## 9f Integration of Process Design and Control through Optimal Control

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Integrated Process Design and Control (IPD&C) has drawn increasing attention over the past decade, as this has given rise to significant economic benefits and improved plant operational performance in applications. However, the multifaceted nature of the problem and the computational burden of the resulting mathematical formulations have restricted progress in this field (Kookos and Perkins, 2001).

The initial works in the field of IPD&C were more focused on designing economically optimal processes that can work efficiently in dynamic mode. These use steady-state response models (such as RGA) or very limited dynamic models for designing the process, and hence generally overlooking the dynamic behavior of the plant under actual disturbances and failing to characterize the behavior of the system in transition between nominal and post-disturbance steady-states. Very recent developments address the need of using dynamic models in IPD&C, but avoid the control-scheme selection step due to near-infinite possibilities that cannot be entirely embedded in an optimization scheme. In general, most available methods fail to adequately assess the controllability of the process through their inability to estimate the closed-loop performance of the design. Further, few existing methods can impose path-constraints (constraints that are active not only at the steady-state but also during the entire operation with short-term disturbances, such as operational constraints and safety-related limitations) within the process design procedure, so that the final design is guaranteed to adhere to these limits in operation.

In this work, a novel optimal process synthesis methodology is proposed. The principal idea is to evaluate the closed-loop dynamic performance of each candidate design directly, during the synthesis stage, under a modified Linear Quadratic Regulator (mLQR) scheme. The control performance evaluations are used in conjuncture with a more conventional static superstructure design approach for process synthesis, as additional constraints and/or objectives. This is accomplished by measuring the control performance of each candidate design with a state-feedback PI controller, which is a simulation step performed for each candidate design. The novelty of the proposed method is that, instead of introducing the controller tuning problem as an additional optimization problem, or additional decision variables in the design problem, it is solved as an optimal control mLOR problem. The solution of the mLQR problem yields an optimally tuned state-feedback PI control scheme. The performance of the optimal controller is the best achievable performance for the given process; hence it is an effective method for comparing the actual control performances that will be displayed by different candidate designs in real operation. The major advantage of the LQR scheme is that the controller equations and parameters can be calculated readily for a linear system. For nonlinear systems, iterative linearization of the nonlinear system models is applied to yield a satisfactory result. The tandem of optimal control and process synthesis enables considering the closed-loop control performance and ensuring the ability to satisfy any path-constraints within the flowsheet design stage.

In formulating an optimization problem for IPD&C, process design variables and manipulated variable adjustments are taken into account as decision variables. Controllability is expressed as a minimum square-error type integral term in the objective function and a number of operational constraints that are to be satisfied for a set of predefined worst-case disturbance vectors. The dynamic optimization problem is solved via a sequential feasible path algorithm, where the original dynamic optimization problem is transformed to a bi-level problem which consists of an outer optimization with respect to design (static) variables subject to an inner optimization with respect to the control (dynamic) variables, a decomposition in parallel with the dual nature of the IPD&C problem. In the inner loop, the optimal control problem is solved for a given design variable vector, where the candidate design is simulated under its optimal control scheme. The simulation in the mLQR step enables evaluation of the entire set of path constraints as well as the actual control performance. The functional evaluations in the inner

loop are fed to the outer loop, where the MINLP optimizer is a quasi-static optimization as the objective and constraints are merely static, though nonlinear, functions. It modifies the design variable vector accordingly, iteratively converging to the optimum design in terms of both cost and controllability.

The proposed IPD&C methodology is exemplified on an evaporator test case, where it is demonstrated to succeed in creating designs that are cost effective and highly controllable. Further refining the algorithm for better computational performance and applications to large scale problems are discussed.

Reference:

1. Kookos, I., & Perkins, J. D. (2001). An algorithm for simultaneous process design and control. Industrial & Engineering Chemistry Research, 40(19), 4079-4088.