Numerical scheme for non-linear model of supercritical fluid extraction from polydisperse ground plant material: Single transport system

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Abstract

© Published under licence by IOP Publishing Ltd.Numerical algorithm is developed for modelling non-linear mass transfer process in supercritical fluid extraction (SFE). The ground raw material is considered as polydisperse, characterized by discrete number of effective particle fractions. Two continuous interacting counterparts separated by permeable membrane are distinguished in plant material build-up. The apoplast plays role of transport channels during extraction, and symplast contains extractable oil. The complete SFE model is non-linear as a result of non-linearity of oil dissolution kinetics. The computational scheme is based on the finite-volume approximation method and Thomas elimination procedure. The resulting system of algebraic equations is solved iteratively. Special attention is paid to polydisperse substrates, when particle scale characteristics of all fractions interact with each other through pore phase concentration on the vessel scale. Stability of the developed algorithm is demonstrated in numerical tests. Special iterative procedure guarantees a monotonic decrease of oil content in individual particles of substrate. It is also shown that in the limit of the so-called shrinking core approach the number of mesh nodes on a particle scale should be increased.