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New iterative method based on the Q-iteration method for robust and rapid determination of concentration distribution in multicomponent separation cascades

摘要

同位素分离级联的浓度分布计算是级联设计与优化的关键，直接影响分离效率与成本。传统 Q 迭代法因其简洁性和快速收敛性被广泛采用，但存在三大缺陷：松弛因子需手动调整且无法自适应级联特性，迭代方向缺乏全局优化易导致震荡，以及在强分离或临界参数下收敛速度极低甚至停滞。

本文提出最小残差 Q 迭代法（MR Q 迭代法），结合传统 Q 迭代与改进的 Q 迭代策略。新方法分两阶段：首先通过 Q 迭代生成近似解，随后切换至 Q 迭代，利用梯度信息动态优化迭代方向与步长，将非线性问题转化为线性求解。该方法通过自适应调整松弛因子与全局梯度引导，有效平衡收敛速度与稳定性，避免局部震荡。

实验表明，MR Q 迭代法显著减少迭代次数与计算耗时，在传统 Q 迭代失效的场景中仍稳健收敛。其自适应机制与全局优化能力提升了复杂级联场景的适用性，为同位素分离的高效优化提供新思路，未来可拓展至瞬态过程与多目标优化领域。

关键词

多组分同位素混合物；分离级联；迭代法；Q 迭代法；牛顿法

Abstract

The determination of concentration distributions in isotope separation cascades is crucial for design and optimization, directly impacting efficiency and costs. While the conventional Q-iteration method is widely used for its simplicity and rapid convergence, it suffers from three limitations: manual tuning of the relaxation factor without adaptability, suboptimal update directions leading to oscillations, and extremely slow or stalled convergence under strong separation or critical parameters.

This study proposes the Minimal Residuals Q-iteration (MR Q-iteration), integrating traditional Q-iteration with an enhanced Q-iteration strategy. The method operates in two phases: generating an initial approximation via Q-iteration, then switching to Q-iteration to optimize update directions and step sizes using gradient information, transforming nonlinear problems into linear solutions. By adaptively adjusting the relaxation factor and leveraging global gradients, the method balances convergence speed with stability while avoiding local oscillations.

Experiments demonstrate that MR Q-iteration significantly reduces iterations and computational time, achieving robust convergence even in scenarios where conventional Q-iteration fails. Its adaptive mechanisms and global optimization capabilities enhance applicability to complex cascades, offering a novel approach for efficient isotope separation. Future extensions may address transient processes and multi-objective optimization.

Keywords

multi-component isotope mixture; separation cascades; iterative method; Q-iteration method; Newton–Raphson method

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