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Methodological framework for choice of intensified equipment and development of innovative technologies

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ABSTRACT

Process intensification is recognized as a promising strategy to satisfy the objectives of sustainable development and economic competitiveness. Unfortunately, no general methodology still enables to choose the best available technologies from the many potential solutions. This work describes a step-by-step methodology that guides engineers from a given problem to a list of existing appropriate intensified devices. The first step of the methodology consists in identifying the process limitation among a list of 16 possibilities that cover a large spectrum of cases. Then, the methodology relates, through a pre-filled connection matrix, the identified limitations to a set of intensification strategies such as geometric (micro)structuring, periodic operation or multi-scale design. The third step relates these strategies to a list of technologies that apply these strategies or in which they can be applied. The matrices enable to sort these technologies by relevance with respect to the initial problem. The final step provides quantitative charts to compare the characteristics of these potential solutions with the specifications of the problem. The methodology not only yields to a short list of appropriate solutions to be technically designed and economically assessed, but also to a list of innovation strategies.

1. Introduction

Since the early developments of chemical engineering, chemical engineers have continuously been caught in the crossfire of two information fluxes. On one side, researchers and chemists keep on proposing new components, operating conditions and synthesis routes. On the other side, technology developers and providers keep on proposing new pieces of equipment with specific operating ranges, constraints and required utilities. In the middle, chemical engineers have kept on developing methodologies and strategies to reconcile both these information fluxes, and find, when no perfect match could be found, compromises that would enable to build an efficient system and reach the production scale without prohibitive losses. These compromises could require for example either to slow down the reaction rates so that the generated heat could be evacuated by a flexible technology, or to choose a thermally under-sized reactor, but whose resistance to corrosion would perfectly fit to the involved chemicals.

Today, the situation has become more difficult for engineers who try to manage these objectives and constraints: the compromises of the past are not acceptable anymore, since they impact the process sustainability and reduce the competitiveness of the company on a world-wide market. In addition, the fundamentals of chemical engineering sciences are also continuously changing, with new concepts and tools, among which one can cite Green Process Engineering [1], globalization and time-to-market acceleration [2], batch-to-continuous conversion [3], New Process Windows [4] and multi-scale approaches [5,6].

To continue developing processes and innovate, chemical engineers proposed strategies to embrace this complexity. One of the most recent approaches is Process Intensification, whose definition has been modified several times since the original proposition by Stankiewicz and Moulijn [7]. The most pioneering idea of this definition is the “significant reduction in the size/capacity ratio” of existing devices, which can be summarized in two words: Acceleration and Miniaturization. This definition has led the chemical engineering community to propose dozens of new designs or reactor concepts: spinning disk reactors, microreactors, reactive distillation, in-line monoliths, and so forth [8–21]. Unfortunately, these propositions have hardened the chemical engineer’s choice among all these potential solutions, and no general methodology has still been made available to help him choose one or several

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Nomenclature

C	concentration (mol/m^3)
Cp	specific heat (J/kg/K)
d_h	hydraulic diameter (m)
D_m	molecular diffusivity (m^2/s)
e	layer thickness (m)
h	heat-transfer coefficient (W/m^2/K)
k_n	Nth-order homogeneous rate constant (m$^{3(1-n)}$/mol^{n-1}/s)
k_d	mass-transfer coefficient (m/s)
L	characteristic length (m)
m	Mark
$mls_{i,j}$	matching coefficient between limitation i and strategy j
$mst_{j,k}$	matching coefficient between strategy j and technology k
n	reaction order
N_L	number of considered limitations
Ns	number of considered strategies
Nu	Nusselt number
Q	volume flow rate (m^3/s)
r	reaction rate
R	characteristic dimension (m)
Re	Reynolds number
S	heat-transfer surface (m^2)
Sc	Schmidt number
Sh	Sherwood number
u	mean flow velocity (m/s)
V	volume (m^3)

Greek letters

$\Delta V^{\neq}$	activation volume (cm^3/mol)
ε	specific dissipated mechanical power (W/kg)
λ	thermal conductivity (W/m/K)
λ_{eff}	effective thermal conductivity (W/m/K)
μ	fluid viscosity (Pa s)
ρ	density (kg/m^3)

Indices and exponents

0	at the reactor inlet
conv	relative to convective heat transfer
cond	relative to thermal conduction
diff	relative to diffusion
hom	relative to homogeneous reaction
het	relative to heterogeneous reaction
mass	relative to mass transfer
mix	relative to mixing

appropriate technologies to solve a given problem or improve the performance of a given process.

This lack of structured methodology has led to the publication of various propositions, based on very different approaches. For specific applications, shortcut methods have been proposed, as well as theoretical-plate based models for reactive separations [22], and dedicated algorithms for batch-to-continuous conversion [23,24]. Numerical approaches have been developed to include the choice between technologies in the optimization step of a process design [25]. Several authors presented fundamental approaches focusing on the search for synergies between elementary units of a process to identify intensification strategies [26–28]. Approaches based on multi-scale analysis and a new interpretation of the unit operations concept have been proposed [18,29–33]. Coupling of these approaches with advanced modeling and optimization methods even yielded to quantitative design of innovative technologies [34–36]. Unfortunately, these methods either require to provide a large amount of information, or to develop modeling or optimization approaches. They cannot be considered as decision tools for the choice of best-available technologies, but more as optimal design methods. The required investment to apply these methods can appear prohibitive to a chemical engineer who just wants to explore the new possibilities of process intensification.

Such a fast-screening methodology is the objective of the present work. It aims at providing the chemical engineer with a decision tool that relates directly and rapidly the specifications of a given problem to the best technologies available commercially. To reach that goal, the methodology is inspired from the approach that rationalized the recent development of microstructured reactors, whose full potentials could be demonstrated by performing Characteristic Time Analysis (CTA). CTA enabled to relate their characteristic dimensions to the efficiency of the involved physical and chemical processes, and to demonstrate how these reactors enable to act on the phenomena hierarchy to control which phenomenon should impose its efficiency to the system [6,37–41]. Dimensions and rates are directly related to miniaturization and acceleration, the both keywords that summarize process intensification. This tool should also be able to help engineers in the frame of process intensification.

The methodology structure is depicted in Fig. 1. Between the initial problem that the engineer intends to intensify, and the best available technologies to solve this problem, two intermediate steps are included. The first one consists in identifying the limitations of the problem, i.e. the chemical or physical phenomena that limit the overall productivity of the system. The second step is based on a set of intensification strategies: this step can be compared to some sort of optical lens that will guide the decision of the engineer from the limitations to the technologies, instead of guiding light. To focus the decision correctly, the front and back faces of this lens have to be polished properly: this shape adjustment is performed thanks to two matching matrices that will be prefilled below. Hence, by selecting the appropriate limitations, the engineer will be automatically guided to a sorted list of technologies. In the same time, a second list of most-appropriate intensification strategies will be provided to offer the possibility to the user to open up his study to an innovation process.

The following paper will first present the set of limitations and strategies that will be considered and the matching matrix between both will be given. For a specific list of technologies, the second matching matrix will be presented. Finally, the application of the methodology will be demonstrated, as well as the automatic tool for its application and the technology diagrams for the final technologies selection.

2. Limitations

To build a decision tool that will enable engineers to solve a large number of potential problems, a set of 17 limitations has been identified (Table 1). These limitations can be classified in two general categories:

- Elementary limitations are well identified since they result from fundamental phenomena, such as heat transfer, mass transfer, reaction kinetics or thermodynamic equilibrium.
- Complex limitations are common process issues, but the underlying reasons why they limit the performance are complex and do not result from one single phenomenon, but from a coupling between various elementary phenomena.