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Optimal Design of Flexible, Operable and Sustainable Processes under Uncertainty: Biorefinery Applications

Extended abstract

Over the last years sustainability has become by far the topic of major concern in the chemical industry domain. The energy challenge is the key point of the environmental friendly policies adopted by all the most developed and industrialized countries worldwide. For this purpose several research programs, such as Horizon 2020, have been funded by the European Union and other institutions for the EU member states. As regards this decarbonisation policy, the International Energy Agency defines renewables as the centre of the transition to a less carbon-intensive and more sustainable energy systems [15]. For all those reasons bio-processes have seen a considerably renewed interest during the last decades. However, in order to be competitive with the petrochemical industry and to replace part of it as soon as possible, the bio-processes need to be able soon to cover a substantial part of the market demand and to be able to adapt with respect to the market needs and the raw material properties. In fact, sustainable raw materials as well as renewable energy sources are characterized by their intrinsic variable nature, both in terms of availability and chemico-physical properties, across the year's seasons.

Based on these premises, it appears evident that the main property required by a process that needs to be competitive in the context of the current chemical industry transition is flexibility. Flexibility is defined as the capability of a system to accommodate a set of uncertain parameters and it has been extensively discussed during the last decades of the 20th century [16, 17]. Flexibility represents a major aspect of the Process Systems Engineering domain in the field of design under uncertainty and suitable indexes for its quantification have been proposed in literature [16-20]. However, the integration of the optimal process design procedure with an a posteriori flexibility assessment is not enough for the energy transition issues to be handled. To achieve this goal the entire reshaping of the conventional optimal design procedure with a flexibility oriented approach is needed.

For this reason, the purpose of this thesis is the reformulation of the optimal process design procedure with a flexibility oriented approach for each of its steps accounting also for the environmental impact analysis. A further ambition of these three years research work is to make a small but relevant step towards the unification of process design, scheduling, and control [21] that still represents the main goal of the PSE community by proposing a sequential methodology that allows to reconsider some decisions taken in the previous phases by means of logical loops based on flexibility related criteria.

To achieve this goal, a suitable case study was set up. Given the particular context, a biorefinery separation process was selected. However, the procedure is focused but not limited to it. In fact, other process units are discussed as well and used as example applications for the proposed procedure. The main case study analyzed throughout this thesis is the product purification section of an Acetone-Butanol-Ethanol fermentation process. The effective recovery (both in terms of recovery ratio and purity) of Acetone and Butanol at least is strictly required for the profitability of the process and, thus, the downstream separation performance plays a critical role for the entire biorefinery. The feed stream to be purified is the process stream at the outlet of a preliminary dewatering operation downstream the fermenter. The dewatering operation is required to remove the major amount of water present in the fermentation broth in order to concentrate the obtained products of interest. In fact the ABE fermentation process, carried out with the

Clostridium Acetobutylicum bacterial strain, suffers from product inhibition causing low concentration at the outlet of the fermenter. The compounds present in the stream to be fed to the purification section are then Acetone, n-Butanol, Ethanol and the remaining amount of water. As uncertain parameters the butanol and water partial flowrates have been selected in order to represent perturbations of feed properties, amount of product to be treated and eventual underperformances of the dewatering section. The selected unit operation for the multicomponent mixture purification into its single species is the distillation since it is the most spread operation in chemical plants and the impact of flexibility on it could be of particular interest even for further applications. As later detailed, both distillation trains and process intensified alternatives (Dividing Wall Column) will be considered to design the separation process.

The results obtained during the three years rely on several studies concerning the different phases and tools for the optimal process design procedure that were carried out during the last century. In particular, for the distillation feasibility assessment under perturbed operating conditions the tool that was used is Residue Curve Mapping based on the methodology introduced by Petlyuk [23]. For the flexibility related part both deterministic [16-17] and stochastic [18-19] indexes available in literature have been compared and exploited to conceive new tools and approaches. As concerns the process integration aspects, the theory behind the Dividing Wall Column is based on the early work of Petlyuk [24] while the design approach accounts for the main advances of recent studies in this domain [25]. Finally, the dynamics and control related aspects were addressed. In particular, the dynamic flexibility assessment was based on the dynamic flexibility index proposed by Dimitriadis and Pistikopoulos [20] and a new switchability index have been conceived on the basis of previous studies concerning the switchability analysis [26].

The outcome of the PhD thesis work organized according to the different steps of the process design procedure is presented in the following paragraphs.

For the full understanding of the implications of the flexibility concept as well as of the flexibility analysis methodology a preliminary literature review to list the available studies and related indicators proposed in the past has been performed. Based on the main works [16-20] in this domain, the indicators and approaches were classified in two main categories, namely deterministic and stochastic flexibility. The first one assesses the maximum allowed deviation magnitude while the second one the probability that a given deviation will be withstood by the system without becoming unfeasible. Both these methodologies have been then applied to a simple distillation unit and a new tool representing the “additional costs vs. flexibility index” was conceived [1]. This tool allows to quantify the required system oversizing related to a more substantial deviation to be accommodated and will be used throughout the entire thesis.

However, in case of bio-processes, such as the ABE/W mixture, some physical constraints related to the separation cannot be overcome with higher investments. That’s why, given that flexibility is a measure of a system feasibility, the discussion concerning the biorefinery case study has been performed starting from the feasibility step. For this purpose, the conventional approach based on residue curve maps for distillation feasibility assessment was reconsidered. In particular, the perturbations of the feed properties in the composition space can be reproduced by shifting the feed and product streams characteristic points accordingly. The methodology, that is usually presented for specifications in terms of purity, has been adapted to specifications in terms of recovery ratio as well by means of the mass balances. Moreover, the single column graphical approach was extended to distillation trains and to the equivalent Dividing Wall Column unit [2, 3]. Beside the proposed algorithm, that was mainly based on the previous theoretical background, also the representation of the new modifications by means of a graphical tool up to 4 component mixtures (i.e. 3D composition space) was provided.

Therefore, the problem of the optimal number of stages in multistage operations accounting for uncertain operating conditions was tackled. The operating costs in fact depend on operating conditions and are affected by upstream perturbations even for a given design. As a consequence, the optimal number of stages given by the best compromise between CAPEX and OPEX might change whether disturbances are likely to occur. To account for uncertainty in the selection of the optimal number of stages, the definition of the OPEX was reformulated as the average value over the disturbance probability distribution function resulting in an increase of the optimal value. This approach was applied not only on distillation columns, that are the main unit discussed in this thesis, but also on other units such as multiple-effect evaporators in order to prove its general validity. Moreover, a higher number of stages results in a lower energy consumption for the same operating conditions. Therefore, the higher investment costs ensure at the same time higher flexibility and lower environmental impacts related to the duty consumption. This outcome was visualized by means of an "emissions vs. flexibility" graphic analogous to the costs related one.

Once addressed the number of stages problem, the analysis has shifted towards the optimal distillation train configuration under uncertain operating conditions. The distillation train optimal design for the ABE/W mixture has been carried out accounting for Acetone and Butanol recovery ratio and purity. For this purpose three configurations are possible, namely indirect, direct (2 units) and midsplit (3 units). The direct configuration proved to be unfeasible with respect to the other two (whose costs are lower by an order of magnitude) due to the very low concentration of Acetone in the feed. The flexibility assessment was then performed on the two remaining alternatives and showed that the indirect configuration is always less expensive for any deviation magnitude. This is due to the fact that the n-Butanol, i.e. the most abundant component, is recovered in the first column preventing the disturbance to affect the following one. In particular, it is worth remarking that the simulation and the flexibility analysis outlined the same feasibility limit conditions that were found by means of the RCM based methodology validating once again its effectiveness.

After that, the effects of process intensification on the operation flexibility were investigated. First of all, a Dividing Wall Column unit for the ABE/W mixture separation was design according to an innovative feasible path-based procedure whose purpose is to maximize the convergence of the simulations used for the unit parameters estimation [6]. Once the optimal design has been performed, the same flexibility analysis methodology was carried out with the DWC unit and compared to the indirect distillation train. The assessment shows that process intensified units keep their higher profitability in proximity of the nominal operating conditions but, for an increasing deviation magnitude, the related additional costs for a higher flexibility requirement increase fast. Inversely, it can be stated that process intensification reduces the flexibility of a unit for a given design with respect to the more expensive conventional solution. Even in this case the environmental impact assessment has been performed as for the previous examples. It can be then concluded that integrating the flexibility and environmental aspects in the design procedure when considering the process intensification alternative allows the decision maker to have a reliable estimation of the expected deviation ranges where it is actually more profitable and sustainable than the conventional one. This assessment was possible thanks to the tools developed during the previous phases of the thesis.

All the design steps discussed so far referred to steady state operations. However, in order to validate the obtained design, the dynamics of the process needs to be analyzed and the control strategy should be selected. The flexibility assessment was then extended to the dynamic operation by including the semi-infinite dimension of time in the uncertain space. The dynamic flexibility assessment of a distillation column was then carried out according to the corresponding indicator proposed in literature [7]. Furthermore, a new switchability index has been conceived [8] for a better analysis of the property of a system to switch between two operating conditions, in this particular case from the nominal to the perturbed one. This indicator is based on the steady state and dynamic indexes and its value ranges from 0 (no dynamic transition is feasible) to 1 (dynamics does not affect the system flexibility). To validate this indicator other case studies (such as a CSTR reactor) have been used as well. This innovative tool proved to be effective for the defined purpose. In particular, it allows the comparison between different control strategies (PID vs MPC), control structures and tuning methodologies.

Given the global overview of the PhD thesis work, the main innovations and achievements provided with respect to the previous state of the art in the available literature by these three research years can be listed according to each section of the manuscript as follows:

- **Feasibility:** Generalization of the Residue Curve Maps conventional procedure for distillation to mass balance related specifications as well as to the distillation column trains and Dividing Wall Column unit;
- **Design:**
    - Coupling between flexibility and economic assessment and conception of an "additional costs vs flexibility" decision-making plot;
    - Inclusion of the environmental impact assessment in the optimal design procedure under uncertain operating conditions;
- **Process intensification:**
    - Definition of a new feasible path-based procedure for the design of the Dividing Wall Column distillation unit;
    - Comparison between process intensifying units and conventional configurations from a flexibility viewpoint;
- **Dynamics & control:** Definition of a new switchability index suitable to assess the flexibility related performances of process design and control configurations accounting for the system dynamics.

In general, combining all those aspects, the PhD thesis work achieves its main goal of reshaping the conventional process design procedure from the feasibility step to the dynamic validation one in a flexibility oriented perspective (cf Figure 1). Moreover, whenever missing, the required tools to carry out the outline methodology have been implemented and proved to be effective for their purpose.

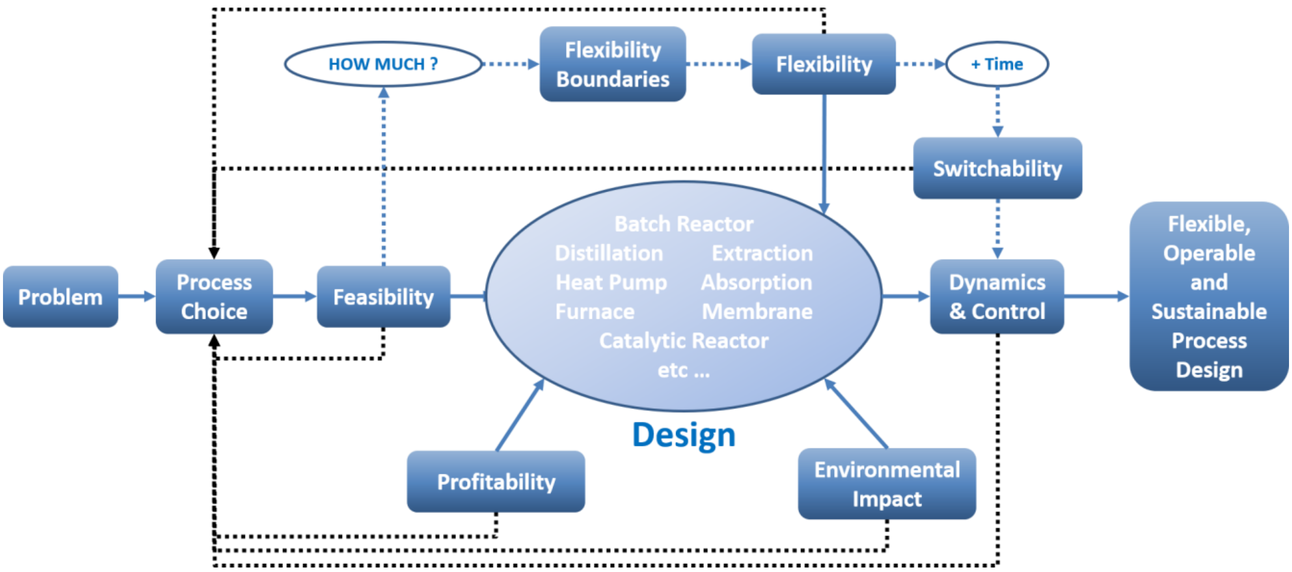

Figure 1 - Flexible Design Procedure

It is finally worth remarking that, although the obtained procedure focuses on chemical processes, it is of general validity and, with some modifications and adjustments to proper steps can be applied to either different problems or systems on which flexibility plays a critical role. In this respect, the author addressed an extensive range of various studies in subsequent publications such as spirits distillation [11], heteroazeotropic distillation [13], optimal cleaning cycles scheduling [9], flexible Demand-Side Management [10, 14] and supply chains flexibility [12].

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SUBSEQUENT APPLICATIONS

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