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Short communication

An easy-to-use calculating machine to simulate steady state and non-steady-state preparative separations by multiple dual mode counter-current chromatography with semi-continuous loading of feed mixtures

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ABSTRACT

Multiple dual mode counter-current chromatography (MDM CCC) separation processes with semi-continuous large sample loading consist of a succession of two counter-current steps: with "*x*" phase (first step) and "*y*" phase (second step) flow periods. A feed mixture dissolved in the "***x***" phase is continuously loaded into a CCC machine at the beginning of the first step of each cycle over a constant time with the volumetric rate equal to the flow rate of the pure "x" phase. An easy-to-use calculating machine is developed to simulate the chromatograms and the amounts of solutes eluted with the phases at each cycle for steady-state (the duration of the flow periods of the phases is kept constant for all the cycles) and non-steady-state (with variable duration of alternating phase elution steps) separations. Using the calculating machine, the separation of mixtures containing up to five components can be simulated and designed. Examples of the application of the calculating machine for the simulation of MDM CCC processes are discussed.

1. Introduction

The counter-current chromatography (CCC) separation methods have been mainly used for preparative purposes to purify large amounts of compounds, especially in natural product chemistry for the separation of bioactive components [1–22]. In solid–liquid analytical chromatography, as a rule, samples are injected at sufficiently low concentrations to achieve elution under linear equilibrium isotherm conditions. In liquid–liquid chromatography, in most cases, the isotherms of the sample components are practically linear in a wider range of concentrations. The ability to load large samples is one of the great advantages of CCC. The requirements of high productivity and resolution in preparative CCC can be met by increasing the sample loading time and application of multiple sample loading and applying effective schemes and operation modes of the separation. The liquid nature of both phases has allowed for the development and implementation of cyclic dual-mode (DM) operating schemes, where the separation consists of a succession of two counter-current steps carried out in series alternating between light and heavy phase flows [20,23–34].

The cyclic DM method with the multiple changes in phase role and elution mode was first proposed by Delannay et al. and called multiple dual-mode CCC (MDM CCC) [23]. One cycle of the MDM CCC process corresponds to two elution steps at opposite ends of the column. The separation power of the MDM CCC is higher than that of conventional CCC, as the shuttle movement of the sample increases its retention in the column, which corresponds to a virtual increase in the length of the column. In the MDM CCC, an increase in productivity can be achieved by the sample re-injection after each cycle as proposed in Ref. [23]. In addition, the performance of the MDM CCC may be further improved by increasing the loading time, i.e. using semi-continuous sample loading.

The theoretical approaches for the MDM CCC with single sample injection were proposed in Refs. [25,27,31]. We have previously developed an analytical description of MDM CCC separations with a single sample loading and variable duration of alternating phase elution steps [31]. A full theoretical treatment of the steady-state (the duration of the flow periods of the phases is kept constant for all the cycles) and non-steady-state (with variable duration

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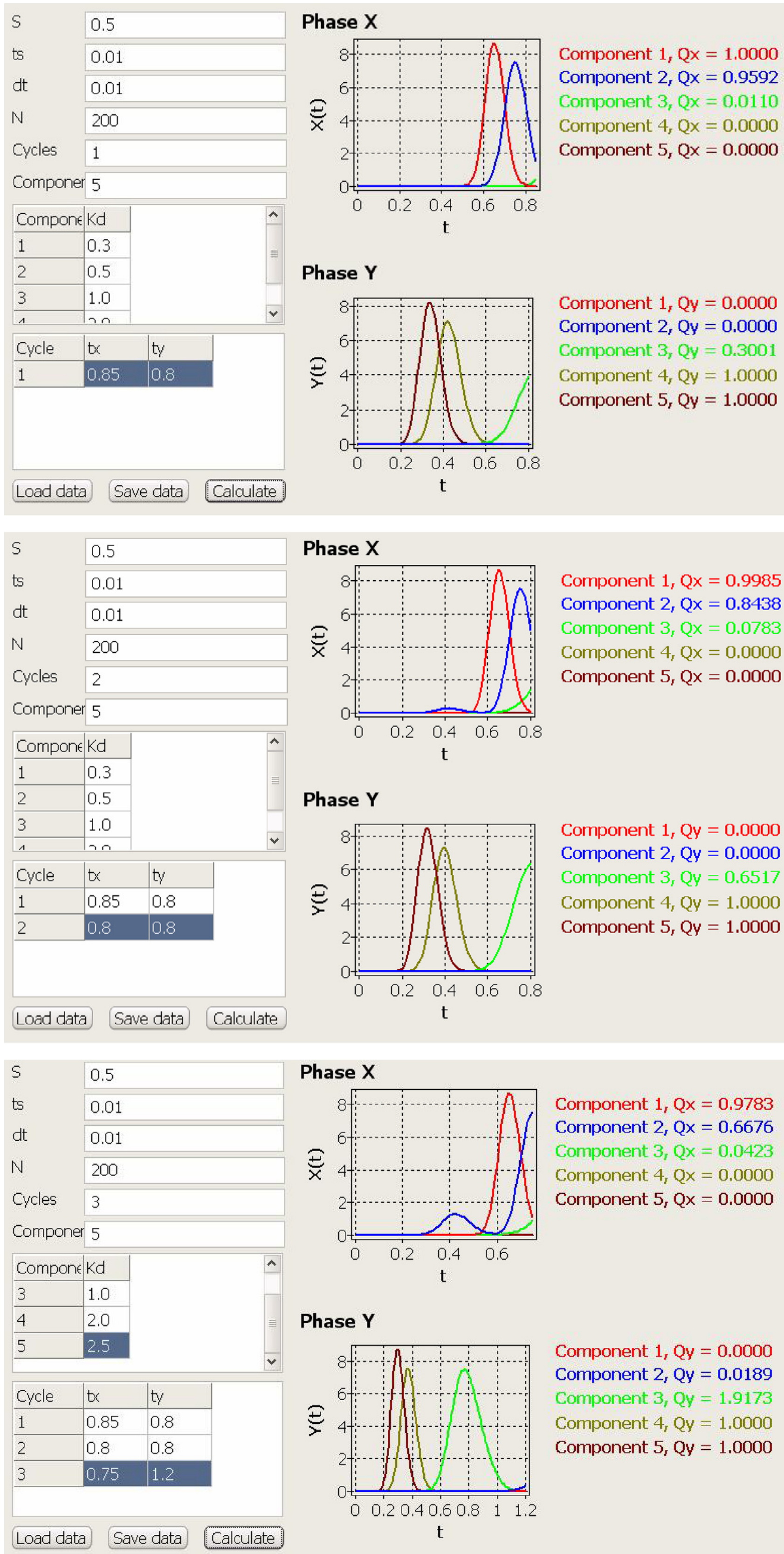

Fig. 1. The screen interface of the calculating machine: Simulation of the isolation and enrichment of the intermediately eluting component (K_{D3} = 1.0) from the five-component mixture K_{D1} = 0.3, K_{D2} = 0.5, K_{D3} = 1.0, K_{D4} = 2.0, K_{D5} = 2.5 in the column with N = 200 within three cycles using adjustable duration of phase elution steps. First cycle: t_x = 0.85, t_y = 0.8; second cycle: t_x = 0.8, t_y = 0.8; third cycle: t_x = 0.75, t_y = 1.2.