DYNAMIC OPTIMIZATION FOR SWITCHING BETWEEN OPERATING MODES IN CRYOGENIC PLANTS

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Abstract

This paper addresses dynamic optimization of a large-scale natural gas processing plant through the formulation of rigorous unit dynamic models. The resulting differential-algebraic equation (DAE) optimization problem is solved with an advanced simultaneous strategy that transforms the original problem into a nonlinear program. Emphasis has been given to detailed thermodynamic and solubility calculations to ensure feasible conditions along the transient.

Keywords

Dynamic Optimization, NGL plant, Large-scale NLP

Introduction

Natural Gas Liquids (NGL) are light hydrocarbons in the range ethane through hexane plus, which may be recovered as liquids from a natural gas source. NGL processing plants provide feedstock, mainly ethane and propane, for production of olefins and other petrochemicals. Turboexpansion processes are currently the most efficient ones for obtaining high ethane recovery. The separation is performed at high pressure and cryogenic conditions. Wilkinson and Hudson (1982) have proposed different turboexpansion plant designs to improve ethane recovery. (Diaz et al., 1997) have solved the debottlenecking problem of an ethane extraction plant as a Mixed Integer Nonlinear Programming (MINLP) model.

Dynamic simulation of complex cryogenic processes has been studied by a few authors. Mandler (2000) has studied dynamic simulation of liquefied natural gas plants and air separation plants for control analysis and design in liquefaction processes. However, dynamic optimization of entire plants has not been addressed until the last decade, mainly due to the lack of reliable large-scale dynamic optimization algorithms (Cervantes et al., 2000). Dynamic optimization problems for chemical processes can be modeled as a differential-algebraic equations (DAE) system.

This work addresses the dynamic optimization of a part of the cryogenic sector in a natural gas processing plant to obtain optimal profiles for control variables through a simultaneous nonlinar programming (NLP) formulation. The demethanizing column, together with the turboexpander, constitutes the main part of the cryogenic separation. The model comprises differential energy and mass balances, hydraulic correlations and rigorous thermodynamic predictions with the Soave-Redlich-Kwong (SRK) equation of state (Soave, 1972) for equilibrium and carbon dioxide solubility calculations.

Natural gas plant description

The cryogenic sector is the core of a turboexpansion natural gas plant. In this sector, inlet gas is cooled by heat exchange with residual gas and demethanizer side and bottom reboilers. The partially condensed gas feed is then sent to a high-pressure separator. The vapor is expanded through a turboexpander to obtain the low temperatures required for high ethane recovery and is then fed to the top of the demethanizer column. The liquid from the high pressure separator enters the demethanizer at its lowest feed point. Methane and lighter components constitute top product and ethane and heavier hydrocarbons are obtain ed

as bottom product. Carbon dioxide is distributed between top and bottom streams.

Optimization strategy

The resulting dynamic optimization problem is solved using a simultaneous approach, with states and control variables represented as piecewise polynomial functions over finite elements in time and the differential-algebraic system discretized using orthogonal collocation over these finite elements. This converts the dynamic problem to an algebraic nonlinear program (NLP), which is solved with a novel reduced space SQP strategy. As described in Cervantes et al. (2000), a barrier approach is applied to convert the inequality constraints in the NLP to a logarithmic penalty term in the objective function. This leads to a parametric NLP with only equality constraints; a penalty parameter on the barrier terms is systematically forced to zero and an NLP is solved for each value of this parameter. Applying Newton's method to the KKT conditions of this equality constrained NLP leads to large, sparse linear subproblems, which are solved using a range and null space decomposition tailored to the structure of the collocation equations. In particular, linearized forms of these equations are eliminated element by element with safeguards employed to ensure the stability of the decomposition. For the remaining degrees of freedom, a quasi-Newton step is calculated in the null space of the constraint gradients. Further details of this method can be found in Cervantes et al. Extensions of this approach have also been described in Biegler et al. (2002).

Model equations

The model includes dynamic MESH equations for the demethanizing column, thermodynamic and solubility predictions with SRK equation of state, hydraulic correlations. The effect of column pressure on turboexpander output is modeled with correlations that relate top feed properties (vaporized fraction, liquid and vapor enthalpy) to demethanizing top pressure. Dynamic energy balances are formulated at each stage and vapor holdup is also taken into account. The resulting DAE system is index one.

The SRK equation of state is used for the estimation of thermodynamic variables: compressibility factor, (z^V, z^L residual enthalpies (ΔH, Δh) , densities (ρ^V, ρ^L) and fugacity coefficients (ϕj^V, ϕ^L) for both vapor and liquid phases. The use of this equation of state has been recommended for representing natural gas mixtures properties at high pressure after extensive comparison of SRK predictions with experimental data (Pedersen et al., 1989). The resulting model is as follows.

Differential equations

Total mass balance at stage i

$$\frac{dM_i}{dt} = F_i + V_{i+1} + L_{i\ 1} \quad V_i \quad L_i$$

Component j mass balance at stage i

$$\frac{dm_{ij}}{dt} = F_i z_{i,j} + V_{i+1} y_{i+1,j} + L_{i\ 1} x_{i\ 1,j} \quad V_i y_{i,j} \quad L_i x_{i,j}$$

Energy balance at stage i

$$\frac{dE}{dt} = V_{i+1} H_{i+1} + L_{i\ 1} h_{i\ 1} \quad V_i H_i \quad L_i h_i$$
$$F_i \left[\varphi_i H_{Fi} + (1 \quad \varphi_i) h_{Fi} \right] + Qsr_i$$

Algebraic equations

Equilibrium ratio

$$K_{i,j} = \frac{\phi_{i,j}^L}{\phi_{i,j}^V}; \qquad y_{i,j} = K_{i,j} x_{i,j}$$

Vapor and liquid enthalpy at stage i

$$H_i = H_i^{ideal} \quad \Delta H_i; \qquad h_i = h_i^{ideal} \quad \Delta h_i$$

Carbon dioxide saturation pressure stage i

It is calculated with a correlation based on carbon dioxide solid-vapor saturation curve (IUPAC, 1973), as function of triple point temperature (T_{CO2}^t) and pressure ($P_{CO2\,t}^t$).

$$ln \frac{P_{i,CO2}^S}{P_{CO2}^t} = 14.568 \ 1 \ \frac{T_{CO2}^t}{T_i} \quad 14.480 ln \frac{T_i}{T_{CO2}^t}$$
$$+ 65.356 \ \frac{T_i}{T_{CO2}^t} \ 1 \quad 47.146 \ \left(\frac{T_i}{T_{CO2}^t} \right)^2 \ 1$$
$$+ 14.540 \ \left(\frac{T_i}{T_{CO2}^t} \right)^3 \ 1$$

Solid carbon dioxide fugacity at stage i

$$f_{CO2}^S = P_{CO2}^S \phi_{CO2}^V$$

Carbon dioxide fugacity in vapor phase at stage i, asumming no solubility of solvent in solid phase

$$\overline{f_{i,CO2}^V} = y_{i,CO2} P_i \overline{\phi_{i,CO2}^V}$$

Summation equations

$$\sum_j K_{i,j} x_{i,j} \quad \sum_j x_{i,j} = 0$$

Vapor volume between stage i and i-1

$$Vol_i^V = \pi \ \left(\frac{D_i}{2} \right)^2 H_{plate,i} \quad \frac{M_i^L}{\rho_i^L}$$

Vapor and total holdup

$$M_i^V = \rho_i^V Vol_i^V; \qquad M_i = M_i^V + M_i^L$$

Component j holdup at stage i

$$m_{i,j} = M_i^V y_{i,j} + M_i^L x_{i,j}$$

Energy holdup at stage i

$$E_i = M_i^V H_i + M_i^L h_i$$

Liquid holdup and hydraulic correlations at stage i

$$M_i^L = 0.896\pi \left(\frac{D_i}{2}\right)^2 \left(Hw_i + Hwo_i\right)\rho_i^L$$

$$Ho_i = 5.56.10^{-4} \left(\frac{V_i}{\rho_i^V Ahole_i Co_i}\right)^2 \frac{\rho_i^V Pmol_i^V}{\rho_i^L Pmol_i^L}$$

$$Hwo_i = 30(0.01495)^{2/3} Fw_i \left(\frac{L_i}{\rho_i^L Weirl_i}\right)^{2/3}$$

$$Hldrop_i = \beta\left(Hw_i + Hwo_i\right)$$

$$P_{i+1} = P_i + 0.24917.10^{-5}\left(Ho_i + Hldrop_i\right)\rho_i^L Pmol_i^L$$

Optimization problem

Model equations have been formulated within a simultaneous dynamic optimization approach, including the the calculation of analytical function derivatives. The objective is to change from a steady state of low ethane recovery to another one with higher recovery, controlling demethanizing top pressure, which is residual gas compressor inlet pressure. Also, reboiler heat duty has been considered as control variable. There are path constraints that correspond to methane content in demethanizing column bottoms (lower than 0.8%, molar basis). However, the most important path constraints are carbon dioxide solubility conditions, both in liquid ancd vapor phase at each stage. Lower demethanizing pressures increase ethane recovery due to an increased expansion ratio in the turboexpander, which produces lower temperatures and a higher liquid content in top demethanizing feed. These cryogenic temperatures may cause carbon dioxide precipitation in both liquid and vapor phases at the upper stages in the column. This condition must be avoided and it can be handled through inequalities in the optimization problem. Carbon dioxide precipitation takes place if its fugacity in solid phase (no solubility of hydrocarbon liquid or vapor mixture is considered in solid phase) is lower than its fugacity in the liquid and vapor mixture. Consequently, these constraints are added to upper stages in the demethanizing column:

The open loop dynamic optimization problem has been formulated as:

$$min \int_0^{tf} \left(\eta_{ethane} - 0.82\right)^2 dt$$

$$st$$

DAE model

$$15 \le Ptop \le 22(bar)$$

$$99 \le Q_{REB} \le 200(MJ/min)$$

$$0 \le x_{B,CH4} \le 0.008$$

$$f_{i,CO2}^V \le f_{i,CO2}^S$$

Numerical results

wo natural gas feeds with different carbon dioxide content are analyzed. Table 1 shows inlet natural gas compositions for the plant. Ten components (up to hexanes) and eight stages have been considered. The problem has been solved by discretization with 20 finite elements and 2 collocation points for all the cases. As a first step, the optimization is performed for natural gas feed A, with top demethanizing pressure as control variable in 40 NLP iterations. Figure 2 shows optimization results; demethanizing pressure is decreased to 15.66 bar, rendering 80.9% ethane recovery in the new steady state. In this case, solubility constraints are not active, neither in the steady state nor in the transient.

The optimization problem has also been solved for reboiler heat duty as control variable. In this case, methane composition in bottom liquid product becomes an active constraint in the new steady state, as it is shown in Figure 3.

Table 1. Alternative natural gas composition

Component	Feed A (%mol)	Feed B (%mol)
Nitrogen	1.44	1.37
Carbon dioxide	0.65	1.30
Methane	90.43	89.40
Ethane	4.61	4.43
Propane	1.76	2.04
Butanes	0.77	0.96
Pentanes+	0.34	0.50

Finally, the optimization has been performed for feed B. Carbon dioxide solubility constraints become active and prevent the decrease in demethanizing column top pressure (19.34 bar), as it is shown in Figure 4. Consequently, ethane recovery cannot be greater than 74.51%. When the optimization problem has been solved without including solubility constraints, a lower optimal pressure is determined (18.02 bar) with an associated increase in ethane recovery (76.57 %). However, this conditions cannot be achieved without carbon dioxide precipitation. For that reason, it is essential to include solubility constraints with accurate thermodynamic predictions to obtain realistic results and to avoid infeasible operating conditions during the transient.

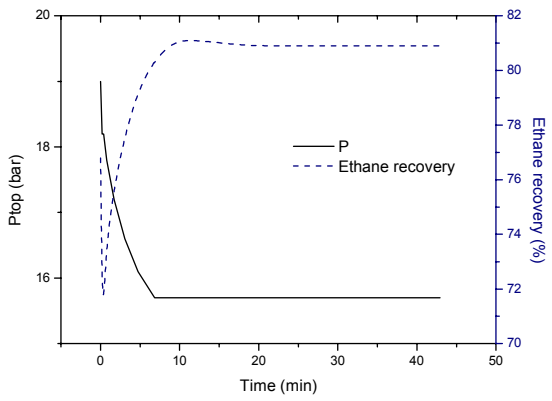

Figure 2. Top pressure and ethane recovery profile for feed A

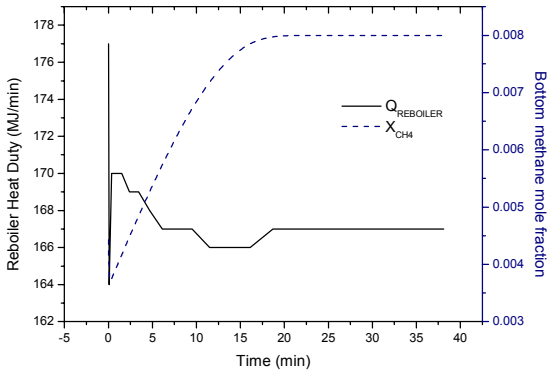

Figure 3. Optimal profiles for reboiler heat duty as control variable (Feed A)

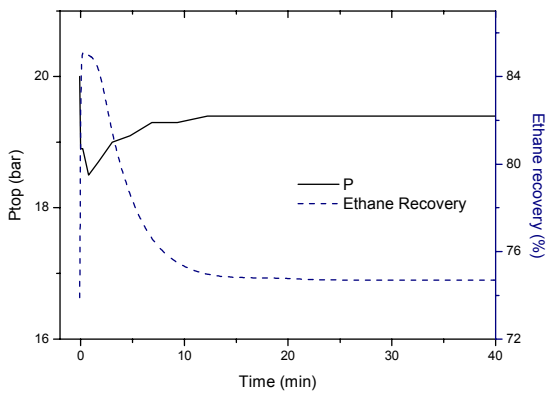

Figure 4. Optimal pressure and ethane recovery profiles for high CO_2 content in feed (B)

Conclusions

The inclusion of rigorous thermodynamic models within a simultaneous approach is a challenging issue due to the high nonlinearity that is added to the problem by thermodynamic equations. Carbon dioxide solubility calculation in both liquid and vapor phases at each column stage has been addressed to keep the process within the feasible operating region (no carbon dioxide precipitation) along the transient period. The resolution of the problem through a simultaneous approach has allowed an efficient handling of these conditions that constitute path constraints in the optimization problem. In this way, a very important practical issue has been addressed The incorporation of different units that constitute the natural gas processing plant is part of current work

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