A SIMULTANEOUS DYNAMIC OPTIMIZATION APPROACH FOR NATURAL GAS PROCESSING PLANTS

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Abstract
In this work we address dynamic optimization of natural gas processing plants through the use first principle models and full discretization of both control and state variables. The optimization problem includes rigorous models for cryogenic countercurrent heat exchangers with partial phase change, separation tanks, distillation columns and turboexpanders. Thermodynamic predictions are made with a cubic equation of state. The partial differential algebraic equation system is transformed into ordinary differential-algebraic equations (DAEs) by applying the method of Lines for the spatial coordinate in cryogenic heat exchangers. The resulting optimization problem is formulated and solved by applying orthogonal collocation on finite elements, and the large-scale Nonlinear Programming (NLP) problem is solved with a Newton-based Interior Point method. The objective is to switch between operating modes to minimize the offset between current ethane recovery and a set point value. Numerical results provide temporal and spatial profiles of controlled and manipulated variables, while fulfilling specific path constraints associated to ethane extraction processes. In particular, the tight integration between process units as well as path constraints has been efficiently handled with low computational time.

Keywords
Simultaneous Dynamic Optimization, Heat exchanger with phase change, Natural Gas Plant.

Introduction
Advances in the development of large-scale optimization algorithms as well as in hardware, have allowed addressing dynamic optimization of entire plants with rigorous models. In particular, natural gas processing plants are examples of highly energy integrated cryogenic processes, with numerous path constraints in transient states. These plants provide ethane as raw material for olefin plants, as well as methane for gas sales, LPG and gasoline. Ethane yield must be high, while minimizing energy consumption and complying with environmental regulations; these are related to carbon dioxide emissions and maximum carbon dioxide content in the residual gas injected to the pipeline. Additional path constraints involve keeping carbon dioxide solubility conditions in the upper stages of the demethanizer column. Mandler (2000) presented Air Products’ dynamic modeling efforts since 1990 for analysis and control of cryogenic liquefied gas plants (LNG). Dynamic optimization models have been proposed for cryogenic columns (Cervantes et al., 2000; Diaz et al., 2003; Raghunathan et al., 2004) and cryogenic heat exchangers (Rodriguez and Diaz, 2007). Vinson (2006) presented recent advances in air cryogenic separation. Finally, Rodriguez et al. (2010) proposed a dynamic model for an entire natural gas plant with a simultaneous optimization approach.

Simultaneous dynamic optimization approaches have seen considerable development over the last two decades. Here, both the discretized differential-algebraic equation (DAE) model and the optimal control problem are formulated as a single nonlinear programming (NLP) problem. In particular, the DAEs are discretized to a set of algebraic equations over finite elements in time, often using implicit Runge-Kutta (IRK) methods, such as
orthogonal collocation on finite elements. Moreover, with
the development of large-scale nonlinear programming
solvers, a number of advantages can be realized. A key
feature of the simultaneous approach is that embedded
solution of the DAE model is no longer required.
Moreover, exact first and second derivative information
for the NLP are readily obtained from the algebraic
equations resulting from the discretization. The
simultaneous dynamic optimization approach is reviewed
in Biegler (2010), where it is also compared with
competing dynamic optimization strategies. In particular,
this approach has been demonstrated to be well-suited to
address highly integrated processes with numerous path
constraints (Biegler and Zavala, 2008).

In this work, we propose a simultaneous dynamic
optimization framework for changing between steady
states to maximize ethane recovery in the cryogenic sector
of a natural gas plant. The problem includes first principle
models for separation tanks, turboexpanders, distillation
columns and countercurrent shell and tube heat exchangers
with partial phase change. The Soave Redlich Kwong
(SRK) equation of state (Soave, 1972) provides
thermodynamic predictions for vapor-liquid equilibrium
and carbon dioxide solubility predictions. These
distributed parameter models are spatially discretized by
the Method of Lines (Schiesser, 1991). The resulting
optimization problem subject to the DAE system is then
discretized by orthogonal collocation on finite elements in
AMPL and solved with IPOPT, a Newton-based Interior
Point method (Waechter and Biegler, 2006). To achieve
enhanced product recovery, this approach has enabled
optimal profiles for the main operating variables to be
obtained with particularly low CPU times.

Natural Gas Plant description
Turboexpansion processes are currently the most
efficient ones for ethane extraction from natural gas
mixtures. Ethane is later provided as raw material for
olefin plants. Methane is delivered as sales, with LPG and
gasoline as the remaining products. The cryogenic sector,
which is shown in Fig. 1, is the most energy intensive part
in a natural gas processing plant. The feed gas is cooled by
heat exchange with the demethanizer top product in
cryogenic heat exchangers (HE1 and HE2), and with side
and bottom distillation column reboilers. After heat
integration, both streams are mixed and sent to a high
pressure separator (HPS). The vapor stream is expanded
through a turboexpander (TE) to achieve the low
temperatures required for demethanization. The liquid
stream from the HPS enters the demethanizer at its lowest
feed point. The top product has mainly methane and
nitrogen, while higher hydrocarbons are obtained in the
bottom product. Carbon dioxide, which has intermediate
volatility between methane and ethane, distributes between
the top and bottom streams.

Figure 1. Cryogenic sector in basic turboexpansion process

Cryogenic conditions in the upper stages of the
demethanizer column may produce carbon dioxide
precipitation, which must be avoided. The top product,
residual gas, is used to cool the feed gas and it is then
recompressed to the pipeline pressure, and distributed for
sale. The bottom product from the demethanizer can be
further processed to obtain ethane, propane, butane and
gasoline. Ethane then undergoes further carbon dioxide
removal prior to its delivery as raw material for ethylene
plants.

Mathematical modeling
A brief description of main features for process unit
models is given below.

Cryogenic heat exchangers with phase change
The main simplifying assumptions for countercurrent
heat exchangers with partial phase change (HE2, in Fig. 2)
are thermodynamic equilibrium between the vapor and
liquid phases. However, they can have different velocities,
and one dimensional flux. A simple scheme of the
cryogenic heat exchanger is shown below.

Figure 2. Cryogenic heat exchanger configuration

Thermodynamic predictions are made with the SRK
equation of state (Soave, 1972). To transform the partial
differential algebraic equation system describing this
distributed parameters problem into a DAE, we have
applied the Method of Lines, using backward finite
differences. In this system, we have selected the fraction of
residual gas flow rate through the bypass valve between HE1 and HE2 as an optimization variable ($X_G$ in Fig. 2), as it is used to achieve a desired outlet natural gas temperature to the high pressure separator. The top heat exchanger where partial natural gas condensation takes place (HE2) has been modeled with 6 cells, while the heat exchanger where only sensible heat is exchanged (HE1) is modeled with 10 cells. A detailed description for the cryogenic system model is given in Rodriguez and Diaz (2007) and Rodriguez (2009). To avoid temperature crosses the following constraints have been included for each cell:

$$T_{S_k} - T_{T_{k+1}} \geq \Delta T_{\text{min}}, k = 1, \ldots, \text{Ncells}1 - 1$$

$$T_{S_k} - T_{T_{IN1}} \geq \Delta T_{\text{min}}, k = \text{Ncells}$$

where $T_{S_k}$ denotes the shell temperature in cell $k$ and $T_{T_{k+1}}$ is the corresponding tube side temperature. Additional constraints ensure monotonic temperature profiles along countercurrent heat exchangers:

$$T_{S_{m,IN}} \geq T_{S_{m+1}}, m = 1, 2$$

$$T_{S_{m,i+1}} \geq T_{S_{m,i}}, i = 1, \ldots, \text{Ncells}; m = 1, 2$$

$$T_{T_{m,i+1}} \geq T_{T_{m,i}}, i = 1, \ldots, \text{Ncells}; m = 1, 2$$

$$T_{T_{m,\text{Ncells}}} \geq T_{T_{m,IN}}, m = 1, 2$$

**High pressure separator**

The model includes an overall dynamic mass balance and geometric equations relating liquid content in the tank to liquid height and liquid flowrate as a function of pressure drop over the liquid stream valve. Detailed equations are presented in Rodriguez and Diaz (2007) and Rodriguez (2009).

**Turboexpander**

The turboexpander is represented with a static model due to its fast dynamics. It is the core unit in cryogenic natural gas processing plants, as it allows achieving low temperatures required for methane/ethane separation. It is modeled as an isentropic expansion, corrected by the expander efficiency. Residual entropy has been calculated with the SRK equation of state. The procedure proposed in GPSA Engineering Data Book (2004) for turboexpander calculation has been implemented and the equation oriented approach efficiently avoids the iterative routine.

**Demethanizing column**

The demethanizer model includes dynamic energy and component mass balances at each stage and equilibrium calculations with SRK equation of state and hydraulic calculations, leading to an index one model. To avoid operating conditions that produce carbon dioxide precipitation in the upper section of the column, additional path constraints on carbon dioxide fugacities have been formulated. They are derived from the isofugacity criterion for phase equilibrium and impose current CO₂ fugacity in the vapor phase at most 80% of the solid fugacity, at each stage $i$:

$$f_i^{CO_2} \leq 0.80 f_i^{S}$$

which can be calculated with low computational effort in a simultaneous approach as:

$$\bar{f}_i^{CO_2} = y_i^{CO_2} P_i^{V}$$

where fugacity coefficients for pure carbon dioxide and in the vapor mixture are calculated with the SRK equation of state at each stage. Further details can be found in Diaz et al (2003).

**Optimization algorithm**

After discretization, the resulting NLP problems are represented in the general form,

$$\min F(x), s.t. c(x) = 0, x \geq 0$$

where $F(x)$ and $c(x)$ represent the objective and constraint functions, and $x$ are all of the discretized state and control variables. The IPOPT solver handles the bound constraints through logarithmic barrier terms added to the objective function and solves the following barrier problem:

$$\min \phi(x) = F(x) - \mu \sum_{j=0}^{n} \ln(x^{(i)})$$

where $x^{(i)}$ denotes the $i$-th component of vector $x$ and $\mu$ is the barrier parameter. Solving a sequence of barrier problems as $\mu \to 0$ results in an efficient strategy to solve the original NLP. The solution of the barrier problems, for fixed $\mu$, is obtained by solving the following Karush-Kuhn-Tucker (KKT) conditions:

$$\nabla F(x) + \nabla c(x) \lambda - \nu = 0$$

$$c(x) = 0$$

$$Xe = \mu e$$

Here $X = diag(x)$, $\lambda$ and $\nu$ are KKT multipliers for the equations and bounds, respectively, and $e$ is a vector of ones. To solve this nonlinear KKT system, IPOPT uses an exact Newton method with a novel filter line search method and efficient sparse linear solvers.

**Optimization problem for Natural Gas Plant**

To demonstrate the above optimization for switching between steady states, we minimize the offset between ethane recovery and a set point value. Here, the optimization variables are demethanizer top pressure ($P_{top}$) and flowrate fraction derived through the bypass valve in cryogenic heat exchangers ($X_G$). The dynamic optimization problem has been formulated in AMPL within a simultaneous approach (Waechter and Biegler, 2006). For accurate approximations with guaranteed convergence properties, even for DAE high index problems, Radau collocation was implemented (Biegler 2010) to discretize the DAE model. We apply this approach to the following dynamic optimization problem:
Numerical results

The dynamic optimization of the entire plant is performed to switch to a steady state with higher ethane recovery. Control variables, corresponding to top pressure in the demethanizer column and the bypass fraction to the first cryogenic heat exchanger, were computed along a time horizon of 100 minutes. A full discretization has been carried out with 15 finite elements with two collocation points, rendering an NLP with 82320 variables and 81720 equality constraints. This led to a reasonably accurate solution. Further extensions that deal with error bounding strategies (see Biegler, 2010) are also planned for future work.

To improve computational performance, we provided exact first and second derivatives along with initializations of the primal variables and bound multipliers through the AMPL environment. In addition, we used the MA57 solver with Metis. Among the IPOPT options, better results have been obtained with the adaptive barrier update and warm starts. The entire plant optimization has been performed in 51 CPUs on an Intel DuoCore 2.2 GHz personal computer.

For this case, ethane recovery is increased from 67% for an initial pressure of the demethanizer of 18 bar, to 75.20% at 15.80 bar, and to an increase in the residual gas flow rate bypassed in the first heat exchanger from 26% to 30%. Figure 3 shows optimal profiles for the control variables: the top demethanizer pressure and bypass fraction. Figure 4 shows the turboexpander outlet temperature profile, which is decreased by an increase of the expansion ratio (TEinlet pressure/Demethanizer top pressure). This leads to the increase in ethane recovery, which is also shown in this figure. Figures 5 and 6 show spatial and temporal profiles for shell side temperature and pressure in the cryogenic heat exchanger where partial condensation takes place. A spatial discretization of six cells has been considered. It can be seen that the increase in the bypassed residual gas flow rate renders a slight increase in the new steady state feed gas outlet temperature (from 213.6 to 214.5 K). Figure 7 shows a decrease in inlet residue gas temperature (from 193 to 191K), associated to the demethanizer column temperature decrease; it also shows an increase in its outlet value in the new steady state due to the warmer feed gas conditions associated to the increase in bypassed residue gas in the second cryogenic heat exchanger. Figure 8 shows the warmer final conditions in the feed gas associated to the increase in bypassed residue gas flow rate.

Figure 3. Bypass fraction in cryogenic heat exchangers and demethanizer top pressure (control variables)

Figure 4. Optimal turboexpander outlet temperature (K) and ethane recovery
Conclusions

This study develops a dynamic optimization formulation to determine transition profiles for changes in steady state conditions for a natural gas processing plant, a highly energy integrated process. Here we consider the formulation of first principles models for process units within a simultaneous dynamic optimization approach. The resulting NLP problem has a large number of variables and equations, but the application of Newton-based Interior Point methods, as well as appropriate handling of the Jacobian and Hessian structure within IPOPT (Waechter and Biegler, 2006) allows for efficient and accurate solution with a considerable reduction of CPU time. This study paves the way for the use of rigorous models for energy minimization, maximization of product recovery and extension within a nonlinear model predictive control environment, which will be investigated in future studies.

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