

RESEARCH NOTES

模拟移动床色谱手性分离过程的非线性非理想模型

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摘要 A non-linear non-ideal model, taking into account non-linear competitive isotherms, axial

dispersion, film mass transfer, intraparticle diffusion, and port periodic switching, was developed to simulate the dynamics of simulated moving bed chromatography (SMBC). The model

equations were solved by a new efficient numerical technique of orthogonal collocation on finite elements with periodical movement of concentration vector. The simulated SMBC performance is in accordance with the experimental results reported in the literature for separation of 1,1'-bi-2-naphthol enantiomers using SMBC. This model is useful for design, operation, optimization and scale-up of non-linear SMBC for chiral separations with significant non-ideal effects, especially for high solute concentration and small intraparticle diffusion coefficient or large chiral stationary phase particle.

关键词 [simulated moving bed chromatography](#) [chiral separation](#) [non-linear isotherm](#) [non-ideal effect](#) [dynamics](#)

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### A Non-linear Non-ideal Model of Simulated Moving Bed Chromatography for Chiral Separations

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**Abstract** A non-linear non-ideal model, taking into account non-linear competitive isotherms, axial dispersion, film mass transfer, intraparticle diffusion, and port periodic switching, was developed to simulate the dynamics of simulated moving bed chromatography (SMBC). The model equations were solved by a new efficient numerical technique of orthogonal collocation on finite elements with periodical movement of concentration vector. The simulated SMBC performance is in accordance with the experimental results reported in the literature for separation of 1,1'-bi-2-naphthol enantiomers using SMBC. This model is useful for design, operation, optimization and scale-up of non-linear SMBC for chiral separations with significant non-ideal effects, especially for high solute concentration and small intraparticle diffusion coefficient or large chiral stationary phase particle.

**Key words** [simulated moving bed chromatography](#); [chiral separation](#); [non-linear isotherm](#); [non-ideal effect](#); [dynamics](#)

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