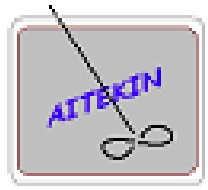

Project no. **506667**

Project acronym: **AITEKIN**

Project title:

Combination of AI techniques and software with advanced reactor equipment for efficient kinetics analysis in the chemical industry

Instrument: **CRAFT Co-operative Research Project**

Thematic Priority: **Horizontal Research Activities involving SMEs**

Title of report

Final activity report
P3 from month 1 to 24
Annexes 7: D5-D6-D8-D10-D11-D12-D13-D14,
Minutes_kick_off
minutes_poznan, minute_berlin_may2006

Period covered: from **25 May 2004** to **24 May 2006**
Date of preparation: **07 July 2006**

Start date of project: **25 May 2004** Duration: 24 months

Project coordinator name **Eugenio Pelosio**
Project coordinator organisation name **Technosind S.r.l.** Revision [1]

INDEX

1 PUBLISHABLE EXECUTIVE SUMMARY 4

1.1 Summary description of project objectives 4
1.2 Contractors involved 6
1.3 Co-ordinator contact details 6
1.4 Project website 6
1.5 Work performed and achieved results. 7
1.6 Use and impact 10

2 SECTION 1 – PROJECT OBJECTIVES AND MAJOR ACHIEVEMENTS 11

2.1 General objectives: 11
2.2 Achievements 11

3 SECTION 2 – WORKPACKAGE 12

3.1 WP 1 Equipment Installation 12
3.1.1 Objectives 12
3.1.2 Tasks 12
- Task 1 – Design and Setup of hardware 12
- Task 2 – Fine tuning 12

3.1.3 Deliverables 13
3.1.4 Milestones 13
3.1.5 Overview of technical progress 13
3.2 WP 2 Expert System Development for Reaction Mechanism Generation 14
3.2.1 Objectives 14
3.2.2 Tasks 14
- Task 3 – Selection of inference rules and pattern matching syntax. 14
- Task 4 – Code development 14

3.2.3 Deliverables 15
3.2.4 Milestones 15
3.3 WP 3 Chemical- algebraic translation software creation 16
3.3.1 Objectives 16
3.3.2 Tasks 16
- Task 5 – Comparison of commercial software for the treatment of algebraic symbols 16
- Task 6- Problem definition 16
- Task 7 – Development of the software code for the translation step 16

3.3.3 Milestones 17
3.3.4 Overview of technical progress 17
3.4 WP4 Reaction tests 18
3.4.1 Objectives: 18
3.4.2 Description of work 18
- Validation using xilene reaction (D10) 19
- Description of the experimental data set for the phenol reaction (D11) 19
- Tsr data treatment for phenol reaction (D11) 19

3.4.3 Deliverables D10 – D11 19
3.4.4 Milestones and result 19
3.5 WP5 Experimental runs and identification 20
3.5.1 Objectives: 20
3.5.2 Tasks 20

3.5.3 Description of work (see deliverable D12) 20
- Kinetics identification: data analysis and model discrimination 20

3.5.4 Deliverables 21
3.5.5 Milestones and result 21
3.6 WP6 Automated reactor design and control 22
3.6.1 Objectives 22
3.6.2 Tasks 22
- Task 11 – Automated reactor design (proprietary system) 22
- Task 12 – Automated reactor design (general purpose simulator) 22

3.6.3 Overview of technical work (see deliverable D13) 22
- Automated reactor design 22

3.6.4 Deliverables 23
3.6.5 Milestones and result 23
3.7 WP7 Project management 24
3.7.1 Objectives 24
3.7.2 Description of work 24
3.7.3 Deliverables 24
3.7.4 Milestones and result 24

4 SECTION 3 – CONSORTIUM MANAGEMENT 28

5 SECTION 4 – OTHER ISSUES 30

6 FINAL PLAN FOR USING AND DISSEMINATING THE KNOWLEDGE 31

6.1 Introduction 31
6.1.1 Strategy in dissemination and exploitation plan 31
6.1.2 Key Words in dissemination 31
6.2 Publishable results 32
6.3 PARTNERS CONTRIBUTION 33
6.3.1 Technosind, Nova System: Exploitation plan 33
Overview table 33
6.3.2 UOM, FE, EVECO and BUTiH: Exploitation plan 34
- Exploitable knowledge and its Use 34
- Dissemination of knowledge: Overview table 36

6.3.3 Polimeri contribution 39

1 Publishable executive summary

1.1 Summary description of project objectives

Reactors are the core elements of chemical processes, which consist of reactors and unit operations for the transformation of feedstocks into final products.

Several advanced commercial products are available for both simulation and optimisation of unit operations under steady and transient conditions.

This is not the case for chemical reactors, due to the variety and complexity of industrial reactions: in most commercial simulators the description of reactions is left to the user. This requires many experiments and the skill of highly qualified theoretical chemists, which can lead to unacceptably high costs. They can be reduced by software tools for the identification of arbitrarily complex kinetics and for the advanced control based on this identification step.

The outcome of Aitekin has been a prototype plug flow reactor with the necessary hardware to carry out temperature scanning kinetic experiments and the AI based software necessary to identify the kinetic mechanism and to design the industrial scale reactor and its control system with limited human involvement.

This objective can be divided into a number of intermediate steps, each of which is an important result of its own:

- A laboratory plug flow reactor for temperature scanning experiments.
- The automatic generation of reaction schemes, given reactants products intermediates and catalytic sites with the possibility of modifying the kinetic mechanisms suggested by this expert system.
- A symbolic translator from a chemical to an algebraic language for further data analysis.
- The rigorous regression analysis of temperature scanning experiments data, based on sensitivity equations, followed by model discrimination, if more than one kinetic mechanism was found.
- The design of an industrial scale reactor, its optimal control system and the automatic generation of computer code for use in a process simulator.

- The installation of a fully equipped temperature scanning reactor TSR
- The kinetic identification: data analysis and model identification
- The automatic reactor design

1.2 Contractors involved

The total consortium consists of five SME proposers and three Research Performers.

Organisation	Type	Role	Size	Country	Business Activity
Technosind S.r.l.	PRC	SME Coordinator	S2	CZ	Engineering enterprise
Eveco Brno, s.r.o	PRC	SME	S3	CZ	Engineering enterprise
Firth Executive	PRC	SME	S2	UK	Service provider
BUTiH	PRC	SME	S3	PL	Engineering Enterprise
Nova Systems Roma S.r.l.	PRC	SME	S3	I	Software house
Polimeri Europa	PRC	RTD Performer	S7	I	Chemical Company
UoM	HES	RTD Performer	S7	UK	Teaching& Research
UOP	PRC	RTD Performer	S7	UK	Chemical company

1.3 Co-ordinator contact details

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1.4 Project website

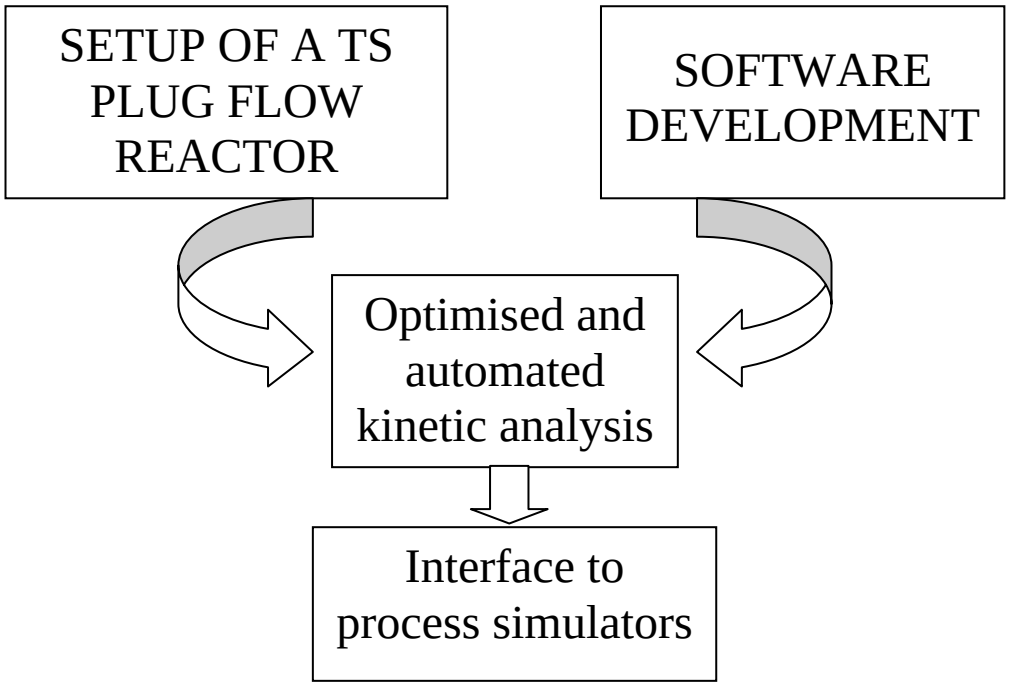
The website is located at The University of Manchester (UoM), Centre of Process Integration, (former UMIST) and includes a public and a confidential part. Access to the latter part is limited to partners and Commission officers.

The link address is:

http://www.cpi.umist.ac.uk/aitekin/

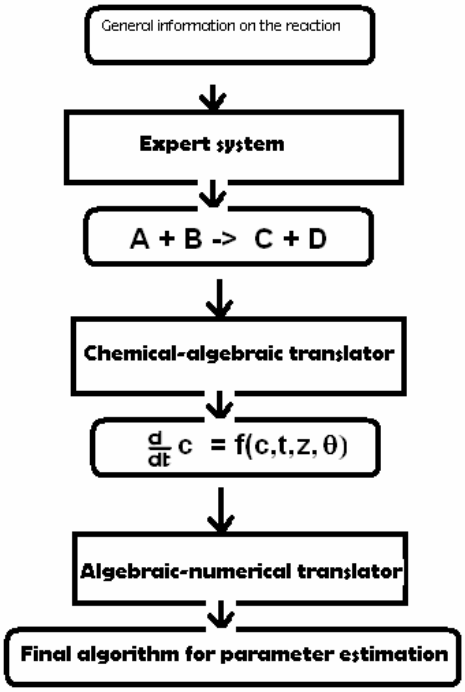
1.5 Work performed and achieved results.

The overall Aitekin project can be visualised as follows:



The setup of the experimental reactor has been completed at the site of the Research Performer Polimeri Europa. A picture of the experimental facilities is reported below.

The software developed can be summarized as indicated in the following graph:



The optimised and automated kinetic analysis, developed in the second year of activities, includes completion of the revision procedure, development of a seamless interface between the various parts of the algorithm and automated analysis of available experimental data and of those data that are presently being generated.

The interface to two largely widespread process simulators has been designed and is fully operational.

1.6 Use and impact

The use of the results obtained in Aitekin by the SMEs partners includes a full range of commercial activities:

1. Hardware, i.e. automated temperature scanning reactors, eventually in collaboration with the present producers of TSRs
2. Software for those laboratories that do not need the implementation of TSRs, either because they already have one or because they use a traditional approach to chemical kinetics (the software developed is largely independent of the approach)
3. Services for those companies that are not able or willing to carry out a full experimentation or analysis of data
4. Development of further interfaces for process simulators and/or inclusion of the software into them
5. A combination of 1) to 4)

A reduction of up to one order of magnitude in both costs and times is expected in the analysis of kinetic data in chemical laboratories, its amount depending largely on the level of integration that each laboratory will choose. The partners are confident that this approach to kinetic data in chemical reaction theory might well become a standard in the course of approximately 5-6 years. In this case a huge impact might be expected.

2 Section 1 – Project objectives and major achievements

2.1 General objectives:

The general objective of Aitekin is a prototype plug flow reactor with the necessary hardware to carry out temperature scanning kinetic experiments and the AI based software necessary to identify the kinetic mechanism and to design the industrial scale reactor and its control system with limited human involvement.

This objective can be divided into a number of intermediate steps, each of which is an important result of its own:

- A laboratory plug flow reactor for temperature scanning experiments.
- The automatic generation of reaction schemes both homogeneous and heterogeneous, using atom-molecule matrices, stoichiometric and thermodynamic feasibility checks with the possibility of modifying the kinetic mechanisms suggested by this expert system.
- A symbolic translator from a chemical to an algebraic language for further data analysis.
- The rigorous regression analysis of temperature scanning experiments data, based on sensitivity equations, followed by model discrimination, if more than one kinetic mechanism was found.
- The design of an industrial scale reactor, its optimal control system and the automatic generation of computer code for use in a process simulator.

2.2 Achievements

- The Execution and preliminary analysis of experiments
- The validation using the phenol reaction
- The validation using xilene reaction
- The kinetics identification: data analysis and model discrimination
- The automated reactor design

3 Section 2 – Workpackage

3.1 WP 1 Equipment Installation

Participant: EVECO, NOVA, POLIMERI, UOP
Lead contractor: Polimeri
Deliverable: D5
(Month: 0 to Month 12)

3.1.1 Objectives

Setup of a plug flow temperature scanning reactor. This include both hardware (plug-flow reactor and control instrumentation) and fine tuning procedures

3.1.2 Tasks

- **Task 1 – Design and Setup of hardware**

  The aim has been to provide an efficient and reliable reactor. This has involved the expertise of Polimeri Europa (Workpackage leader), where the actual reactor has been implemented, UOP and Eveco. The three partners have used their past experience in traditional experimental reactors, as well as the information gained from an accurate literature survey.

- **Task 2 – Fine tuning**

  Implementation of instrumentation equipment (measurement and control). Temperature scanning reactors require a careful design of input and environmental thermal conditions for the measurements to be statistically reliable. Additionally, measurements equipment, data logging, storage and retrieval have been carefully implemented by Nova Systems in close collaboration with Polimeri Europa.
  As per schedule the complete setup of a fully equipped TSR has been accomplished (see D5).

3.1.3 Deliverables

Setup of both temperature scanning reactor and control instrumentation (D5)

3.1.4 Milestones

The temperature scanning reactor is working flawlessly

3.1.5 Overview of technical progress

The test-reaction has been identified and the necessary chemical information has been collected (see D5 of this Report).

The setup of the plug flow temperature scanning reactor, including the control and acquisition system, has been completed (D5 of this Report).

3.2 WP 2 Expert System Development for Reaction Mechanism Generation

Participant: TECHNO, NOVA, POLIMERI ,UOP

Lead contractor: UoM

Deliverable: D6

(Month: 0 to Month 12)

3.2.1 Objectives

Development of an expert system for generating candidate reaction mechanisms

3.2.2 Tasks

- **Task 3 – Selection of inference rules and pattern matching syntax.**

Implementation of the inference rules into the selected shell, based on pattern matching. The inference rules include:

- Reactions with radical intermediates
- Reactions with homogeneous catalysts
- Reactions with heterogeneous catalysts

This part has been completed by UoM, supported by Technosind thanks to its experience in catalytic kinetics.

As per schedule the complete algorithm has been identified (see Annex 2). UoM was able to deliver more PMs without increasing the contracted cost which enhanced the quality of the deliverables presented. SME partners have been satisfied with this progress.

Identification of the algorithm for the expert system. This part of the programme was carried out jointly by UoM (Workpackage leader) for the chemical part and Nova System (for the computer science aspects).

- **Task 4 – Code development**

The operating system selected is Windows 95/98/NT/2000/XP. Guidelines for porting it to other operating systems have been provided.

3.2.3 Deliverables

Manual of the software (D6)

3.2.4 Milestones

Test cases are worked out satisfactorily

3.3 WP 3 Chemical- algebraic translation software creation

Participant: TECHNO, EVECO, FE, BUTiH, NOVA, POLIMERI
Lead contractor: POLIMERI
Deliverable: D8
(Scheduled: →Month: 5 to Month 14 Actual → Month: 3 to Month 16)

3.3.1 Objectives

Development of a software tool for the automatic translation from the chemical into the algebraic language. The implementation of a chemical-algebraic translator has been completely carried out. This part of the programme has been carried out jointly by all partners, except UoM, with which, however strict contacts have been maintained, so as to guarantee a consistent and seamless interface to the expert system and the automatic chemical-algebraic translator.
The complete algorithm has been implemented ahead of schedule.

3.3.2 Tasks

- **Task 5 – Comparison of commercial software for the treatment of algebraic symbols**

  Cost evaluation and optimisation.

- **Task 6- Problem definition**

  Selection of symbols and syntax rules for reactions with radical intermediates, homogeneous and heterogeneous catalysts. The result is that the kinetic mechanisms generated in Workpackage 2 are written in a suitable notation

- **Task 7 – Development of the software code for the translation step**

  - Implementation of the software for translating the symbols and syntax rules defined in Task 6 into the algebraic equations corresponding to the relevant

reaction rates (differential algebraic set of equations) according to the rules of the commercial software selected in Task 5

- Report describing the commercial software available for the transformation of algebraic strings into software code

- Software code and manual of the translator of the chemical notation into algebraic strings (input to the commercial software)

3.3.3 Milestones

- **The software necessary for the estimation of the kinetic parameters and for model** discrimination is now available. It consists of four steps:

- Automatic kinetic mechanism generation

- Symbolic representation of the reaction kinetics

- Translation of the symbolic chemical notation into a differential-algebraic set of equations (using the symbolic notation of a commercial software)

- The software containing the set of differential-algebraic equations is interfaced to the equipment developed in Workpackage 1

3.3.4 Overview of technical progress

The commercial software (Eas_stimate) for the treatment of algebraic language has been selected.

According to the rules of the commercial software selected, the new software (Chemnet) for translating the chemical symbols into the algebraic equations has been defined and implemented (see D6). The software code has been validated using the experimental data obtained from the temperature scanning reactor for the phenol reaction by Polimeri Europa (see D6).

3.4 WP4 Reaction tests

Participant: TECHNO, EVECO, BUTiH, POLIMERI, UoM

Lead contractor: POLIMERI

Deliverable: D10, D11, see annexes.

(Scheduled: →Month: 13 to Month 18 Actual → Month: 12 to Month 19)

3.4.1 Objectives:

Obtaining the amount of data, necessary for the kinetics identification step. Both temperature scanning and traditional plug flow reactors have been utilised for comparison

3.4.2 Description of work

A fully description of the performed work is in the annexed deliverable D10 and D11

A main target for the AITEKIN project is the development of integrated software packages. The first element of this software is a Chemical-Algebraic translator (Chemnet), in which reaction mechanisms are written using the traditional chemical notation. Its output are the corresponding kinetic model equations, which are directly fed to the Algebraic-Numerical translator (Eas-stimate, a commercial software that has been modified to fit the purposes of the project).

Chemnet performs the automatic transformation of the set of the kinetic steps that describe the full reaction scheme into the corresponding set of sensitivity differential equations (both ordinary and partial). This corresponds to moving from chemical to algebraic symbols.

Then Eas_stimate translates the equations into FORTRAN language followed by a non-linear parameter estimation which minimizes a suitable objective function, finding the most likely estimate of parameters. It provides also a statistical analysis for the values founded.

The experimental data from the temperature scanning reactor for the Phenol reaction reported in Paragraph 3 have been used for the validation of Chemnet.

Step-reactions are identified by Chemnet, which expresses their rate equations as functions of the concentrations of the adsorbed intermediates. Two examples have been considered for the validation of this complex mechanism identification.

- **Validation using xilene reaction (D10)**

The experimental data from the temperature scanning reactor for the UOP Xylenes reactions are reported in Annex 2 of the Sixth Month Report allowable in the AITEKIN Website. We have used these data for the validation of Chemnet.

The UOP test reaction may be summarized for the main compounds in the overall reaction:

- **Description of the experimental data set for the phenol reaction (D11)**

TSR experiments have been performed using benzene and H_2O_2 as reactants and water and sulfolane as solvents**.** The temperatures scanned, range from 70 to 100°C at a pressure of 4 atm to keep reagent mixture in the liquid state; 3.75 g of catalyst (Titanium – Silicalite 1 bounded with 20% of silica), diluted with quartz where loaded in the isothermal zone of the reactor. The flow rate of the feeding stream has been changed in order to obtain contact time $\tau w = 0.3 \div 4$ min, referred to the weight of active phase of catalyst (3g). The reaction is relatively exothermic (ΔH = -68.82 Kcal/moles).

In this way reagents and products concentration trends, have been collected performing various TSR runs at different flow rates.

- **Tsr data treatment for phenol reaction (D11)**

The reaction mechanism and the relevant kinetic model assumed to account for the data of the phenol reaction have been introduced in the Chemical-Algebraic translator (Chemnet) and the Algebraic-Numerical translator (Eas-stimate).

To this purpose both the original Wojciechowski method (fitting components rates) and a direct concentration-fitting method were used and compared.

3.4.3 Deliverables D10 – D11

A report with the experimental data obtained.

3.4.4 Milestones and result

Reaction test results – assessment of data consistency

3.5 WP5 Experimental runs and identification

Participant: EVECO, FE, BUTiH, POLIMERI, UoM

Lead contractor: EVECO

Deliverable: D12.

(Scheduled: →Month: 18 to Month 24 Actual → Month: 19 to Month 24)

3.5.1 Objectives:

Data analysis and model discrimination software using the previously developed tools

3.5.2 Tasks

- **Task 9 – Identification of the kinetic mechanisms for the reactions selected using the commercial software**

Kinetic parameter estimation through statistical analysis of results.
Estimation of preexponential factors, activation energies and radical intermediates.

- **Task 10 – Model discrimination**

Comparison of results obtained using all the kinetic mechanisms suggested by the inference machine developed in Workpackage 2 and selection of the most likely mechanism.

3.5.3 Description of work **(see deliverable D12)**

- **Kinetics identification: data analysis and model discrimination**

The chemical-algebraic translator *Chemnet* and algebraic-numerical translator *Eas_stimate* have been validated on a test reaction performing a model discrimination analysis.
The chosen test reaction is the catalytic xylenes reaction with ethyl-benzene and a strong excess of hydrogen.
The reaction was performed in the UOP laboratories in a plug-flow reactor with the Temperature Scanning technique. The experimental data are reported in Annex 2 of the Sixth Month Report allowable in the AITEKIN Website.

The reaction mechanism has been simplified by taking into account only the main compounds. Since the system was far from equilibrium, all reactions were treated as reversible.
Four different models have been compared to describe the overall reaction in terms of different single reactions.
For a complete description see annex D12

3.5.4 Deliverables

Technical reports (contained in the quarterly report D12) with the results obtained (mechanism selection and kinetic parameters identification) for the test cases.

3.5.5 Milestones and result

The whole procedure for the proper identification of the elementary reactions of complex kinetic mechanisms has been validated.

3.6 WP6 Automated reactor design and control

Participant: TECHNOSIND, EVECO, BUTiH, POLIMERI, UoM, UOP

Lead contractor: UOP

Deliverable: D13, see annex.

(Scheduled: →Month: 18 to Month 24 Actual → Month: 19 to Month 24)

3.6.1 Objectives

Automated reactor design and control

3.6.2 Tasks

- **Task 11 – Automated reactor design (proprietary system)**

Procedure for the automated development of the code describing the reactor with the kinetics resulting from the previous analysis for insertion into a proprietary process simulation.

- **Task 12 – Automated reactor design (general purpose simulator)**

The ASPEN environment has been selected as general purpose simulator.

3.6.3 Overview of technical work (see deliverable D13)

- **Automated reactor design**

The objective of the activity automated design of reactors is the development of suitable FORTRAN code for the insertion of the kinetic models into process simulators.
This part of the project has been assessed using the corresponding code developed previously (Reaction, Chemnet and Eas_stimate) for the proprietary simulator CHEOPE by Polimeri Europa. The automated procedure has been validated for CHEOPE using the Phenol reaction as the test case. This validation work allows the procedure to be extended to a widespread commercial simulator (e.g.: Aspen Plus).
This report describes the procedure for the automated development of the code describing the reactor with the Phenol kinetics for insertion into the Polimeri Europa proprietary process simulator and the results obtained.
The described reaction has been extensively studied inside this project using the Temperature Scanning Reactor and the collected experimental data have been used for

the development of the kinetics of the reaction as well as for the validation of the packages Chemnet and Eas_stimate.

In Cheope as well as in AspenPlus, users can provide subroutines for the definition of kinetic model for various reactor and unit operation models (RPlug, RBatch, RCSTR). For the reactor models, the kinetics subroutine calculates the rate of generation for each component in each substream. If solids participate in the reactions, the kinetics subroutine also accounts for changes in the outlet stream particle size distribution, and in the component attribute values. Parameters are usually passed to the user subroutine through the argument list and/or the common blocks to access parameters specific to the different unit operation models. In addition the reaction stoichiometry and the associated user-supplied kinetics subroutine name must be defined.
For a more complete description see annex D13.

3.6.4 Deliverables

A technical manual containing design specifications and procedures.

3.6.5 Milestones and result

The overall procedure for a completely automated reactor design has been validated and the final goal of the project has been attained.

3.7 WP7 Project management

Participant: Technosind, Eveco, FE, BUTiH, Nova Systems, Polimeri, UMIST, UOP.

Lead contractor: Technosind

Deliverables: D1, D2, D3, D4, D7, D11, D14

3.7.1 Objectives

Project Management

3.7.2 Description of work

- **Project presentation**
- **Reporting**

5 quarterly reports

1 mid-term report

1 final report

- **Review and assessment**

Technical assessment of results vs. project objectives.

Financial review of expenditures vs. project budget

- **Task required by SMEs to acquire the technical know-how and to protect the knowledge generated.**
- **Exploitation and dissemination task.**

3.7.3 Deliverables

5 quarterly reports D2, D3 (sixth month report), D4, (D9*), D11

8 interim report D1, D5, D6, D8, D10, D12, D13, D14.

2 annual reports D7, D15

1 final report D15

* the content of D9 is in the First annual Report D7

3.7.4 Milestones and result

Accurate project management.

Table 1: Deliverables List

Del. No.[1]	Deliverable name	WP no.	Lead participant	Nature[2]	Dissemination level[3]	Delivery date (proj. month)[4]
D1	Project Presentation	7	UMIST	O	PU	3
D2	First Quarterly Report: description of • Selection of inference rules for D6 • Selection of algorithms for variable mesh grids • Comparison of commercial software	7	Technosind	R		3
D3	Second Quarterly Report: description of • Definition of chemical-algebraic translation rules • Degree of advancement of D5 and D6	7	Technosind	R		6
D4	Third Quarterly Report: description of • Degree of advancement of D2 and D3	7	Technosind	R		9
D5	Design and installation of a fully equipped temperature scanning reactor	1	Polimeri	P	PP	12
D6	Reaction generation software	2	UMIST	O	RE	12
D7	Annual Progress Report: description of: • Complete equipment • Reaction generation software (with manual)	7	Technosind	R	PU	12
D8	Software for translating chemical kinetic notation into algebraic- (partial) differential equations	3	Technosind	O	RE	14
D9	Fourth Quarterly Report: description of • Degree of advancement of D10 • Translation	7	Technosind	R		15

	software (with manual)					
D10	Execution and preliminary analysis of experiments on the two test cases selected	4	Polimeri	R	CO	18
D11	Fifth Quarterly Report: description of • Experimental data sets	7	Technosind	R		18
D12	Kinetics identification (data analysis and model discrimination)	5	Eveco	R	CO	24
D13	Automatic reactor design	6	UOP	R	CO	24
D14	Exploitation plan	7	Technosind	R	PU	24
D15	Final Report	7	Technosind	R	PU	24

[1] Deliverable numbers in order of delivery dates: D1 – Dn

[2] **R** = Report
P = Prototype
D = Demonstrator
O = Other

[3] **PU** = Public
PP = Restricted to other programme participants (including the Commission Services).
RE = Restricted to a group specified by the consortium (including the Commission Services).
CO = Confidential, only for members of the consortium (including the Commission Services).

Table 2: Milestones List

Workpackage	Timing (Month No)	Type	Assessment Criteria
A. Equipment Installation	12	Reactor vessel and equipment	Reactor and instrumentation fully operational
B. Expert System for generation of kinetic mechanisms	12	Software code	Full debugging and testing
C. Chemical-algebraic translation software creation	14	AI software	Full debugging and testing
D. Reaction tests	18	Reaction tests results	Data consistency
E. Parameter estimation and model discrimination	24	Final kinetic mechanism identification	Statistical analysis
F. Reactor design	24	Full design using the new methodology	Comparison with traditional design techniques

4 SECTION 3 – CONSORTIUM MANAGEMENT

The good agreement between partners allowed a smooth and successful management. A detailed explanation of main questions is reported in Periodic Management Report.
The distribution of the first and second tranches is detailed in the Annexes.
Some minor changes were necessary for accomodating two unforeseen financial audits

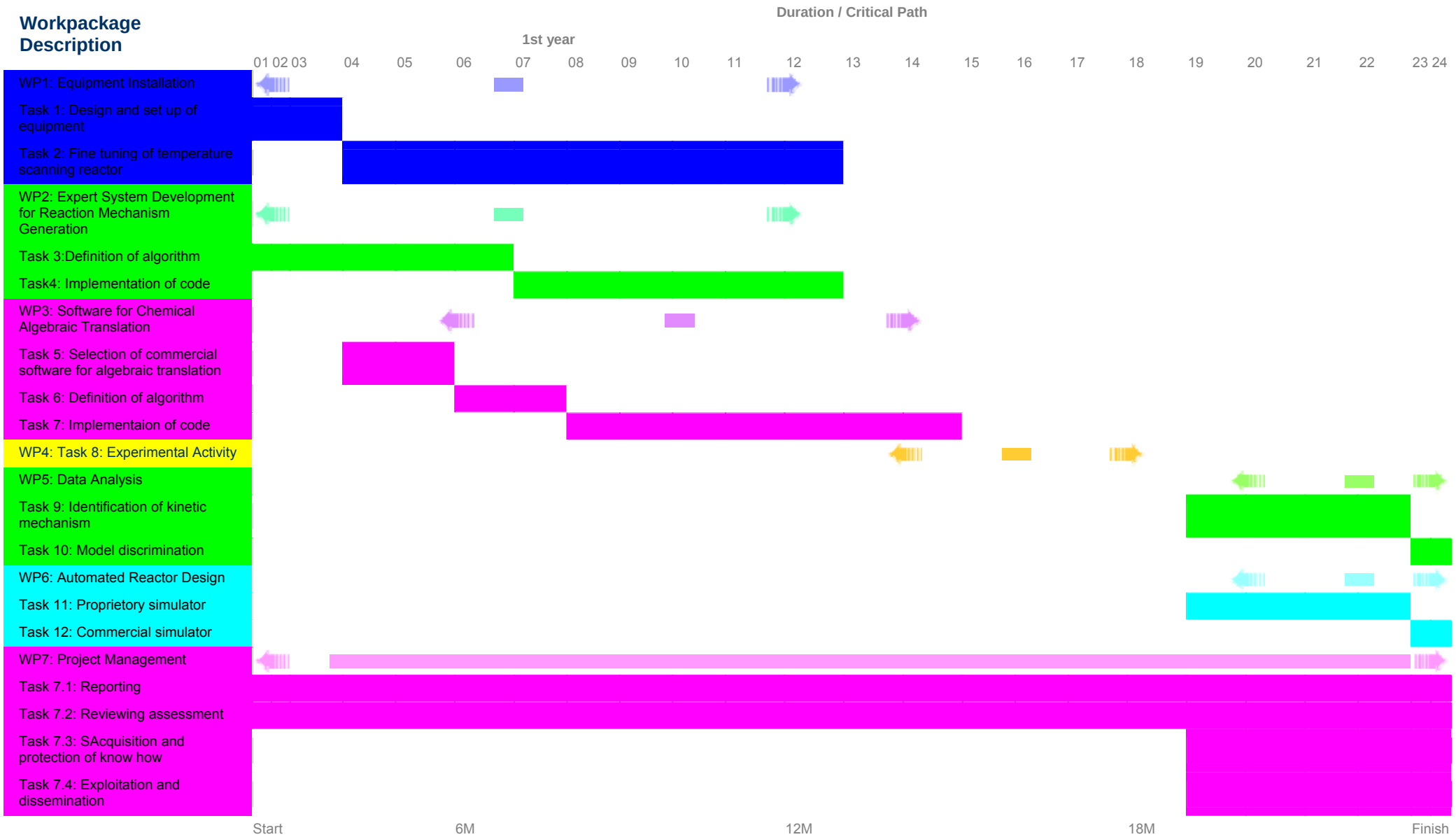
All main data are published in the AITEKIN web site.

The flow of information has taken place in a flawless and efficient manner. Communications among partners have relied largely on the interactive web service set up by UOM and, occasionally, on electronic mail. Both public (more than 600 visits from the scientific and industrial public) and confidential website (again more than additional 500 visits) has been very frequently visited which is a proof of a considerable interest and already started dissemination
There have been five meetings:

- CASTEL GANDOLFO (ROME) 27 – 28 May 2004, hosted by TECHNOSIND (see minutes_kick_off)
- PORTHDAFARCH, WALES - 15-19th November 2004, hosted by FIRTH EXECUTIVE
- NOVARA - 20/21 June 2005, hosted by POLIMERI EUROPA
- POZNAN, Poland – 27/28 January 2006 hosted by BUTiH (see minutes_poznan)
- BERLIN, Germany – 16/17 May 2006 hosted by TECHNOSIND (see minutes_berlin_may2006)

See annexed minutes of Rome, Poznan and Berlin meetings (minutes_kick_off , minutes_poznan and minute_berlin_may 2006).

Table 3: Workpackages - Plan and Status Barchart



5 Section 4 – Other issues

The project has greatly benefited from the excellent complementarity between all the partners (both SMEs and RTD performers), as was experienced in the previous 12 months.
The distribution of activities among the partners has taken place as foreseen in the project.

While the co-ordination and the general supervision of the project rest with the SMEs, which first developed the inception of Aitekin, the actual implementation of the activities in the second twelve months of the project has been mainly the responsibility of the three RTD performers, with the important contribution of all SMEs. In particular, Polimeri Europa and UOP concentrated on the reactor experimental activities, whereas UOM's main task has been, as per schedule, the implementation of the expert system. The UoM delivered more PMs without increasing the contracted cost which has been appreciated by the project partners.
The main experimental tests have been carried out by Polimeri Europa with the assistance of other partners, who have provided literature data for optimal experimental settings.
The balance of the work in terms of resources and personmonths between SMEs and RTD performers agrees very well with the one foreseen by the approved Revised Workplan (approx. a ratio of 1.5).

6 final plan for using and disseminating the knowledge

see deliverable D14 for a detailed explanation.

6.1 Introduction

6.1.1 Strategy in dissemination and exploitation plan

Two strategies for the exploitation plan are presently being considered.
First, we are trying to estimate the degree of acceptance of the new tools by professional chemists. Thus, beta versions of the algorithms have been delivered to selected groups of chemists working at Polimeri Europa and UOP (both entitled to use the software according to the Consortium agreement) in departments other than those involved in the project. A periodic three month evaluation period has been allowed.
It was decided not to submit a questionnaire, but rather to prompt for comments on perceived difficulties and suggested improvements. The only request is to provide an order-of-magnitude estimate for the value of the software, based on their experience. Using these comments a full-fledged questionnaire will be developed for other users out of the Consortium, who will be given a demo version for evaluation. These users will be selected from the list of members of Eurokin willing to participate in this evaluation. The pricing policy will be decided upon the information provided by these users.

Secondly, contacts are presently underway to try to establish an agreement with the spin-off company SE Reactors.

The basis for some kind of collaboration with the Institut für Angewandte Chemie Berlin-Adlershof eV, where there is the only TSR provided by SE Reactors in Europe, have been informally settled in the last meeting (contact of FE, UOP and Technosind with the Institute).
This is precisely the reason for having the last meeting in Berlin.

6.1.2 Key Words in dissemination

- **DEVELOPMENT NEW COMMERCIAL AREAS**
- **INTERNATIONAL BUSINESS LINKS**
- **REFERENCES RELIABILITY IN INTERNATIONAL TENDERS & BIDDINGS**
- **IMPLIED WARRANTY FOR MARKETING NEW PRODUCTS**

6.2 Publishable results

An abstract has been submitted to the 9th Conference on Process Integration, Modelling and Optimisation for Energy Saving and Pollution Reduction PRES 2006.

This first presentation of Aitekin has been accepted for Oral presentation.

The following journals are presently being considered for the submission of papers related to Aitekin and the results obtained in this project.

1. Applied Thermal Engineering
   Editor-in-Chief: Prof David A Reay, DRA Ltd, Tyne and Wear, UK

2. Heat Transfer Engineering
   Editor-in-Chief: Prof. Afshin J. Ghajar, School of Mechanical and Aerospace Engineering, Oklahoma State University, Stillwater, USA

3. Journal of Cleaner Production
   General Editor: Prof. Don Huisingh, Center for Cleaner Products and Clean Technologies, University of Tennessee, Knoxville, USA

4. Resources, Conservation and Recycling
   Journal Chief Editor: Dr Ernst Worrell, Lawrence Berkeley National Laboratory, Berkeley, CA, USA

5. Integrated Processes and Energy Saving
   Member of the Editorial Board: Prof Petro Kapustenko, Kharkiv Polytechnic Institute University, Kharkiv, Ukraine

6. Drying Technology - an International Journal
   Member of the Editorial Board: Dr Tadeusz Kudra, CANMET Energy Technology Centre, Canada

7. ENERGY - The International Journal
   Editor-in-Chief: Prof. Noam Lior, University of Pennsylvania, Philadelphia, PA 19104-6315, USA

8. Clean Technologies and Environmental Policy
   Editor-in-Chief: Dr. Subhas K. Sikdar, National Risk Management Research Laboratory, United States Environmental Protection Agency, 26 West Martin Luther King Drive, Cincinnati, OH, 45268, USA

On a very competitive scientific world-forum the actual publication is a result of a severe selection procedure. However as the leading RTD personalities have an excellent track record we are confident that the project results will find their way to one or more of these high impact journals.

However, following the IPR procedure for CRAFT projects, publications will be subject to the approval of those SMEs that are exclusive owners of the research results and would agree to publish only parts which would not undermine their IPRs.

Since the appropriate measures to protect IPRs are still underway, a publishable summary of exploitable results is not provided.

6.3 PARTNERS CONTRIBUTION

6.3.1 Technosind, Nova System: Exploitation plan

This consideration has been jointly written by Technosind and Nova System.

Exploitable Knowledge	**Exploitable product(s) or measure(s)**	**Sector(s) of application**
Expert RXN Software Chemnet	Expert System AI Based Software & Control System	Chemical Industry, Research
Timetable for commercial use	**Patents or IPR protection**	**Owner & Partners**
2007	Copyright planned for 2007	SME….others

Overview table

DATES	TYPE	AUDIENCE	SIZE of Audience	Partner Responsable involved
Current publications	*AITEKIN: A new software tool for enhanced kinetics studies…..more*		*1500 researchers academics decision makers*	*SME RTD others*
2007 Future publications	*1.An Effective Algorithm for complex Reaction Network Construction 2. Sensor Placement for Systems with Model Uncertainty*	*World wide Research, Industry, Higher Education*		*UoM Polimeri*
Exhibition	*Industry Sector*	*World wide Research & Industry*		
Internet web	*General Public, Academia*	*World wide*	*Appr. 5000/7000*	*UoM*

6.3.2 UOM, FE, EVECO and BUTiH: Exploitation plan

- **Exploitable knowledge and its Use**

  This section will only present exploitable results, defined as knowledge having a potential for industrial or commercial application in research activities or for developing, creating or marketing a product or process or for creating or providing a service.

Exploitable Knowledge (description)	**Exploitable product(s) or measure(s)**	**Sector(s)** of application	Timetable for commercial use	Patents or other IPR protection	**Owner** & Other Partner(s) involved
1. Expert_RXN software	Expert system	Chemical Industry	2007	Copyright planned for 2007	FE Ltd

- Exploitable result: Expert_RXN is useful software product that combines the novel reaction generation algorithm and expert system into an industrial strength vehicle for building sound mathematical models to help suggest alternative models, to select the most suitable model and to discriminate rival models.
- Firth Executive Ltd will be the owner of the Software and will carry out the commercial exploitation of the package. It will be able to license the Software and/or to conduct its own consulting activities using the Software
- The result will be exploited either directly by FE Ltd, or by licensing the Software to third parties.

- Future work will be focus on developing new approaches to minimise the uncertainty in the kinetic model parameters and to maximise the information for model discrimination by the design of new experiments when appropriate.
- A copyright for Expert_RXN will be obtained.
- Several potential users have been informed about Software and their responses have been positive.
- Development of reaction and combustion processes based on Expert_RXN will lead to economically and environmentally more efficient technological solutions which in their turn will have positive socio-economic impact.

- **Dissemination of knowledge: Overview table**

Planned /actual Dates	Type	Type of audience	Countries addressed	Size of audience	Partner responsible /involved
	Press release(press/radio/TV)	*General public*			
2006-2007	*Publication of a leaflet English and Polish versions*	*General public, Industry*	European countries	*2000*	*FE Ltd, BUTiH*
	Media briefing	*Higher education*			
2006, 2007	***Conferences:*** *PRES, CHISA, ESCAPE, CISAP annual and bi-annual conferences*	*Research, Industry, Higher Education*	European and other countries	*3000-5000 researchers, academics and decision-makers*	*UoM, FE Ltd*
	Exhibition	*Industry (sector x)*			
	Current publications				
2006	*Bagatin, Palmery, Theodoropoulos*, Klemes, Galloway, Pelosio, Dovi, Firth, Kowalska, Urbaniec AITEKIN: A new software tool for enhanced kinetics studies, PRES2006, #1455, Prague, 2006*	*Research, Industry, Higher Education*	European and other countries	*1500*	*UoM, FE Ltd*
	Future publications				
2006-2007	*1. An Effective Algorithm for Complex Reaction Network Construction, Wenling Zhang, Costas Theodoropoulos and Robin Smith, prepared for submission to Journal of Combinatorial Chemistry* *2. Sensor Placement for Systems with Model Uncertainty, Wenling Zhang and Costas Theodoropoulos, in preparation* *3. Publishing a communication on AITEKIN results and relevant contact data (in Polish) professional journal Przemysl Chemiczny (Chemical Industry)*	*Research, Industry, Higher Education*	World wide		*UoM* *UoM* *BUTiH*

Planned /actual Dates	Type	Type of audience	Countries addressed	Size of audience	Partner responsible /involved
2004	***Project web-site:*** *http://www.cpi.umist.ac.uk/aitekin/ with the full information about EXPERT_RXN*	*General public, Industry, Academia*	World wide	*Appr. 5000-7000*	*UoM*
2006	*Publishing a communication on AITEKIN results and relevant contact in:* *- BUTiH website www.butih.pl* *- website of the Department of Process Equipment, Warsaw Univ Tech.* *www.zap.pw.plock.pl* *- website of the Institute of Process and Environmental Engineering, Faculty of Mechanical Engineering at Brno University of Technology http://www.upei.fme.vutbr.cz/*	*General public, chemical engineering and industrial communities*	*Central and East European countries*	*Appr. 2000* *Appr.500* *Appr. 2000*	*BUTiH* *EVECO*
	Posters				
	Poster at conference	*Research, Industry, Higher Education*	Europe	*500*	*???*
	Flyers				
	Direct e-mailing				
	Film/video				

Every opportunity will be exploited to inform potential users of the Software. Annual and bi-annual ***conferences*** such as CHISA, PRES, CISAP, ESCAPE are the perfect spot for dissemination activities among the target audience.

The results are reported in PRES 2006 Proceedings: *Bagatin, Palmery, Theodoropoulos*, Klemes, Galloway, Pelosio, Dovi, Firth, Kowalska, Urbaniec AITEKIN: A new software tool for enhanced kinetics studies, PRES2006, #1455, Prague, 2006.* The target audience is about 500 chemical engineering experts from 49 countries.

Contribution is being prepared for

- Journal of Combinatorial Chemistry: W. Zhang, K. Theodoropoulos and R. Smith, An Effective Algorithm for Complex Reaction Network Construction
- Another publication being prepared: W. Zhang and K. Theodoropoulos, Sensor Placement for Systems with Model Uncertainty
- Publishing a communication on AITEKIN results and relevant contact data (in Polish) professional journal Przemysl Chemiczny (Chemical Industry)

- A website (http://www.cpi.umist.ac.uk/aitekin/) is being in functional almost from the beginning of the Project and will stay functioning after the end of the project. Complete information about EXPERT_RXN is posted on this website (2004)

Publishing a communication on AITEKIN results and relevant contact in:

- BUTiH website, www.butih.pl (2006)
- website of the Department of Process Equipment, Warsaw University of Technology, www.zap.pw.plock.pl (2006)
- EVECO website http://www.evecobrno.cz/vyzvy_e.html (2006)
- website of the Institute of Process and Environmental Engineering, Faculty of Mechanical Engineering at Brno University of Technology http://www.upei.fme.vutbr.cz/ (2006)

6.3.3 Polimeri contribution

Many aspects of the AITEKIN project are of interest to Polimeri Europa internally and also results of Polimeri Europa can be applied and exploited by others.

Based on the experience of making use of kinetic design simulation tools Polimeri Europa believes that by using the advanced and validated AITEKIN capability a substantial amount of money can be saved in two main areas:

- Minimising the chemical process development time by using advanced design tools
- Minimising the development phase equipment and test runs costs

The AITEKIN project also provided Polimeri Europa with an extended network of contacts in the field of kinetic modelling, which information can be shared and discussed in future occasions.

Therefore Polimeri Europa will:

- use the knowledge gained in internal research and design projects
- publish technical papers and reports about the AITEKIN test cases, results, and knowledge
- establish the AITEKIN test cases as benchmark tests for kinetic software tools in the scientific community with the objective of accelerating and improving kinetic modelling development.