Abstract
Modelling and simulation of a process flowsheet usually involve identifying the structure of the flowsheet, deriving model equations to represent each operation, and solving the resulting total model equations according to one of various available simulation strategies. The flowsheet synthesis problem determines the type of operations and their sequence needed to achieve the conversion of raw materials to some specified set of products. The flowsheet design problem determines the optimal values for the conditions of operation and other operation/equipment related variables for the synthesized flowsheet. The flowsheet modelling, synthesis and design problems are related since for generation and screening of alternatives, some form of flowsheet models are needed. Also, flowsheet models are needed for verification of the synthesis/design problem solution.

In contrast, a group-contribution (GC) based pure component property estimation of a molecule requires knowledge of the molecular structure and the groups needed to uniquely represent it. The needed property is estimated from a set of *apriori* regressed contributions for the groups representing the molecule. Having the groups and their contributions together with a set of rules to combine groups to represent any molecule therefore provides the possibility to “model” the molecule and/or a mixture of molecules. This also means that the reverse problem of property estimation, that is, the synthesis/design of molecules having desired properties can be solved by generating chemically feasible molecular structures and testing for their properties. This reverse problem is also known as computer aided molecular design.

Let us now imagine that each group used to represent a fraction of a molecule could also be used to represent an operation in a process flowsheet. Just as in chemical property estimation, groups may have one or more free attachments, in flowsheet “property” estimation, process-groups may also have similar number of free attachments. In this way, a set of process-groups representing different types of operations may be created and the “properties” of a specified flowsheet may be estimated by first identifying the process-groups that will uniquely represent it and then by computing their contributions to the needed “property”.

Having a set of process-groups and their combination rules together with their contributions for a set of properties therefore allow simultaneous modelling/simulation, synthesis and
design of process flowsheets. If the flowsheet needs to be optimized based on maximizing or minimizing an estimated flowsheet “property”, it is easy to determine the optimal flowsheet, since it is simply a question of determining the feasible flowsheet structures and ordering them in terms of the estimated “property”. For performance functions defined as a function of more than one “property”, the feasible structures need to be ordered in terms of a calculated performance function.

Based on the above ideas, an initial set of process-groups representing separation operations, mixing operations and some reaction operations have been created to represent a range of process flowsheets. Tables of process-groups and their contributions for a limited set of flowsheet “properties” have been generated. Examples of flowsheet “properties” are driving forces for different types of separation and reaction. A set of combination rules similar to those used in generating chemically feasible molecular structures has also been derived. The proposed paper will present the process-groups, their combination rules, the regressed process-group contribution tables, and illustrate through examples, aspects of the flowsheet modelling/simulation, synthesis and design.

**Keywords**: process synthesis, process design, group contribution method