Interior Point Solution of Integrated Process and Control Design Problems with Embedded MPC

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Introduction

The potentially significant impact that the design of a process plant can have on its ability to be satisfactorily controlled has led to the development of integrated formulations in which dynamic performance requirements are included as constraints within an optimal design framework. Failure to account for the dynamic operation of a process could lead to reduced profits or even safety and environmental constraint violations. This motivates the need to design the process and its associated control system in an integrated manner. Prior work in simultaneous process and control system design has focused primarily on the use of linear controllers such as proportional-integral control (Mohideen et al., 1996; Bahri et al., 1997; Schweiger and Floudas, 1998; Kookos and Perkins, 2001; Pistikopoulos and Sakizlis, 2002). Baker and Swartz (2004a) considered actuator saturation effects in integrated design and control. This results in model discontinuities, and to avoid potential difficulties with a sequential solution approach in which the integration of the model differential-algebraic equation system is separated from the optimization, they follow a simultaneous solution approach in which the actuator saturation is handled through mixed-integer constraints. They demonstrated that failure to account for actuator saturation could lead to suboptimal designs. The growth in solution time with problem size led to the development of an alternative approach in which saturation was modeled using complementarity constraints, and the resulting problem solved using an interior-point approach (Baker and Swartz, 2004b).

The Integrated Design Problem with Constrained MPC

In this paper we consider integrated design and control with constrained model predictive control (MPC) as the regulatory control system. MPC has become the advanced control method of choice in the chemical process industry, thus direct accommodation of MPC within the integrated design framework is important. The resulting problem shares the characteristic of model discontinuity with the actuator saturation problem above, but is more complex, since the control calculation involves the solution of a quadratic programming (QP) problem at every sampling period. When embedded within a design optimization problem, this results in a multi-level optimization problem. We follow a simultaneous solution approach in which the MPC optimization sub-problems are replaced by their Karush-Kuhn-Tucker (KKT) optimality conditions. In recent work (Baker and Swartz, 2005), we have considered this formulation for the constraint back-off calculation problem with constrained MPC as the regulatory control system. This results in a single-level optimization problem, but with complementarity constraints. IPOPT-C (Raghunathan and Biegler, 2003), an interior point algorithm designed for mathematical programs with complementarity constraints, was found to solve these problems reliably and significantly faster than a mixed-integer quadratic programming formulation. Here, we extend the formulation to integrated design and control. Our approach differs from that of Sakizlis et al. (2003) who use a parametric formulation of the predictive controller in an integrated plant and control system design strategy. They use a sequential solution approach in which the Boolean algebraic conditions defining the regions of applicability of the explicit control laws are replaced with steep hyperbolic tangent functions.

Formulation

The general form of an integrated design and control problem consists of:

An objective function:	$\min \Phi(x, y, u, d, t)$
Dynamic equations:	$\dot{x} = f(x, u, d, t)$
Initial conditions:	$x(0) = x_0$
Algebraic constraints:	$h(y, x, u, d, t) = 0$,
	$g(y, x, u, d, t) \leq 0$
Control equations:	$u = \mathsf{fn}(x, y, d)$

where d represent the design variables including set-points, y represent the controlled outputs, x represent the states and u represent the inputs to the system.

We consider here linear constrained MPC applied to a nonlinear dynamic plant. This is a commonly occurring situation in practice, and is reasonable for operation close to a desired steady-state and/or for processes that are not strongly nonlinear. The internal dynamic model used by the predictive controller is based on a linearization around the nominal operating point; thus it is a function of both the design variables and the operating point. The nonlinear dynamic plant model is discretized using orthogonal collocation on finite elements, and the resulting equations included as constraints in the overall optimization problem. The controller equations comprise the KKT conditions of the MPC open-loop optimization problems (QP problems) corresponding to each sampling period.

The general form of a QP problem is:

$$\begin{aligned} \min_{x} \quad & \frac{1}{2}x^T H x + g^T x \\ \text{Subject to} \quad & \\ Ax &= b \\ x &\geq 0 \end{aligned}$$

The KKT conditions of this QP problem can be written as:

$$\begin{aligned} Hx - A^T\lambda + g - \nu &= 0 \\ Ax &= b \\ x_i \nu_i &= 0 \\ (x, \nu) &\geq 0 \end{aligned}$$

From this it can be seen that the transformation of the MPC QP optimization problem into its KKT optimality conditions results in a set of constraints that is linear except for the complementarity constraints.

Together with the discretized plant model, these equations define the closed-loop dynamic response of the system. The complementarity constraints resulting from the KKT conditions of the QP sub-problems are handled through the application of an interior point solution approach.

Case study: CSTR

The first case study under investigation is the design of a single-input, single-output, continuously stirred tank reactor based on the model presented in (Schweiger and Floudas, 1998).

The reaction taking place is a first-order, exothermic, irreversible reaction A $\rightarrow$ B. The reactor is cooled by means of a cooling jacket surrounding the tank. It is assumed that the contents of the reactor and the cooling jacket are perfectly mixed and that the volume and density of the contents of the reactor and the cooling jacket remain constant and are independent of the temperature and concentration of the mixture.

The controlled variable in this system is the temperature of the reactor, and it is controlled by manipulating the flow-rate of cooling water through the jacket. Changes in the feed temperature to the reactor act as disturbances to the process. The flow-rate required to negate the effect of the disturbance is determined by a model predictive controller. It will be assumed that valve dynamics can be neglected.

The nominal operating point of the temperature in the reactor and the nominal cooling water flowrate are included as decision variables in the problem. The height and diameter of the tank are initially unknown and are also included as design variables in the integrated process and control design. Also, the optimal value of the controlled variable tuning parameter for the model predictive controller is unknown. The tuning parameter is assumed to be constant over the reference trajectory. The design is generated for a single disturbance scenario, a step increase of 17K in the feed temperature. The following restriction is imposed on the dimensions of the reactor: $0.5 \leq L/D \leq 2$.

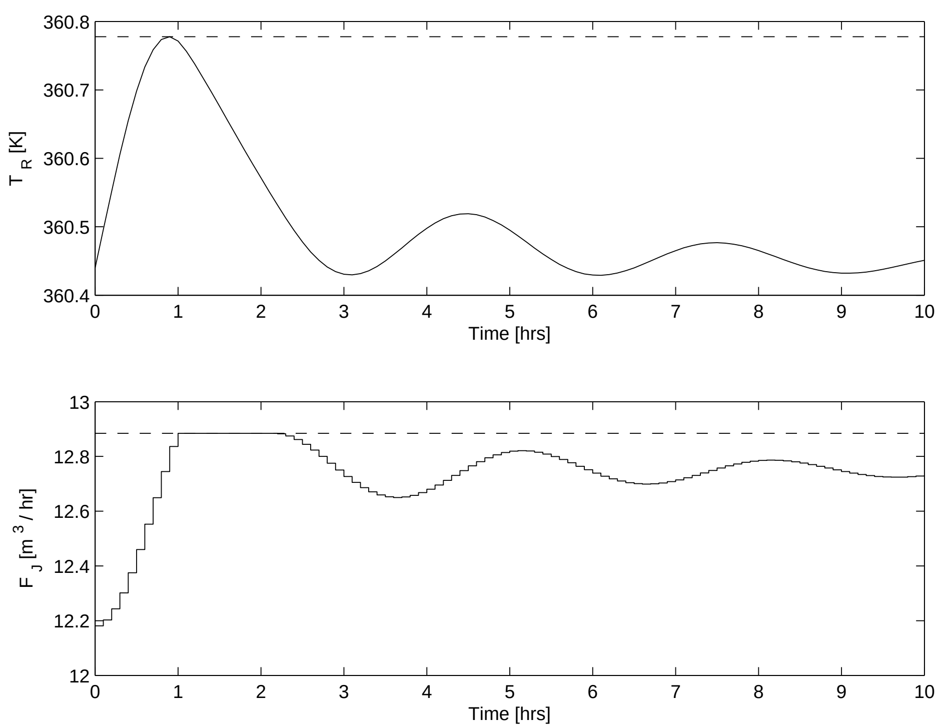

Figure 1: Optimal trajectory obtained for the CSTR problem for a disturbance of 17K .

The problem was solved using IPOPT-C, with the internal linear MPC model integrated simultaneously using a backwards difference strategy. The optimization determined optimal operating points

Table 1: Optimal solution to case study 1

Variable	Description	Value	
Objective	Objective	339.8	000 $
T_R	Temperature	360.4	K
F_R	Jacket flow-rate	12.18	m^3/hr
H_R	Height of reactor	2.98	m
D_R	Diameter of reactor	5.95	m
Q	MPC CV Weight	7.18	

for the reactor temperature, flow-rate, the diameter and height of the tank, and controlled variable weighting for the MPC controller as reported in Table 1. The resultant optimal trajectory is illustrated in Figure 1.

Conclusion

In this paper an optimization strategy is proposed for simultaneous process and control design that allows for model predictive control. The explicit inclusion of the KKT optimality conditions that comprise the controller optimization at each time step allows for incorporation into the optimization-based design framework. The resulting mathematical program with complementarity constraints (MPCC), which arises from the direct inclusion of the KKT optimality conditions, is solved using IPOPT-C.

The discrete time controller model is obtained from a linearization around the nominal operating point, which changes based on the outcome of the optimization. To overcome this, the internal model is formulated as a backwards difference integration problem that is integrated simultaneously within the optimization.

We have shown that this approach combined with IPOPT-C can successfully solve the integrated process and control design problem with a constrained model predictive controller with a single-input, single-output case study. Application to additional case studies is in progress.

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