

Homotopy Continuation Enhanced Branch and Bound Algorithms for Process Synthesis Using Rigorous Unit Operation Models

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October 6, 2021

Abstract

Process synthesis using rigorous unit operation models is highly desirable to identify the most efficient pathway for sustainable production of fuels and value-added chemicals. However, it often leads to a large-scale strongly nonlinear and nonconvex mixed integer nonlinear programming (MINLP) model. In this work, we propose two robust homotopy continuation enhanced branch and bound (HCBB) algorithms (denoted as HCBB-FP and HCBB-RB) where the homotopy continuation method is employed to gradually approach the optimal solution of the NLP subproblem at a node from the solution at its parent node. A variable step length is adapted to effectively balance feasibility and computational efficiency. The computational results demonstrate that the proposed HCBB algorithms can find the same optimal solution from different initial points, while the existing MINLP algorithms fail or find much worse solutions. In addition, HCBB-RB is superior to HCBB-FP due to lower computational effort required for the same locally optimal solution.

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