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Robust multi-objective dynamic optimization of chemical processes using the Sigma Point method

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HIGHLIGHTS

- We present a novel method for robust dynamic optimization via the sigma point.
- The proposed method outperforms a linearization approach for a large-scale problem.
- The method is integrated into a dynamic multi-objective optimization framework.
- The trade-off between increased robustness and decreased productivity is studied.
- A reduction in reactor performance and in the Pareto front width is observed.

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ABSTRACT

Dynamic optimization solutions largely rely on the accuracy of the underlying mathematical models. However, these models only represent an approximation of the real dynamic process and their predictions are dependent on a set of parameter values. These parameter values can be hard to estimate exactly (e.g., thermal conductivity) or vary over time (e.g., due to fouling) potentially leading to hazardous situations when applying a model based optimal solution. Robust dynamic optimization deals with the uncertainty related to these parameters in order to quantify their effect and deliver safer (i.e., more robust) operating conditions. This paper discusses a computationally efficient robust dynamic optimization approach based on the Sigma Point method and shows how it outperforms a linearization-based method for a nonlinear dynamic chemical vapor deposition reactor case-study with multiple uncertainties. Moreover, by accounting for uncertainty a trade-off between process safety and performance of the reactor is introduced. This aspect is cast in a multi-objective dynamic optimization framework. In particular, it is illustrated how an increasing robustness (i.e., process safety) induces a worsening of other investigated objective functions and results in robustified Pareto sets.

1. Introduction

Chemical processes are often described by complex and dynamic mathematical models. Model based approaches enable to systematically devise appropriate plant designs and operational policies via tailored simulations and the solution of well-defined dynamic optimization problems. However, these optimal solutions heavily rely on the model accuracy. Unfortunately, every model suffers from inherent uncertainties due to difficulties in correctly estimating key model parameters or to drifting of the plant from its original conditions.

Uncertainty can appear under the form of parametric uncertainty which has ideally to be accounted for in the optimization of these processes (e.g., Sahinidis, 2004). Generally, uncertainty can be treated based on different strategies: (i) via the formulation of expected values and *chance constraints* that take into consideration the uncertainty's probability distribution (see, e.g., Wendt et al., 2002; Mitra, 2009; Recker et al., 2012; Li et al., 2002, 2008; Schenkendorf et al., 2009) or, (ii) via the formulation of a *worst-case* scenario optimization when the uncertainty is known to lie within a given set, e.g., a box or ellipsoid (see, e.g., Nagy and Braatz, 2004; Houska et al., 2012; Nagy and Braatz, 2003; Telen et al., 2013).

Particular challenges relate in the probabilistic framework to an integration over the probability distribution. Different variance quantification and analysis approaches can be found for example

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in Diwekar and Kalagnanam (1997); Nagy and Braatz (2007). In the worst-case framework, the challenges arise from the hard-to-solve robust counterpart problem, i.e., a worst-case scenario or min–max optimal control problem which has to be solved by approximation strategies (see Hermanto et al., 2007 for an application to optimal control). For example, the approximation strategy adopted in Diehl et al. (2006) is based on first order Taylor series linearization of the model with respect to the uncertainty and the robust counterpart problem is solved with the use of Lyapunov equations. In these cases no measurement information is assumed, while other methodologies – which are not considered in the current paper – make use of available measurements to ensure robustness (Srinivasan et al., 2003).

Moreover, there is a price to pay in order to increase robustness. Typically, this is reflected in a performance reduction (Datskov et al., 2006) and an increased computational burden. This trade-off between the nominal performance and robustness can be investigated using *multi-objective optimization* (MOO). Main groups of methods to solve multi-objective optimization problems include (i) *vector based approaches* (e.g., Deb, 2001) and (ii) *scalarization approaches* (e.g., Miettinen, 1999). The former class treats the MOO problem directly and often makes use of evolutionary algorithms. This class of methods requires a significant amount of function evaluations and typically cannot efficiently handle a large number of degrees of freedom. However, a high number of successful applications has been reported in the literature, e.g., in Zhang et al. (2002), Sarkar et al. (2007), Rangaiah and Bonilla-Petriciolet (2013). The latter class converts the MOO problem in a series of parametric *single objective optimization* (SOO) problems. Each of the SOO problems can be efficiently solved with fast gradient-based optimization methods. The most common approach is the classic Weighted Sum (WS). However, these methods suffer from some intrinsic drawbacks (Das and Dennis, 1997), to overcome them other advanced scalarization approaches are used in this work: (i) Normal Boundary Intersection (NBI) (Das and Dennis, 1998) and (ii) the (Enhanced) Normalized Normal Constraint ((E)NNC) (Messac and Mattson, 2004; Sanchis et al., 2008). It has been shown that the integration of direct dynamic optimization methods with the latter scalarization methods leads to an efficient solution of dynamic optimization problems with multiple objectives (Logist et al., 2012).

In this paper the probabilistic framework is used to formulate an approximate but computationally tractable solution approach for *robust dynamic optimization problems* (RDOPs) involving *expected value dynamic optimization* and additional *chance constraints*. The approach is based on the *sigma point method* (SP) (Julier and Uhlmann, 1996), which allows the accurate approximation of the probability distribution through any nonlinear mapping via a sampling technique. In particular, the proposed approach is compared with the linearization method used in Logist et al. (2011). Moreover, the developed approach is incorporated in a *multi-objective dynamic optimization problem* (MODOP) frame as developed in, e.g., Logist and Van Impe (2012) by explicitly including robustness as an additional objective. This framework for *robust multi-objective dynamic optimization problems* (RMODOP) finally leads to a robustified Pareto sets (Logist et al., 2011).

The developed framework is tested for the model based multi-objective optimization of a Chemical Vapor Deposition (CVD) reactor case-study for the production of high-grade polysilicon. Polysilicon consists of high purity silicon crystals, according to Del Coso et al. (2011) up to 99.99% purity, and is mainly produced for the micro-electronics and photo-voltaic (PV) market (Del Coso et al., 2011). Moreover, the PV industry has been expanding in the last years and it is expected to keep this trend in the near future (Masson et al., 2013; Solangi et al., 2011). The amount of PV capacity installed worldwide in 2013 has been 24% higher than that of 2012 and by 2017 it is expected to be between 55% and 170% higher than that of 2012.

The classic way to produce crystal-grade polysilicon is via Chemical Vapor Deposition (CVD). A thin high-purity silicon bar is placed inside the reactor and it is used as a seed for the crystal growth. The deposition reaction is endothermic. Higher temperatures enhance the thermodynamics and the kinetics of the process leading to higher productivity. The rods are heated by the Joule effect, i.e., an electric current induces a heating effect due to the electric resistance of the silicon. The Joule effect enables a fine temperature control but excessive temperatures in the center of the rod must be avoided at all times.

For the CVD case-study, the MODOP is formulated to quantify the underlying trade-off between: (i) maximizing productivity (i.e., the volume of the rods) and (ii) minimizing the energy consumption. The aim is to reduce the excessive electricity consumption due to the Joule heating. The RDOP deals with the uncertainty on the emissivity and the electric conductivity of the silicon rods.

This paper is structured as follows: Section 2 introduces the mathematical background including the MODOP (see Section 2.1), the RDOP formulation (see Section 2.2) and the integration of both formulations in the RMODOP (see Section 2.3). Section 3 introduces the dynamic model of the CVD reactor case-study. Then, Section 4 presents and discusses the obtained results. Finally, Section 5 draws the conclusions for the presented work.

2. Mathematical formulation

In this section, the mathematical formulations at the base of this work are presented. In particular, this work is centered around the numerical solution of *dynamic optimization problems* (DOPs). This formulation is in the following subsections extended to include multiple objectives and uncertainties:

$$\min_{\mathbf{x}(\xi),\mathbf{u}(\xi),\xi_f} \quad J, \tag{1}$$

subject to

$$\frac{d\mathbf{x}}{d\xi} = \mathbf{f}(\mathbf{x}(\xi), \mathbf{u}(\xi), \xi, \mathbf{p}) \quad \xi \in [0, \xi_f], \tag{2}$$

$$\mathbf{0} = \mathbf{b}_c(\mathbf{x}(0), \mathbf{p}), \tag{3}$$

$$\mathbf{0} \geq \mathbf{c}_p(\mathbf{x}(\xi), \mathbf{u}(\xi), \xi, \mathbf{p}), \tag{4}$$

$$\mathbf{0} \geq \mathbf{c}_t(\mathbf{x}(\xi_f), \xi_f, \mathbf{p}). \tag{5}$$

Here, $\mathbf{x}$ are the state variables, $\mathbf{u}$ the time-varying control variables, $\mathbf{p}$ are the time-invariant model parameters. The vector $\mathbf{f}$ represents the dynamic system equations (on the interval $\xi \in [0, \xi_f]$) with initial conditions given by the vector $\mathbf{b}_c$. In particular $\mathbf{f}$ can comprise Ordinary Differential Equations (ODE), Differential Algebraic Equations (DAE) as well as Partial Differential Equations (PDE). The vectors $\mathbf{c}_p$ and $\mathbf{c}_t$ indicate, respectively, path and terminal inequality constraints on the states and controls. Each individual objective function can consist of both Mayer (M) and Lagrange (L) terms:

$$J = \mathrm{M}(\mathbf{x}(\xi_f), \xi_f, \mathbf{p}) + \int_0^{\xi_f} \mathrm{L}(\mathbf{x}(\xi), \mathbf{u}(\xi), \xi, \mathbf{p})\, d\xi. \tag{6}$$

Two main classes of methods exist to solve dynamic optimization problems: (i) *direct* and (ii) *indirect* methods. *Direct* methods are also known as *"first discretize, than optimize"* in contrast with *indirect* methods which follow the route "*first optimize, than discretize*". *Indirect* methods are based on the first order necessary conditions for optimality and reformulate the dynamic