

Executive Summary

EU FP7 project “Process Intensification methodologies applied to Liquid-Liquid Systems in structured equipment” (PILLS)

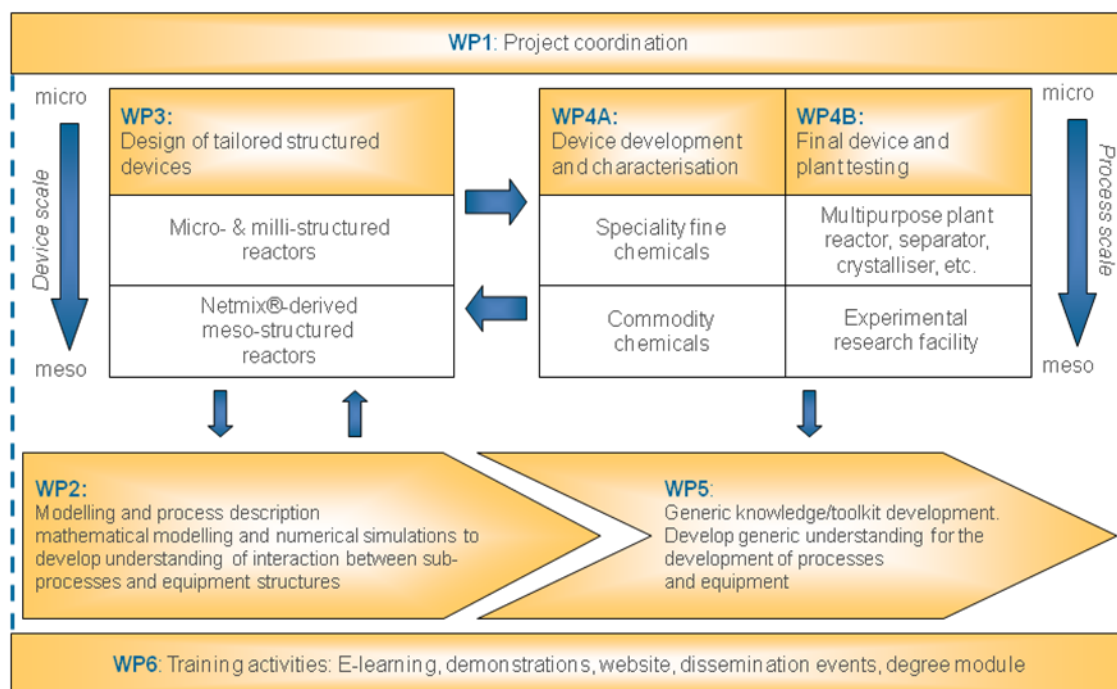


Figure 1: Schematic summary of Work Package contributions

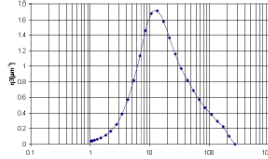
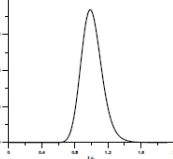
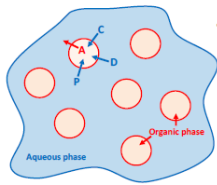
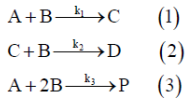


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Figure 2: Multiphase Reactor Models

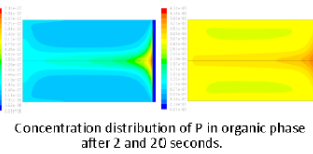
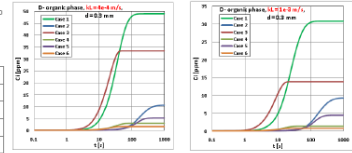
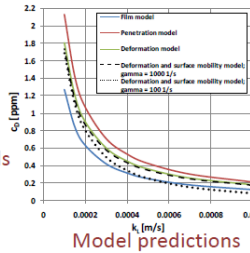
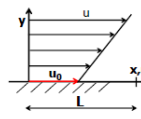
Integration of predictive models using CFD and hybrid modelling methods. Consider following set of complex reactions in the liquid-liquid system and predict drop RTD and drop size



Case	Inlet Temp (°C)	W _B	W _A	W _{cat}	W _{Co}	aqueous Flow (kg/h)	organic Flow (kg/h)	Total Flow (kg/h)
1	100	1	0.03	0.65	0.32	250	10.2	260.2
2	70	1	0.03	0.65	0.32	250	10.2	260.2
3	100	1	0.03	0.7	0.27	250	10.2	260.2
4	70	1	0.03	0.7	0.27	250	10.2	260.2
5	70	1	0.03	0.65	0.32	250	12.1	262.1
6	70	1	0.03	0.7	0.27	250	12.1	262.1

predicted RTD and drop size distribution

Mass transfer scheme and model fundamentals and comparison of models



Model predictions

Concentration distribution of P in organic phase after 2 and 20 seconds.

Figure 3: Micro- and meso-structured devices for two-phase liquid-liquid reactions

Micro-structured reactor (IMM)



Pilot-scale StarLam micromixer made from tantalum

Meso-structured reactor (FLU)



Machining of the Stainless Steel plates (top) and one of the reactor plates after machining (right)



Reactor plate coated with tantalum to prevent corrosion issues (below)

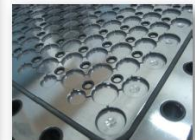
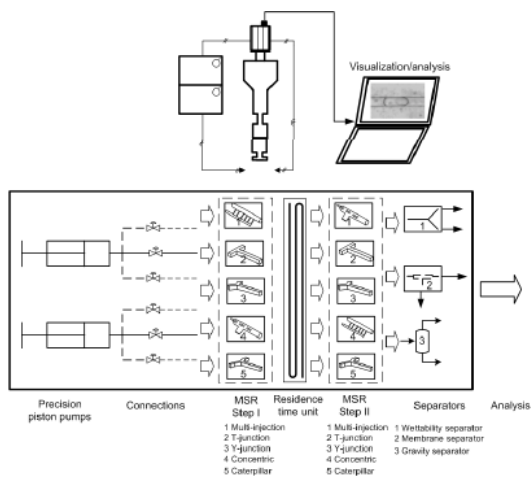
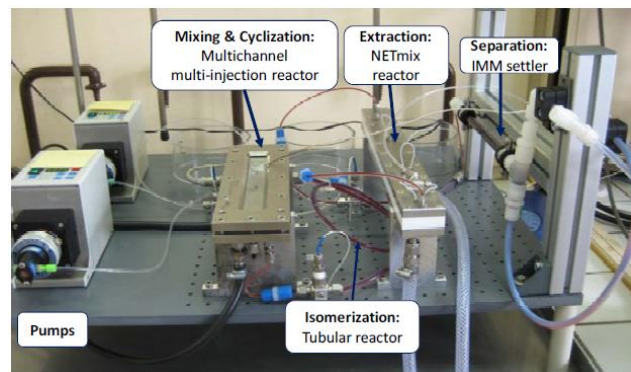


Figure 4: Multipurpose plant for fine chemical production

Schematic overview of multipurpose plant



Photograph of multipurpose plant



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Figure 5: Experimental Research Facility for bulk chemical production

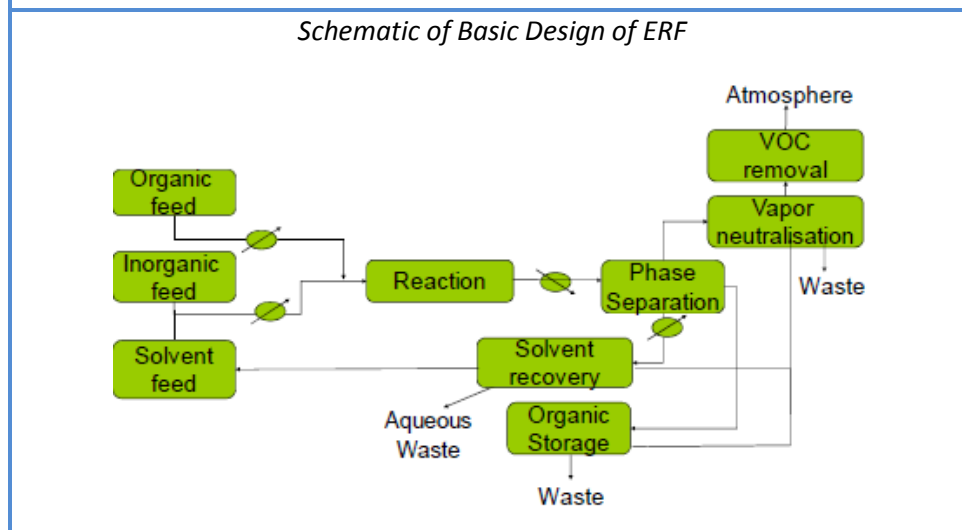
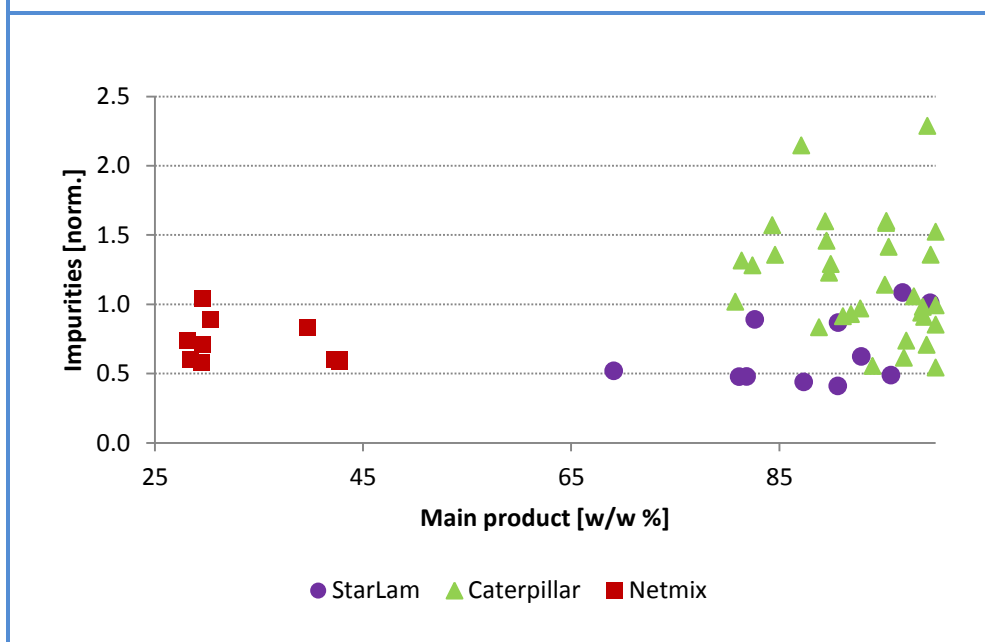


Figure 6: Comparison of main product concentration and impurity levels for structured reactors



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Figure 7: Generic Knowledge Codification

Processes likely to benefit from Intensified Structured Equipment



- ✓ **Reaction is fast / mixing sensitive**
- ✓ **Undesired side reactions or consecutive reactions**
- ✓ **Highly exothermic or endothermic reaction**
- ✓ **Difficult separation after reaction**
- ✓ **Intractable emulsion generated**
- ✓ **Business benefits such as distributed production**



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Potential Impact and main dissemination activities and exploitation results

Table 1. Peer Reviewed Publications

Title	Main Author	Title of the periodical or the series	Date of publication	Relevant pages
Influence of flow regime on mass transfer in different types of microchannels	Madhvanand N. Kashid	Industrial and Engineering Chemistry Research	21/12/2011	6906-6914
Cyclization of Pseudoionone to β -Ionone: Reaction Mechanism and Kinetics	Madhvanand N. Kashid	Industrial and Engineering Chemistry Research	21/12/2011	7920-7926
Gas-liquid and liquid-liquid mass transfer in microstructured reactors	Madhvanand N. Kashid	Chemical Engineering Science	01/12/2011	3876-3897
Analytical method to predict two-phase flow pattern in microstructured reactors	Madhvanand N. Kashid	Chemical Engineering Science	01/12/2011	219-232
Mixing efficiency and energy consumption for five generic microchannel designs	Madhvanand N. Kashid	Chemical Engineering Journal	01/12/2011	436-443
EFFECT OF MODEL STRUCTURE ON COMPLEX LIQUID-LIQUID HETEROGENEOUS REACTIONS	Jerzy Baldyga	SYMPOSIUM SERIES NO. 157, EPIC 2011	01/10/2011	175-181
Analytical method to predict two-phase flow pattern in horizontal capillaries	M.N.Kashid and J Baldyga	Chemical Engineering Science	28/05/2012	219-232
Effect of model structure on complex liquid-liquid heterogeneous reactions	J Baldyga	Symposium Series IChemE	20/06/2011	175-181
Effect of multiphase flow on mass transfer and chemical reactions	W Kowalinski	PhD Thesis at Warsaw University of Technology	01/03/2012	1-220
Nowy model wnikania masy do kropli fazy rozproszonej New model of mass transfer to dispersed phase	J Baldyga	Proceedings of XIIth Polish Seminar on Mixing	06/06/2011	22-27
Wnikanie masy w układach dwudazowych ciecz-ciecz w mikroreaktorach. Mass transfer in two-phase flows in microreactors	W Kowalinski	Proceedings of XIIth Polish Seminar on Mixing	06/06/2011	103-109



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Table 2: Dissemination activities of PILLS at conferences and events

Type of activities	Main leader	Title	Date	Place
Conference	IMM	CHISA 2010 - 19th International Congress of Chemical and Process Engineering	28/08/2010	Prague
Conference	EPFL	Two-phase micro-structured reactors for intensification of instantaneous exothermic cyclization	28/08/2010	Prague
Conference	FCTUC	Insights in heterogeneous liquid-liquid reactions against the background of bulk chemical production	01/09/2010	Prague
Conference	WUT	Modelling of complex liquid-liquid heterogeneous reactions	06/09/2010	Prague
Presentations	CIN	PILLS Mid-term Dissemination Event	09/12/2010	Coimbra
Workshops	FCTUC	Open days for ERF	23/02/2011	University of Coimbra
Conference	WUT	New model of mass transfer to dispersed phase	06/06/2011	11th Polish Seminar on Mixing - Szczecin-Miedzyzdroje
Conference	WUT	Mass transfer in two-phase flows in microreactors	06/06/2011	11th Polish Seminar on Mixing - Szczecin-Miedzyzdroje
Conference	EPFL	Intensification of catalytic reactors (keynote)	20/06/2011	International Scientific Conference, Manchester
Conference	EPFL	Process intensification via continuously operated microstructured reactors	20/06/2011	International Scientific Conference, Manchester
Conference	WUT	EPIC 2011: Application of test reactions to study micromixing in the rotor-stator mixer	20/06/2011	Manchester
Conference	WUT	EPIC 2011: Effect of model structure on complex liquid-liquid heterogeneous	20/06/2011	Manchester
Conference	FCTUC	ENBIS Conference	06/09/2011	Coimbra
Conference	WUT	Effect of mass transfer on complex liquid-liquid heterogeneous reactions	22/09/2011	8th European Congress of Chemical Engineering - Berlin
Presentations	WUT	Effect of mass transfer on complex liquid-liquid heterogeneous	25/09/2011	8th European Congress of Chemical Engineering, Berlin
Conference	EPFL	Microstructured Reactor	27/12/2011	Bangalore
Conference	IMM	IMRET 2012	20/02/2012	Lyon
Presentations	CIN	PILLS End of Project Dissemination Event	22/03/2012	Brussels
Workshops	WUT	Mass transfer in PILLS Project	03/04/2012	Warsaw Poland



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Mid-term dissemination event – 10th December 2010, Coimbra, Portugal

14:00	Registration
14:30	Steve Fletcher, Chemistry Innovation & Patrick Löb, IMM <i>“Process Intensification methodologies applied to Liquid-Liquid Systems in structured equipment – concept, objectives and status of the EU project PILLS”</i>
15:00	Jeremy Double, Britest <i>“Whole process design for liquid-liquid reaction systems”</i>
15:30	Jerzy Baldyga, Warsaw University of Technology <i>“Description and Modelling of complex liquid-liquid heterogeneous reactions”</i>
16:00	Coffee
16:30	Albert Renken, Ecole Polytechnique Fédérale Lausanne <i>“Intensification of instantaneous exothermic cyclisation of pseudoionone: process development, two phase meso- and micro-structured reactors and derived concept of a multipurpose plant for fine chemical synthesis”</i>
17:10	Cristina Gaudêncio, University of Coimbra <i>“Insights in heterogeneous liquid-liquid reactions against the background of bulk chemical production: process development, two phase meso- and micro-structured reactors and introduction to the Experimental Research Facility as pilot installation”</i>
17:45	Posters & Networking
19:00	Close of day 1
	Day 2
09:00	Rebecca Farnell, Chemistry Innovation <i>Welcome and Introduction to the day</i>
09:20	University of Coimbra, Huntsman, CUF & Ecole Polytechnique Fédérale Lausanne <i>*Tour of the Experimental Research Facility and model demonstration of Multipurpose Plant</i>
10:25	IMM & Warsaw University of Technology <i>*Laptop simulations and model micro-reactors</i>
12:00	Fluidinova <i>*Demonstration and simulation of NETmix® reactor</i>
13:00	Chemistry Innovation <i>Summary</i>
13:15	Lunch and networking
14:00	Event Close

Final dissemination event – 22nd March 2012, Brussels, Belgium



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For more information about the PILLS project contact Rebecca Farnell, Chemistry Innovation (rebecca.farnell@ciktn.co.uk).

10:00	Registration
10:30	Steve Fletcher, Chemistry Innovation & Patrick Löb, IMM <i>Process Intensification methodologies applied to Liquid-Liquid Systems in structured equipment – concept, objectives and results of the EU project PILLS</i>
11:15	Albert Renken, Ecole Polytechnique Fédérale de Lausanne & Petra Prechtel, Givaudan <i>Process Intensification of Liquid-Liquid Systems for specialty chemical production: overview of the pilot scale multipurpose facility and capability and its application to β-ionone production</i>
12:00	Cristina Gaudêncio, University of Coimbra; Paulo Araújo, CUF & Asier Rodriguez, Huntsman <i>Process Intensification of Liquid-Liquid Systems for bulk chemical production: learnings from demonstrator scale testing of structured reactors</i>
12:30	Lunch and Networking
13:10	Patrick Löb, IMM & Paulo Quadros, Fluidinova <i>Introduction to micro– and meso-structured reactors developed within the PILLS project</i>
13:30	Madhav Kashid, Ecole Polytechnique Fédérale de Lausanne <i>An overview of the PILLS training material for higher educational institutes</i>
13:45	Jeremy Double, Britest <i>Generic lessons for the development and design of liquid-liquid processes</i>
14:00	Demonstration & Poster Exhibition (with coffee) Warsaw University of Technology - <i>Exhibit of modelling animations</i> Fluidinova and IMM - <i>Exhibit of micro– and meso–structured reactors and animations</i> Ecole Polytechnique Fédérale de Lausanne - <i>Demonstration of educational training manuals and animations</i> Britest - <i>Demonstration of e-learning content</i>
15:30	Close



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Project Team & Dissemination Activities

PILLS project team and some delegates at the final dissemination event



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