Abstract. This presentation is aimed to introduce the EXTRAPOLIS project, subsidised by the CNRS (France) in the frame of the “Energy 2006-2009” program (PR1-2-22). The general purpose of this project is to promote the use of multifunctional exchangers-reactor at industrial scale. Some aspects will be the subject three communications in this GPE congress.

Key-words: extrapolation, micromixing, process intensification, vortex generators, static mixer-reactor, multifunctional heat exchanger.

INTRODUCTION

The concept of multifunctional exchanger-reactors is born from the development of the process intensification, consisting in the use of innovative geometries designed for the sake of:

- energy gain (intensified transfers)
- better productivity (less diluted reagents)
- better safety (local control of temperature)
- reduction of effluents (best selectivity)

A previous CNRS research project on “Multifunctional Heat Exchangers (MHE)” (“Energy 2003-2006”, AC PR2.1), has confirmed the feasibility and the benefits of such systems, consisting in the achievement of various highly exothermic chemical reactions in open loop reactors. An increase by a factor 100 to 10000 of the thermal power exchange with the secondary flow, compared to the batch processes, allows a sufficient temperature control to effectively prevent the runaway risk. They ensure a good and homogeneous mixing,
which is the key parameter for the process efficiency. All this makes possible to increase the concentrations, and spare a part of the costly product separation. Actually, MHE are convenient for the objectives of sustainable development.

These features have been established at laboratory scale, for flow rates about 1L/h. In order to meet the industrial needs, the productivity has to be increased a factor 1000. This objective cannot be attained by simple homothetic geometry of the laboratory reactor, because of the degradation of all the performances (mixing efficiency, heat transfer) in the size increase. It is well known that the dimensionless numbers governing the physical mechanisms of (turbulence, macromixing, heat transfers, mass transfers, micromixing, and chemical reactions) cannot be in the whole maintained at the same level in a size up, while the transfers are systematically penalized. The general purpose of exchangers extrapolation in industrial situations needs geometrical modifications especially to retain the surface density factor. The practical skill in this domain of the CEA partner has been a food for though in this research program. In order to master and optimize the scaling operation, it arises in particular the need of fundamental investigations for a better understanding of the governing transfer mechanisms, in the idea of favoring systems that provide palliative solutions to counteract the unfavorable effects of the scale up.

The broad outline of the EXTRAPOLIS project consists hence in a theoretical axis and an experimental one. The theoretical section is focused on fundamental aspects: the conceptual aspects of extrapolation, an innovative approach for the description of the fundamental mixing mechanisms, and the implementation in CFD programs of a micromixing model, to account for the small turbulence scales part in the molecular contact between the chemical species, especially for high Schmidt numbers. The experimental section consists in the study of selected geometries, a plate type exchanger DEANHEX, and a HEV exchanger, to understand and optimize their behavior in extrapolation. Finally, making the most of the previous investigations, the realization of a set of prototypes specifically designed for extrapolation purposes is planned to conclude this project.

GENERAL DESCRIPTION OF THE EXTRAPOLIS PROJECT

The main objective of the EXTRAPOLIS project is the contribute to the development of multifunctional exchangers-reactors in the chemical industries, and for that:

- Understand the evolutions of performances in the scale up of multifunctional exchangers-reactors
- Explore solutions for the retain of laboratory performances at industrial scale, especially for rapid and exothermal reactions
- Design and build-up of original prototypes able to maintain the mixing abilities in the scale up

Principle of multifunctional heat exchangers

Multifunctional heat exchangers are basically heat exchangers or static mixer providing a high level of transfers, especially suitable for the heat removal of highly exothermal reactions, and that could be classified in “intensified systems”1,2,3.

Intensification can be yielded by different contrivances that have in common to disrupt the flow. As shown in figure 1 for a wide variety of MHE geometries, these disturbances can be induced by obstacles, like fins, vortex generators, solid foams filling the flow section, but also by bends or flux recombination. Understanding the action mode of these different systems towards the mixing properties is quite important to propose firstly a good recommendation for extrapolation rules, and secondly to conceive a good design for an optimal behavior in the scale up.

The first kind of flow disturbances are of dynamical origin, as far as they are the result of vortices and wake effects due to the flow derivation. In a good design, they considerably intensify the transfer without increasing substantially the pressure drop. To the contrary, a bad design will be in favor of “useless pressure drop” by the generation of excessive dead zones in the flow. Another trap would be the idea of saturating the flow with the insets: beyond a certain cluttering, the transfers are damped and the over energy consumption is in this case wasted. The other type of disturbances is of kinematical type: the mixing is ensured by the advection and the cross over of stream lines. This kind of mixing must be profitable for extrapolation because it can be achieved independently of the Reynolds number, so that the system is not tamed by the
dynamic similitude. This is the fundamental idea of the DEANHEX mixer, conceived in the LGC laboratory, where the mixing is ensured by the Dean flow in the bends, and the intensity of the mixing is governed by the curvature radius and the bend angle. Different geometries corresponding to this criterion were till now studied by our research team in the previous program, as well in laminar, inertial or turbulent regimes, examples are given in fig 1.

![Figure 1- Examples of multifunctional exchangers-reactors](image)

**Good working knowledge of extrapolation for heat exchangers**

The approach of the extrapolation of MHE can be transposed of the actual practice for heat exchanger as worked out in the CEA. To ensure the same thermal exchange power for large size exchanger, some compromise have to be done in the size of the primary and secondary flow sections, but the geometry of the components have to be chosen for maintaining the same flow features at laboratory scale and industrial scale, like illustrated in figure 3. In this approach, it clearly appears that the same geometry cannot be used with satisfactory results in the size up.

![Figure 2- From the elementary scale to the industrial plant](image)
Hence, following the method of the CEA\textsuperscript{3} research department, the main idea that will be developed in the EXTRAPOLIS project is to target the best systems to make up for the loss of performances in the scale up. The main leads that will be explored for the intensification of the mixing are the following:

- the potentiality of kinematical mixing
- the use of inserts like vortex generators
- the design of bends
- the corrugation of walls
- the use of nonstationary flow, like pulsed flows

These topics will be investigated in the different steps of the project, either in a theoretical approach or in an experimental one.

**Outline of the EXTRAPOLIS project**

The research program takes place in the 2006-2009 period, hence comes in its last year. All the topics presented in figure 4 are nearly completed, except for the development of the pilot EXTRAPOLEX that needs the finalization of the other themes. The two sections of the project, the theoretical and experimental ones, involve the complementary competences of all the partners.
THEORETICAL SECTION OF EXTRAPOLIS

The problematic of extrapolation

The problem of extrapolation is generally asserted in terms of dimensional analysis. From the fundamental transport equations and chemical kinetics, the role of the Reynolds number, Peclet number and of the two Damköhler numbers can be analyzed. This work was carried out by Dr. Philippe Carrière (LMFA) in different configurations: batch and open loop reactors, slow and fast reactions, laminar, chaotic or turbulent regime, for a scale up based on flow section increase or flux division. This exhaustive review provides relevant information for the understanding of the evolution of each mechanism in the extrapolation.

Mixing and local stirring

Mixing is considered through the kinematics of the local, instantaneous gradient of a passive tracer or scalar quantity, such as concentration. The rise of the tracer gradient, which is equivalent to the stretching of material surfaces, results in the enhancement of mixing through acceleration of molecular diffusion. This is caused by the mechanical action of straining, a matter of strain intensity and orientation of the gradient with respect to the local strain principal axes. In particular, increase of the tracer gradient is promoted by alignment with the most compressive strain direction. The question indeed comes to understanding how the tracer gradient behaves under the combined effects of molecular diffusion, strain and rotation. In addition, since stirring most often occurs in time varying flows, local stirring properties are determined by the dynamics of the tracer gradient, namely its response to any nonstationary mechanical actions or forcing. The approach is based on universal mechanisms and is thus valid for explaining local stirring in different flow regimes. Through analytical and numerical studies, we specifically investigate the case of nonstationary forcing and its possible effect on promotion of stirring. This topic will be presented by in the present conference by Dr. Gonzalez (CORIA) in “Investigation of local stirring through the behavior of tracer gradient”.

Micromixing in CDF

Micromixing is actually accounted for in numerous commercial CFD programs for the needs of combustion simulations, which occur for the most in turbulent regime in gas phase. In liquid phase, the available models are not adequate because the molecular contact takes place at much smaller scales than the Kolmogorov scale, and appears hence as the limiting factor in the chemical reaction. As recommended by Fox, the transport of a passive tracer and its variance are added to those of reactive species, in order to compute the reaction rate. This model will allow reliable numerical simulation in a wide scale range. It will be validated and tested by comparison with measurements carried out in the CEA. This aspect is developed in the LTN, in collaboration with the CORIA.

EXPERIMENTAL SECTION OF EXTRAPOLIS

The performances of the MHE are supported by some flow properties that have to be characterized: the macromixing (RTD), the global heat and mass transfer coefficient, the friction factor and Colburn factor, and the micromixing efficiency. This requires a set of methods that have been carried out partly in the “Multifunctional exchangers” program, as well as in the present program.

Extrapolation of a “good candidate”: the DEANHEX reactor

A plate-type heat exchanger/reactor, namely DEANHEX, including one process plate and one utility plate, seems a promising configuration for operating an extrapolation. A wavy channel is mechanically...
etched on each plate with a numerical robot. The present work aims at optimizing the geometry of the process channel by correlating its geometrical parameters (curvature radius and bend angle) with hydrodynamic criteria. An optimization of the straight length is made for the “relaxation” of the secondary flow, in the aim of minimizing the pressure drop. This work will be the subject of the communication in the actual congress of Z. Anxionnaz in “Hydrodynamic study and optimization of the geometry of a Heat Exchanger/Reactor”, in the frame of a PhD thesis in the LGC and CEA.

Extrapolation of a “good candidate”: the HEV mixer

The HEV mixer has been studied for a few years in the LTN. The tube equipped with vortex generators provides a very efficient mixing in turbulent flow for a small pressure drop. Typically, this device is difficult to extrapolate on several orders of magnitude. Based on LDA turbulence measurements, the purpose here is to investigate the evolution of the turbulent length scales for a 2.5 extrapolation factor. This will be the subject of a communication in the GPE-EPIC 2009 conference of T. Lemenand: “Evolution of length scales and turbulence spectra in the extrapolation of HEV exchanger size”.

Design of a new EXTRAPOLIS component

The new pilot will be designed and constructed in the CEA (june-september 2009), with the collaboration of the LGC and LMFA. The operating principle will be based on a kinematical mixing, probably a flux recombination, although this issue has not been settled at the present time.

CONCLUSIONS AND FUTURE WORKS

The main issues of this project are to propose a practical answer based on scientific investigations. The EXTRAPOLEX prototype will be designed on the base of the flow properties considerations. The global performances in the scale up will be studied experimentally and tested for an industrial chemical reaction.

REFERENCES