



NMP2-CT-2003-505862

INSERT

Integrating Separation and Reaction Technologies

STREP

Thematic priority 3 - NMP

PUBLISHABLE FINAL ACTIVITY REPORT

PERIOD COVERED : FROM February 1, 2004 TO January 31, 2007

PROJECT START DATE : February 1, 2004 DURATION : 36 Months

PROJECT COORDINATOR: PROF. EUGENY KENIG

ORGANISATION: UNIVERSITY OF DORTMUND

Introduction

At the heart of the chemical, petrochemical, fine chemicals, pharmaceuticals, biochemicals and electronics industries is the chemical conversion of raw materials to higher value products. Usually one or more separation steps are needed to isolate the desired products, prepare the feed mixtures, recover useful material from waste streams, etc. Recycles are also commonplace, allowing unconverted materials to be reused, rather than wasted. ***The overall chemical conversion process is thus a reaction and separation (R&S) system.*** These two phenomena interact strongly: as a result, process designs should aim to exploit synergies between them.

The general issue of process design and optimisation, taking into account reaction, separation and recycle, is an ongoing area of research, with applications for both chemical and biochemical reactions. Advanced process technologies across the spectrum of industries are exploiting beneficial interactions between R&S. In a number of cases, ***combining of the R&S steps within processing equipment leads to step changes in the state of the art.*** Examples include reactive distillation processes, membrane reactors, simulated moving bed reactors, reaction in supercritical fluids, reactive liquid-liquid extraction, reactive absorption and reactive stripping

In the recent years, the demand in the development of novel processes integrating traditional unit operations into more complex process combinations has been progressively increasing. These combinations lumping together functionalities of different type and nature bring about several important advantages among which are capital cost reduction, increase of product yield and considerable reductions in energy, water and solvent consumption as required by the EU Council Directive 76/769/EEC. To meet this demand, ***new integration concepts have to be developed.***

On the other hand, a range of issues form obstacles to the wide-spread adoption of advanced R&S technologies. These issues include:

- lack of systematic tools for generating and evaluating alternative processes at the initial stages of process design and of accurate experimental data
- uncertainty regarding scale-up of processes
- cost and fragility of materials used for membranes
- lack of understanding of the underlying physical and chemical phenomena and suitable models of processes and chemical systems and
- limited number of demonstration projects

Therefore, the full potential of a range of combined R&S separation devices has not been adequately addressed to date.

This situation has predestined the objectives of the INSERT project.

Main INSERT objectives are

- to provide better understanding of R&S processes by creating and using adequate and predictive process models
- to establish generic models and methods for rapid screening of alternative process sequences to best exploit interactions between the reaction, separation and mixing processes
- to develop entirely novel processes and novel process configurations that will outperform conventional processes with respect to energy consumption, waste generation, environmental impact, capital investment, product yield and product quality
- to develop a novel methodology for estimation of the optimal degree of integration of R&S steps
- to design, model, analyse and demonstrate the feasibility of promising new process equipment, accounting also for issues relating to scale-up and catalysis

- to validate the new methodology based on an extensive experimental programme
- to initiate and support close co-operation between industrial and academic Partners aimed at the optimisation of existing and creation of new economically beneficial R&S processes.

Contractors involved

Partic. No.	Participant name	Country
1	University of Dortmund (Co-ordinator)	Germany
2	University of Manchester Institute of Science and Technology	United Kingdom
3	EniTecnologie	Italy
4	SULZER AG	Switzerland
5	BASF AG	Germany
6	University of Stuttgart	Germany
7	Bayer Technology Services GmbH	Germany
8	National Oil Corporation "PETROM" S.A.	Romania
9	Research and Development Center for Refining Industry in Plock	Poland
10	University "POLITEHNICA" of Bucharest	Romania
11	University of Genoa	Italy
12	University of Pisa	Italy
13	Process Design Center B.V.	Netherlands
14	Eveco Brno, s.r.o.	Czech Republic

The Co-ordinator contact details

Prof. Eugeny Kenig

University of Dortmund, Department of Biochemical and Chemical Engineering

Mail address: Emil-Figge-Str. 70, D-44221 Dortmund, Germany

Phone: +49-231-755-2357,

Fax: +49-231-755-3035

Email: e.kenig@bci.uni-dortmund.de

<http://www.bci.uni-dortmund.de/tv/>

Work performed

INSERT activities comprised both theoretical and experimental work performed in parallel, with established close links between the Partners involved in the relevant tasks.

The main goal of the theoretical part was to develop an integration methodology and software tools, whereas the experimental part was mainly directed to provide necessary data for the model development and validation. In the first stage of the project, computer hardware/software facilities and interfaces were agreed and corresponding chemical test systems, catalysts, internals and equipment necessary for the project accomplishment were established. Besides, metrics on environmental impact, process economics, safety, etc. were specified.

Next, generic models and methods were developed to allow a range of alternative processes to be screened to best exploit interactions between the R&S processes. This work was supported by the investigation of swelling and shrinking behaviour of catalyst and scale-up methods.

Finally, the R&S integration methodology was developed that comprises two major steps (Figure 1):

- generation of suitable process alternatives for R&S processes, based on fundamental physicochemical data such as vapour-liquid equilibrium, chemical reaction properties, etc. as well as heuristic analysis, simplified process models and engineering experience
- detailed simulation and evaluation of the suggested alternatives and establishment of the optimal degree of unit integration using the rate-based process modelling.

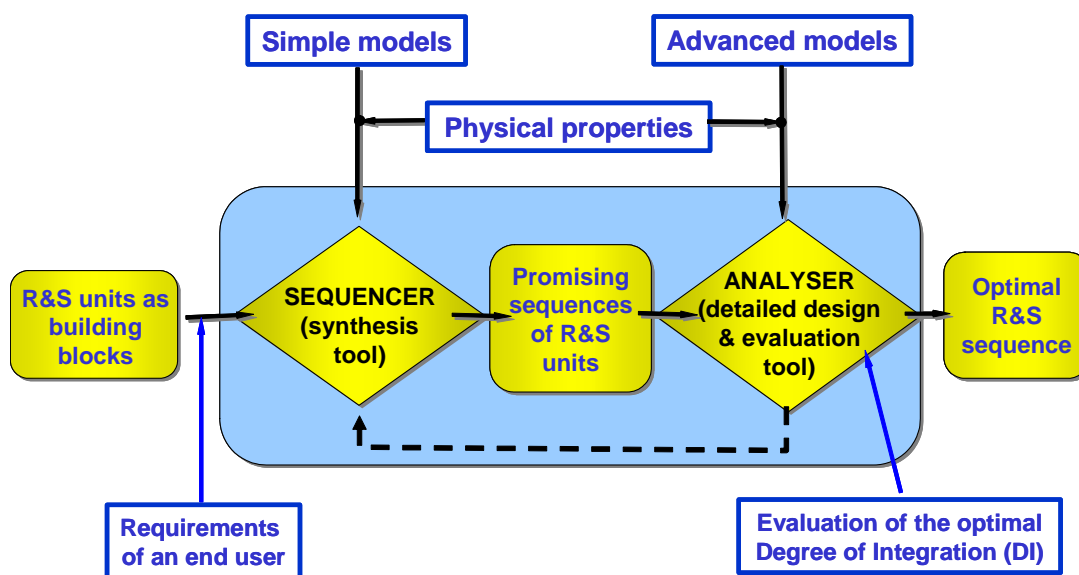


Figure 1. INSERT Methodology

These steps are supported by the relevant computer-aided methods and software tools. The first one represents a synthesis tool to provide promising process sequences (and therefore it is called SEQUENCER). The second tool is the process simulator with the advanced rate-based modelling framework. The latter provides the necessary process variables and allows a rigorous analysis of the sequences suggested by SEQUENCER. This tool is called ANALYSER.

With these steps performed, a user can estimate and apply the optimal degree of integration regarding the R&S steps and determine an ultimate optimal process configuration with possible innovative integration solutions.

The new models and methods were applied to industrial case studies relevant to a range of industries (e.g. pharmaceutical and biochemical, as well as petrochemical and chemical) and thoroughly evaluated.

Much effort was done to collect physicochemical and operational parameters necessary for the simulations. Missing data were measured, some other were estimated. All these data were collected in the relevant data base. Simultaneously, the equipment for mini-plant and pilot plant experiments was commissioned and pilot plant experimental investigations were performed. Reactions integrated with distillation, adsorption, membranes and dividing wall columns were investigated. Six chemical systems with modifications, different sequences were investigated at different partners' sites.

These complex and interrelated activities were based on a carefully designed work plan (Figure 2) as well as on a good communication flow, and close collaboration of all partners and co-ordinating team.

At the end of the project, promising process equipment was designed, modelled, analysed and the designs and models were tested. Highly novel processes, including the reactive dividing wall column, were developed and evaluated, and several relatively immature technologies were further advanced, potentially resulting in step changes in processing technologies. The models and methods developed formed the basis of generic computer-aided process-engineering tools for synthesis and optimisation of reaction-separation sequences.

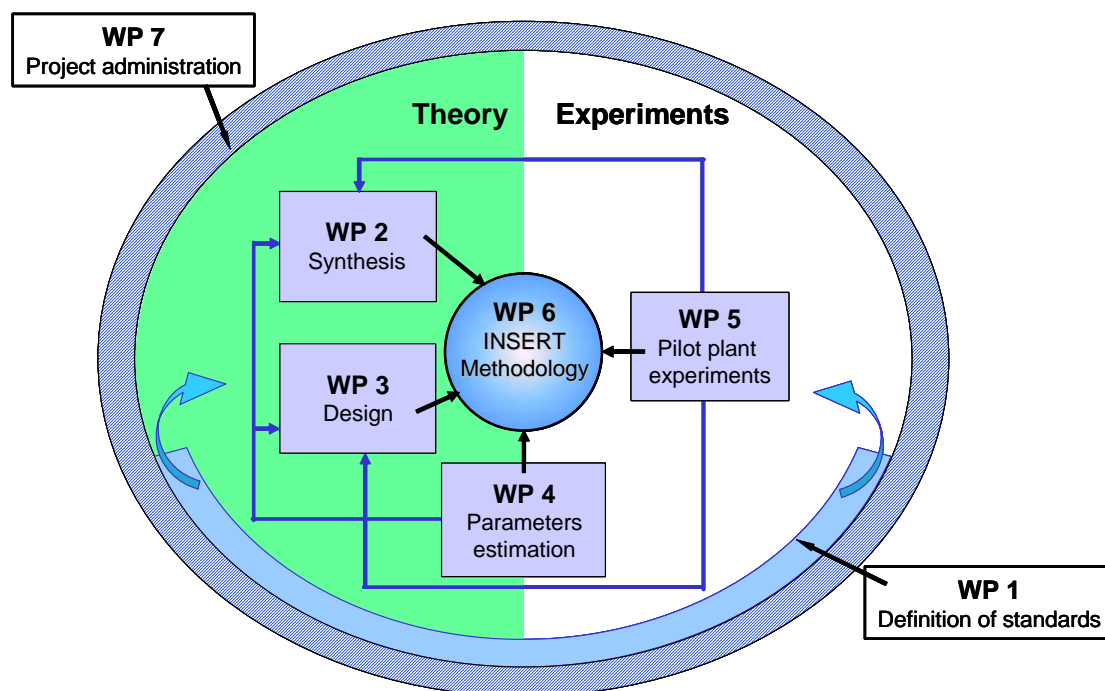


Figure 2. Work plan structure and work packages

All objectives of the project were reached, and even an extension of INSERT programme by an adsorption-based system was made possible.

The project results are disseminated in over 60 publications in high reputation scientific journals and at established conferences and workshops. This number will further grow.

Impact

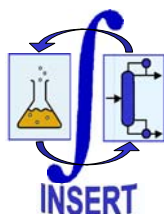
The results obtained in the Project help to

- shorten the time required from product idea to commercial plant by up to 50%;
- significantly reduce time and focus on laboratory, bench and pilot scale experiments (from 8 to 4 years in average), thus saving energy and resources in the design phase
- improve the possibilities of optimal process design and operation
- provide the foundations for continued collaborative research in this field.

INSERT also found a way to the integration of equipment based on the integration of efforts, skills and resources of the Partners. The Project results will facilitate

- a move from incremental to breakthrough strategy in process synthesis and design via integration of reaction and separation units
- an establishment of a long term research area related to the innovative integrated processes and process sequences
- an integration of research excellence via close collaboration of large industrial companies, SMEs, research institutions and universities from different parts of Europe and
- an integration of education and skills via incorporating the new methods into students courses and professional courses for engineers and executives

Project Website



The activities conducted in the frame of the INSERT Project are presented on an interactive website (www.insert-eu.de), which is maintained by the Coordinator and located at the Department of Biochemical and Chemical Engineering, University of Dortmund, Germany. The site has been established in order to provide an efficient and effective way of communication between project partners, if required also with the EC, and to disseminate information to the public.

The **Public** section of the INSERT site contains:

- ❑ a short project information and links to partners web sites as pop-up logos,
- ❑ link to the previous project INTINT and list of publications prior to the start of the project,
- ❑ non-confidential presentations, deliverables and publications,
- ❑ contact data of the EC and partner institutes.