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DYNAMIC OPTIMIZATION WITH A SIMULTANEOU METHOD: APPLICATION TO A HEAT EXCHANGER

Mariela A. Rodríguez, Maria Soledad Díaz, Alberto J. Bandoni

Planta Piloto de Ingeniería Química, PLAPIQUI (UNS – CONICET)
Camino La Carrindanga, Km.7 (8000) Bahía Blanca, ARGENTINA
Tel.: +54 291 486 1700 Fax: +54 291 486 1600
E-mails: {marodriguez, sdiaz, abandoni}@plapiqui.edu.ar

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Abstract. *In this work we use a numeric method based on a combined discretization and simultaneous dynamic optimization approach to solve a system consisting of partial differential and algebraic equations. The spatial derivatives are discretized by finite differences while the resulting DAE (Differential-Algebraic Equations) optimization problem is transformed into a large-scale NLP (Nonlinear Programming) problem through collocation over finite elements. This method is implemented in a computer package resident in a remote computer located at the Department of Chemical Engineering Carnegie Mellon University, which is accessed via a high-speed internet connection (Internet 2) from a client computer at the Centro Regional de Investigaciones Basicas y Aplicadas Bahia Blanca (CRIBABB).*

We have applied this strategy to the resolution of the dynamic optimization model of a gas - gas heat exchanger, which is part of a larger model under development. The goal is to minimize the transient between two set points of an outlet stream temperature. The dynamic model provides profiles of controlled and manipulated variables which are in agreement with available data, and the remote optimization system performed very well.

1 INTRODUCTION

Natural Gas Liquids processing plants provide feedstock, mainly ethane and propane, for production of olefins and other petrochemicals. In our country, there are several natural gas processing plants, two of which currently provide raw material for the most important petrochemical complex in the country, located next to Bahía Blanca.

The extraction of ethane and heavier hydrocarbons from natural gas can be efficiently performed through turboexpansion processes. The separation is carried out at high pressure and cryogenic conditions. However, cryogenic processes involve intensive material and energy integration, complex process flowsheet, small driving forces for flow and heat exchange, tight operational requirements and very high product purities. These attributes place them on the complex side of the spectrum of potential simulation, optimization and control applications. During the last two decades, much research and development work has been devoted to the determination of more efficient expansion processes and their optimal operating conditions. Bandoni et al.[1] have developed a methodology based on an energy analysis in the cryogenic sector for the selection of natural gas processing plant designs. Diaz et al.[2] have solved the debottlenecking problem of an ethane extraction plant as a Mixed Integer Nonlinear Programming (MINLP) model. They have shown that significant improvement in the plant operation and economics could be achieved by simultaneously considering minor structural modifications. Diaz et al.[3] have studied the detailed design of a turboexpansion plant for a wide range of natural gas mixtures by means of an MINLP strategy integrated to rigorous process and costs models. They have also analyzed similar process technologies that can be used to obtain propane as the main product and re-inject ethane to pipeline. More recently, Diaz et al.[4] have studied dynamic behavior of main units in the plant, in particular the cryogenic high-pressure demethanizing column, through a simultaneous approach to solve the DAE optimization problem. As part of this project we are now modeling cryogenic heat exchangers in the NGL processing plant. The complete model will comprise heat exchangers, a high-pressure separator, a turboexpander and a demethanizing column.

2 OPTIMIZATION ALGORITHM

Dynamic simulation problems are increasingly used to model control and scheduling of batch processes; startup, transient and shutdown analysis; safety studies and evaluation of control schemes. A few authors have addressed dynamic simulation of complex cryogenic 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[5]. Dynamic optimization problems for chemical processes can be modeled as a differential-algebraic equations (DAE) system.

DAE optimization problems can be solved using a variational approach[6] or by applying a Nonlinear Programming (NLP) solver to the DAE model. The variational approach is good for problems without bounds. However, if the problem has active constraints, it is very difficult to determine the correct switching structure and suitable initial guesses for state and adjoint

variables. There are two types of methods that apply NLP solvers: sequential and simultaneous. In the first strategy, the control variables are parameterized using a finite set of control parameters. The objective and constraint functions are evaluated for a given set of parameters by integration of the dynamic model using a DAE solver. The sensitivities with respect to the parameters are obtained from the same DAE solver and a small optimization problem is solved in the space of the parameters. Vassiliadis[7] and Cervantes and Biegler[8] present a thorough review on these methods.

Simultaneous approaches solve the DAE system together with the optimization problem. Both state and control variables are discretized and the original DAE optimization model is transformed into a large-scale NLP problem that may require special solution strategies. Simultaneous approaches have advantages for problems with path constraints and for systems where instabilities can occur for a range of inputs. In addition, the simultaneous approach solves the DAE system only once, at the optimal point, and therefore can avoid intermediate solutions that may not exist or may require excessive computational effort.

The large-scale NLP problems that arise from the full discretization of the DAE system are usually solved using Sequential Quadratic Programming (SQP) methods. These methods can be classified into full-space and reduced space approaches. Full-space methods take advantage of the DAE optimization problem structure and the sparsity of the model and they are very efficient for problems with many degrees of freedom[9,10] as the optimality conditions can be easily stored and factored. Characteristics of these methods are that second derivatives of the objective function and constraints are usually required, and special precautions are necessary to ensure convergence properties.

The DAE system is discretized using collocation on finite elements. The variables are then partitioned into dependent and independent variables in each element. A Newton step for the dependent variables is obtained by solving small square systems of equations for each element. The step for the discretized independent variables is obtained by solving a QP for all the elements.

The general formulation of the DAE optimization problem is as follows:

$$
\begin{gathered}
\text{Min } \Phi(z(t_f), y(t_f), u(t_f), t_f, p) \\
s.t.: \\
\mathrm{d}\, z(t)/\mathrm{d}\, t = \mathrm{f}(z(t), y(t), u(t), p, t) \\
\mathrm{h}(z(t), y(t), u(t), p, t) = 0 \\
\mathrm{z}(0) = \mathrm{z}_0 \\
\mathrm{h_s}(z(\mathrm{t_s}), y(\mathrm{t_s}), u(\mathrm{t_s}), p, \mathrm{t_s}) = 0 \\
z(t) \in [z_l \; z_u] \quad , \quad y(t) \in [x_l \; x_u] \\
u(t) \in [u_l \; u_u] \quad , \quad p \in [p_l \; p_u] \\
t_f \in [t_{fl} \; t_{fu}]
\end{gathered}
\tag{1}
$$

where Φ is a scalar objective function; **f** is the right hand side of differential equations

constraints; **h** are algebraic equation constraints, $\mathbf{h_s}$ are additional point conditions at times t_s; $\boldsymbol{z}$ are differential state variables; $\boldsymbol{z_o}$ are the initial values of $\boldsymbol{z}$; $\boldsymbol{y}$ are algebraic state variables; $\boldsymbol{u}$ are control variables; $\boldsymbol{p}$ are time independent variables and t_f is the final time. This system presents initial condition and point conditions at time t_s.

The differential-algebraic equation optimization problem is transformed into a nonlinear programming (NLP) problem by collocation on finite elements[11,12,13]. The resulting large-scale NLP will be solved with a reduced space interior point algorithm, incorporating recent advances in the interior point strategy that includes adjusting and adding finite elements in the simultaneous approach[14,15].

3 OCC METHODOLOGY

With the development of superior model-based control strategies and more efficient numerical solvers, dynamic optimization has become a viable tool for process systems engineering. A number of modeling systems, including commercial tools, have also increased the awareness and activity in dynamic simulation and optimization based on first principles models. As a result, very large optimization models can be formulated that represent complex process systems.

The representation and solution of the differential-algebraic equation (DAE) model is a key part of this formulation. The relative merits of these strategies are discussed in Biegler et al.[14], and there are active research efforts in the refinement of these strategies.

In the past decade, NLP tools have advanced rapidly for real-time optimization. Currently, it is not uncommon to formulate and solve NLP problems with 10^5 variables and constraints. Moreover, the availability of second derivates in same platforms allows more sophisticated methods to be used. Jockenhövel et al.[16] classify these methods into the following categories: active set versus barrier methods to handle bounds and inequality constraints, providing second order information and exploiting problem structure through full space or reduced space methods and line search and trust region methods to enforce global convergence. The environment includes automatic differentiation facilities to construct Jacobian and Hessian information from DAE model, a rich choice of discretization schemes for DAE models and graphical utilities to observe and assess the performance of the optimization strategy.

Jockenhövel et al.[16] discuss the above features and combine them into a novel dynamic optimization package, called OptControlCentre (OCC). OCC implements a simultaneous optimization approach for real-time optimization.

The software platform OptControlCentre (OCC) was developed for the implementation of dynamic optimization. Built on a MATLAB framework and using MAPLE for the generation of exact derivates, OCC allows its users to perform dynamic optimization of complex problems with a powerful graphical user interface. The continuous process model is defined as a set of DAEs using a relatively simple syntax in the first stage of OCC. In the second stage, the MAPLE-based code generator OCOMA[16] transforms the continuous DAE optimization problem to an NLP problem through a full discretization of state and control variables.

OCOMA then automatically writes the FORTRAN subroutines that contain the NLP problem, including symbolic first and second derivatives. In the third stage, these codes are then linked with a large-scale reduced Successive Quadratic Programming (rSQP) algorithm that solves the NLP problem. OCC allows off-line optimization, and the optimization result can be visualized using the graphical interface built with MATLAB tools.

4 HEAT EXCHANGER

Among a variety of types of heat exchangers, shell-and-tube heat exchangers are widely used in almost all-industrial branches. A number of thermal simulation and design methods have been developed for shell-and-tube exchangers operating in steady state. Because of various reasons such as start-up or shutdown, heat exchangers often endure transient response. Variations of external loads that lead to disturbances of inlet temperatures and flow rates of fluid streams and changes of heat transfer conditions also induce a transitory process in heat exchangers.

Knowledge of transient response of shell-and-tube heat exchangers is required for process control and optimum operation.

In this section we examine the procedure for optimizing the transient response of a baffled shell-and-tube single-pass counterflow heat exchanger, in which the fluid circulating in the tubes is residual gas and the fluid in the shell is natural gas. The shell-and-tube heat exchanger illustrated in Figure 1 has one shell pass and one tube pass. The inner stream flows through several tubes and the outer stream is confined by a large-diameter vessel.

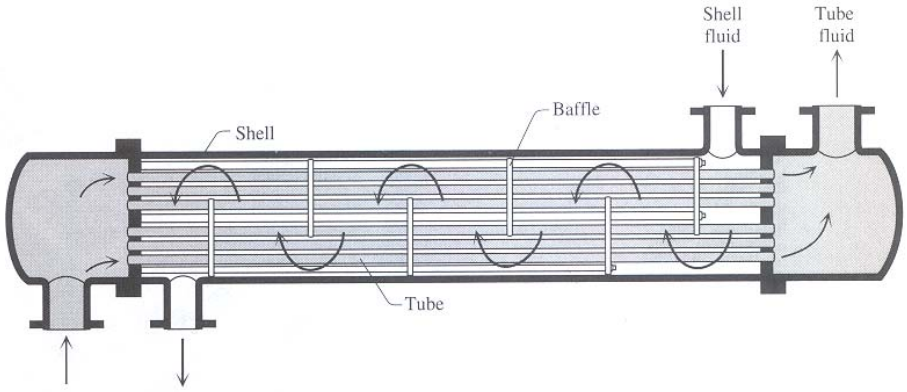

Figure 1: Shell-and-tube heat exchanger

As shown in Gaddis and Schlunder[17], an effective way to model a shell-and-tube heat exchanger with baffles is to break it up into several linked subsystem or cells. The number of baffles in the shell and the number of tube passes determine the number of cells. Figure 2 shows the diagram of the multicell model.

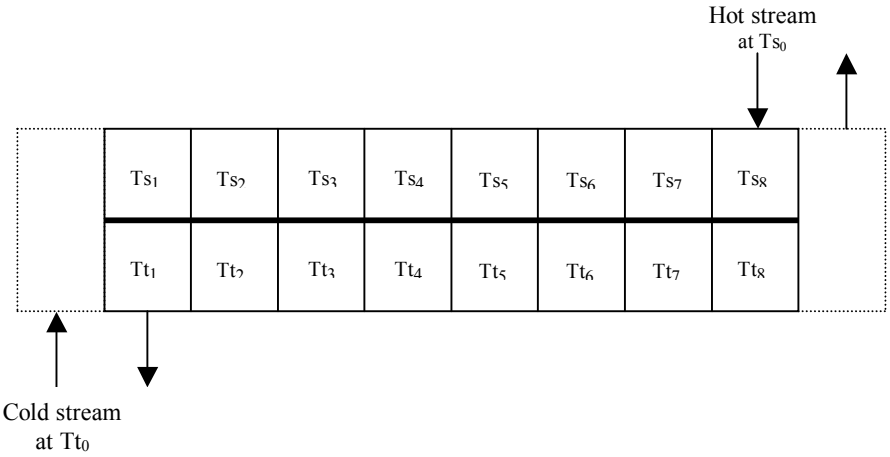

Figure 2: Multicell model

5 MODEL DESCRIPTION

The shell-and-tube heat exchanger is a particular case of a distributed parameter system. The fluid temperatures vary not only just along the length of the heat exchanger but also with time at each point along the exchanger. This process is modeled by a partial differential equation (PDE) system. To solve it, we transform it into an ordinary differential equation (ODE) system. We have used the finite difference method to discretize partial derivatives with respect to exchanger length.

The finite difference method begins with the discretization of space such that there is an integer number of points in space at which we calculate the field variable. In this way, the partial differential equation system becomes an ODE.

5.1 Differential Equations

The heat exchanged between the shell-side and tube-side fluids can be found by performing an energy balance.

Energy balance in the tubes:

$$\frac{dTt(i)}{dt} = \frac{v(i)}{\Delta z}\left(Tt(i-1) - Tt(i)\right) + \frac{h * A_{\text{sup}}}{\rho(i) * Cp * A * L}\left(T_s(i) - Tt(i)\right) \tag{2}$$

Energy balance in the shell

$$\frac{dT_s(i)}{dt} = \frac{v_s(i)}{\Delta z}\left(T_s(i-1) - T_s(i)\right) + \frac{h_s * A_{\text{sup}}}{\rho_s(i) * Cp_s * A_s * L}\left(Tt(i) - T_s(i)\right) \tag{3}$$

The initial conditions are:

$$\begin{aligned} Tt(0) &= Tt_0 \qquad t = 0 \\ Ts(0) &= Ts_0 \qquad t = 0 \end{aligned} \tag{4}$$

The temperatures of each inlet stream at the initial time are known. The heat exchanger is divided into 8 cells of equal length each one.

5.2 Algebraic Equations

To formulate a rigorous model we consider that the density of both fluids change with the temperature and calculate these as:

$$\begin{aligned} \rho(i) &= \frac{M * P}{zt(i) * R * Tt(i)} \\ \rho_s(i) &= \frac{M_s * P_s}{zs(i) * R * T_s(i)} \end{aligned} \tag{5}$$

Compressibility factors are computed as linear functions of temperature that have been obtained through phase equilibrium calculations with Soave Redlich Kwong equation of state.

$$\begin{aligned} zt(i) &= 0.734680 + 0.000821 * Tt(i) \\ zs(i) &= 0.262774 + 0.002069 * Ts(i) \end{aligned} \tag{6}$$

We consider that heat capacity is constant along the heat exchanger. The velocity of each stream is calculated as:

$$\begin{aligned} v(i) &= \frac{F}{\rho(i) * A} \\ v_s(i) &= \frac{F_s}{\rho_s(i) * A_s} \end{aligned} \tag{7}$$

Cell length is calculated as:

$$\Delta z = \frac{L}{n} \tag{8}$$

where n is the number of elements in which the heat exchanger is divided.

5.3 Objective Function

The objective is to minimize the offset between the outer stream temperature of natural gas and a set point value.

$$Objective\ function = \min \int_0^{tf} \left(Ts(1) - Tsp\right)^2 \tag{9}$$

The control variable is the inner flow of the cold stream.
The optimization problem is as follows:

$$\begin{gathered} Min \int_0^{tf} \left(Ts(1) - Tsp\right)^2 \\ s.t. \\ \{Eq.(2)\ to\ Eq.(8)\} \\ -\infty \le z(t) \le +\infty \quad , \quad -\infty \le y(t) \le +\infty \\ 900 \le u(t) \le 1300 \\ 0 \le tf \le 40 \end{gathered} \tag{10}$$

6 SIMULATION RESULTS

The previously described model consists of a system of algebraic-differential equations.

The solution of the system of Eq.(2) to (9) is obtained with OCC program. This software discretized automatically the differential-algebraic system, makes the calculation of first and second order derivatives in a symbolic way and then solves the large-scale nonlinear programming optimization problem[16].

The number of discretized variables is 1320 and the number of discretized equations is 1320. The CPU time is 20 minutes in an UltraSparc 250 Workstation.

Even though final time was 40 minutes, we plot the following figures up to 20 minutes because steady state is achieved at this time value.

Now, we present two scenarios that are possible in this plant. The system is working at steady state with a fixed set point temperature that controlled the outer stream of natural gas. This set point has to be changed to another value. In the first case we consider that the new set point is lower than the current value. In a second case the new set point is greater than this value. In both cases we analyze what happens with the inner flow of residual gas (control variable). As the outer temperature of residual gas has fixed upper and lower bounds, the behavior of this variable is plotted too.

6.1 Case 1

Figure 3 shows outer residual gas temperature and flowrate profiles in the first analyzed scenario. The optimization variable (u(t)) oscillates and then reaches a new steady state. Residual gas outer temperature falls down to the lower bound and keeps this value.

In Figure 4 it can be seen that both fluids temperature profiles grow along the exchanger. They show that the temperature reach a steady state in less than 20 minutes.

Natural gas outer temperature is the controlled variable. This temperature has to achieve the set point value. Figure 5 shows its optimum profile.

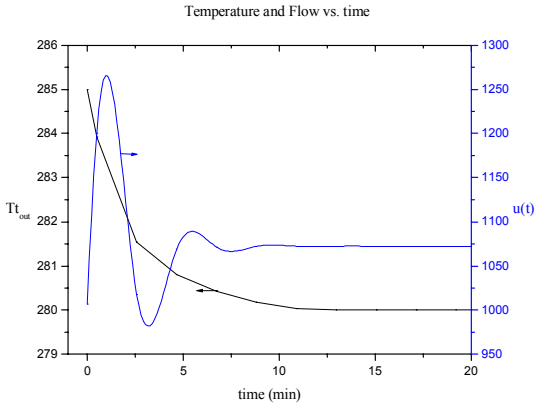

Figure 3: Temperature and Flow vs. time

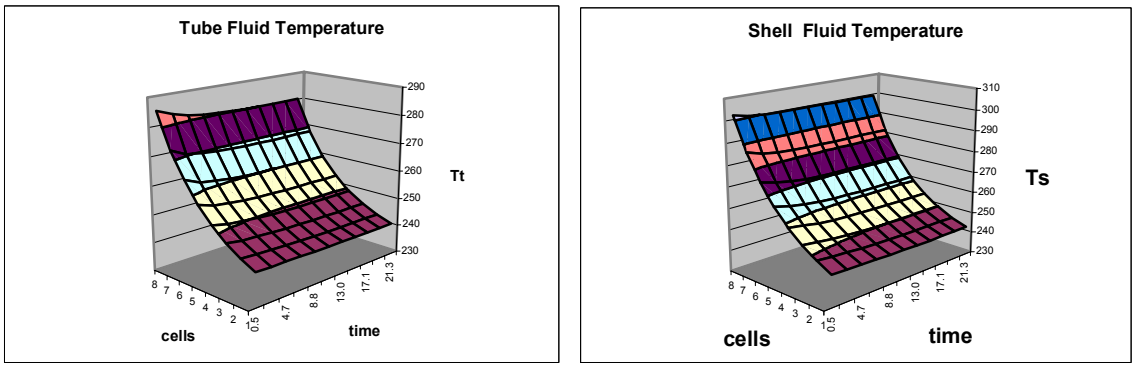

Figure 4: Optimal fluid temperature profiles in tubes and shell.

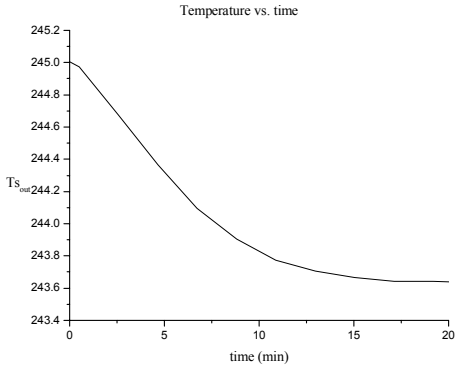

Figure 5: Natural gas temperature vs. time

6.2 Case 2

In the second scenario a set point value greater than the initial one is considered for outer natural gas temperature. Figure 6 shows outer temperature and flowrate optimal profiles. The optimization variable oscillates a little before reaching the new steady state value. Residual gas outer temperature gets to its upper bound.

In Figure 7 it can be seen that both fluids temperature profiles increase along the exchanger. Finally, Figure 8 shows optimal natural gas outer temperature profile.

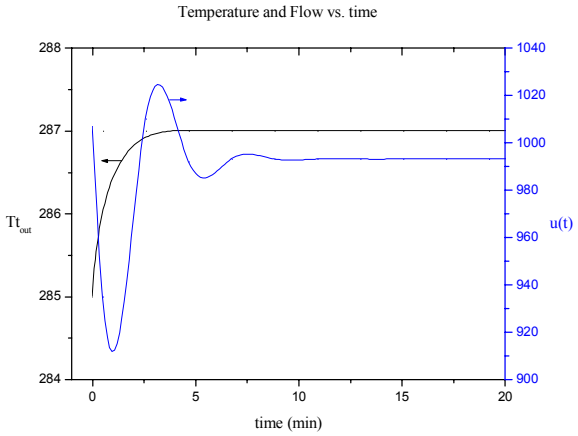

Figure 6: Optimal Residual gas temperature and Flowrate vs. time

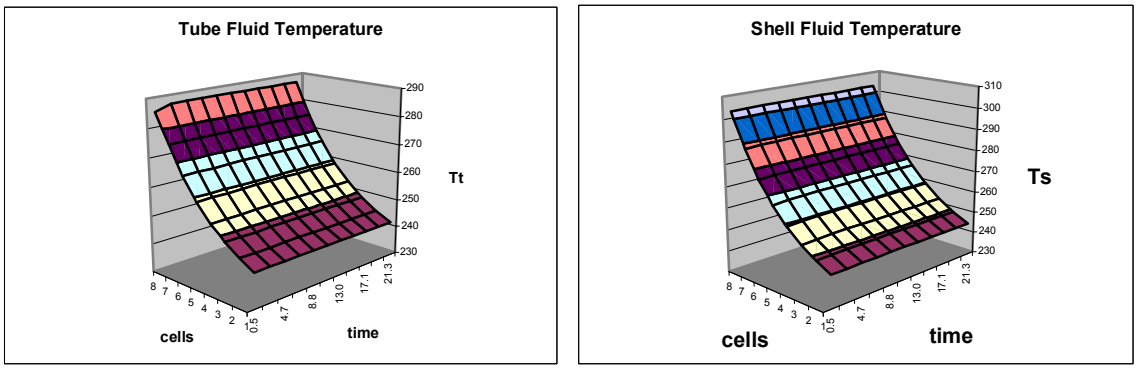

Figure 7: Optimal fluids temperature profile in tubes and shell

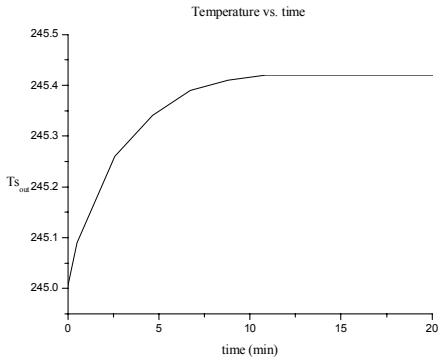

Figure 8: Optimal natural gas temperature vs. time

7 CONCLUSIONS AND FUTURE WORK

The developed model allows the prediction of optimal cooling gas flowrate (optimization variable) to achieve a set point temperature value in the warm stream (natural gas) in a countercurrent gas-gas heat exchanger.

DAE system with partial derivatives with respect to length and time that constitutes the optimization problem set of constraints is first transformed into an ordinary differential equation system by discretization by finite differences. The resulting DAE is then discretized by collocation on finite elements and transformed into a nonlinear system of equations that gives rise to a large-scale nonlinear programming problem. A full space Successive Quadratic Programming algorithm is applied to solve it within OCC environment.

The model is used to analyse the dynamic response of the gas – gas heat exchanger evaluating the trend of natural gas outlet temperature due to variations on set point temperature. The computational analysis provided numerical values of response times showing how the mathematical model is adequate to analyse, in the design approach, the heat exchanger dynamic behaviour.

This work was feasible through the use of high-speed Internet 2 that made possible this problem resolution using OCC, from a remote computer.

A preliminary model for the cryogenic heat exchanger in the NGL plant has been presented. In current work, we are modeling a second heat exchanger where natural gas phase change takes place. The final model will comprise main units in the cryogenic sector: demmethanizing column, heat exchangers, high-pressure separator and turboexpander.

8 NOMENCLATURE

A	cross-sectional area, m^2
A_{sup}	surface area per unit length, m^2/m
Cp	heat capacity, MJ/Kmol K
F	mass flow rate, Kg/min

h	heat transfer coefficient, W/(m^{2}K)
L	length of heat exchanger, m
M	molecular weight, Kg/Kmol
n	number of cells
P	pressure, bar
R	universal constant of gases, m^3 bar/(Kmol K)
t	time, min
T	temperature, K
T_{sp}	set point temperature, K
v	velocity, m/min
z	compressibility factor
ρ	density, Kg/m^3
Δz	cell length

Subscripts

t	tube side
s	shell side
0	inlet

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