hand there is a need for further development of sensors for online measurement of molecular property and conversely, that there is a need to develop models that correlate polymer properties to existing measurement techniques. Overall, the project has resulted in an intensification of the semi-batch emulsion polymerisation process. This intensification could result in more efficiency in terms of resource usage and energy consumption, thus reducing the strain of the manufacturing industry on the environment.
Increased resource-usage and energy efficiency would also result in increasing the standing of the European polymer industry in the global market. By implementing the results of the project in industry, natural resources can be saved by higher process efficiency.

WP4

WP4 researchers developed fast and robust model providing predictions of monomers conversion, heat generated by the reaction, latex solid content and average molecular weights of the produced copolymer in a good agreement with experimental data from both laboratory and pilot-plant reactors. And further improved the model speed by the rational reduction of model equations and by the translation of model from MATLAB into C++ code.
To the best of our knowledge, model-based predictive control of latex quality implemented in such complex system at industrial scale has not been published yet. This work thus represents state-of-the-art in the field of emulsion copolymerisation real-time optimisation/control with immediate impact on the economic benefits and energy savings of the industrial processes.

WP5

Continued tests should be conducted using the “Novel MPC” at pilot plant in order to adequately determine the full potential of the new technology.
The vision was to move from recipe based to optimisation based production.
Using the novel MPC for emulsion polymerisation, expected benefits include:

- Accurate temperature control:

  - Rapid variations in reaction heat → Can be predicted and counteracted.
  - Offset free tracking of non-isothermal temperature reference trajectory.
  - Faster temperature set point changes.
- Optimal feeding of reactants:
  - Minimise polymerisation times.
  - Short dosing times might be important for product quality.
- Fulfil constraints during the batch:
  - Available cooling capacity.
  - Temperature constraints.
  - Pressure constraints.
  - Constraints on the amount of reactants or intermediate products in the reactor.
  - Quality constraints.
  - Safety related constraints.
- Terminal constraints on product quality.

In summary, these measures yields an opportunity to produce the desired product (with high accuracy) in the shortest possible time. For fully developed applications, a reduction in batch time is expected to be from 5 to 20 %.

WP6

WP 6 focused on the implementation and demonstration and is based on the development of methods and techniques as well as outcomes of all other work-packages i.e., WP 2- WP 5. This work-package concentrates on adoption of the developed control and sensors methods on pilot plant reactor in BASF, as well as demonstration of the closed loop control models developed in the project. Hence, a demonstration (WP 6) illustrates successful completion of the project, thereby exhibiting the importance of WP 6.

In order to implement state-of-art closed loop methods on pilot-plant reactor, there are necessary prerequisites, which are developed during the project in other work-packages or employed on reactor in order to realise process intensification of semi-batch polymerisation process by model based control. These prerequisites can be summarised as:

- Detailed mechanistic kinetic model of the polymerisation process, incorporating product/polymer properties
- Reactor periphery model with cooling circuit, coupled with kinetic model
- Modern DCS (Distributed Control System) - allows for external connection via OPC server
- Enclosed energy balance of the reactor by hard-sensors of temperatures, flow-rates, in to and out of the reactor and cooling circuit
- An external server, hosting model based soft-sensor and real time optimisation tool box.

During the project, all these prerequisites were accomplished, thereby ensuring successful demonstration of model based closed-loop control and optimisation for semi-batch polymerisation process at pilot scale. The results were reported in the work package deliverables. The benchmarking between conventional and intensified polymerisation process by comparison of process data for two processes was reported under WP5 deliverables.

4.1.5 Dissemination activities

Throughout its entire lifespan, COOPOL partners spent much effort on dissemination, both towards the scientific community and relevant target groups in the industry. Main target of these efforts was to encourage the uptake and exploitation of the project's outputs and results, which was one of COOPOL's main long-term objectives. KTN/CIKTN provided their expertise in innovative networking processes to enable COOPOL to achieve its dissemination and exploitation strategy.

The project was able to develop a robust, accurate process model and, real-time process control system over its 36 months of collaborative research; and use its dissemination tools in an effective manner. This was reported in more detail in the project's periodic progress reports (deliverables mid-term event and final dissemination event).

COOPOL researchers defined several dissemination activities (publications, posters, oral presentations, etc.) during the lifespan of the project. Further dissemination activities are planned after the project's end date – 28 February 2015 – either as joint or individual activities. One such publication is: "Robust process model for styrene and n-butyl acrylate emulsion copolymerisation in smart-scale tubular reactor", authored by Pokorny R., Zubov A., Lüth F., Matuska P., Pauer W., Moritz H.-U., Kosek J., to be published in June 2015 in the Industrial & Engineering Chemistry Research Journal. This is joint effort between VSCHT and UHAM.

KTN/CIKTN delivered two large-scale dissemination events to release COOPOL researchers' results deemed to be non-sensitive for the Industry partners' exploitation plans and both received excellent feedback on organisation and content.

In general Academic partners will drive fundamental process result dissemination through publications to demonstrate state of the art advances and maintain their high scientific standing. Industry partners will focus on result dissemination through marketing departments and the launch of new improved products to gain sales revenue and advance their standing in the market place. Specific process results at end-user facilities may well be extremely sensitive and so, as the approaches mentioned previously meet at a critical mid-point, many discussions in this area are envisaged as the project progresses to ensure all partners requirements are met.

A public website was created and maintained to publicise the project and facilitate raising its profile. (http://www.coopol.eu/) Google Analytics was installed in the final year of the project and recorded over 900 different users from over 35 countries visiting the site indicating a high public profile. Dissemination of project outputs to stakeholders and the wider scientific community has been through press releases, presentations at conferences and tradeshows, articles in peer reviewed journals etc. The public website has provided a central place to signpost interested parties to the relevant outputs.

Control and timing of disclosures has been actively managed through strict procedures to avoid release of sensitive material such that protection of advantage is lost. Results assessment to identify novelty and value to a) the partners and b) the wide community has been addressed through an approval procedure followed by all partners to ensure everyone has been consulted prior to any COOPOL results passing outside the project.

4.1.6 Exploitation of results

The identification of and recordal of new inventions was achieved through the secure website where a dedicated dissemination area managed by CIKTN/KTN is present. The invention itself along with ownership and potential use was highlighted and the appropriate exploitation strategy explored. The value of the result and its protectability were considered and the Industry partners decided to take further or release for publication. In all cases maximising the project impact was key.

Two themes for industrial commercialisation were identified and the partners BASF/Cybernetica intend to follow through with plans to implement new products and procedures in these areas to benefit polymer manufacture.

A. Robust, accurate process model incorporating soft sensor algorithms
B. Real time process control system incorporating robust methodologies

It is predicted that a 7-10% gain in efficiency can be obtained by introducing predictive model control and the results from COOPOL will allow BASF to make a compelling case for uptake and accelerate its introduction to their polymerisation plants.

A detailed assessment of foreground generation and dissemination approaches has been performed. A rigorous control procedure has been implemented to ensure information disclosure is not performed without approval. Dissemination of non-sensitive data has been encouraged and will be actively pursued in the remainder of the project to raise awareness of the scientific excellence achieved. Overall the Project partners have disseminated their results widely and gained scientific recognition for the advances made. It is envisaged that a number of presentations after the end of the project will be made that can continue the process of detailing progress. In addition submissions to peer review journals including COOPOL work will be made. All releases will continue to be approved by all partners to ensure exploitation value is retained by the partners and fully deployed for gain. Selected releases have been held due to commercial sensitivity and the industrial partners will exploit these advantages in their products and services in the future.

Based on EC Technology Readiness Level (TRL) rating depicted in Table 1, TRL of COOPOL project is rated as 7, which indicates the integration of developed methods and techniques into pilot system as well successful demonstration of prototype at pilot plant level (illustrated in table 1).

EC - Technology Readiness Level Definition	
TRL 1	Basic Research: Initial scientific research has been conducted. Principles are qualitatively postulated and observed. Focus is on new discovery rather than applications.
TRL 2	Applied Research: Initial practical applications are identified. Potential of material or process to solve a problem, satisfy a need, or find application is confirmed.
TRL 3	Critical Function or Proof of Concept Established: Applied research advances and early stage development begins. Studies and laboratory measurements validate analytical predictions of separate elements of the technology.
TRL 4	Lab Testing/Validation of Alpha Prototype Component/Process: Design, development and lab testing of components/processes. Results provide evidence that performance targets may be attainable based on projected or modeled systems.
TRL 5	Laboratory Testing of Integrated/Semi-Integrated System: System Component and/or process validation is achieved in a relevant environment.
TRL 6	Prototype System Verified: System/process prototype demonstration in an operational environment (beta prototype system level).
TRL 7	Integrated Pilot System Demonstrated: System/process prototype demonstration in an operational environment (integrated pilot system level).
TRL 8	System Incorporated in Commercial Design: Actual system/process completed and qualified through test and demonstration (pre-commercial demonstration).
TRL 9	System Proven and Ready for Full Commercial Deployment: Actual system proven through successful operations in operating environment, and ready for full commercial deployment.

Table 1: EC definition of Technology Readiness Level (TRL)

Please provide the public website address (if applicable), as well as relevant contact details

http://coopol.eu/

Use and dissemination of foreground

2 Use and dissemination of foreground

Section A

TEMPLATE A1 SCIENTIFIC PUBLICATIONS

No	Title / DOI	Main author	Title of the periodical or the series	Number, date or frequency	Publisher	Place of publication	Date of publication	Relevant pages	Is open access provided	Type
1	Modeling the Mechanism of Coagulum Formation in Dispersions dx.doi.org/10	Martin Kroupa, Michal Vonka, Juraj Kosek	Langmuir	Vol. 30/Issue 10	American Chemical Society	United States	18/03/2014	2693-2702	No	Peer reviewed
2	Poly(acrylate s) via SET-LRP in a continuous tubular reactor 10.1039/C3PY0 0833A	James A. Burns, Claudia Houben, Athina Anastasaki, Christopher Waldron, Alexei A. Lapkin, David M. Haddleton	Polymer Chemistry	Vol. 4/ Issue 17	Royal Society of Chemistry	United Kingdom	01/01/2013	4809	No	Peer reviewed
3	Styrene–butadiene rubber (SBR) production by emulsion polymerization: Dynamic modeling and intensification of the	Alexandr Zubov , Jiri Pokorny, Juraj Kosek	Chemical Engineering Journal	Vol. 207-208	Elsevier	Netherlands	01/10/2012	414-420	No	Peer reviewed
4	Properties of Smart-Scaled PTFE-Tubular Reactors for Continuous Emulsion Polymerization Reactions 10.1002/masy. 201300086	Fabian Gabriel Lueth, Werner Pauer, Hans-Ulrich Moritz	Macromolecular Symposia	Vol.333/ Issue 1	Wiley-VCH Verlag	Germany	01/11/2013	69-79	No	Peer reviewed

No	Title / DOI	Main author	Title of the periodical or the series	Number, date or frequency	Publisher	Place of publication	Date of publication	Relevant pages	Is open access provided	Type
n/a	Application of the Two-Model Approach to a Semi-Batch Emulsion Copolymerization Process in two different software environments : OptoEcon and Cybernetica CE NIT	Kölle, Konstanze			RWTH Aachen University	Aachen, Germany	01/09/2013		No	Thesis
n/a	Experimentelle Untersuchungen und numerische Simulationen eines Smart Scale Prozesses zur Intensivierung der Emulsions polymerisation	Lüth, Fabian			UNIVERSITÄT HAMBURG	Germany	16/10/2014		No	Thesis
n/a	A Modeling Framework for Control of Smart-Scale Tubular Polymerization Reactors. A Case Study on Nonlinear Model-based Predictive Control of an Emulsion Copolymerization Process	Gjertsen, Fredrik			Cybernetica AS (host institution) in cooperation with NTNU, Trondheim	Norway	10/06/2015		Yes	Thesis

TEMPLATE A2 (DISSEMINATION ACTIVITIES, ALL OTHER DISSEMINATION ACTIVITIES NON PEER REVIEWED PUBLICATIONS)

No.	Type of activities	Main Leader	Title	Date	Place	Type of audience	Size of audience	Countries addressed
1	Oral presentation to a scientific event	UNIVERSITAET HAMBURG	Process Intensification of Continuous Emulsion Polymerisation	15/01/2015	Control of Emulsion Polymerisation Symposium, Frankfurt, Germany	Scientific community (higher education, Research) - Industry	100	International

No.	Type of activities	Main Leader	Title	Date	Place	Type of audience	Size of audience	Countries addressed
2	Oral presentation to a scientific event	BASF SE	Intensification of Semi-Batch Emulsion Polymerisation Processes – A Demonstration Case Study @ BASF	15/01/2015	Control of Emulsion Polymerisation Symposium, Frankfurt, Germany	Scientific community (higher education, Research) - Industry	100	International
3	Posters	THE CHANCELLOR, MASTERS AND SCHOLARS OF THE UNIVERSITY OF CAMBRIDGE	Online Monitoring of Emulsion Polymerisations using Ram an Spectroscopy	14/01/2015	Control of Emulsion Polymerisation Symposium, Frankfurt, Germany	Scientific community (higher education, Research) - Industry	100	International
4	Posters	RHEINISCH-WESTFAELISCHE TECHNISCHE HOCHSCHULE AACHEN	Effect of Sensor Network Configuration on Identifiability an d Observability of Semi-batch Emulsion Polymerisation Processes	14/01/2015	Control of Emulsion Polymerisation Symposium, Frankfurt, Germany	Scientific community (higher education, Research) - Industry	100	International
5	Posters	RHEINISCH-WESTFAELISCHE TECHNISCHE HOCHSCHULE AACHEN	Modelling, Parameter and State Estimation of a Continuous Emulsion Polymerisation Process	14/01/2015	Control of Emulsion Polymerisation Symposium, Frankfurt, Germany	Scientific community (higher education, Research) - Industry	100	International
6	Posters	VYSOKA SKOLA CHEMICKO-TEC HNOLOGICKA V PRAZE	Coagulation and Fouling in Sheared Emulsions: Mode ling by Discrete Element Method	14/01/2015	Control of Emulsion Polymerisation Symposium, Frankfurt, Germany	Scientific community (higher education, Research) - Industry	100	International
7	Posters	UNIVERSITAET HAMBURG	Optimised Process Properties of a S mart Scale Tubular Reactor for Emulsion Polymerisation	14/01/2015	Control of Emulsion Polymerisation Symposium, Frankfurt, Germany	Scientific community (higher education, Research) - Industry	100	International

No.	Type of activities	Main Leader	Title	Date	Place	Type of audience	Size of audience	Countries addressed
8	Posters	VYSOKA SKOLA CHEMICKO-TEC HNOLOGICKA V PRAZE	Mathematical Modelling of Emulsion Copolymerisation in a Smart-Scale Tubular Reactor	14/01/2015	Control of Emulsion Polymerisation Symposium, Frankfurt, Germany	Scientific community (higher education, Research) - Industry	100	International
9	Posters	RHEINISCH-WESTFAELISCHE TECHNISCHE HOCHSCHULE AACHEN	Robust Dynamic Real-Time Optimisation of the Semi-Batch Emulsion Polymerisation Process with Un certainties in the Parameter Values	14/01/2015	Control of Emulsion Polymerisation Symposium, Frankfurt, Germany	Scientific community (higher education, Research) - Industry	100	International
10	Posters	UNIVERSITAET HAMBURG	Influence of Parameter Variation on Chemical Properties of Copolymers Produced in a Continuous Smart Scale Reactor	14/01/2015	Control of Emulsion Polymerisation Symposium, Frankfurt, Germany	Scientific community (higher education, Research) - Industry	100	International
11	Posters	VYSOKA SKOLA CHEMICKO-TEC HNOLOGICKA V PRAZE	Dynamic Model and On-line Monitoring of 4-Monomer Emulsion Copolymerisation in Semi-Batch Reactor	14/01/2015	Control of Emulsion Polymerisation Symposium, Frankfurt, Germany	Scientific community (higher education, Research) - Industry	100	International
12	Posters	UNIVERSITAET HAMBURG	Particle Size Monitoring of Batch and Se mi-Batch Emulsion Polymerisations by using RAMAN- and Turbidity Sensors	14/01/2015	Control of Emulsion Polymerisation Symposium, Frankfurt, Germany	Scientific community (higher education, Research) - Industry	100	International
13	Oral presentation to a scientific event	RHEINISCH-WESTFAELISCHE TECHNISCHE HOCHSCHULE AACHEN	From Sensor Tips to State and Parameter Estimates	14/01/2015	Control of Emulsion Polymerisation Symposium, Frankfurt, Germany	Scientific community (higher education, Research) - Industry	100	International

No.	Type of activities	Main Leader	Title	Date	Place	Type of audience	Size of audience	Countries addressed
14	Oral presentation to a scientific event	VYSOKA SKOLA CHEMICKO-TEC HNOLOGICKA V PRAZE	Modelling of Emulsion Copolymerization Reactors: from Kinetics and Thermodynamics to the Dispersion Stability	14/01/2015	Control of Emulsion Polymerisation Symposium, Frankfurt, Germany	Scientific community (higher education, Research) - Industry	100	International
15	Oral presentation to a scientific event	THE UNIVERSITY OF WARWICK	Monitoring aqueous SET-LRP reactions using an advanced polymerization react or	18/11/2014	AiCHE, Atlanta, USA	Scientific community (higher education, Research) - Industry		International
16	Posters	RHEINISCH-WESTFAELISCHE TECHNISCHE HOCHSCHULE AACHEN	A data processing framework for online monitoring and optimization of emulsion polymerization processes	19/11/2014	AiCHE, Atlanta, USA	Scientific community (higher education, Research) - Industry		International
17	Oral presentation to a scientific event	THE UNIVERSITY OF WARWICK	Aqueous living radical polymerisation using copper comp lexes: The Perrier effect	17/11/2014	AiCHE, Atlanta, USA	Scientific community (higher education, Research) - Industry		International
18	Oral presentation to a scientific event	VYSOKA SKOLA CHEMICKO-TEC HNOLOGICKA V PRAZE	Intensification of Emulsion Copolymerization – Development and Application of Mathematical Model for Nonlinear Model Predictive Control	18/11/2014	AiCHE, Atlanta, USA	Scientific community (higher education, Research) - Industry		International

No.	Type of activities	Main Leader	Title	Date	Place	Type of audience	Size of audience	Countries addressed
19	Oral presentation to a scientific event	VYSOKA SKOLA CHEMICKO-TEC HNOLOGICKA V PRAZE	Properties of Charge-Stabilized Dispersions Under High Shear Modeled By Discrete Element Method	18/11/2014	AiCHE, Atlanta, USA	Scientific community (higher education, Research) - Industry		International
20	Oral presentation to a scientific event	RHEINISCH-WESTFAELISCHE TECHNISCHE HOCHSCHULE AACHEN	Robust Dynamic Real-Time Optimization of a Semi-Batch Emulsion-Co polymerization Process with Un certainties in the Parameter Values	17/11/2014	AiCHE, Atlanta, USA	Scientific community (higher education, Research) - Industry		International
21	Posters	UNIVERSITAET HAMBURG	Process Intensification through Smart Scale Technology in Continuous Emulsion Polymerization	12/09/2014	3rd working party on Polymer Reaction Engineering (WPPRE III), San Sebastian, Spain	Scientific community (higher education, Research) - Industry		International
22	Oral presentation to a scientific event	VYSOKA SKOLA CHEMICKO-TEC HNOLOGICKA V PRAZE	Mathematical model for on-line control of emulsion copolymerization in semi - batch and smart-scale reactors	23/08/2014	CHISA, Prague	Scientific community (higher education, Research) - Industry		International
23	Oral presentation to a scientific event	VYSOKA SKOLA CHEMICKO-TEC HNOLOGICKA V PRAZE	Coagulation and fouling in dispersions modeled by discrete element method	23/08/2014	CHISA, Prague	Scientific community (higher education, Research) - Industry		International

No.	Type of activities	Main Leader	Title	Date	Place	Type of audience	Size of audience	Countries addressed
24	Oral presentation to a scientific event	THE CHANCE LLOR, MASTERS AND SCHOLARS OF THE UNIVER SITY OF CA MBRIDGE	Online monitoring of emulsion polymerization with Raman spectroscopy, conductivity an d mass spectroscopy	23/08/2014	CHISA, Prague	Scientific community (higher education, Research) - Industry		International
25	Web sites/Applications	CHEMISTRY INNOVATION LIMITED	Dissemination event details added, literature list updated	30/07/2014	http://www.coopol.eu/	Scientific community (higher education, Research) - Industry - Civil society- Policy makers - Medias		International
26	Web sites/Applications	CHEMISTRY INNOVATION LIMITED	New webpage developed for 2015 conference registration - flyer developed for promotion across KTN members	30/07/2014	https://www.eventbrite.co.uk/e/intensifying-a-100- year-old-process-control-of-emulsion-polymerisation	Scientific community (higher education, Research) - Industry - Civil society- Policy makers - Medias		International
27	Web sites/Applications	CHEMISTRY INNOVATION LIMITED	Coopol researchers article added - literature list updated	14/05/2014	http://www.coopol.eu/	Scientific community (higher education, Research) - Industry - Civil society- Policy makers - Medias		International
28	Oral presentation to a scientific event	VYSOKA SKOLA CHEMICKO-TEC HNOLOGICKA V PRAZE	Discrete element model of agglomeration and fouling of emulsions	16/05/2014	Hangzhou, China	Scientific community (higher education, Research) - Industry		International
29	Posters	UNIVERSITAET HAMBURG	Model-based online Monitoring of Se mi-Batch Emulsion Polymerizations with combined hard-sensors	14/05/2014	Hangzhou, China	Scientific community (higher education, Research) - Industry		International

No.	Type of activities	Main Leader	Title	Date	Place	Type of audience	Size of audience	Countries addressed
30	Posters	VYSOKA SKOLA CHEMICKO-TEC HNOLOGICKA V PRAZE	Modelling of Emulsion Copolymerization in Semi-batch and Continuous Tubular Reactors	14/05/2014	Hangzhou, China	Scientific community (higher education, Research) - Industry		International
31	Posters	THE CHANCE LLOR, MASTERS AND SCHOLARS OF THE UNIVER SITY OF CA MBRIDGE	Online monitoring of emulsion polymerization with Raman spectroscopy, conductivity an d mass spectroscopy	06/05/2014	Europact, Dechema, Frankfurt	Scientific community (higher education, Research) - Industry		International
32	Web sites/Applications	CHEMISTRY INNOVATION LIMITED	Google Analytics added, literature list updated, home page updated	06/04/2014	http://www.coopol.eu/	Scientific community (higher education, Research) - Industry - Civil society- Policy makers - Medias		International
33	Organisation of Workshops	Cybernetica AS	Cybernetica CENIT training event - for Coopol researchers	31/03/2014	Cybernetica AS, Trondheim	Scientific community (higher education, Research)	10	International
34	Posters	UNIVERSITAET HAMBURG	Process intensification of continuous emulsion polymerization reaction using smart scale PTFE tubular reactors	17/03/2014	Continuous Flow Technology in Industry II, Robinson College, Cambridge, UK	Scientific community (higher education, Research) - Industry		International
35	Web sites/Applications	CHEMISTRY INNOVATION LIMITED	Women in science article added, literature list updated	25/11/2013	http://www.coopol.eu/	Scientific community (higher education, Research) - Industry - Civil society- Policy makers - Medias		International

No.	Type of activities	Main Leader	Title	Date	Place	Type of audience	Size of audience	Countries addressed
36	Oral presentation to a scientific event	THE UNIVERSITY OF WARWICK	Online monitoring of emulsion polymerizations using Raman Spectroscopy	06/11/2013	AiCHE 2013 Annual Meeting, San Francisco, USA	Scientific community (higher education, Research) - Industry - Civil society- Policy makers - Medias		International
37	Web sites/Applications	CHEMISTRY INNOVATION LIMITED	Dissemination event details added, literature list updated,	22/10/2013	http://www.coopol.eu/	Scientific community (higher education, Research) - Industry - Civil society- Policy makers - Medias		International
38	Oral presentation to a scientific event	VYSOKA SKOLA CHEMICKO-TEC HNOLOGICKA V PRAZE	Engineering insight into thermodynamic of emulsion polymerizations	14/10/2013	CHISA 2013, 14- 17 October 2013, Srni, Sumava, Czech Republic	Scientific community (higher education, Research) - Industry		International
39	Oral presentation to a scientific event	VYSOKA SKOLA CHEMICKO-TEC HNOLOGICKA V PRAZE	Mathematical modelling and on-line control of emulsion copolymerization - process model and optimization	14/10/2013	CHISA 2013, 14- 17 October 2013, Srni, Sumava, Czech Republic	Scientific community (higher education, Research) - Industry		International
40	Oral presentation to a scientific event	VYSOKA SKOLA CHEMICKO-TEC HNOLOGICKA V PRAZE	Discrete model of ag glomeration and fouling of emulsions	14/10/2013	CHISA 2013, 14- 17 October 2013, Srni, Sumava, Czech Republic	Scientific community (higher education, Research) - Industry		International
41	Oral presentation to a scientific event	VYSOKA SKOLA CHEMICKO-TEC HNOLOGICKA V PRAZE	Fouling of emulsions simulated by discrete element modelling	09/09/2013	APST 2013, Johannes Kepler University Linz, Altenberger Straße 69 4040, Linz, Austria	Scientific community (higher education, Research) - Industry		International

No.	Type of activities	Main Leader	Title	Date	Place	Type of audience	Size of audience	Countries addressed
42	Web sites/Applications	CHEMISTRY INNOVATION LIMITED	Changes to website - Partner details amended - Cambridge added - Project Flyer revised - News Item added	10/06/2013	http://www.coopol.eu/	Scientific community (higher education, Research) - Industry - Civil society- Policy makers - Medias		International
43	Oral presentation to a scientific event	VYSOKA SKOLA CHEMICKO-TEC HNOLOGICKA V PRAZE	Meso-scale Mode ling of Transport an d Reaction in Reconstructed Porous Polyolefin Particles	25/05/2013	2nd Working Party on Polymer Reaction Engineering, Frankfurt, Germany	Scientific community (higher education, Research) - Industry		International
44	Oral presentation to a scientific event	VYSOKA SKOLA CHEMICKO-TEC HNOLOGICKA V PRAZE	Mathematical Modelling of Heat Transfer in Polymer Foams: Morphology Optimization	25/05/2013	2nd Working Party on Polymer Reaction Engineering, Frankfurt, Germany	Scientific community (higher education, Research) - Industry		International
45	Posters	VYSOKA SKOLA CHEMICKO-TEC HNOLOGICKA V PRAZE	Meso-scale Mode ling of Transport an d Reaction in Reconstructed Porous Polyolefin Particles	24/05/2013	2nd Working Party on Polymer Reaction Engineering, Frankfurt, Germany	Scientific community (higher education, Research) - Industry		International
46	Posters	VYSOKA SKOLA CHEMICKO-TEC HNOLOGICKA V PRAZE	Mathematical Modelling of Heat Transfer in Polymer Foams: Morphology Optimization	24/05/2013	2nd Working Party on Polymer Reaction Engineering, Dechema, Frankfurt, Germany	Scientific community (higher education, Research) - Industry		International
47	Posters	VYSOKA SKOLA CHEMICKO-TEC HNOLOGICKA V PRAZE	Emulsion Copolymerization Mode ling: Coagulum Formation and Process Optimization	21/05/2013	11th Workshop on Polymer Reaction Engineering (PRE 2013), Dechema, Frankfurt, Germany	Scientific community (higher education, Research) - Industry		International

No.	Type of activities	Main Leader	Title	Date	Place	Type of audience	Size of audience	Countries addressed
48	Posters	UNIVERSITAET HAMBURG	Advantages of Milli-Structured PTFE -Tubular Reactors for Continuous Emulsion Polymerization Reactions	21/05/2013	11th Workshop on Polymer Reaction Engineering, Dechema, Frankfurt, Germany	Scientific community (higher education, Research) - Industry		International
49	Web sites/Applications	CHEMISTRY INNOVATION LIMITED	COOPOL	18/05/2012	http://www.coopol.eu/	Scientific community (higher education, Research) - Industry - Civil society- Policy makers - Medias		International
50	Posters	VYSOKA SKOLA CHEMICKO-TEC HNOLOGICKA V PRAZE	Dynamic Model of SRB production by emulsion polymerization	06/05/2012	Polymer Reaction Engineering VIII- Engineering Conferences International, Cancun, Mexico	Scientific community (higher education, Research) - Industry		International
51	Posters	UNIVERSITAET HAMBURG	Advantages of Milli-Structured PTFE -Tubular Reactors for Continuous Emulsion Polymerization Reactions	16/04/2013	2nd Working Party on Polymer Reaction Engineering, Hamburg, Germany	Scientific community (higher education, Research) - Industry		International
52	Posters	VYSOKA SKOLA CHEMICKO-TEC HNOLOGICKA V PRAZE	Interactions of polymer particles investigated by a discrete element model	19/11/2012	LAGEP - Meetings of the Centre Jacques Cartier 2012, Lyon, France	Scientific community (higher education, Research) - Industry		International
53	Posters	VYSOKA SKOLA CHEMICKO-TEC HNOLOGICKA V PRAZE	Dynamic modelling of styrene-butadiene rubber production by emulsion polymerization	19/11/2012	LAGEP - Meetings of the Centre Jacques Cartier 2012, Lyon, France	Scientific community (higher education, Research) - Industry		International

No.	Type of activities	Main Leader	Title	Date	Place	Type of audience	Size of audience	Countries addressed
54	Web sites/Applications	THE UNIVERSITY OF WARWICK	Project Website restructure and update	24/10/2012	http://www.coopol.eu/	Scientific community (higher education, Research) - Industry - Civil society- Policy makers - Medias		International
55	Oral presentation to a scientific event	VYSOKA SKOLA CHEMICKO-TECHNOLOGICKA V PRAZE	SBR production by emulsion polymerization: Dynamic modeling and intensification of the process	02/09/2012	International Symposium on Chemical Reaction Engineering ISCRE 22, Maastricht, Netherlands	Scientific community (higher education, Research) - Industry		International
56	Press releases	THE UNIVERSITY OF WARWICK	Project Start Details Released	29/05/2012	http://www2.warwick.ac.uk/fac/sci/eng/news/coopol_sustainable_manufacturing	Scientific community (higher education, Research) - Industry - Civil society- Policy makers - Medias		International
57	Posters	VYSOKA SKOLA CHEMICKO-TECHNOLOGICKA V PRAZE	Discrete Element Model for Prediction of Coalescence and Agglomeration	21/05/2012	SSCHE12, 39th International Conference, Hotel Hutník, Tatranské Matliare, Slovak Republic	Scientific community (higher education, Research) - Industry		International
58	Press releases	CHEMISTRY INNOVATION LIMITED	Project Funded Details Released	08/02/2012	https://connect.innovateuk.org/web/collaborative-projects/article-view/-/blogs/coopol-driving-processing-industries-towards-a-more-sustainable-model-of-	Scientific community (higher education, Research) - Industry - Civil society- Policy makers - Medias		International

Section B

TEMPLATE B1: LIST OF APPLICATIONS FOR PATENTS, TRADEMARKS, REGISTERED DESIGNS, UTILITY MODELS, ETC (CONFIDENTIAL)

TEMPLATE B2: OVERVIEW TABLE WITH EXPLOITABLE FOREGROUND (CONFIDENTIAL)