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A systems engineering approach for managing the complexity in sustainable chemical product-process design

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Abstract

This paper provides a perspective on model-data based solution approaches for chemical product-process design, which consists of finding the identity of the candidate chemical product, designing the process that can sustainably manufacture it and verifying the performance of the product during application. The chemical product tree is potentially very large and a wide range of options exist for selecting the product to make, the raw material to use as well as the processing route to employ. It is shown that systematic computer-aided methods and tools integrated within a model-data based design framework can manage the complexity associated with product-process problems very efficiently. Three specific computer-aided tools (*ICAS*, *Sustain-Pro* and *VPPDLab*) have been presented and their applications to product-process design, highlighted.

1. Introduction

Chemical product-process design consists of finding the identity of the candidate chemical product, designing the process that can sustainably manufacture it and verifying the performance of the product during application [1]. The chemical product tree is potentially very large; starting from a set of basic raw materials, which gives a bigger set of basic chemicals that leads to an even bigger set of intermediate chemicals, and finally ending with a very large number of refined chemicals and consumer products. At the top of the product tree, the chemical products are usually from the life sciences, pharmaceutical, food and related industries while at the lower-middle levels, the chemical products are usually from the oil, petrochemical and chemical industries. These lower-middle level chemicals are usually produced in large amounts and the use of model (knowledge) based tools in the design/analysis of their processes are quite common. The product-process design problems differ in terms of the type of chemical(s) being produced.

The products (and the processes that make them) from petrochemical and chemical industries are usually commodity chemicals, which could be classified as small and/or structurally simple molecules, produced in large amounts. In this case, process optimization in terms of operational efficiency and cost is usually a defining factor for a candidate product-process. The products (and the processes that make them) from life sciences, pharmaceutical, food and related industries, on the other hand, are usually large and/or complex molecules, produced in small amounts. Here, process optimization in terms of operational reliability and time of operation is usually a defining factor for a candidate product-process. This means that although the steps in systematic product-process design could be the same, the models-data and the methods and tools that employ them in the various solution steps may be very different for design problems involving different types of chemicals.

Product-process design in the life sciences, pharmaceutical, food and related industries, as opposed to the oil and petrochemical industries, is principally dependent on experiment-based trial & error approaches, providing thereby, opportunities to develop model-based solution approaches to reduce some of the experiment-based steps. However, concerns related to increasing industrial activities accompanied by rapid depletion of resources and increase in pollution and waste, provide opportunities to improve energy-water management, supply chain and sustainability within an enlarged system boundary for product-process design problems within the oil, petrochemical and related industries. This means that solution approaches for product-process design need to address many inter-related issues, such as,

- Multi-scale: important data related to the chemicals may come from different sources, at different scales of time and size; for example, the properties that define the product characteristics could be based on the microstructure of the molecule or material, while the process behaviour that needs to be monitored and controlled during operation may be defined by the macroscopic (end-use) properties of the chemical system; the supply chain and sustainability issues need to be addressed at the mega-scale.

- Multidiscipline: the conversion, for example, of resources such as the biomaterials through biocatalysis requires knowledge of organic synthesis, enzymes, reaction catalysis, bioreactor design and operation – information about these topics come from different disciplines; sustainability analysis requires data, methods and tools also from different disciplines.

- Integrated computer-aided techniques: lack of models to predict the behaviour of chemicals at different scales, of enzymes during organic synthesis, of reaction kinetics, *etc.*, means that appropriate model-based computer aided techniques have not been developed and therefore, use of experiment-based techniques is the only option for these problems, until reliable model based systems become available. Also, the multi-scalar and multi-disciplinary nature of problems point to the need for integration of appropriate methods, tools and data.

In principle, product-process design (and development) needs to consider the demand for improved chemical-based products, made from more sustainable raw material resources and employing more efficient processes to make them. Therefore, methods and tools suitable for current and future product-process design need to manage a collection of sub-problems that require efficient and consistent handling of data and knowledge from different sources and at different scales of time and size. A systems approach that can efficiently "manage the complexity" becomes therefore a very desirable option [2].

This paper provides a perspective on the opportunities for the development and use of a hybrid model-data based framework for systematic solution of chemical product-process design problems through efficient management of the involved complexities. Three specific computer-aided methods and tools are presented: *ICAS* (integrated computer-aided system); *Sustain-Pro* (sustainable process design); *VPPD-Lab* (virtual product-process design laboratory). Examples illustrating the application of these tools to solve typical product-process design problems are discussed.

2. Product-Process Design: Problem Definition

The generic mathematical definition of the product-process design problem is given by,

$$\textit{Minimize/maximize } F_{obj} = \{\boldsymbol{S}^T \underline{y} + f(\underline{x})\} \tag{1}$$

Subject to

$$\underline{D}_1 = \underline{h}_1(\underline{x}, \underline{z}, \underline{p}) \tag{2}$$

$$\underline{D}_2 = \underline{h}_2(\underline{x}, \underline{z}, \underline{p}) \tag{3}$$

$$0 \geq \underline{g}_1(\underline{x}, \underline{z}, \underline{p}, \underline{\theta}) \tag{4}$$

$$0 \geq g_2(\underline{x}, \underline{z}, \underline{p}, \underline{\theta}) \tag{5}$$

$$\boldsymbol{B}\underline{y} + \boldsymbol{C}\underline{x} \leq \underline{d} \tag{6}$$

In the above generic problem definition, the performance index (Eq. 1) needs to be minimized or maximized and may include multiple terms; the process model (Eq. 2) satisfies the conservation of mass and/or energy as a function of the product-process variables ($\underline{x}$), design variables or process parameters ($\underline{z}$) and model parameters ($\underline{p}$); the product performance model (Eq. 3) predicts the behaviour of the product during its application; the product-process structure equations (Eq. 6) generate the feasible molecular-flowsheet structures as a function of decision (integer) variables ($\underline{y}$) and process variables ($\underline{x}$); and finally, the product-process constraints (Eqs. 4-5) define operational and/or chemical functional constraints ($\underline{\theta}$). Considering that the models maybe multi-scalar, non-linear and the variables involved may be integer as well as real, the generic problem defined above could represent a complex multi-dimensional problem of the MINLP (mixed integer non linear programming) type. Several variations of the above problem have also been formulated and solved in process optimization [3], heat-mass exchange networks [4], and in product-process design [5].

3. Framework for Managing the Complexity

To solve the generic product-process design problem defined above, several issues need to be addressed. For example, how to generate (or create) the product-process model objects for a large range of chemical systems? How to collect the necessary data for process parameters ($\underline{z}$) and property model parameters ($\underline{p}$) for a wide range of systems? How to find a good initial estimate for process variables ($\underline{x}$) and decision variables ($\underline{y}$) for different types of problems? One way to manage this complexity would be to provide a hybrid model-data based framework for handling a diverse set of design work-flows corresponding to a wide range of problems, through a suit of computer-aided methods and tools. This framework would need to have a knowledge base of data, a library of models, a collection of algorithms (the work-flow and data-flow guiding the engineer/scientist through the solution steps), and, other associated methods-tools (such as a tool to analyze data; a tool to create the missing model; a tool to screen feasible alternatives). An important question here is what would be the role of models?

3.1 Modelling & Roles of Models-Data

As illustrated in Fig. 1, models and data play a very important role in the solution of product-process related problems. Various types of problems involving products and/or processes are

listed on the right hand side of the figure. These problems are solved through corresponding methods of solution (algorithms) when enough knowledge and/or data are available. Since in most cases, the necessary knowledge and/or data may not be available, models are needed to supplement the available information. For example, models are needed to predict the behaviour of the product-process, to evaluate the performance of the product-process, to monitor and/or control the product-process, and many more. These models are of different type (different types of equations are used to represent the system); scales (involve sub-systems requiring different size and time scales); complexity (number of equations, degree of non-linearity, dimension, *etc.*) and simulation mode (steady state, dynamic, batch, identification, *etc.*).

Based on the above discussion, the role of models within the context of product-process design is briefly discussed below. Should the model be used to simply replace the experiment, or, should the model play a more active role in finding truly innovative solutions? That is, should models be used mainly to verify a design (for given process parameters, property model parameters, design constraints and decision variables, verify if the optimal process variables have been identified and if the value of the corresponding objective function is really optimal?); or, should they be used as part of a trial & error solution approach (assume values for process parameters, calculate the process variables and the measured variables, and, check if the target properties are satisfied and if the objective function is optimal, if not, repeat the procedure for another set of process parameters); or should the problem be decomposed into sub-problems and solved according to a derived hierarchy?

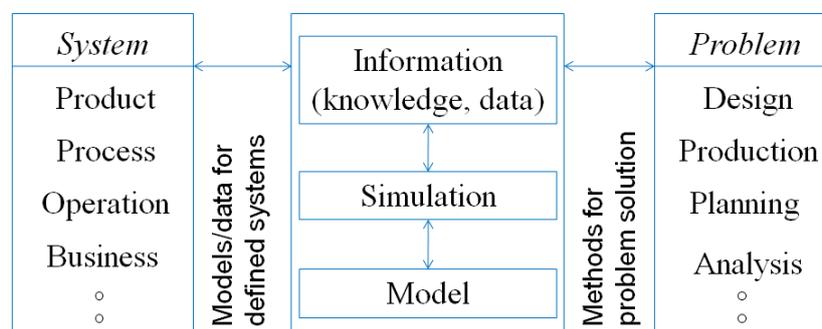| *System*		Information		*Problem*
Product		(knowledge, data)		Design
Process	Models/data for defined systems		Methods for problem solution	Production
Operation		Simulation		Planning
Business				Analysis
○ ○		Model		○ ○

Figure 1: Need for models/data in problem solution

For the verification role, a validated model (in the form of a process simulator) performs the same function as experiments. The design decisions, are however, obtained separately (using

the same models in a different role). For the trial & error solution approach, a model-based simulator simply replaces the experiment. While experiment based trial and error is sometimes the only alternative to solve a specific product-design problem, if the appropriate models are available, the search can be conducted over a larger space and the time and resources used to obtain a design can be significantly reduced. In this case, the experimental resources are reserved for the verification step in the final stages of the design process, rather than using them in the early stages of the design process. Here, the process model is used to define design targets (in terms of optimal process variables and their corresponding target properties) for the chemical product, while a collection of property models are used in the search for a match of the target. The method is called "reverse design" because first the optimal solution is located and from it, the design constraints are defined [6]. Then, the set of values for the process parameters matching the targets (the optimal solution) is determined.

The application range of the hybrid model-data based framework depends on the application range of the available models. Therefore, to achieve a wide search space during the early stages of the design process, the corresponding models need to be predictive by nature. In the later stages of the design process when specific values of the design variables (process parameters) are required, the models need to be quantitatively correct but the application range does not need to be wide. In this respect, a multi-scale modelling scheme that can generate the necessary model(s) would be an interesting option, especially if the necessary model parameters could be predicted on-line without the need for additional experimental data. The main idea here is to use the same set of experimental data to regress model parameters at different scales. The models at the lower scales need less parameters to represent the same dataset and the model descriptors for the lower scales can be used to estimate the missing parameters in the adjacent higher scale. In this way, the predictive power of the model-based framework for product-process design is extended without the need for new data.

Data, generated and/or measured, provide needed information about the product-process for their design/analysis. The larger the collection of the available data, the more useful they become for model development and for model-data based solution strategies. For this, however, a good representation of the knowledge (data) is necessary. Examples of ontology based knowledge representation for model-based design frameworks can be found in Singh et

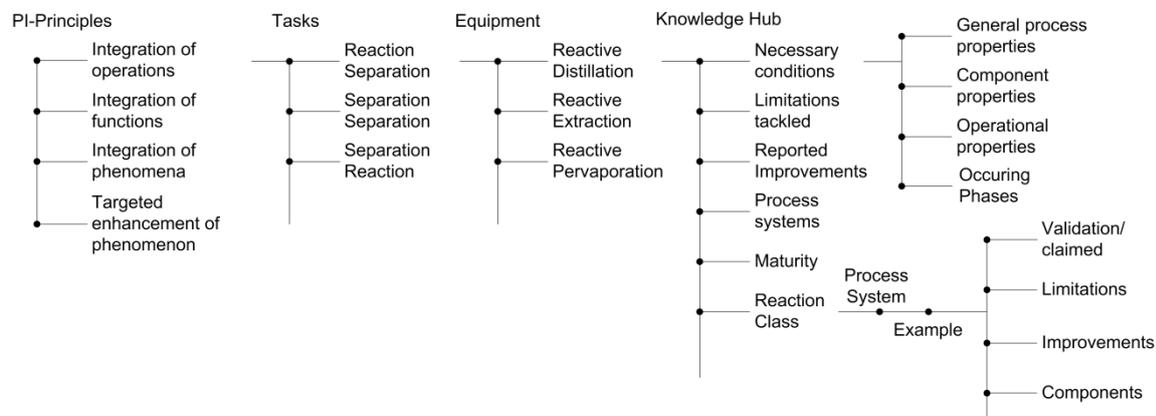al. [7] and Lutze et al. [8]. Figure 2 provides an illustration of ontology based knowledge representation.

Figure 2: Ontology-based structure of the process-intensification (PI) knowledge base [8].

3.2 Solution Strategy

The mathematical problem represented by Eqs. 1-6 can be large and complex, depending on the specific problem details, and therefore, may be difficult to solve. An alternative is to decompose the problem (see Figure 3) into a set of more easily solvable sub-problems and to identify those that can be solved through model-based solution approaches. As illustrated through Figure 3, solving these sub-problems according to a pre-determined sequence would then help to reduce the search space of the synthesis-design problem because each sub-problem has a corresponding area of application and the solution hierarchy orders the sub-problems in increasing order of the area of application. When the final sub-problem is reached, experiments may be employed to verify and test the few remaining (feasible) solutions of the problem. The advantage of this systematic approach is that during the early stages, where enough data and models are available, the search space is rapidly reduced by using simple qualitatively correct models. In the later stages, where quantitative values become important and data/models become more unreliable, the experimental resources are employed to evaluate a few feasible alternatives to identify the truly innovative and best solution.
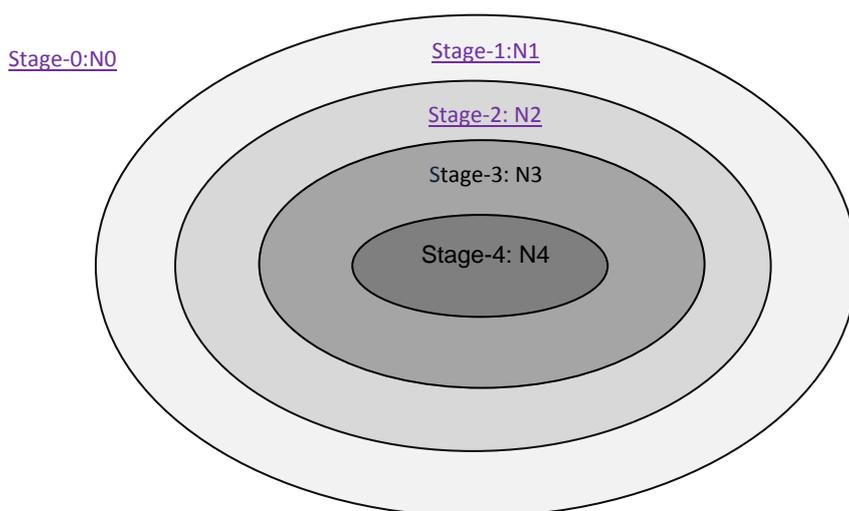
Figure 3: Number of alternatives reduced with the decomposition approach [5].

Note: N0 > N1 > N2 > N3 > N4, where Ni indicate the number of feasible alternatives.

3.3 Integrated Computer Aided System: ICAS

An integrated computer aided system (*ICAS*) has been developed to efficiently manage the complexity for sustainable chemical product-process design [9, 10]. *ICAS* combines computer-aided tools for modelling, simulation (including property prediction), synthesis/design, control and analysis into a single integrated system. These tools are present in *ICAS* as toolboxes. During the solution of a problem, the user may move from one toolbox to another to solve problems requiring more than one tool. For example, in process synthesis, one option is to define the feed stream, then analyse the mixture (analysis and utility toolbox), then generate a flowsheet (synthesis toolbox), then optimise the flowsheet (design toolbox), and finally verify the design (analysis toolbox). From any toolbox it is possible to invoke the simulation engine to perform steady state and/or dynamic simulation for batch and/or continuous process operations. From the synthesis toolbox, it is possible to invoke the solvent design tool (design toolbox) if a solvent is needed for a specific separation task. There is also a utility toolbox, which determines properties, phase diagrams, *etc.*, that can be used by the other toolboxes or by the user to analyze the behaviour of the specified system. Figure 4 highlights the idea of integration and the advantages that can be obtained through this integration.

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- ICAS combines computational tools for modelling, simulation (including property prediction), synthesis/design, control and analysis for chemical products and their processes in a single integrated and flexible system.
- ICAS employs algorithms based on a systematic solution approach.
- ICAS allows single- and multi-dimensional problems to be solved efficiently, reliably, consistently and robustly.
- ICAS improves productivity by allowing sharing of common knowledge between different groups of people.
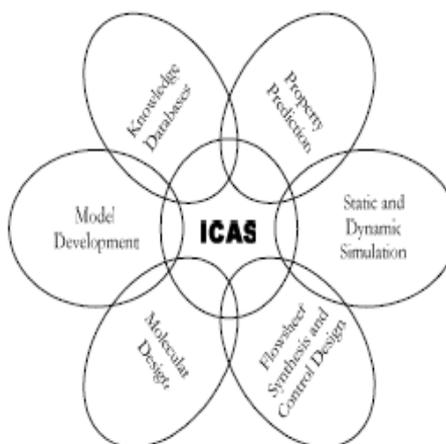

Figure 4: The idea of integration within ICAS

The main tools of *ICAS* are the following: *ProPred* (pure component property prediction, including product analysis; *ProCAMD* (design of molecules and mixtures); *MoT* (modelling test-bed); *CAPEC_Database* (large collection of data of different types of chemicals); *ICAS-PDS* (separation process synthesis & design, including reactive separations) and *ICAS-Utility* (generation of different types of phase diagrams). In addition, options for steady state and dynamic process simulations and optimization are also available in *ICAS*.

3.4 Sustainable Process Design: Sustain-Pro

The tool *Sustain-Pro* allows the systematic design of sustainable chemical processes. It can be applied for sustainable design of new processes or retrofit (sustainable) design of existing processes. *SustainPro* is based on the work-flow, data-flow and calculations corresponding to the methodology developed for continuous (Carvalho *et al*. [11]) as well as batch operations (Carvalho *et al*.[12]). *SustainPro* is able to generate, screen and then identify sustainable alternatives in any chemical process by locating the economic, operational, environmental, and safety related bottlenecks inherent in the process. In order to evaluate the generated alternatives it employs a set of performance criteria, consisting of sustainability metrics, safety indices and environmental impacts. The implemented methodology allows the study of continuous, semi-batch and batch processes.

The starting point for design methodology is the process specification in terms of prices, operation conditions and the respective process flowsheet. A knowledge base and collection

of external tools (*ICAS-ProPred*; *ICAS-ProCAMD*; process simulators; *CAPEC_Database*, *etc.*) have been incorporated into *Sustan-Pro* as supporting tools. As shown in Figure 5, the starting point for a problem is process specifications followed by the creation of problem specific data. The calculations in *Sustain-Pro* are divided into three parts:

- Part I – Indicator analysis (represents the process in terms of open- and close-paths; for each path computes mass and energy indicators).

- Part II – Evaluation (different sustainable alternatives are generated based on the effect of the indicators on the process specifications).

- Part III- Generation and comparison of new alternatives (computations of sustainability metrics, safety indices, environmental impact).

Sustain-Pro has been applied to a wide range of chemical processes such as refineries, gas processing, and pharmaceuticals.
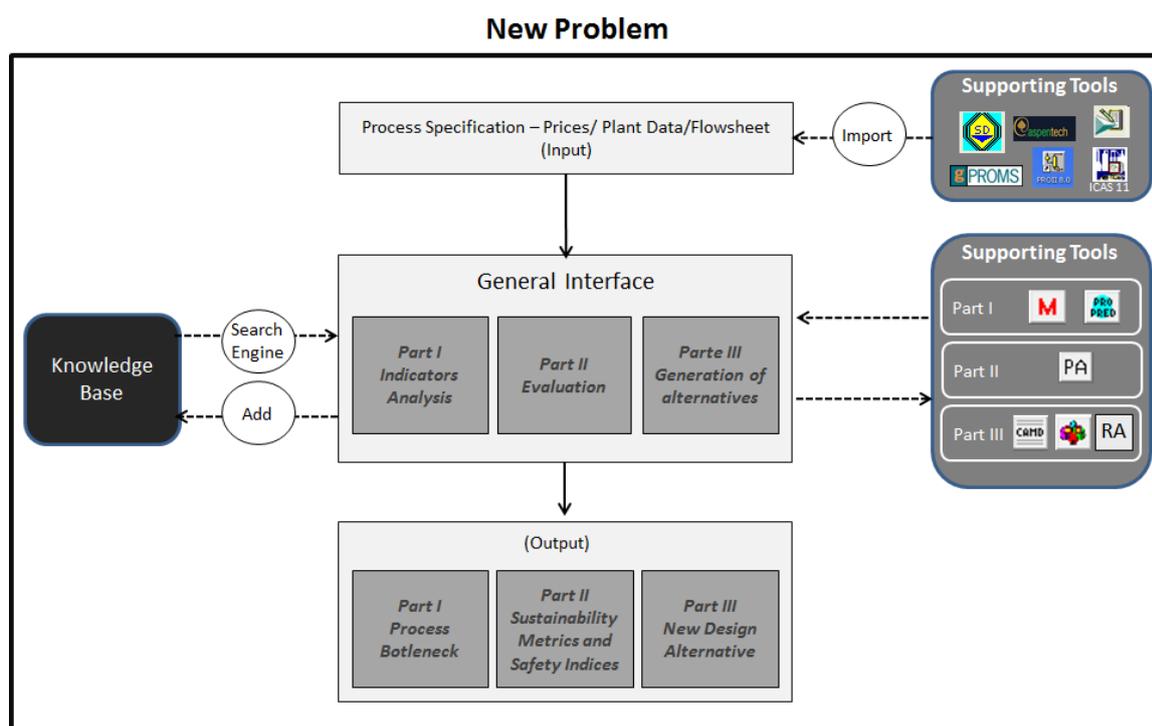

Figure 5: Architecture of *Sustain-Pro*

3.5 The Virtual Product-Process Design Lab: VPPD-Lab

The virtual product-process design lab, *VPPD-Lab*, is a tool for design and analysis of various chemicals based formulated products through virtual experiments [13]. The idea behind the

virtual product-process design lab is the following: instead of doing the experiments needed to search for a product and its process to manufacture it, the engineer / scientist performs virtual experiments, through the *VPPD-Lab* software. The forward and the reverse solution approaches (for design problems) are available. The software contains a large knowledge base of data (of chemicals, of solvents, of plants, of microcapsule devices, *etc*.); a large collection of models (models for property prediction, models for controlled release, models for mixing, *etc*.); of design algorithms (methods for formulation design, methods for molecule design, methods for polymer design, methods for process flowsheet synthesis, *etc*.); other tools (property prediction software; model generation software; equipment design software; design of experiments software, *etc*.). These are organized through a framework for efficient management of the complexity. Figure 6 gives an overview of the main features of *VPPD-Lab*, which has been used in the design and evaluation of the controlled release of a drug active ingredient through a polymeric microcapsule, pesticide formulation, paint formulation, fuel-cells, and many more.
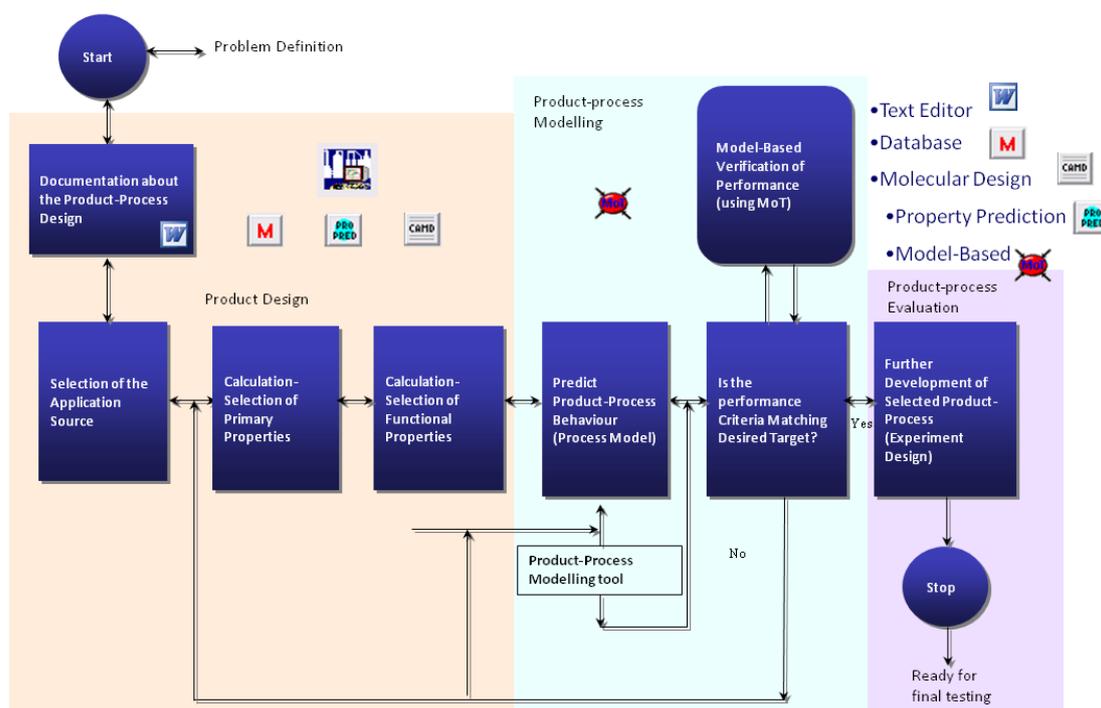

Figure 6: Flow-diagram of the VPPD-lab software [13].

In the first step the problem is defined (for example, identity of the active ingredient; the desired controlled release parameters, *etc*.). In the second step the selection of the application source (for example, active ingredient released into the body) and the primary properties of

solvent and the polymer (needed by the controlled release model) are made. If the user is unable to provide this information, methods for solvent design and polymer design are used to generate a list of candidates to select from. In the next step the selection and calculation of the functional properties needed to evaluate the controlled release design is made (if models are not available, the modelling software helps to generate new models). In the next steps, the product performance model is used to predict the product behaviour. If the desired (target) performance is matched, then the last step of verifying the product performance through experiments is performed. If the target is not matched, it is possible to repeat from any of the earlier steps with a new design alternative.

Important issues to note from this example are that multi-scale models have been used, data and knowledge from different disciplines have been used and, design / evaluation problem has been effectively used by solving a collection of sub-problems according to a pre-determined sequence. The final step (not shown) would be to select a few of the alternatives and perform the necessary experiments to validate the selection. Therefore, the experiments are done not to design the product but to verify the product. This approach has the potential to save time and money in bringing a chemical based product to the market. Obviously, the accuracy and range of application of the *VPPD-Lab* software depends on the available data and models in the software.

4. Application Examples

A wide range of problems related to product-process design have been successfully solved with the model-data based tools presented above. A brief overview of some of these problems is given below (a list of application examples together with their solution details can be obtained from the author):

- Solvent design – Solvents for separation as well as for promoting organic synthesis have been designed and analyzed (solvents for separation [14], solvents for organic synthesis [15], industrial solvent selection [16]. Tools used: *ProPred*, *ProCAMD* and *CAPEC_Database*.

- Liquid formulated product design: A systematic methodology has been developed and applied to design consumer products such as insect repellent lotion, hair spray and other liquid cosmetic products [17]. Tools used: *VPPD-Lab* and from it, *ProPred*, *ProCAMD* and *MoT*.

- Modelling of crystallization processes – a generic model from which different types of needed crystallization models can be generated, evaluated and used developing model-data based design frameworks [18]. Tools used: *ProPred*, and *MoT*.

- Modelling of short-path evaporators – a generic model from which different types of needed crystallization models can be generated, evaluated and used developing model-data based design frameworks [19]. Tools used: *ProPred*, and *MoT*.

- Sustainable design of chemical processes – a wide range of chemical processes has been analyzed in terms of their sustainability and more sustainable retrofit design alternatives have been proposed [11, 12]. Tools used: *Sustain-Pro* and from it, *CAPEC_Database*, *ProPred*, *ProCAMD*, *Process Design Studio* and any process simulator.

5. Conclusions and future work

Systematic computer-aided model-data based solution approaches are ideally suited to manage the complexity related to the analysis and solution of various types of product-process design problems. For the methods and tools to be able to solve a wide range of problems, models valid for a wide range of problems need to be available. The various methods and tools need to be integrated through a hybrid model-data based framework, which can play a major role in advancing the state of the art in product-process design. The role of the model, however, needs to be clearly defined. This paper highlighted some of the opportunities and needs related to the development and use of systematic model-data based solution approaches for chemical product-process design.

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