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Process design based on physicochemical properties for the example of obtaining valuable products from plant-based extracts

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ABSTRACT

Herbal ingredients for use in the food, cosmetic and pharmaceutical industry are mainly gained from plant extracts. The challenge of producing these ingredients is the economic optimization of the design for the corresponding technical processes. To achieve this goal, a systematic, model-based approach is necessary, which is not yet available for complex mixtures (Bart and Pilz, 2010 [11]). The general basis for modeling and simulation of industrial processes is the knowledge of the physical properties of the system. A cost-effective option to get hold of separation factors of mixtures is the direct characterization of the multicomponent system, which has been the subject of earlier publications (Josch et al., 2012 [2]; Josch and Strube, 2012 [3]; Bart and Pilz, 2010 [11]). In this work, a systematic approach is illustrated on how to effectively characterize complex mixtures for a first process design. In addition, physical properties for individual plant components can be determined for modeling to optimize industrial processes. For this purpose, those processes which are well established in the chemical industry, including the use of substance databases and calculation of properties by means of thermodynamic theories, will be discussed. In addition, limitations of these approaches and resulting research requirements are shown.

1. Introduction

Selective extractions of active pharmaceutical ingredients from plant-based materials have increased in recent years due to the high consumer demand. The world trading volume of phytopharmaceuticals was approximately 100 billion US Dollars in 2011 [1]. In other areas, such as the cosmetic and food industry, growth rates of up to 6 % for the coming years are expected [1]. Benefits of plant extracts compared to synthetic products are, in addition to the public acceptance, the opportunity to obtain complex compounds economically. One example is the production of secondary metabolites, such as mono-, di- and sesquiterpenes, which can either not be produced synthetically or not economically. Extraction of these valuable materials and the subsequent purification are not carried out target-oriented and are mostly empirically driven with only few experimental examinations [2]. Thus, there is no systematic procedure for the design of the overall processes.

To meet economic and environmental requirements for the production of herbal substances, also in future, needs optimized processing. Therefore, this publication will focus on the purification of plant extracts as representative for the efficient handling of complex mixtures.

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In general, design and set up of industrial processes are divided into several development phases, like basic and detail engineering, equipment procurement, installation and start-up, and system operation [3]. The aim is to arrive at optimal process conditions at an early stage, since changes become more expensive the further development has progressed [3]. Therefore, an attempt is made using a conceptual process design (CPD) to arrive at an optimal process design for the separation sequence very early in process development, and in spite of still low information content (Fig. 1).

For this to happen, the process design has to be model-based, because this is the only way to find the process optimum fast and cost-effectively [4–6]. Depending on the modeling depth, either physicochemical properties or only separation factors are needed. These can either be retrieved from databases (e.g. Dortmunder Datenbank [DDB], DIPPR or Reaxys), calculated by means of thermodynamic theories (UNIFAC and COSMO-RS) or determined experimentally.

This approach has already been established for multi-component mixtures with small molecules and is considered state of the art [7–9]. In this work, it will be assessed how this methodology can be transferred to complex mixtures with the objective to generate an optimal separation sequence relatively early in process design. This task is complicated by the fact that those multicomponent mixtures consist of many compounds from a variety of compound classes, for which at least in part neither substance data nor molecular structures are known. Therefore, a systematic approach is to be developed for characterization and determination of the required physical properties for complex mixtures. This systematic process for determination of physical properties will be performed on technical sample systems from industry. The sample systems including yew needles, fennel fruits and sage leaves were chosen to represent several industries in an optimal way. The target component from yew needles (10-deacetylbaccatin III) provides the starting material for semi-synthesis of the breast cancer drug taxol [10]. Fenchone and anethole are target components from the fennel fruit which are mainly used in the cosmetic and phytopharmaceutical industry. Most valuable substances in sage leaves are carnosol and carnosic acid, which are predominantly applied as anti-oxidants and preservatives in the food industry.

2. Materials for the determination of physicochemical properties

2.1. Raw materials

In this paper, the raw material systems yew needles, fennel fruits, and sage leaves were considered as examples, representing different parts of a plant as main sources and at the same time displaying different chemical classes (e.g. mono- and di-terpenoids, alkaloids or phenolic substances) for the determination of product properties for complex molecules.

In the following chapter the utilized raw materials yew, fennel and sage are defined and the compounds to be isolated from the individual plant matrix are shown in Table 1. The experimental methods for characterization of complex mixtures have been published in detail in earlier publication and are therefore not described in this work [2,3,11].

2.1.1. European yew

Basically, yew represents a plant category containing a variety of yew species. Literature, for example, differentiates between the European, Pacific, Canadian, Japanese, Mexican, or Chinese yew [12]. All of them have in common to contain toxic components, like taxin B, or therapeutic compounds 10-deacetylbaccatin III and taxol [13]. Until 1990, the breast cancer therapeutic taxol was extracted from the bark of the pacific yew (*Taxus brevifolia*), where it can reach concentrations up to 0.1 mg/g [14]. As the tree grows slowly and does not survive the removal of the bark,

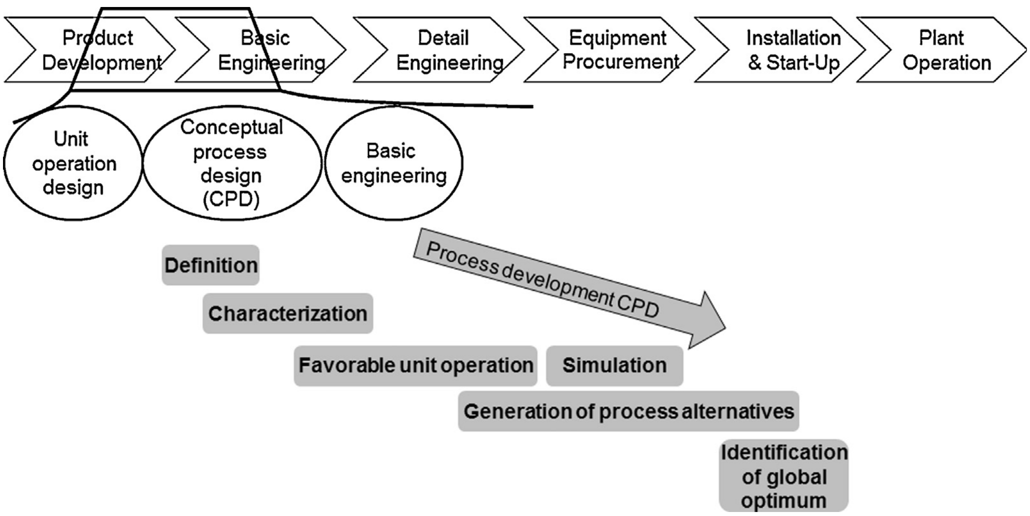

Fig. 1. Conceptual process design according to Josch and Strube [3].