An integrated approach for the design of emulsified products

Consumer oriented chemical based products, including emulsified ones, are structured products constituted by numerous chemicals, and they are used every day by millions of people. They are still mainly designed through trial-and-error based experimental techniques. A systematic approach, integrating model-based as well as experiment-based techniques, for design of these products could significantly reduce both time and cost connected to product development by doing only the necessary experiments, and ensuring chances for innovation. In this work we present an integrated methodology for the design of emulsified formulated products. The methodology consists of three stages: the problem definition stage, the model-based design stage, and the experiment-based verification stage. In the problem definition stage, the consumer needs are translated into a set of target thermo-physical properties and into a list of categories of ingredients that are to be included in the formulation via a robust knowledge base. In the model-based design stage, structured databases, dedicated algorithms and a property model library are employed for designing a candidate base case formulation. Finally, in the experiment-based verification stage, the properties and performances of the proposed formulation are measured by means of tailor-made experiments. The formulation is then validated or, if necessary, refined thanks to a systematic list of actions. All these tools have been implemented as a new template in our in-house software called the Virtual Product-Process Design Laboratory and have been illustrated via a case study (a hand-wash detergent) where the complete methodology (all three stages) is for the first time applied.

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A Comprehensive Framework for Surfactant Selection and Design for Emulsion Based Chemical Product Design

The manufacture of emulsified products is of increasing interest in the consumer oriented chemical industry. Several cosmetic, household and pharmaceutical products are in the emulsified form when sold and/or they are expected to form an emulsion when used. Therefore, there is a need for the development of a methodology and relevant tools in order to spare time and resources in the design of emulsion-based chemical products, so that the products can reach the market faster and at a reduced cost. The understanding and modeling of the characteristic behavior of emulsions and their peculiar ingredients is consequently necessary to tackle this problem with computer-aided methods and tools. A comprehensive framework for the selection and design of surfactants, the main responsible for the formation and the stability of emulsions, is presented here together with the modeling of the cloud point, a key-property of nonionic surfactants, with a group-contribution model. The mathematical formulation of a standard product design problem is presented, together with the list of both the pure component properties (related to nonionic surfactants) and the mixture properties (relevant to the overall products as an emulsion) needed for the solution of the design algorithm. These models are then applied together with established predictive models for pure component properties of ionic surfactants and for standard mixture properties such as the density, the viscosity, the surface and the interfacial tension, but also the type of emulsion expected (through the hydrophilic–lipophilic balance), and its stability (through the hydrophilic–lipophilic deviation), forming a robust chemical product design tool. The application of this framework is highlighted for the design of some emulsion based chemical products.

An Integrated Methodology for Emulsified Formulated Product Design

The consumer oriented chemical based products are used every day by millions of people. They are structured products constituted of numerous chemicals, and many of them, especially household and personal care products, are emulsions where active ingredients, solvents, additives and surfactants are mixed together to determine the desired emulsified product. They are still mainly designed and analysed through trial-and-error based experimental techniques, therefore a systematic approach, integrating model-based as well as experiment-based techniques, for design of these products could significantly reduce both time and cost connected to product development by doing only the necessary experiments, and ensuring chances for innovation. The main contribution of this project is the development of an integrated methodology for the design of emulsified formulated products. The methodology consists of three stages: the problem definition stage, the model-based design stage, and the experiment-based verification stage. In the problem definition stage, the consumer needs are translated into a set of target thermo-physical properties and into a list of categories of ingredients that are to be included in the formulation. In the model-based design stage, structured databases,
dedicated algorithms and a property model library are employed for de- signing a candidate base case formulation. Finally, in the experiment - based verification stage, the properties and performances of the proposed formulation are measured by means of tailo - made exp eriments. The formulation is then validated or, if necessary, re- fined thanks to a systematic list of action. The problem definition stage relies on a robust knowledge base, which needs to system- atically generate quantitative, useful input information for t he model - based stage, starting from the consumer assessments. In the model - based stage, comprehensive chemical da- tabases, consistent property models and a dedicated algorithm for the design of emulsified solvent mixtures are needed. Finally, for the experi ment - based stage, an efficient planning of the experiments is required, together with the systematic generation of a list of actions to be taken, in case some of the experiments do not validate the candidate formulation generated in the previous stage. All the above mentioned issues are addressed in this PhD work: the necessary property models have been retrieved and organized in a model library; new property models have been developed for a set of thermo - physical properties of surfactants; a robust, system atic knowledge - base has been developed in relation to emulsified formulated products; chem- ical databases have been improved and generated; and an algorithm for the model - based design of emulsified solvent mixtures has been developed. All these tools have been im- plemented as a new template in the virtual Product - Process Design laboratory software. To illustrate the application of the proposed methodology, three case studies have been developed. For one of these case studies, the whole methodology has been ap plied, while for the other two, only the first two stages and part of the experiment - based verification iv stage have been applied, that is, the experimental work has been planned, a list of actions has been generated, but no actual measurement has been taken.

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The Virtual Product-Process Design Laboratory for Structured Chemical Product Design and Analysis
The objective of this paper is to present new methods for design of chemicals based formulated products and their implementation in the software, the Virtual Product-Process Design Laboratory. The new products are tailor-made blended liquid products and emulsion-based products. The new software employs a template approach, where each template follows the same common steps in the workflow for design of formulated products, but has the option to employ different product specific property models, data and calculation routines, when necessary. With the new additions, the software is able to support the design and analysis of a wide range of homogeneous formulated products: tailor-made blends, single phase liquid formulations and emulsion-based products. The decision making process is supported by dedicated property models and structured databases, specifically developed for each design problem scenario. Output from the software is a small set of most promising product candidates and a short list of recommended experiments that can validate and further fine-tune the product composition. The application of the new features is highlighted through two case studies relative to an emulsion-based product and a tailor-made blend

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Design of an Emulsion-based Personal Detergent through a Model-based Chemical Product Design Methodology

An extended systematic methodology for the design of emulsion-based Chemical products is presented. The methodology consists of a model-based framework involving seven sequential hierarchical steps: starting with the identification of the needs to be satisfied by the product and then adding one-by-one the different classes of chemicals, until a formulation is obtained, the stability of which as an emulsion is finally checked with appropriate models. Structured databases, appropriate pure component as well as mixture property models, rule-based selection criteria and CAMD techniques are employed together to obtain one or more candidate formulations. A conceptual casesudy representing a personal detergent is presented to highlight the methodology.

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Contributors: Mattei, M., Hill, M., Kontogeorgis, G., Gani, R.
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Design of a Tank Cleaning Blend through a Systematic Emulsified Product Design Methodology

Commercial and industrial detergents, formulated liquid blends, have recently become extremely sophisticated, in order to address a broad range of cleaning tasks and to deliver superior performances with a minimum of effort and time. These products, by definition, consist of different chemicals, each with a specific function related to the needs of the product: surfactants, builders, bleaching agents, enzymes and minors, usually mixed together with a carrier, necessary to keep the blend as a homogeneous liquid formulation. A system approach and associated tools can help to virtually generate and test different candidates in order to identify the most promising formulations before a detailed experimental stage for final selection and product development is applied. In this way, the whole design procedure speeds up, saving time and money, and the optimum formulation is identified, since a broad range of alternatives are investigated. The approach adopted for the design of emulsion-based chemical products consists in a systematic model-based methodology employing seven hierarchical steps: starting with the identification of the product needs and their transposition into appropriate target properties, then building the formulation by adding, one-by-one, the different classes of chemicals needed for each function: from the active ingredients, to the solvents, the emulsifiers and the additives, and finally determining the optimal composition of the formulated product. The design of the ingredient, driven by selection criteria based on the functional properties of each category of chemicals as well as by consideration of effectiveness, safety, toxicity and cost, is done through a data-model based computer aided molecular design technique. When a model-based design is not applicable since the functional properties needed to perform a rigorous choice are not readily available for consideration in a product design methodology, rule-based selection criteria are applied. These are centered on structured databases, where some relevant properties (e.g. saf
ety or toxicity-related), if not available, are predicted through dedicated pure component property models. Once all the most advantageou s ingredients have been chosen, the recipe candidates are identified through a knowledge-based mixture design method, where economic considerations are included together with appropriate boundaries related to solubility, stability, toxicity and safety issues. A special database of chemicals, classified according to their function and associated properties, has been developed. Also, a model library consisting of pure component and mixture property models has been developed so that the needed functional properties can be reliably predicted when their data cannot be found in the database. The abovementioned methodology and related tools are generic, in the sense that many different emulsified products can be designed through this framework once the needs-property relations are established, and they are here highlighted through a case-study dealing with the design of a tank cleaning blend. The main focus of this contribution is on the design of surfactants, primary responsible for the cleaning activity, thanks to a comprehensive framework based on newly developed both pure component and mixture property models. The workflow methodology with associated models, tools, databases and algorithms will be implemented into a computer-aided framework for emulsion-based formulation design.

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**Development of a New Comprehensive Framework for Surfactant Selection and Design for Emulsion-based Chemical Product Design**

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**Modeling of the Critical Micelle Concentration (CMC) of Nonionic Surfactants with an Extended Group-Contribution Method**

A group-contribution (GC) property prediction model for estimating the critical micelle concentration (CMC) of nonionic surfactants in water at 25 °C is presented. The model is based on the Marrero and Gani GC method. A systematic analysis of the model performance against experimental data is carried out using data for a wide range of nonionic surfactants covering a wide range of molecular structures. As a result of this procedure, new third order groups based on the characteristic structures of nonionic surfactants are defined and are included in the Marrero and Gani GC model. In this way, those compounds that exhibit larger correlation errors (based only on first- and second-order groups) are assigned to more detailed molecular descriptions, so that better correlations of critical micelle concentrations are obtained. The group parameter estimation has been performed using a data set of 150 experimental measurements covering a large variety of nonionic surfactants including linear, branched, and phenyl alkyl ethoxylates; alkanediols; alkyl mono- and disaccharide ethers and esters; ethoxylated alkyl amines and amides; fluorinated linear ethoxylates and amides; polyglycerol esters; and carbohydrate derivative ethers, esters, and thiols. The model developed consists of linear group contributions, and the critical micelle concentration is estimated using the molecular structure of the nonionic surfactant alone. Compared to other models used for the prediction of the critical micelle concentration, and in particular, the quantitative structure–property relationship models, the developed GC model provides an accurate correlation and allows for an easier and faster application in computer-aided molecular design techniques facilitating chemical process and product design.
Prediction of thermo-physical properties of liquid formulated products

The objective of this chapter is to give an overview of the models, methods and tools that may be used for the estimation of liquid formulated products. First a classification of the products is given and the thermo-physical properties needed to represent their functions are listed. For each property, a collection of the available models are presented according to the property type and the model type. It should be noted, however, that the property models considered or highlighted in this chapter are only examples and are not necessarily the best and most accurate for the corresponding property.

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Systematic Approach for Conceptual Process Design: Production of Styrene From Benzene and Ethylene

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Use of Water-Oil-Surfactant System Phase Behavior Data/Model for Emulsion-based Chemical Product Design

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A Systematic Methodology for Design of Emulsion Based Chemical Products

A systematic methodology for emulsion based chemical product design is presented. The methodology employs a model-based product synthesis/design stage and a modelexperiment based further refinement and/or validation stage. In this paper only the first stage is presented. The methodology employs a hierarchical approach starting with the identification of the needs to be satisfied by the emulsified product and then building up the formulation by adding one-by-one the different
classes of chemicals. A structured database together with dedicated property prediction models and evaluation criteria are employed to obtain a list of formulations that satisfy constraints representing the desired needs (target properties). Through a conceptual case study dealing with the design of a sunscreen lotion, the application of this new methodology is illustrated.

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A Systematic Methodology for Design of Emulsion Based Chemical Products

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Design of an Emulsified Hand Wash Through a Systematic Model-Based Methodology

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Property Prediction for Emulsion based Chemical Product Design

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Systematic methodology for design of emulsion based chemical products
Mattei, M., PhD Student, Department of Chemical and Biochemical Engineering
Gani, R., Main Supervisor
Kontogeorgis, G., Supervisor
Gernaey, K. V., Examiner
Kate, A. J. B. T., Examiner
Wiebe, L., Examiner
Technical University of Denmark
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Project: PhD

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Design of a Tank Cleaning Blend through a Systematic Emulsified Product Design Methodology
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Michele Mattei (Lecturer)
Department of Chemical and Biochemical Engineering
Computer Aided Process Engineering Center
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Description
Oral conference presentation: Michele Mattei, Peter Krogh, Bo Depner, Georgios M. Kontogeorgis and Rafiqul Gani, 2013, “Design of a Tank Cleaning Blend through a Systematic Emulsified Product Design Methodology”
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