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Dynamic optimization of an Intensive Energetically Integrated Large-Scale Process

Mariela A. Rodriguez, J. Ignacio Laiglecia, Patricia M. Hoch, M. Soledad Diaz

Planta Piloto de Ingeniería Química, PLAPIQUI, Universidad Nacional del Sur, CONICET. Camino La Carrindanga km 7, 8000 Bahía Blanca, ARGENTINA
sdiaz@plapiqui.edu.ar

Abstract

In this work we propose a first principles dynamic optimization model for an intensive energetically integrated process, a natural gas processing plant, within a simultaneous dynamic optimization framework. We have developed rigorous models, including thermodynamics with a cubic equation of state, for separation tanks, distillation columns, turboexpanders and cryogenic countercurrent heat exchangers with partial condensation. The resulting partial differential algebraic equation system is transformed into an ordinary differential algebraic equation one (DAE) by applying the method of Lines for the spatial coordinate. The high integration between process units as well as path constraints have been efficiently handled by a simultaneous dynamic optimization approach in which the DAE is transformed into a large nonlinear programming problem through orthogonal collocation over finite elements in time and solved with an interior point algorithm. In the case study, we maximize ethane recovery under a ramp change in natural gas feed flowrate. The model provides temporal and spatial profiles of controlled and manipulated variables that are in good agreement with plant data.

Keywords: Dynamic Optimization, Simultaneous Approach, Heat exchanger with phase change

1. Introduction

Dynamic optimization of entire plants has proven to be of great importance for properly studying process operation and control. Recent advances in dynamic optimization algorithms have paved the way to entire plant optimization, being the simultaneous approach (Biegler and Zavala, 2008) the most appropriate one to address highly integrated processes with numerous path constraints. Natural gas processing plants are examples of highly integrated cryogenic processes. They provide ethane as raw material for olefin plants. Ethane yield must be high, while minimizing energy consumption and complying with environmental regulations related to carbon dioxide emissions and maximum carbon dioxide content in the residual gas injected to the pipeline. Mandler (2000) presents Air Products dynamic modeling efforts since 1990 for analysis and control of cryogenic liquified gas plants (LNG). Dynamic optimization models have been proposed for cryogenic demethanizing columns (Diaz et al., 2003; Raghunathan et al., 2004) and cryogenic heat exchangers (Rodriguez and Diaz, 2007). Vinson (2006) has presented recent advances in air cryogenic separation.

In this work, the dynamic optimization of the entire cryogenic sector of a natural gas plant, which includes separation tanks, turboexpanders, distillation columns and countercurrent shell and tube heat exchangers with partial phase change, has been addressed. The distributed parameter model has been spatially discretized by the Method of Lines (Schiesser, 1991) and the optimization problem subject to the DAE system has been solved through a simultaneous dynamic optimization approach (Biegler and Zavala, 2008) in which the resulting Nonlinear Programming (NLP) problem is solved with an Interior Point method (Waechter and Biegler, 2006). Optimal profiles have been obtained for main operating variables to achieve an enhanced product recovery under a ramp change. Numerical results have been compared to available plant data.

2. Case study

The cryogenic sector is the most important part in a natural gas processing plant, being the core of the turboexpansion process. As it is shown in Fig. 1, part of the feed gas is used for heat exchanging with the demethanizer top product in cryogenic heat exchangers (HE1 and HE2), while the rest of it is heat integrated with the distillation column reboilers.

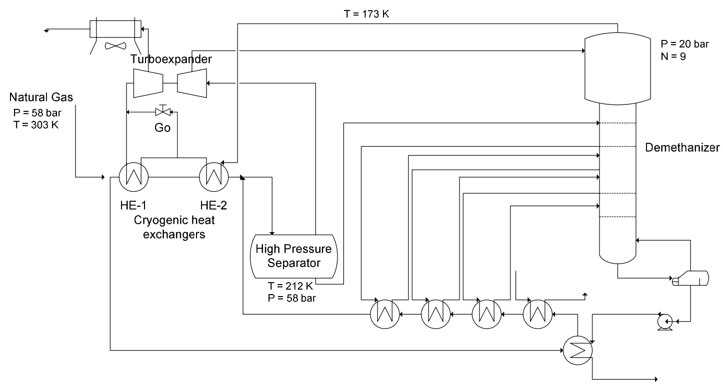

Figure 1 Basic turboexpansion process

After heat integration, both streams are mixed and sent to a high pressure separator (HPS). The vapor stream is expanded through a turboexpander in order to achieve the low temperatures required for demethanization. The liquid stream from the HPS enters the demethanizer in its lowest feed point. The top product has mainly methane and nitrogen, while higher hydrocarbons are obtained in the bottom product. Carbon dioxide distributes between top and bottom streams. It is necessary to verify that the operating conditions of the columns are such that carbon dioxide does not solidify in the top stages. Top product, referred to as 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 gasolines.

3. Mathematical modeling

In previous work, we have developed first principles dynamic models for countercurrent heat exchangers with partial phase change (Rodriguez and Diaz, 2006, 2007) and cryogenic distillation columns (Diaz et al., 2003; Raghunathan et al., 2004). In this work, we have formulated horizontal vessel dynamic models and static models for turboexpanders and we have integrated process unit models within a simultaneous dynamic optimization framework. A brief description of main features for process unit models is given below.

3.1 Cryogenic heat exchangers with phase change

Main simplifying assumptions for countercurrent heat exchangers with partial phase change (HE2, in Fig. 1) are that we assume thermodynamic equilibrium between the vapor and liquid phases, but they can have different velocities, and one dimensional flux. Thermodynamic predictions are carried out with the Soave, Redlich, Kwong cubic equation of state (Soave, 1972) and analytical derivatives of thermodynamic functions (compressibility factor, fugacity coefficient, residual enthalpy) with respect to temperature, pressure and compositions are included in the model. To transform the resulting partial differential algebraic equation system describing this distributed parameters problem into a DAE, we have applied the Method of Lines (Schiesser, 1991), using backward finite differences. In this system, we have selected the residual gas flowrate through the bypass valve between HE1 and HE2 as an optimization variable (Go in Fig. 1), as it is used to achieve a desired outlet natural gas temperature to the high pressure separator. The 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).

3.2 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 function of pressure drop over the liquid stream valve. Detailed equations are presented in Rodriguez and Diaz (2007) and Rodriguez (2009).

3.3 Turboexpander

The turboexpander is the main process unit in cryogenic natural gas processing plants, as it provides the low temperatures required for methane/ethane separation. Due to its fast dynamics, it can be represented with a static model. A pressure-temperature diagram is shown in Fig. 2.

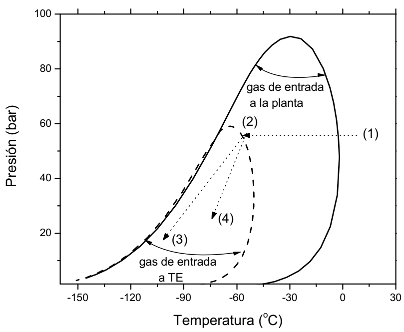

Figure 2. P-T diagram for natural gas in turboexpansion process

Natural gas enters the turboexpander at point 2 and, as it undergoes expansion, it moves from 2 to 3, which represents the turboexpander outlet conditions. It has been modeled as an isentropic expansion and corrected by the expander efficiency. Residual entropy calculations with SRK equation of state have been included. 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. Details can be found in Rodriguez (2009).

3.4 Demethanizing column

The demethanizer model includes dynamic energy and component mass balances at each stage, equilibrium calculations with SRK equation of state and hydraulic calculations, rendering an index one model. It also includes solubility calculations for carbon dioxide with SRK at each stage, as the low temperatures in the upper section of the column can produce carbon dioxide precipitation. Path constraints on CO_2 fugacities have been included to avoid precipitation as:

$$\overline{f^V_{i,CO2}} \leq f^S_{i,CO2}, \tag{1}$$

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

$$\overline{f^V_{i,CO2}} = y_{i,CO2} P_i \overline{\phi^V_{i,CO2}} \tag{2}$$

Further details can be found in Diaz et al (2003), Raghunathan et al. (2004).

4. Optimization model and algorithm

We have formulated the following dynamic optimization problem:

$$\min \int_0^{tf} \left(\eta_{ethane} - \eta_{SP}\right)^2 dt$$

$$\textit{st DAE system + Solubility constraints (1)-(2)} \tag{3}$$

$$15 \leq P_{top}(t) \leq 22(bar)\,;\; 0 \leq X_{bypass}(t) \leq 1\,;\; 0 \leq x_{methane-bottoms}(t) \leq 0.005$$

$$y_L \leq y \leq y_U\,;\; z_L \leq z \leq z_U\,; z(t=0) = z_0$$

where the objective function is the minimization of the offset between ethane recovery and a target value; optimization variables are demethanizer top pressure (Ptop) and flowrate fraction derived through the bypass valve in cryogenic heat exchangers (Xbypass). The dynamic optimization problem has been formulated in Fortran 90 environment within a simultaneous approach in which both control and state variables are approximated by piecewise polynomials and the DAE system is discretized by orthogonal collocation over finite elements (Cervantes abd Biegler, 1998; Biegler and Zavala, 2008). The large scale nonlinear programming model is solved with an Interior Point method with reduced SQP techniques within program IPOPT (Waechter and Biegler, 2006).

5. Numerical results

To validate the optimization model, we have compared model results for a ramp perturbation with available plant data from an actual turboexpansion plant in operation (Cia. Mega SA). The objective is to analyze model performance to represent the type and speed of response of main plant variables under a 3.5% increase of natural gas feed flowrate ramp perturbation, corresponding to a current plant situation, as shown in Figs. 3 and 4. Due to confidentiality, it is not possible to report actual values for data, but for analysis purposes the pressure scale was divided into 1 bar ticks and flowrates in 20 kmol/h ticks. Figure 3 shows profiles for feed gas flowrate and demethanizer top pressure; it can be seen that at time=128 min a ramp type perturbation is introduced, reaching a final value 3.5% higher than the initial one. Figure 4 shows the response of a controlled variable, the outlet temperature of the cryogenic heat exchangers, which is controlled through opening the bypass valve between HE1 and HE2. The top temperature of the demethanizer column is also shown.

To compare plant data with model results, the dynamic optimization problem posed as Eqn. (1) has been solved for a natural feed flow rate perturbation represented as a ramp that approximates very well the real plant perturbation (Figure 5, solid line).

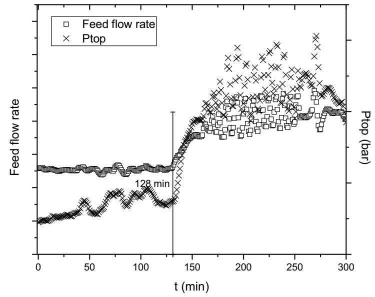

Figure 3 Natural gas feed flowrate and top pressure of demethanizer (plant data)

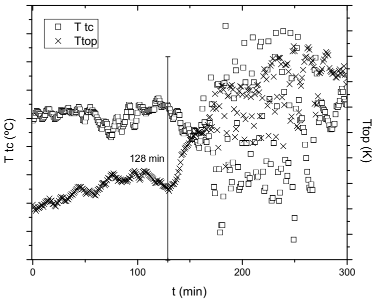

Figure 4 Cryogenic HE temperature and demethanizer top temperature (plant data)

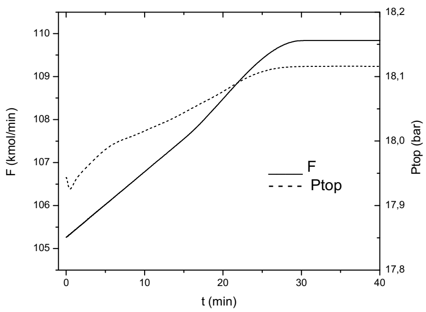

Figure 5. Feed flowrate to each train of cryogenic heat exchangers (solid line) and top pressure profile of demethanizer

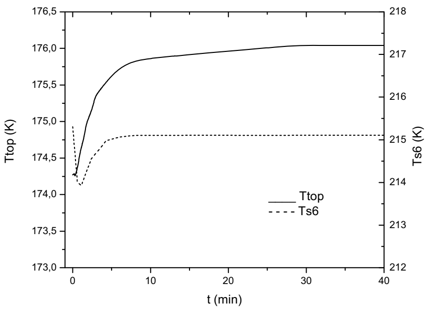

Figure 6. Demethanizer top temperature (solid line) and outlet temperature of cryogenic heat exchangers

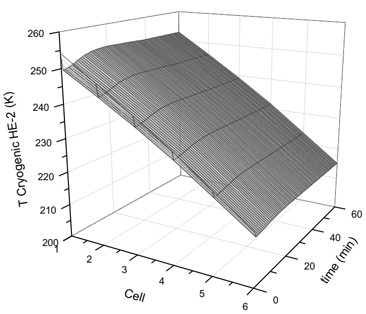

Figure 7: Condensate flowrate profile in HE2

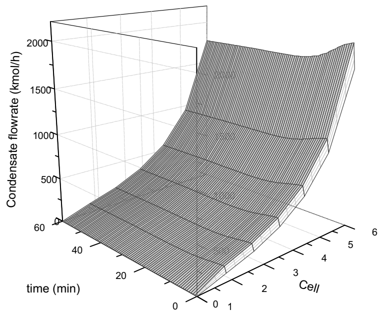

Figure 8: Temperature profile in HE2

The discretization has been carried out with 20 finite elements with two collocation points, rendering an NLP with 39550 variables and 39510 equality constraints. Numerical results are shown in Figures 5 to 10. The main variables show a behavior comparable to plant data. Figures 5 and 6 show the responses of top pressure and temperature of the demethanizer column, as well as the temperature of the partially condensed natural gas entering the HPS (Ts6). They do not show delay and follow the shape of the feed gas profile, reaching the new steady state at approximately 30 minutes. Figure 6 shows that the temperature of the partially condensed vapor from the cryogenic heat exchangers (Ts6) shows an initial decrease due to the instantaneous shut-down of the bypass control valve (in the initial steady state 10% of the stream is deviated to the first cryogenic heat exchanger). The model determines the immediate shut-down of the valve, emulating the behavior of the control system regulating the cold tank temperature. Then, the increasing demethanizer top flow rate to a higher thermal level gives rise to a new steady state, where the temperature is 2K higher than the initial one(215.10K). The behavior is analogous to plant behavior reported in Fig. 4, starting from T=128 min. Figures 7 and 8 show temporal and spatial profiles of condensate flow rate and temperature for the cryogenic heat exchanger with phase change, respectively. Total CPU time has been 864 s. The objective function, ethane recovery has changed from an initial value of 73.64% to 75.76%.

Conclusions

We have addressed dynamic optimization of a highly energy integrated large-scale process through the formulation of first principles models for process units within a simultaneous dynamic optimization approach. Even though the resulting NLP problem has a large number of equations, the Interior point method with reduced SQP techniques, as well as appropriate handling of the Jacobian structure within program IPOPT (Waechter and Biegler, 2006; https://projects.coin-or.org/Ipopt) allows an efficient resolution. Numerical results have been favorably compared to plant data of an actual plant in operation.

6. Acknowledgements

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References

Biegler,L.T., V.M. Zavala (2008), Large-scale nonlinear programming using IPOPT: An integrating framework for enterprise-wide dynamic optimization. Computers and Chemical Engineering 33 (2009) 575–582

Cervantes A. M., L. T. Biegler (1998). Large-scale DAE optimization using a simultaneous NLP formulation. AIChE Journal,44,1038-1050.

Diaz, S., S. Tonelli, A. Bandoni, L.T. Biegler (2003), "Dynamic optimization for switching between steady states in cryogenic plants", Found Comp Aided Process Oper 4, 601-604.

Mandler J.A. (2000). "Modelling for control analysis and design in complex industrial separation and liquefaction processes", J. Process Control, 10, 2, 167-175.

Raghunathan, A., M.S. Diaz, L.T. Biegler (2004). An MPEC Formulation for Dynamic Optimization of Distillation Operations", Computers & Chemical Engineering, 28, 2037-2052.

Rodriguez, M., (2009) "Dynamic Modeling And Optimization of Cryogenic Separation Processes", PhD Dissertation, Universidad Nacional del Sur, Bahia Blanca, Argentina.

Rodríguez, M., M. S. Diaz, (2007), "Dynamic Modelling And Optimisation of Cryogenic Systems", Applied Thermal Engineering (ISSN 1359-4311), 27, 1182-1190.

Schiesser, W.E., (1991), "The Numerical Method of Lines", San Diego, CA: Academic Press

Soave G. Equil. Constants for a Modified Redlich-Kwong Eq. of State. Chem. Eng. Sci. 1972; 27: 1197-1203.

Vinson, D.R., (2006), Air separation control technology, Computers & Chemical Engineering, 30, 10-12, 1436-1446.

Waechter, A., Biegler, L.T. (2006), On the implementation of an interior-point filter-line search algorithm for large-scale nonlinear programming Research Report RC 23149, IBM T.J. Watson Research CenterYorktown, New-York.