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Naphthalene sublimation. Experiment and optimisation based on neuro-evolutionary methodology

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ABSTRACT

This paper presents experimental and simulation studies on spherical samples of naphthalene sublimation in the presence of air as driving agent. The mass transfer rates and the influence of air flow characteristics on mass transfer are investigated. The degree of sublimation and sublimation front position as function of time are also determined. A modelling and optimisation strategy based on neural networks and genetic algorithms, designed in simple and adaptive variants, is developed and applied for determining optimal working conditions which lead to the maximisation or minimisation of sublimation rate. Accurate results are obtained proving the efficiency of the neuro-evolutionary methodology.

1. Introduction

Naphthalene sublimation technique is one of the most convenient method to study heat and mass transfer with multiple applications such as: determining the coefficients of heat and mass transfer for various configurations of flow space, for various forms of the surface samples fixed or moving [1–4], estimation of vapour pressure [5], studying the heat transfer for complex geometric objects [6–8].

To investigate this type of process by simulation has a series of advantages related to the possibility of obtaining accurate predictions or optimal working conditions. With this purpose, artificial intelligence tools, especially artificial neural networks (ANN) and genetic algorithms (GA), are often applied [9–13].

The present paper examines the sublimation of naphthalene spherical samples under atmospheric pressure in air as entrainer, without recycle. The sample weight was measured continuously as a function of time, at different air flow characteristics. The experimental data were used to calculate the mass transfer rate, the degree of sublimation, and the sublimation front position. The influence of air flow characteristics has also evaluated in order to determine optimal process conditions. The optimisation of the naphthalene sublimation process was performed using an ANN–GA methodology which related the rate of sublimation in the minimum or maximum values with optimal working conditions (process time, entrainer temperature, and entrainer flow rate). A feed-forward neural network with high performance was developed as a process model to be included into the optimisation procedure. An efficient GA with adaptive parameters, *i.e.* adaptive crossover and mutation rates, was used to solve the optimisation problem. In an ANN–GA methodology, original adaptive elements, own implementation, and a new application related to the naphthalene sublimation define and distinguishe this approach from those known in the open literature.

2. Experimental

2.1. Materials and methods

The experiments used in the present work consisted in the sublimation of naphthalene spherical samples under atmospheric pressure in air as entrainer, without recycle, with the goal to investigate the mass transfer rates and evaluate the influence of air flow characteristics on mass transfer.

Fig. 1 shows schematically the experimental equipment employed in this study. The installation is constituted by a sublimation chamber (1), a heat exchanger for air (2), a centrifugal fan (3), an analytical balance (4), and a thermostat (5). The

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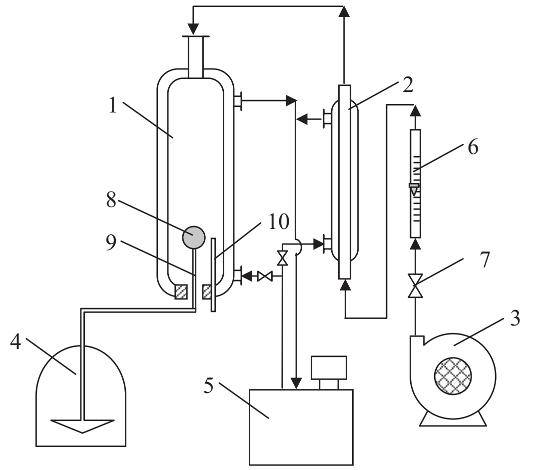

Fig. 1. Schematic of test installation: (1) sublimation room; (2) heat exchanger; (3) centrifugal fan; (4) analytical balance; (5) thermostat; (6) rotameter; (7) valve; (8) sample; (9) shaft and (10) digital thermometer.

experiments were carried out in a sublimation chamber, a jacketed vertical column from thermoresistant glass with 55 mm internal diameter, and 600 mm height. A double pipe from glass is used as heat exchanger for air. The entrainer heated with electrical resistance in the heat exchanger enters at top of the sublimation chamber and passes through the sample. The volumetric flow rate of the air through the sublimation chamber is measured by a rotameter (6) and controlled with the valve (7).

The samples were created by cooling molten naphthalene poured into stainless steel moulds with about 20 mm diameter. The spherical sample (8) was attached to the end of vertical shaft (9) placed in the sublimation chamber. During each experiment, the temperature in sublimation chamber was kept constant with hot water circulated in the column jacket. Sample weight was measured continuously as a function of time with an analytical balance. The sample temperature was measured with a digital thermometer (10) placed in the vicinity of the sample. The duration of the experiments was measured with a digital chronometer.

The experimental determinations were made for four values of air temperature (50 °C, 60 °C, 65 °C, and 70 °C) and, for each temperature, four values of air flow rate (2000 L h^{-1}, 3000 L h^{-1}, 4000 L h^{-1}, and 5000 L h^{-1}) were considered. The weight of the sample during the sublimation process was measured with an analytical balance. 150 experimental data resulted from experiments constituted the data set for modelling and optimisation of the sublimation process.

To calculate the rate of naphthalene sublimation, the amount of sublimated naphthalene in time, the particle radius, and its surface area have been determined.

2.2. Modelling and optimisation strategy

In this paper, artificial neural networks were chosen to model the sublimation process of naphthalene based on the fact that they possess the ability to learn what happens in the process without actually modelling the physical and chemical laws that govern the system.

Our experimental data fulfil a necessary condition for ANN modelling: a sufficient number of data (150) was obtained which uniformly cover the investigated domain. Feed-forward multilayered neural network type (multilayer perceptron, MLP) was chosen and tested for naphthalene sublimation based on its simple structure, ease of designing and training, good predictions it provides, and the possibility to combine it with other simulation techniques (in this case, genetic algorithms). The modelling purpose was to evaluate the performance of the process, quantified by the sublimation rate, ν_s, (output variable) depending on process time, t, entrainer temperature, T, and entrainer flow rate, M_ν (the three input variables of the neural model).

The developed neural model was included into an optimisation procedure, designed for obtaining maximum/minimum values for the sublimation rate, which was solved with GA. This algorithm was chosen based on a series of benefits given by the flexibility, ease of operation, minimal requirements, or global perspective offered. In the present work, GA was applied comparatively in two variants: simple and adaptive.

Following the biological analogy, an individual is represented by a chromosome, composed of a number of genes, codified, in this work, by real values. The fundamental operators of a genetic algorithm are: selection, crossover, and mutation. Roulette-wheel selection, arithmetic real-values crossover, and mutation by resetting a gene to a random value in its domain were applied here for optimising the rate of naphthalene sublimation. The stop condition of the procedure was determined by a pre-established maximum number of generations.

Number of individuals in the population, maximum number of generations, crossover and mutation rates are control parameters of GA which influence the algorithm performance. Generally, it is difficult to choose the most appropriate values for these parameters, the method often applied being trial-and error. A solution to alleviate this problem is proposed in this work and is consisted in the use of adaptive rates for crossover and mutation. To be able to dynamically adjust these rates, it is important to identify the moment when the algorithm begins to converge into an optimum, *i.e.* to observe the average value of the fitness of the population $\overline{f}$, in conjunction with the maximum fitness $f_{\max}$. For a population which has converged into an optimum, $f_{\max} - \overline{f}$ should have a lower value than in the case when the population is dispersed in the search space. Thus, the main idea of the adaptive genetic algorithm is that the values of the crossover rate, p_c, and the mutation rate, p_m, should be varied depending on the difference $f_{\max} - \overline{f}$. The rates p_c and p_m should increase when the algorithm tends to converge, and thus increase the genetic diversity and lower the chances of converging into a local optimum. However, even if the GA may no longer get stuck into a local optimum anymore, its performance, in terms of generations needed for convergence, may decrease.

In order to eliminate this problem, good solutions in the populations must be kept. This translates into low values for p_c and p_m for individuals with good fitness functions, and large values for individuals with poor fitness functions. The crossover rate should be proportional to $f_{\max} - f_p$, where f_p is the largest fitness value out of the two parents. The mutation rate should be proportional to $f_{\max} - f$, where f is the fitness value of the current individual.

Therefore, the expressions used to adaptively determine the crossover and mutation rate, respectively, are:

$$p_c = \frac{k_1 \cdot (f_{\max} - f_p)}{f_{\max} - \overline{f}} \qquad (1)$$

$$p_m = \frac{k_2 \cdot (f_{\max} - f)}{f_{\max} - \overline{f}} \qquad (2)$$

In the above equations, k_1 and k_2 are constants, $k_{1,2} \in \mathrm{R}^+$ and $k_{1,2} \leq 1$.

3. Results and discussion

3.1. Processing of the experimental data

The sublimation rate, the degree of sublimation, and sample radius were calculated as a function of time for various