Faculty of Engineering and Applied Science
Chemical Engineering Seminar Series

Discrete-Steepest Descend: A new Mixed-Integer Nonlinear Programming (MINLP) Algorithm for Chemical Process Optimization

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Dupuis Hall, Room 217

The aim of this talk is to introduce a novel optimization model and algorithm for the solution of Mixed Integer Nonlinear Programming (MINLP) and Generalized Disjunctive Programming (GDP) problems that emerge in chemical process optimization. The algorithms incorporate concepts from discrete convex analysis (DCA) that allow a more efficient exploration of the integer and some binary or Boolean variables in the formulation known as ordered discrete decisions. In this talk, the method will be formally introduced first followed by a discussion on the advantages of the proposed method from the point of view of computational costs and solution quality when compared to conventional GDP and MINLP solvers. Multiple case studies from different fields in chemical engineering will be used throughout the talk to demonstrate the versatility and potential of the method. One of these problems will involve the rate-based optimal design of catalytic distillation columns. To our knowledge, this optimization problem has not been solved using deterministic MINLP optimization strategies due to their complex nature. Moreover, the application of the proposed method was extended to address GDP problems through a new DCA-based technique referred to as logic-based Discrete-Benders Decomposition (LD-BD). To our knowledge, LD-BD is the first algorithm that combines DCA theory with logic-based Benders Decomposition (LBBD) principles. Furthermore, we also extended the application of DCA-based optimization tools to the Mixed-Integer Dynamic Optimization domain. Two case studies involving the optimal design and operation of catalytic distillation units and simultaneous scheduling and control will be presented to demonstrate the key features of the proposed algorithms. Overall, the proposed DCA-based algorithms bring advances to the field of MINLP optimization by solving challenging problems in the fields of optimal process design, optimal process scheduling, and optimal process integration.