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Model-based equipment-design for plant-based extraction processes – considering botanic and thermodynamic aspects

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ABSTRACT

The growing demand for plant-based products in the food, cosmetics and pharmaceutical industry leads to the need for a systematic process and equipment-design for the potentially applicable extraction techniques. Therefore, in this article, the classification of plant-based raw materials according to their characteristics is discussed. Furthermore, physicochemical modelling via distributed plug flow approach is applied and its possible fields of application are examined. Here, especially the extraction of water from the plant-based raw material as well as the entailed effects on the equilibrium and the mass transport kinetics are concerned. In addition to that, an evaluation method for the examined and generally available equipment through spider diagram is proposed. The relation to the initially argued botanic systems is discussed in particular. The extraction of vanillin from vanilla beans serves as exemplary system for this.

1. Introduction

Nowadays, the extraction of ingredients from plant-based raw materials mainly proceeds without systematics and is thus primarily empirical. This leads to processes, which are not designed optimal concerning energy and solvent consumption as well as yield, purity and time effort. In contrast, there is an increasing demand for plant-based nutrition, flavours, drugs and cosmetics [1]. In addition, the optimal design of these processes is a crucial factor for the implementation of profitability because of the increasing competition. Despite the vast demand, a systematic approach that combines the botanic characteristics – like for example, the structure of the raw material – and the technical implementations is not established so far [2,3]. In the chemical industry, such an approach is state of the art. Here, the processes are designed and optimized in a model-based way. This design is time saving and cost-effective. For the design of extraction processes, these models are not yet approachable with sufficient accuracy because of the complexity of the systems.

First approaches for the systematic design and optimization are primarily developed in universities. These approaches are most often based on the statistical experiment design or physicochemical modelling. The extraction of oleaonolic acid and ursolic acid from sage [4,5] as well as the extraction of vanilla beans and pepper [6] or the extraction of sugar beets can be named as examples here [7].

Statistical modelling is a method based purely on experiments for the identification of factors, e.g. temperature, pressure, corn size or extraction time, which have a sensitive influence on a target, such as yield or purity. Thereby, the statistical model of the process can be created by using polynomial regression. These statistical models are able to describe and visualize the process in a predefined factor range by curve fitting of the experimental results. For every plant-based system to be examined the same experimental effort is required and

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further, due to lack of a physicochemical process base, a learning curve cannot be generated [6].

For the predicative description of extraction processes, primarily for the extraction using supercritical CO_2, different physicochemical models are to be found in literature. These form a basis for a systematic approach. Thereby, the extraction equipment can be designed with small experimental effort and hence, time saving and cost-effective. Particularly, the three physicochemical approaches (1. shrinking core model [8,9], 2. model of broken and intact cells [10,11] and 3. desorption model [12,13]) can be mentioned here. A summary of the three modelling approaches with the respectively regarded substance systems is given in [5,14,15].

The effect of chemical properties as a starting-point for all process development has already been broadly described [3,6,14,16–18]. This paper focuses additionally on botanical and thermodynamic properties. Hence, a systematic approach is revealed, discussed and combined with the examinations of the botanic characteristics; the focus is on the integration of botanic and thermodynamic aspects as well as the selection and evaluation of the extraction equipment through physicochemical models.

2. Material and methods

The experimental setup for the process design and/or optimization consists of different methods for 1. pre-treatment of the raw material, 2. a standard apparatus for measuring phase equilibrium in maceration, 3. extraction kinetics in percolation equipment as well as 4. necessarily analytics. With these robust means, the solid–liquid extraction process step can be investigated.

The used raw material, *Vanilla planifolia*, as well as the equipment and the accompanying analytics are described in earlier publications [6]. To close the mass balances, the compositions of the two phases, the solid- and liquid phase, have to be determined. The target and side components are determined through HPLC. To close the mass balance for water and the solvent, the water content is determined through Karl–Fischer titration in the extract phase and through toluene distillation and moisture analyzer in the solid phase. [6].

3. Botanic basics and modelling approaches

The optimized design of the extraction as well as the influence of the remaining water in the raw material are discussed using the example of vanillin from *V. planifolia*. Fig. 1 illustrates the botanical influencing variables extended by the target function, the equipment. The most common instruments for solid–liquid extraction and the raw materials processed therein are tabulated in [3]. According to today's state of knowledge, an optimal process design is possible in a model-based way or with extremely high experimental effort. Hence this is a time and money-consuming process.

For the process design, botanical as well as economic factors have to be considered. Therefore, these factors are briefly illustrated in the following. For the selection of the extraction equipment, the raw material and its characteristics are crucial. Primarily, the botanical values 1. accessibility of the ingredients for the solvent, 2. structure of the matrix as well as 3. moisture content and swelling behaviour of the raw material can be named here. [16] In addition to the botanical characteristics mentioned, the characteristics of the target and side components are decisive as well. Essential oils, for example, are most often extracted via water steam distillation [19], whereas vanillin is won by solvent extraction [6].

The parameters to be determined for the process design are primarily the equilibrium, the mass transport kinetics and the fluid dynamic. Hereby, the former (equilibrium and mass transport kinetic) depend on the regarded substance system. The fluid dynamics is depending on the equipment. Hence, for optimizations of existing apparatuses as well as the design of apparatus on industrial scale, the fluid dynamic of the respective apparatus has to be

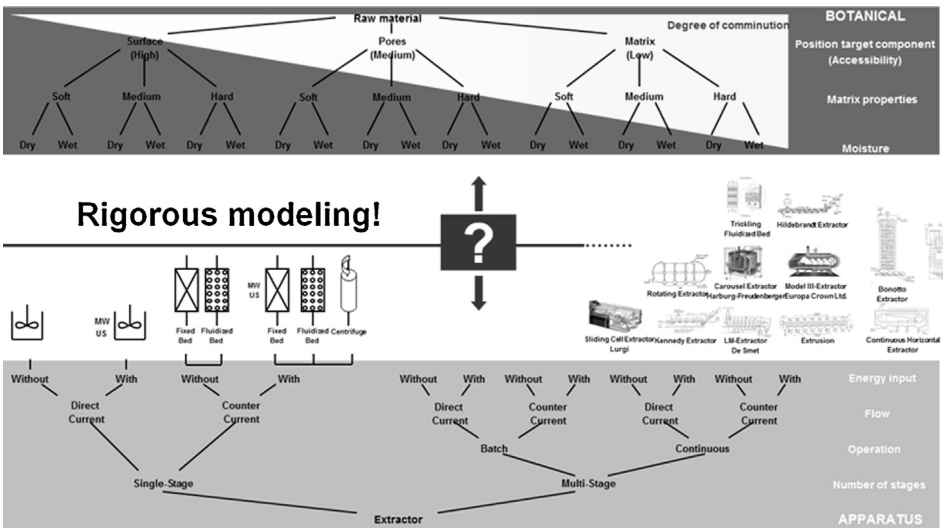

Fig. 1. Classification of botanical systems [16].