Globally optimal scheduling of an electrochemical process via data-driven dynamic modeling and wavelet-based adaptive grid refinement

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Abstract

Flexible operation of an electrochemical recovery process of succinic acid can potentially yield economic benefits. We conduct experiments on the process and retrieve data for data-driven dynamic modeling. We then perform offline dynamic scheduling with discrete-time Hammerstein-Wiener (HW) models to obtain the globally optimal process schedule. We acknowledge the high computational requirements of the solution approach and propose a wavelet-based adaptive grid refinement algorithm for global optimization (GO) (AGRAGO), which employs a refinement criterion based on Lagrangian multipliers. AGRAGO is implemented in our in-house software for deterministic GO, MAiNGO. It is, then, used to automatically allocate the available control parameters in the grid to provide superior solutions in less CPU time. We demonstrate the applicability of AGRAGO and observe improved results compared to uniform control sampling while still detecting high computational expenses for dynamic GO. Overall, global dynamic scheduling (GDS) with AGRAGO leads to 14.1% economic savings.

**Keywords**: electrochemical acid recovery, demand-side-management, global dynamic scheduling, Hammerstein-Wiener model, adaptive grid refinement

* 1. Introduction

Optimal process scheduling provides economic savings to electricity-intensive processes (Mitsos et al., 2018). When process dynamics are time-relevant to electricity price fluctuations, they are accounted for to ensure schedule accuracy, resulting in a dynamic optimization (DO) problem (Bhatia and Biegler, 1996). Although typically solved with local optimization methods or model simplification techniques (Dias and Ierapetritou, 2019), optimal dynamic scheduling is often applied to complex processes necessary to be considered to avoid intractable scheduling objectives (Yang et al., 2014). Nonconvex global dynamic optimization (GDO) is considered among others (Floudas and Gounaris, 2009) by Kappatou et al. (2022), who introduce an approach of deterministic GDO using a HW nonlinear process model. The optimization problem is solved after control parametrization and time discretization using ODE relaxations (Singer and Barton, 2004) and a branch-and-bound (B&B) algorithm. The high computational demands of the method favor grid refinement approaches (e.g., Chen et al., 2012) that optimally decide on the control discretization to use fewer optimization variables (DoFs) and reach high-quality solutions. Schlegel et al. (2005) introduce an adaptive refinement algorithm based on wavelets to solve continuous-time DO problems sequentially. Schäfer et al. (2020a,b) extend their work to quasi-steady-state scheduling problems introducing a refinement criterion based on Lagrangian multipliers.

We here give a summary of our latest work (Papadimitriou et al., 2023), where we perform GDS to a downstream electrochemical process of succinic acid recovery (Schröder et al., 2022) using HW models (Kappatou et al., 2022) trained on experimental data. To reduce the computational expenses, we then propose a wavelet-based adaptive grid refinement algorithm for GO (AGRAGO), applicable to DO problems, based on previous works (Schlegel et al., 2005; Schäfer et al., 2020a,b), which we include in our software for deterministic GO, MAiNGO (Bongartz et al., 2018).

* 1. Data-driven dynamic modeling

We focus on a downstream process (Fig. 1) of bio-based succinic acid recovery (Schröder et al., 2022) as a promising candidate for scheduling application. We perform experiments on the first electrolysis cell and obtain data on the power consumption (model output) over the process molar throughput (model input) by applying current density variations while reaching full acid protonation. The data are used to identify a single-input, single-output HW model. Discrete-time dynamics and an ANN trained on the H function are used to decrease computational expenses. The model uses a 4th- (H,) and a 2nd-degree (W) polynomial, and a 4th-order LTI. The resulting model fitting is 95 % (*1 - NMSE*).

* 1. Deterministic global dynamic scheduling

We consider the scheduling problem of flexible operation of the process of Fig. 1 to adjust the molar throughput (**u**) leading to varying power consumption levels (**y**) while reaching a fixed daily acid production under one-day hourly changing German spot electricity prices of February 7, 2023. The problem is formulated, according to Kappatou et al. (2022), as a GDO problem, and is solved for a piecewise constant control parametrization and varying control time series - discretization (*n*), using MAiNGO (Bongartz et al., 2018)). The ANN relaxations are provided by MeLOn (Schweidtmann and Mitsos, 2019).

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| Figure 1. Succinic acid recovery process flowsheet (Schröder et al., 2022) and Hammerstein-Wiener (HW) process model representation. The HW model consists of a linear dynamic block (LTI) placed between two nonlinear static blocks (H and W). |

The results indicate an overall increasing objective value improvement and an exponential scaling of the computational expenses over the number of control discretization points (*n*). The latter poses limits to the real-time applicability of the method, considering a 12-hour gap between price announcement and implementation. The highest economic benefit of the solution accepting this limit is 13.1 %. The corresponding schedule gives the dynamic process response to the price fluctuations.

* 1. Wavelet-based adaptive grid refinement algorithm for global optimization (AGRAGO)

We propose an adaptive control grid refinement algorithm for GO (AGRAGO) based on discrete wavelet transformations (Schlegel et al., 2005; Schäfer et al., 2020a,b) for full exploitation of the price fluctuations while decreasing computational expenses or equivalently using fewer DoFs. AGRAGO works iteratively (Fig. 2); first performing (D)GO given a certain control grid, then post-processing the optimization results evaluating the coefficient values and the Lagrangian multipliers associated with the deactivation and activation, respectively of a coefficient to, last, construct the grid of the next iteration. The algorithm terminates heuristically.

AGRAGO is integrated into MAiNGO (Bongartz et al., 2018) for automatic refinement and, in contrast to previous works, allows for application to a wide selection of problems, including GDS. It, additionally, incorporates the concept of *batches* (subhorizons of the same power-of-two grid intervals) to allow matching setpoint and problem parameter (i.e., price) changes and suggests GO in the space of the original control parameters rather than the wavelet coefficients (Schäfer et al., 2020b). The adaptations improve the results in terms of objective value and CPU time, respectively.

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|  Figure 2. Simplified graphical representation of AGRAGO.  |

We solve the problem using AGRAGO, similar to Section 3, considering three *batches* and a set of equality constraints related to the coefficients’ deactivation. We note a similar computational scaling and improved savings for the same *n* compared to uniform control sampling. AGRAGO exhibits high savings for only a few DoFs (1.7 % higher compared to equidistant sampling for five *n*). The best solution achieved with AGRAGO respecting the computational time limitations gives 14.1 % savings. The resulting optimal schedule suggests higher benefits from lower production during the high and medium prices and more flexible adjustments during the lower prices to fulfill the daily production demand.

* 1. Conclusions

We perform experimentation and data-driven dynamic modeling for an electricity-intensive process for electrochemical acid recovery. We consider the flexible operation of the process for participation in a day-ahead electricity market and solve the dynamic optimization problem to global optimality. We note the high economic savings attained and the high computational demands of the approach. We propose a wavelet-based adaptive grid refinement algorithm for global optimization (AGRAGO) for automatic control discretization refinement applied to global dynamic scheduling. AGRAGO application results in higher savings, reached in less computational time and an overall economic gain of 14.1 %.

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