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Phenomena-Based Approach for Automated Generation of Process Options and Process Models

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Abstract : Due to global challenges of increased competition and demand for more sustainable products/processes, there is a rising pressure on the industry to develop innovative processes. Through Process Intensification (PI) the existing and new processes may be able to attain higher efficiency. However, very few PI options are generally considered. This is because processes are typically analysed at a unit operation level, thus limiting the search space for potential process options. PI performed at more detailed levels of a process can increase the size of the search space. The different levels at which PI can be achieved is unit operations, functional and phenomena level. Physical/chemical phenomena form the lowest level of aggregation and thus, are expected to give the highest impact because all the intensification options can be described by their enhancement. The objective of the current work is thus, generation of numerous process alternatives based on phenomena, and development of their corresponding computer aided models. The methodology comprises: a) automated generation of process options, and b) automated generation of process models. The process under investigation is disintegrated into functions viz. reaction, separation etc., and these functions are further broken down into the phenomena required to perform them. E.g., separation may be performed via vapour-liquid or liquid-liquid equilibrium. A list of phenomena for the process is formed and new phenomena, which can overcome the difficulties/drawbacks of the current process or can enhance the effectiveness of the process, are added to the list. For instance, catalyst separation issue can be handled by using solid catalysts; the corresponding phenomena are identified and added. The phenomena are then combined to generate all possible combinations. However, not all combinations make sense and, hence, screening is carried out to discard the combinations that are meaningless. For example, phase change phenomena need the co-presence of the energy transfer phenomena. Feasible combinations of phenomena are then assigned to the functions they execute. A combination may accomplish a single or multiple functions, i.e. it might perform reaction or reaction with separation. The combinations are then allotted to the functions needed for the process. This creates a series of options for carrying out each function. Combination of these options for different functions in the process leads to the generation of superstructure of process options. These process options, which are formed by a list of phenomena for each function, are passed to the model generation algorithm in the form of binaries (1, 0). The algorithm gathers the active phenomena and couples them to generate the model. A series of models is generated for the functions, which are combined to get the process model. The most promising process options are then chosen subjected to a performance criterion, for example purity of product, or via a multi-objective Pareto optimisation. The methodology was applied to a two-step process and the best route was determined based on the higher product yield. The current methodology can identify, produce and evaluate process intensification options from which the optimal process can be determined. It can be applied to any chemical/biochemical process because of its generic nature.

Keywords : Phenomena, Process intensification, Process models , Process options
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