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Time for a New Class of Methods and Computer Aided Tools to Address the Challenges Facing Us?

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This paper highlights the need for a new class of computer aided tools applicable for a wide range of chemicals-based product synthesis-design and the sustainable design of their corresponding manufacturing processes. The new tools are needed to meet the current and future challenges through innovative and more sustainable solutions that the currently available tools may not be able to provide. For example, even though process simulators are among the most used computer-aided tools in industrial research and development as well as in education, they may have reached their limit in terms of the problems they can solve. Since the process simulators are based on unit operations and predefined process flowsheets, they are unable to find innovative new solutions with new unit operations. Also, employing process simulators as the basis for synthesis, design and/or operation-control of processes does not appear to be the most desirable option. While in the area of process engineering at least several computer-aided tools have been developed and are used routinely, in the area of product engineering, the development of computer-aided tools with similar functions as the process simulator have only recently been reported. This paper gives an overview of a new class of computer-aided tools, using two recently developed tools as illustrative examples. The basis for this new class of tools are software components that can be configured according to the specific needs of the user or problems. Also, through their predictive model-based solution techniques, they are able to provide innovative and more sustainable solutions to a wide range of problems of interest.

1. Introduction

The need for innovative and significantly better solutions than we currently can obtain has become critical and urgent because of the grand challenges of health, food, water, energy and environment that we are facing (Negro et al., 2018). The way we convert our resources to the chemicals-based products that we need for the survival of our society is clearly not working as evidenced by the sharp drop of earth's biocapacity, measured in terms of hectares per person (Global Footprint Network, 2017). The solution of this complex problem offers the opportunity for fundamental advances in science and technology. However, one area that needs urgent attention is our solution approach where we predominantly either use experiment-based trial and error approaches, or model-based computer aided techniques. While the former guarantees an experimentally verified solution but does not guarantee that better solutions do not exist, the latter is able to quickly find the best solution within a defined search space using validated models. Both, however, lack predictive capabilities. That is, ability to find solutions beyond the scope of the technologies they are employing. This paper focuses on issues related to model-based computer aided techniques and what must be done to overcome them.
The development and use of the so-called process simulator has without doubt achieved great success. The petroleum and related industries have made significant progress towards achieving reliable design, safer operation, with for example, lower energy consumption and higher profit. This success, however, has led to a negative trend, that is, replacement of the trial and error experiment-based solution approach to a trial and error simulator-based solution approach, which is a faster and less expensive option. However, does it lead to the innovative and significantly better solution that we now need? The current unit-operation based process simulators have an inherent deficiency that they do not have the capability to find new and innovative processing

routes involving newly developed technologies. That is, should we look for solution approaches that are not so simulator specific? Are simulators able to solve the problems of current interest? If not, should we develop new methods & tools, or, should we wait until process simulators have the needed capabilities, such as the ability to find innovative solutions?

Clearly, a new class of methods and associated model-based computer aided tools are needed, and through which, predictive and innovative capabilities are provided. Also, the many current and future needs, which may change with time, must be satisfied. For example, capabilities to synthesize new processing routes; to design chemicals-based products; to integrate resource management-utilization; to synthesize new intensified operations; to generate sustainable process alternatives and many more need to be provided. Therefore, rather than provide large, complex and rigid process simulators, it could be useful to provide smaller and flexible tailor-made problem specific tools configured from a library of different software components (databases, models, design work-flows, analysis tools, solvers, etc.) according to the needs of the user. Note that here, the process simulator is one of many components in the developed tool. The models in the component library needs to have predictive capabilities. It should be possible to generate tailor-made tools of different scales with smooth transition from one scale to the other for similar applications. The paper highlights the scope and significance of this new class of computer-aided tools and associated methods with several illustrative examples of new tools that are able to achieve significant improvements through innovative, new and more sustainable solutions.

2. The challenges

The challenges are illustrated through the following two problem definitions involving sustainable process-product development and their integration, proposed recently by Zhang et al. (2016).

Problem 1: Given a set of raw material (resources) and a set of desired products (single species chemicals), determine the optimal processing route together with the design of the operations involved subject to minimization of energy and waste, risk of unsafe operation, environmental impacts, costs (operational and capital) as well as supply chain issues.

Problem 2: Given a set of desired product functions, determine the identity of the chemical product (single species, mixtures, blends or formulations) that provide the desired functions as well as a sustainable processing route to manufacture and/or deliver the product.

A general mathematical problem formulation for the above problems has also been proposed by Zhang et al. (2016). It can be noted that problem-1 is a special case of problem-2 when a set of candidate chemicals represent a set of likely products and the objective is to find which product should be made from which raw material and through which processing route? Figure 1a illustrates problem definition-1, where the objective is not only to find the optimal process but also to minimize the waste streams and the release of GHG (greenhouse gases). Recently, Bertran et al. (2017) have shown that considering issues such as, geographical location dependent factors such as product demand, raw material resources availability, utility (energy, water) availability and prices, aspects of supply chain can also be incorporated into the overall sustainability criteria. Even though specific examples of conversion of renewable resources to useful products through energy efficient processes have been reported by many (Vooradi et al. (2018) provides several examples), there is still a lack of data, theory, models, methods and model-based computer aided tools that are needed to solve a wide range of problems that are of current and future importance.

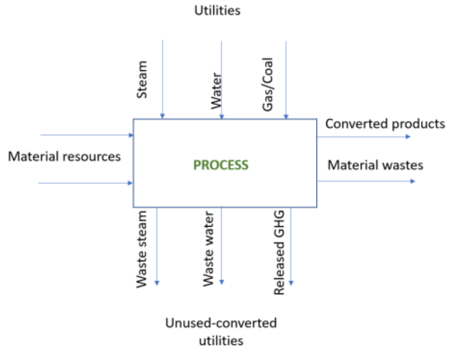
3. Need for new methods & tools

To offer the solution of a wide range of problems (1 and 2 and other related problems), current as well as new methods and associated tools require to address issues such as:

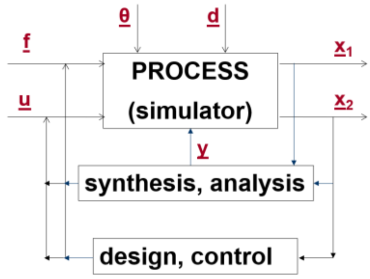
- problem size and complexity (difficulties in numerical solution arise when model complexity increases with problem size),
- dimensionality and multi-discipline (functions of the product and process need to be evaluated at different scales but their data come from different disciplines),
- lack of data and models (ability to solve a wide range of problems depends on the application range of the available data and models),
- significantly better and more sustainable solutions (predictive model-based techniques that lead to new, innovative and sustainable solutions are needed).

Are the current model-based methods and associated tools able to meet the challenges as outlined above and in Figure 1a? Or, where are the deficiencies?

One of the most used computer-aided tools in Chemical Engineering are the so-called Process Simulators with several commercial versions that are routinely used by oil & gas, petrochemical, chemical and related industries to solve a range of process engineering problems. A process simulator, however, by definition is a modelling and simulation tool and therefore, it can only be used indirectly for synthesis, design, analysis, control, etc., purposes through iterative (or trial-and-error) approaches where it generates simulated data in the inner-loop for each trial, while techniques for synthesis, design, analysis, control, etc., generate new alternatives in the outer-loop. Figure 1b highlights this iterative technique, which relies on the process simulator to model and simulate the process alternatives.



(1a)



(1b)

Figure 1: Overview of the sustainable product-process synthesis, design, analysis and control problem. 1a: process with input-output relations; 1b: iterative solution approach.

In Figure 1b, $\underline{f}$ = feed stream variables; $\underline{u}$ = input manipulated (design) variables; $\underline{d}$ = equipment-operation parameters; $\underline{\theta}$ = model parameters; $\underline{x}_1$= process variables; $\underline{x}_2$= measured (specification) variables; $\underline{y}$ = decision-logical (integer) variables.

The difficulties with this iterative approach are the following (to name a few):

- different types of problems require different types of models-solvers (steady state process design-optimization require steady state process models; controller system design-verification need dynamic process models of various complexity; detailed equipment design need distributed parameter models with partial differential equations; also, different types of models need their corresponding numerical solvers);
- different industrial sectors need different data and/or models to represent their product-process (while the unit operations employed in different processing routes may be similar in different industrial sectors, the chemical systems are usually different and therefore, they need different property data and models; also, process operation type (batch or continuous) depends on the product being manufactured);
- values of different types of variables are decided in the outer-loop (see Figure 1b) when the process simulator is employed in iterative solution approaches (while changes in real variables that define alternative process operations for design and control problems can be easily handled, changes in integer variables that may alter the processing route are difficult to handle as the process flowsheet details need to be changed);
- different analysis tools need to be considered (these are tools for economic analysis, safety and hazards analysis, environmental impact analysis, LCA indicator calculations, etc, that need to be incorporated).

To address the above issues, it is possible to add more data, more models, more solvers, etc., to existing process simulators thereby creating large monolithic inflexible and highly complex tools that would be difficult to maintain and/or update and may also become less efficient and robust. Even after these additions, there could still be processes that would not be possible to model and therefore to simulate. This means new processes cannot also be synthesized, designed, analysed and/or operated-controlled. As Chen and Grossmann (2017) have pointed out, currently there are no commercial software tools to determine optimal processing routes even though there are established tools for other process synthesis problems, such as heat and energy integration (Klemeš et al. 2013). In the area of chemical product synthesis and design, the authors do not have knowledge of any general purpose commercial software tool for chemicals-based product synthesis or design.

Therefore, a new class of model-based computer aided tools are needed that can increase the application range in terms of the chemical systems as well as the types of problems (synthesis, design, analysis, control and, simulation) that can be solved, while providing significantly better (or more sustainable) solutions.

4. Software component-based computer-aided tool development

The main features of this new class of computer-aided tools are that they are based on software components that can be assembled through a flexible environment (software framework) according to the needs of a class of well-defined problems related to process-product synthesis, design, analysis, control and many more. Thus, instead of a large monolithic tool with many unwanted features and without many needed features, it should be possible to tailor-make computer-aided tools according to specific needs. Another important feature is that these software components use predictive models and so have the capability to obtain new and innovative solutions.

4.1 General framework

The framework provides the architecture to upload software components such as databases, property models, process models of different types, and method-templates (for example, synthesis, design, analysis, control) with their specific work-flows (for example, step by step algorithms), the associated data-flows and computer-aided tools. An example of the general framework is illustrated through Figure 2, where it can be seen that adding the needed software components, it is possible to develop (tailor-make) problem specific software tools. Any number of tools, components as well as templates may be used in a specific tool. While some of the features of the framework are similar to what can be found in many process simulators, the important new features are the method templates with their problem specific work-flow, data-flow, software components and associated tools.

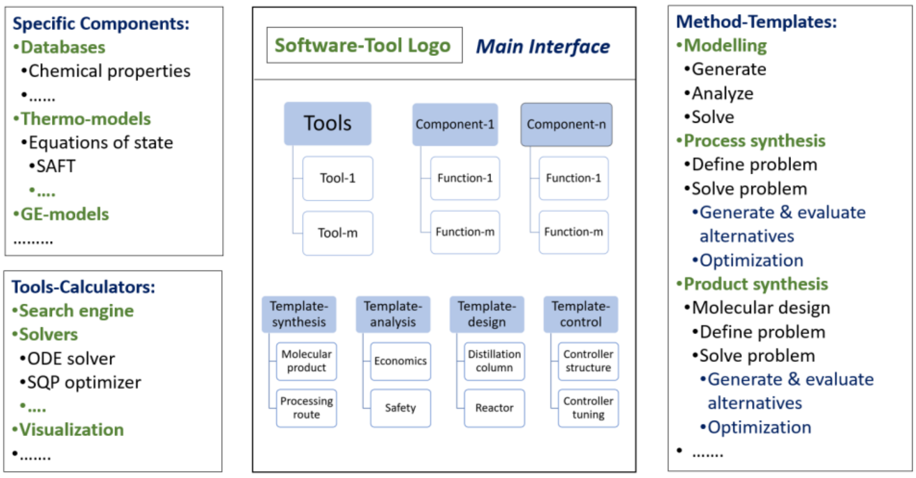


Figure 2: Illustration of the framework for software component-based computer-aided tool

4.2 Component library

A software component is obtained through a collection of basic-tools and associated methods. A collection of components leads to a computer-aided tool. For example, a process simulator may be constructed through the following software components: database, model library, flowsheet representation system, solver library, etc., configured within a simulation environment. Table 1 lists some examples of software components together with their basic-tools and associated methods.

Table 1: Examples of software components created through basic-tools and associated methods

Basic-tools	Associated method	Software components
Data storage	Search-retrieve method	Database
Model equations	Analysis-solution method	Model library
Molecular structure	Representation by groups & group contribution tables	Group contribution-based property model package
Unit operations	Flowsheet representation-evaluation	Superstructure creator
Superstructure-models	Analysis-optimization solver	Process synthesis
Property models	Reverse property calculation method	Molecular and/or mixture design

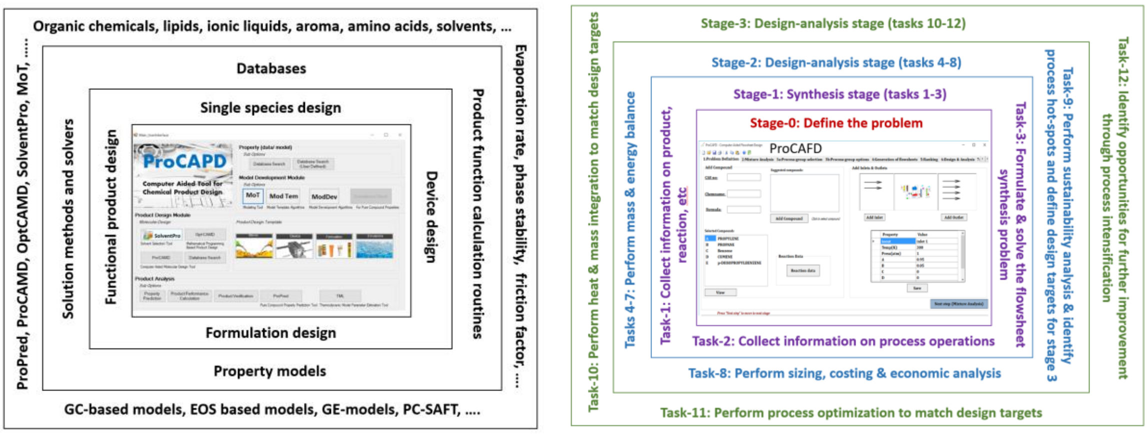
From Table1, it can be noted that different sets of software components can be created if the basic-tools and the associated methods are available. The combination of basic-tools and the associated method defines the application range of the created software component. Through a library of software components, tailor-made problem specific computer-aided tools can be generated, on demand, for the user.

4.3 Application examples

Two recent developments in the area of computer-aided tools for process-product synthesis, design, analysis and simulation are highlighted in this section together with a brief discussion on how other problem specific computer-aided tools can be generated.

ProCAPD (Kalakul et al. 2018) is an integrated tool for computer aided product design. Similar to a process simulator, ProCAPD can be used to simulate the behavior of a known chemical product. However, unlike a process simulator, it can also be used to design different types of products (using different in-house synthesis-design templates). It also has property-process modelling options, a large collection of databases for different classes of chemicals and properties and an interactive design template developer for new products and/or design methods. Figure 3a highlights the architecture of ProCAPD, where the main interface is at the inner core, then the method-template, then the associated software components and finally, the basic-tools. ProCAPD has been applied to design solvents & refrigerants (Kalakul et al., 2018), surrogate fuel blends (Choudhury et al., 2017) and formulated liquid products (Conte et al., 2011).

ProCAFD (Tula et al., 2017) is an integrated software component-based computer-aided tool that has been tailor-made for synthesis, design, analysis and optimization of chemical and related processes employing 12 hierarchical tasks based sustainable design methodology. It has only one design-template where the work-flow consists of 12 tasks organized into 4 stages. Each task has its associated list of software components, where the user has multiple options to carry out the task. For example, processing route generation may be performed based on well-known heuristics, group contribution based generate and test or superstructure optimization. It can be noted that process simulators are only used in stage-2 (tasks 4-7). Figure 3b illustrates organization of the hierarchy of tasks within PtoCAFD. Bertran et al. (2017) gives examples of successful applications of stages 1-3 involving renewable resources conversion and CO2 capture-utilization. Tula et al. (2017) illustrates the use of stages 1-3 for sustainable chemical process synthesis and design where new innovative solutions have been found. Figure 4 highlights three innovative alternatives obtained for the well-known methyl-acetate process.



(3a) (3b)

Figure 3: Software architecture for ProCAPD (3a); Organization of the hierarchy of 12 tasks distributed within 4-stages in ProCAFD.

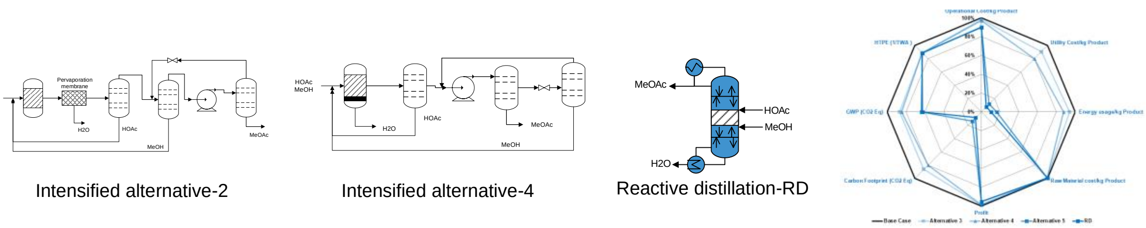


Figure 4: Innovative process synthesis-design results (methyl-acetate production). The 3 flowsheets from the left are sustainable alternatives; figure on the right highlights the nontrade-off solutions through a spider-plot.

5. Conclusions

Chemical engineering and in particular, process systems engineering can play a leading role to address the current and future challenges of energy, water, food and health. New and better technologies needed for improved conversion, separation, heating-cooling, etc., (developed from other disciplines) can be incorporated through new software component-based computer aided tools that have the ability to find innovative and more sustainable solutions. A critical issue here is to understand the role and function of the individual software components so that problem specific computer-aided tools can be created and applied with minimal effort. The architecture of the software component-based computer-aided tools must allow flexibility to handle large and complex problems by breaking them down into smaller solvable problems (as in the case of 12 tasks based sustainable process design) while at the same time, designing different chemicals-based products through similar design templates but having different software components (for example, database and property models). Examples of applications of these computer-aided tools have been cited and the development of new computer-aided tools have been explained. However, like all computer-aided tools, the framework, software components library and the associated tools and methods need to be continuously extended, improved and tested. Tutorial examples illustrating the use of ProCAFD and ProCAPD for exercise problems from the product and process design textbook of Seider et al. (2017) have been developed. Finally, yes it is definitely time for a new class of computer-aided tools that can do more than process simulation.

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