A strategy for simulation and optimization of gas and oil production

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Abstract

A new formulation to easy simulation and optimization of gas and oil production systems is presented in this work. The problem of interest corresponds to the typical daily gas and oil production calculation, i.e. a one-day time period planning. The simulation problem considers determination of oil and gas production for the current topology. The optimization problem is established by considering that the instantaneous production of the gas/oil network must optimally satisfy a given demand. Non-linear behavior and reverse flow is assumed for wells and cubic equations of state are used to estimate thermodynamic properties. The resulting model contains differential and algebraic equations for a given fixed topology of interconnected wells coupled with surface pipeline networks. The model combines DASSL to solve the inner set of differential–algebraic equations, and Knitro to solve both the optimization problem and the overall set of non-linear equations. The good performance of the model and the numerical strategy is illustrated with real cases of study.

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1. Introduction

Petroleum, either as gas or oil, is a finite and scarce resource upon which modern society is strongly dependent. Hence, mankind is forced to rationalize and optimize its production and consumption to make them safer, more efficient, and cheaper. Indeed, the complexity of gas and oil production systems represents a unique challenge. A typical production infrastructure, either offshore or onshore, can be described as a number of fields containing several reservoirs where wells have been or may be perforated for production or even injection when recovery actions are performed. Surface facilities are also included to, among other purposes, allow well streams interconnectivity via manifolds. In offshore oilfields, gas and oil production is concentrated in different platforms from where it is transported to sales or storage points. A typical well may consist of either a single pipe or two pipes. If the well contains two pipes then one pipe, which is called the tubing line, goes inside the other one, which is called the casing line. The entry point of gas and oil from the reservoir into the well is referred to as the wellbore. Valves represent an important part in production systems to allow individual flowrate control. Thus, the resulting pipeline network includes reservoirs, wells, manifolds, and valves (Fig. 1). The main target of integrated reservoir management should be to maximize oil and gas recovery within the current economic and technical limits. The target is not easy to achieve since a reasonably good development plan, even for a single well, involves several stages in a traditional approach (Morooka, Guilherme, & Mendes, 2001). Attempts to optimize petroleum production have evolved in different directions. Considering just the reservoir, the optimization problem implies an analysis of the production–injection operation system where geological parameters become variables to optimize (Yang, Zhang, & Gu, 2003). Efforts to optimize based on building intelligent systems has also demonstrated to be a potentially fertile technique to increase petroleum production (Morooka et al., 2001). On other direction, it was observed that a schedule of operations is typically demanded from the production planning point of view. This analysis leads naturally to establish a multiperiod optimization problem. Linear programming (LP) models have...
been used to solve planning of some coordinated operations in petroleum production (Aronofsky & Williams, 1962; Garvin, Crandall, John, & Spellman, 1957; Lee & Aronofsky, 1958). To improve the accuracy of LP, an iterative scheme has been suggested where non-linear simulation and LP are wisely combined (Eieg & Herring, 1997). More recently, a multiperiod mixed-integer linear programming (MILP) model has been proposed for the planning and scheduling of oil investment and operation of offshore facilities (Iyer, Grossmann, Vasantharajan, & Cullick, 1998). They applied piecewise linear approximations to model each source of non-linearity in equations. Though avoiding direct dealing with the difficulty of non-linear equations eases the computational burden, the result is not entirely appropriate.

Mixed-integer non-linear programming (MINLP) has also been applied for oil production. Van den Heever and Grossmann (2000) proposed a MINLP model for offshore oilfield production planning where non-linearities are incorporated. A bilevel decomposition technique and the aggregation of time periods, allowing logic structures, were combined into a so-called aggregation/disaggregation algorithm to deal with the problem. Complex business rules such as tax and royalty calculations were later added to this model (Van den Heever, Grossmann, Vasantharajan, & Edwards, 2001). In this case, operating conditions are assumed constant across the whole planning horizon. However, it is well known that well and reservoir conditions change as a function of several variables such as the volume of gas and oil extracted/injected and geological parameters (Horne, 1998). Ortiz-Gómez, Rico-Ramírez, and Vázquez-Román (2001) have incorporated this effect in a short-term planning of oil production.

Yet, the daily oil and gas production problem has received little attention. It has been reckoned that significant uplift in gas and oil production can be achieved by means of continuous production system optimization on a daily basis (Heinemann, Lyons, & Tai, 1998). However, only a few papers have been reported to optimize production in the most immediate term. In the past, decisions regarding production considered process simulation where nodal analysis (Beggs, 2003), which is not a robust approach and fail for complex networks, has been typically applied and fluid properties were normally estimated via correlations (Abdel Waly, El-Massry, Darwesh, & El Sallaly, 1996). More recently, Handle-Schachler, McKie, and Quintero (2000) proposed an optimization approach that includes property evaluation based on cubic equation of state but serious simplifications were imposed on the model. This approach has been implemented in a commercial package for both simulation and optimization of gas production. More recently, a model has been developed that includes flow correlations to determine gas-lift allocation where gas injection rates are discretized and solved via special order sets (Kosmidis, Perkins, & Pistikopoulos, 2004).

In the daily gas and oil production problem, petroleum engineers are typically requested to exactly produce as to satisfy a given demand with the existing wells network, having a fixed topology and associated valves to adjust each well production. A difficulty of satisfying the programmed schedule produced by LP, MILP, or MINLP planning schemes arises because the interconnectivity of wells has never been considered during planning stages. Even when productive wells belong to the same reservoir, pressure at each wellbore can be radically different and the associated cost of production may also be different in each well. Hence, individual well productivity is substantially affected because of the interconnectivity. As a result of the interconnectivity, a well might also attempt to inject into another well rather than contributing to the overall production. It is then important to include the prediction of flow direction in each well. It is of course expected that the given demand, rather than maximizing production, be optimally satisfied.

This paper deals with the typical daily gas and oil production calculation. This problem can be visualized as a one-day time period planning. Both simulation and optimization problems of oil and gas production are considered in this paper. The KNITRO code (Byrd, Gilbert, & Nocedal, 2000; Waltz, Morales, Orban, & Nocedal, 2003) is applied to solve these problems. This code implements an interior method for non-linear programming that uses trust regions and a merit function to promote convergence. The oil and gas production problem is established in Section 2 to identify all process units involved in this process. Basic conceptual process units are detected from the process description and modeled in Section 3. Section 4 gives the solution strategy to obtain convergence in both simulation and optimization problems. Cases of study are analyzed in Section 5. Finally, our conclusions are contained in Section 6.

2. Problem statement

The daily gas and oil production simulation and optimization problems are established here as follows: for a given configuration of a production system the purpose of simulation is to calculate the contribution of each well in the overall production; the purpose of optimization concerns determination of the contribution of each well when operating to satisfy a given demand but minimizing the total cost. The production system consists of a fixed topology, i.e. a process flowsheet, containing a number of reservoirs where several wells have been already drilled. All wells must be considered ready to produce and are interconnected via surface pipeline facilities where gas and oil is
distributed to sale and/or storage points. Once the wells topology is established, the problem solved in this study answers questions such as if the network can satisfy a given demand to eventually take further appropriate actions. It is assumed that all parameters in the model described later remain constant on a time period of one day. A cost coefficient is associated to each well and the problem is then formulated as minimizing the production cost subject to technical constraints that come from the topology and the constraint because of the given demand. Constraints for the optimization problem include mass, energy and momentum balances, pipes’ diameters and valve’s parameters to control the flow. Reverse flow is allowed so that injection from one well into another well is an unknown to determine. Neither drilling nor close down of wells is considered in this study. The system must not produce more than the demand to avoid storage problems, i.e. it becomes an equality constraint. It is felt here that incorporating the demand constraint is a more realistic problem since petroleum production is often limited by international agreements. Next section contains a description of the mathematical model.

3. Mathematical models

To ease both network description and the solution procedure, two main types of conceptual process units are proposed: well and manifold (Fig. 1). The conceptual well represents the pipe connecting the reservoir to allow gas and oil flow from the reservoir to the surface where it is connected to a manifold. Since a well has already been drilled and connected in one side to a reservoir, it has only one point left for connection that corresponds to the outlet point of the pipe. The manifold then represents a pipe where several pipes, wells or manifolds, can be interconnected and in which the mass may be transported certain distance. For simplicity, we assume that the manifold may interconnect several wells or manifolds at the entry (input) point but just another manifold may be connected at the outlet point (output) of the manifold. A pipe has always an input point and one output point associated so that a calculated negative flow means that the flow direction is opposite to the expected one. There is also a valve associated to each well or manifold. The underlining idea is that the valve in the well/manifold may not only represent the so called “choke” valve of wells but also can be used for the purpose of production control. Since both conceptual units well and manifold contain two common parts, pipe and valve, the following subsections start by describing the model with assumptions for each common part. Models for whole conceptual units are described latter. For the sake of simplicity in representation, subindexes in several variables are only used during the conceptual units description.

3.1. Pipe

Considering a homogeneous mass flowrate \( m \) flowing across a pipe segment with diameter \( D \), inclined a \( \theta \) angle, and total length \( L \) (Fig. 2), then it has been shown that applying momentum and energy balance the resulting equations are

\[
\frac{dP_{\text{pipe}}}{dL} = -\frac{m g}{A_{\text{avg}}} \sin \theta - \frac{f m v^2}{2 A_{\text{avg}}} \\
\frac{\Delta H_{\text{pipe}}}{dL} = -m g \sin \theta - \frac{dQ}{dL} - m v \frac{dH}{dL}
\]

(Vázquez-Román, 1998):

\[
\frac{dP_{\text{pipe}}}{dL} = -\rho g \sin \theta - \frac{f m v^2}{2 D} - \rho \nu \frac{d}{dL} \\
\frac{\Delta H_{\text{pipe}}}{dL} = -m g \sin \theta - \frac{dQ}{dL} - \rho \frac{d}{dL}
\]

where \( P \) is the pressure, \( \rho \) the fluid density, \( g \) the acceleration due to gravity, \( f \) the friction factor, \( v \) the fluid velocity, \( H \) the enthalpy, and \( Q \) is the heat transfer.

According to Gibbs, given the mass and two independent properties it is possible to determine the complete thermodynamic state. Eqs. (1a) and (1b) suggest that pressure and enthalpy represent the most natural independent variables for the thermodynamic state evaluations. Thus, it is convenient to express the velocity variable in (1a) and (1b) as a function of these two variables, i.e. \( v = v(P, H) \) so that,

\[
v = \frac{m}{\rho A} \frac{dH}{dL}
\]

In addition, velocity can be expressed in terms of flowrate, density, and the cross-sectional area of the pipe, \( A \),

\[
v = \frac{m}{\rho A}
\]

Eqs. (1a), (1b), (2), and (3) can be combined for the pipe to produce,

\[
[1 + \frac{m}{A_{\text{avg}}} \left( \frac{\Delta H}{dL} \right)_H] \frac{dP_{\text{pipe}}}{dL} + \left( \frac{\Delta H_{\text{pipe}}}{dL} \right)_H = \frac{m g}{A_{\text{avg}}} \sin \theta - \frac{f m v^2}{2 A_{\text{avg}}} \\
\frac{\Delta H_{\text{pipe}}}{dL} = -m g \sin \theta - \frac{dQ}{dL} - m v \frac{dH}{dL}
\]

Assuming constant average values in selected terms, Eqs. (4a) and (4b) have been often integrated to determine outlet conditions in a pipe (Vázquez-Román, 1998). Furthermore, energy balance (Eq. (4b)) is normally over simplified and it is even removed. These integrations, with constant values in most involved variables, have generated several models consisting of pure algebraic equations. These models tend to contain
Species mol%  

<table>
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<tr>
<th>Species</th>
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<tr>
<td>Nitrogen</td>
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<tr>
<td>Carbon dioxide</td>
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</tbody>
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Fig. 3. Results with algebraic pressure drop models.

Heat transfer in production systems is another complex problem. The best assumption to make for heat transfer coefficients around the wellbore is to consider them as buried pipelines. Methods to estimate heat transfer coefficients can be found, for instance, in Incropera and De Witt (1996). The overall heat transfer coefficients in wells range from 0.5 to 50 Btu/(h ft² R) for instance, in Incropera and De Witt (1996). The overall heat transfer coefficient is required to achieve the same answer. This tends to occur when results are very sensitive to temperature. The best solution is to segment the well according to the geologic manifold. To apply this solution in this approach, the conceptual well should be connected to a series of interconnected manifolds where one manifold is connected to another one having different properties in the surroundings. The heat transfer equation can easily be inserted in Eq. (1b) so that no extra equation has to be considered for the model.

The friction factor required in Eqs. (4a) and (4b) is an extremely complex surface physics phenomenon. Empirically based correlations to “fit” the observed behavior have been developed using the friction factor as a function of the relative roughness of the pipe wall and the Reynolds number (Re). The Re is a dimensionless number which measures the “smoothness” of the flow: a low Re indicates smooth or laminar flow, and a high number, indicates mixed or turbulent flow. The following equations are often used for friction factor (Perry, Green, & Maloney, 1988):

\[ f = \frac{64}{Re}, \quad \text{if } Re < 700 \]  

\[ f^{1/2} = \left[ 1.74 - 2 \log \left( \frac{D}{L} \frac{18.7}{Re^{1/2}} \right) \right]^{-1}, \quad \text{if } Re > 3000 \]  

\[ f = \frac{64}{Re} + 1.008 \times 10^{-3} (Re - 700), \quad \text{if } 700 < Re < 3000 \]  

It is worth noting that these correlations are discontinuous at the two boundaries (Re=700 and 3000) although in most cases pipes are operated in turbulent conditions. However, the above correlations have been slightly modified to ensure that the friction factor is continuously differentiable, prevent friction factor blow up, to improve smoothness at small Re and continuity at intermediate values. The main problem with Eqs. (5a)-(5c) appears when it is applied to two-phase systems because it is difficult to assign a universal definition for the viscosity in the Re. The most commonly used form due to McAdams, Woods, and Heroman (1942) is used for this purpose here. In addition, absolute values for Re in Eqs. (5a)-(5c) are used to allows reverse flow calculations.

Having the capability of evaluating the thermodynamic state and the friction factor, the pipe model essentially provides two differential equations. Thus, Eqs. (4a) and (4b) can be integrated to produce the pressure drop and enthalpy change in the pipe for given inlet conditions, mass flowrate, and all parameters such as the existence of multiple numerical solutions such as multiple solutions and a high number, indicates mixed or turbulent flow. The following equations are often used for friction factor (Perry, Green, & Maloney, 1988):

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as pipe diameter, pipe length, and heat transfer coefficient. The result is,

$$\Delta \Pi_{pipe} = \int_{0}^{L} \left( \frac{\partial P}{\partial a_{12}} - \frac{\partial P}{\partial a_{121}} \right) \, dL \quad (6)$$

$$\Delta H_{pipe} = \int_{0}^{L} \left( \frac{\partial H}{\partial a_{12}} - \frac{\partial H}{\partial a_{121}} \right) \, dL \quad (7)$$

where

$$a_{11} = 1 + m \frac{\partial \nu}{\partial T} \quad (8a)$$

$$a_{12} = m \frac{\partial \nu}{\partial H} \quad (8b)$$

$$a_{21} = m \frac{\partial \nu}{\partial P} \quad (8c)$$

$$a_{22} = 1 + m \frac{\partial \nu}{\partial H} \quad (8d)$$

$$b_1 = -m \frac{\partial g}{\partial C_{v}} \frac{s_0}{s} - f_{min} \frac{\partial P}{\partial A d_{C}} \quad (8e)$$

$$b_2 = -m \frac{\partial g}{\partial C_{v}} \frac{s_0}{s} - \frac{\partial Q}{\partial T} \quad (8f)$$

It is not possible to obtain analytical solutions to Eqs. (6) and (7) since all terms in these equations change with length. Hence, they have to be integrated numerically. The given initial conditions could be the pressure and enthalpy at inlet point or even measurable properties such as pressure and temperature in which case calculation of the thermodynamic state would produce enthalpy among other variables.

### 3.2. Valves

Valves perform an important part in production systems. In particular, the so-called choke valves produce effects in flow that deserve a separated analysis. Flow across a choke is divided in two groups: subcritical and critical. Subcritical flow occurs when the associated mixture velocity at the choke throat is less than the sonic velocity. The practical implication is that the flowrate depends on the downstream pressure when subcritical flow occurs at the choke throat, whereas this dependency is radically eliminated in critical flow. It means that after achieving critical flow, downstream pressure could be decreased further but the volumetric flowrate would remain constant. Supercritical condition cannot occur in reality. Choke valves are strategically placed in wells to avoid the blow up of the formation.

Most flow simulators do not reproduce this effect and either abort the iteration or calculates a lower flowrate value because of the above-mentioned inconsistency in simplified integrated models where multiple solutions may appear. In this work, an isentropic process is considered in all valves and the pressure drop, $\Delta P_{valve}$, is modeled using a simplified linear expression (Smith & Corripio, 2008):

$$\Delta P_{valve} = \frac{C_{valve} m}{\pi P} \quad (9)$$

where $C_{valve}$ is a constant parameter and $\pi P$ is the aperture of valve which has a restricted value $\pi P \in [0, 1]$. Using the aperture of valve allows that flow becomes nil when the valve is closed though there may be a pressure difference between the downstream and upstream pressures. In some cases, the $C_{v}$ can be used to fit experimental information. An important feature of this equation is that it can be used without any change for reverse flow calculation.

In addition, speed of sound is evaluated to detect critical flow. From physics, the speed of sound $c$ is obtained from thermodynamic properties (see, for instance, Smith, Van Ness, & Abbot, 1996). The maximum flowrate, $m_{max}$, is then calculated from,

$$m_{max} = V \left( \frac{\partial P}{\partial V} \right)_{S} \quad (10)$$

where $V$ is the molar volume, $P$ the pressure, and $S$ is the entropy.

For the sake of simplicity, it is assumed here that valves operate under pure Joule–Thompson effect, i.e. the enthalpy is the same at valve inlet and outlet. For given inlet pressure and enthalpy conditions at valve inlet point and a positive flowrate, the outlet pressure is then calculated with Eq. (9) while the enthalpy remains constant. If the flow is reverse then the known pressure and enthalpy correspond to the outlet point conditions and Eq. (9) can be used to calculate the pressure at the so defined entry point.

It must be observed that Eq. (9) is valid only for subcritical flow. When critical flow is detected then the calculation is reduced to determine the energy content at outlet stream, i.e. the thermodynamic state. Hence, the valve model, as well as the pipe model, demands the evaluation of thermodynamic states. Next section contains a description of how the evaluation of thermodynamic states is visualized in this model.

### 3.3. Thermodynamic state

During production system operations, the state of aggregation of fluid mixtures can be liquid, gas or a mixed liquid–gas as a result of the various pressure and temperature conditions. An equation of state is then required to model the thermodynamic behavior for both liquid and gas pure phases and mixtures. Using cubic equations of state is very attractive because they can be applied in all fluid phases and they also cover a sufficient range of pressure. The main disadvantage is that it aggregates extra numerical difficulties because of the highly non-linear equations added to the phase equilibrium problem. Several methods have been developed to solve the phase equilibrium problem. The Gibbs energy function is the most widely thermodynamic function used to determine the equilibrium state at given temperature and pressure. However, other energy functions could be more conveniently used for a different combination of independent variables such as pressure and volume.
In general, methods can be classified as those using direct minimization of the Gibbs energy function or those based on satisfying the necessary conditions for the minimum. Seider, Gautam, and White (1980) present a good review of these approaches. More recently, global optimization strategies have been applied to guarantee that the obtained numerical solution corresponds to the overall minimum. McDonald and Floudas (1995a, 1995b) applied activity coefficient models to address global optimization. Harding and Floudas (2000) analyze the most conventional cubic equations of state to provide convexity by reformulating each non-linear expression and hence to obtain the global minimum.

It is clear from above that calculating the thermodynamic state is a challenging task. If the state calculation were directly incorporated into the production model then the possibility of failure is high. Geoffrion (1972) has observed while solving optimization problems that some non-linearity difficulties may ease by sub divisions. Hence, the calculation of the thermodynamic state is considered here as a black box to overcome the numerical difficulties that cubic equations of state could introduce in the model. Thus, an ad hoc method is used to produce appropriate values in all required variables when given two independent properties, pressure and enthalpy, or temperature and the molar fraction of the system. A recent cubic equation of state (Poling, Prausnitz, & O’Connell, 2001) has been programmed to calculate the thermodynamic states when up to two phases are in equilibrium. The resulting subroutine was named TState. The following subsections describe how the above models are used in the present approach for the so-called here conceptual wells and manifolds.

3.4. Conceptual well

The conceptual well model is divided here in three main parts as indicated above: mass flowing from the reservoir to the wellbore, flowrate in the pipe, and the valve associated to the outlet point of the pipe. The main assumption considered here is that the system operates under steady-state conditions because the reservoir and pipe dynamics are irrelevant for the gas and oil production problem in a daily basis.

Gas and oil flowrate from the reservoir to the wellbore depends on several factors such as geological properties of well surroundings like fractures, permeability, thickness, porosity, etc. Modeling these factors is a considerable difficult task and it is beyond our goals. It is a normal practice to indirectly evaluate them and incorporate their effects in terms of productivity indexes for each well. Thus, well production generates an pressure drop between the reservoir pressure and the flowing pressure at wellbore. \( \Delta P_{rw} \), given by (Horne, 1998):

\[
\Delta P_{rw} = P^p - P^r\\n= \frac{141.2Bh}{k} \left( \frac{1}{\eta} \ln \frac{0.000264k}{\Phi} + 0.80907 \right) \tag{11}
\]

where \( B, \mu, k, h, \eta, \Phi \), and \( \Phi \) are experimentally determined parameters associated to the reservoir and the well, \( P^r \) the reservoir pressure, \( P^p \) the wellbore or bottom hole flowing pressure, \( q \) the volumetric production flow, and \( t \) is the operation time that starts when all parameters were determined. The original reference should be consulted for appropriate units.

Since all parameters and operation time are known for the daily production problem then Eq. (11) can be simplified as:

\[
\Delta P_{rw} = c_t \Delta H \tag{12}
\]

where \( c_t \) is the result of combining the parameters from Eq. (11). Lastly, Eq. (12) indicates that pressure drop can be approximated in the short time as a linear function of flowrate. In addition, each well has a maximum production flow, which may depend on geological properties. This maximum is normally determined from experimental work. Experience indicates however that the maximum production for a well will rather depend on the choke valve performance.

To evaluate the change of enthalpy from the reservoir to the wellbore, it is assumed here that an isothermal process is carried out. Then, the change of enthalpy is given by,

\[
\Delta H_{rw} = H(P_r, T_r, x) - H(P^p, T^p, x), \tag{13}
\]

where \( P_{r} \) is the reservoir pressure, \( T_{r} \) the reservoir temperature, and \( x \) the reservoir composition.

Lastly, Eq. (12) indicates that pressure drop can be approximated as indicated above: mass flowing from the reservoir to the wellbore, \( \Delta P_{rw} \), is the pressure drop from the reservoir to the wellbore that is calculated with Eq. (13).

Similarly, the total change in enthalpy for a well, \( \Delta H_{w} \), is obtained as follows:

\[
\Delta H_{w} = H_{inlet,w} - H_{outlet,w}; \tag{14}
\]

where \( \Delta H_{inlet,w} \) is the enthalpy at inlet conditions, \( H_{inlet,w} \) the enthalpy at outlet point, \( \Delta H_{inlet,w} \) the enthalpy change from the reservoir to the wellbore that is calculated with Eq. (13), \( \Delta H_{inlet,w} \) the enthalpy change in the pipe that is calculated by simultaneous solution of Eqs. (6) and (7), and \( \Delta H_{inlet,w} \) is the enthalpy change in the valve that is considered nil.
3.5. Conceptual manifold

The conceptual manifold allows that several pipes become interconnected but it is itself a pipe where a valve is incorporated to control flowrate. As above indicated, mixture of all inlet streams occurs at the inlet extreme point of this pipe. Then, the inlet pressure of a manifold is equivalent to the outlet pressure for each interconnected conceptual well or even another manifold. Thus, a manifold would provide as many equations of same type as interconnected units:

\[ P_{\text{inlet},m} = P_{\text{outlet},j}, \quad \forall m \in M \text{ and } j \in J_m \]  

where \( M \) is the set of manifolds \( J_m \), the set of conceptual units \( j \) connected at the inlet point of manifold \( m \), \( P_{\text{inlet},m} \) the pressure at inlet point of conceptual manifold \( m \), and \( P_{\text{outlet},j} \) is the outlet pressure of the conceptual unit \( j \).

Mass and energy balances are also required at inlet of each manifold:

\[ x_{\text{inlet},m} = \sum_{j} x_{j,m}, \quad i = 1, \ldots, c, \quad \forall m \in M \text{ and } j \in J_m \]  

\[ m_{\text{inlet},m} H_{\text{inlet},m} = \sum_{j} m_{j} H_{\text{inlet},j}, \quad i = 1, \ldots, c, \quad \forall m \in M \text{ and } j \in J_m \]  

\[ \forall i \in J_m \]

where \( c \) is the number of chemical species, \( x_{j,m} \), the molar fraction of species \( i \) in conceptual unit \( j \), \( m_{j,m} \), the total molar rate in conceptual unit \( j \), \( H_{\text{inlet},j} \) the enthalpy at inlet point of conceptual unit \( j \), and \( H_{\text{inlet},m} \) is the enthalpy at inlet of conceptual unit \( m \).

The overall pressure drop in the manifold \( m \), \( \Delta P_m \), from the inlet to the outlet is,

\[ \Delta P_m = P_{\text{inlet},m} - P_{\text{outlet},m} = \Delta P_{\text{pipes},m} + \Delta P_{\text{valve},m}, \quad \forall m \in M \]  

where \( \Delta P_{\text{pipes},m} \) is the pressure drop in the pipe of the manifold from the inlet point to the valve that is calculated by simultaneous solution of Eqs. (6) and (7) and \( \Delta P_{\text{valve},m} \) is the pressure drop in the valve that is calculated with Eq. (9). Indeed, the effect of pressure drop in the valve can be not only fitted but also cancelled by setting the parameter \( C_{\text{valve}} \) to zero. This might particularly be desirable when a manifold interconnect several manifolds.

The overall change of enthalpy for the manifold \( m \), \( \Delta H_m \), is obtained from,

\[ \Delta H_m = H_{\text{outlet},m} - H_{\text{inlet},m} = \Delta H_{\text{pipes},m} + \Delta H_{\text{valve},m}, \quad \forall m \in M \]  

where \( \Delta H_{\text{pipes},m} \) is the enthalpy at outlet conditions, \( H_{\text{outlet},m} \) the enthalpy at inlet conditions, \( \Delta H_{\text{valve},m} \) the change of enthalpy in the valve that is assumed nil.

4. Solution strategy

The Knitro code (Byrd et al., 2000; Waltz et al., 2003) is applied to solve both simulation and optimization problems. This code implements an interior method for non-linear programming that uses trust regions and a merit function to promote convergence. A detailed description of the algorithm is given in Waltz et al. (2003). In this work, gradients are approximated with forward finite differences and the Hessian is approximated with the BFGS method. Even the resulting set of non-linear equations is solved in Knitro where, to specify a non-linear equations problem, the objective function is specified as zero and all equations are considered as equality constraints. Numerical integration of Eqs. (6) and (7) is performed by applying the code DASSL (Brenan, Campbell, & Petzold, 1989) to the set of differential equations.

To start, a production system has to be described in terms of conceptual wells and manifolds. A dialog-based computer program, called WellNet, was developed to easy this description. Fig. 4 shows this program where the topology of a production system consisting on eight wells and two manifolds has been incorporated. Each well is represented with a circle, whereas each manifold is represented with a rectangle. Associated parameters to each conceptual unit are defined in descriptive dialogs that are activated by clicking in the representative circle or rectangle.

WellNet provides facilities to define the chemical species in the mixture via a database that contains several pure chemical species. Were it required, these properties could easily be modified to use other values. In addition, several cubic equations of state could also be selected. WellNet was programmed in Visual Studio C++ 6.0 and all cases presented here were tested in a PC Pentium 4, 2.40 GHz.

Once the topology of a production system and all required information are appropriately incorporated, users should select what problem to solve. Next sections describe both simulation and optimization problems.

4.1. The simulation problem

Several simulation cases are possible to evaluate in WellNet. In all simulation problems, the topology and physical parameters such as the aperture of valves remain constant. The most typical case in production systems consists of determining all flowrates for given conditions at reservoir and sales or storage points. Two types of process simulation can be identified in this work: standalone and overall simulation.

In a standalone situation for wells, at least the molar composition of the flowing mixture and aperture of the valve must be given as well as all parameters, shown in the model above, such as length, diameter, etc. An analysis of degrees of freedom based in the most simplified model indicates eight unknowns and four equations to result in four degrees of freedom (Table 2). More equations are involved in the model but they do not modify the actual value for degrees of freedom. In fact, all of them have been coded to configure the subroutine TState that calculates the whole thermodynamic state. Eqs. (3), (4a), and (4b) from
Table 2
Degrees of freedom in wells for standalone simulation

<table>
<thead>
<tr>
<th>Equation</th>
<th>Probable unknowns</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$P_{\text{inlet},w} - P_{\text{outlet},w} - \int_0^L (b_{1} a_{22} - b_{2} a_{12} a_{11} a_{22} - a_{12} a_{21}) dL - C_{\text{valve},w} \dot{m}_w = 0$</td>
</tr>
<tr>
<td>2</td>
<td>$w \left( H_{\text{outlet},w} - H_{\text{inlet},w} \right) - \int_0^L (b_{1} a_{21} - b_{2} a_{11} a_{22} - a_{11} a_{21}) dL = 0$</td>
</tr>
</tbody>
</table>

Subroutines in TState

3: $T_{\text{outlet},w} = T_{\text{outlet},w}(P_{\text{outlet},w}, H_{\text{outlet},w}, x_w)$

4: $T_{\text{inlet},w} = T_{\text{inlet},w}(P_{\text{r},w}, H_{\text{inlet},w}, x_w)$

Number of equations: 4; number of unknowns: 8; degrees of freedom: 4.

Table 2 are also included in this code. Thus, TState calculates all thermodynamic states required to calculate the residuals for Eqs. (1) and (2) from Table 1, which are used to converge the simulation problem using Knitro.

A typical scenario for a current standalone simulation in a well consists in determining the outlet pressure and temperature for given flowrate, and inlet temperature and pressure. The thermodynamic state at the reservoir can be calculated for given experimental pressure, temperature, and molar composition at the reservoir. Then, the thermodynamic state at the wellbore can be calculated assuming an isothermal process and the pressure calculated with Eq. (12) for a given flowrate. The pipe model is then applied for the given flowrate and the thermodynamic state at the wellbore to calculate the pressure drop and final enthalpy for a given length. Simultaneous solution to Eqs. (6) and (7) requires several calculations of thermodynamic states at different lengths that are carried out in TState. The valve model is finally solved to calculate the thermodynamic state at the wellbore outlet. If the flowrate is unknown then the outlet (surface) pressure should be defined and an iterative procedure could be used to calculate the flowrate. The procedure is repeated under Knitro control until convergence is achieved.

Another typical standalone simulation implies exchanging the flowrate with the outlet pressure in the above problem so that...
the flowrate becomes an unknown while the pressure is given. In this case, $T_{\text{State}}$ would again calculate the inlet thermodynamic state and Eqs. (1) and (2) from Table 1 are used to converge flowrate and outlet temperature.

In all standalone simulations, WellNet calculates the maximum flowrate, according to Eq. (10), to report this value and flagging on if the demanded or calculated flowrate results bigger than the critical value. Both residuals for Eqs. (1) and (2) from Table 1 and $T_{\text{State}}$ are prepared to use negative flowrate to allow reverse flow.

The standalone simulation for a manifold is similar to the well. Table 3 indicates also four degrees of freedom to result in a set of options similar to the standalone simulation for wells. It is important in this case that the thermodynamic state at inlet point be previously calculated and then the similarity to wells is maintained. Two cases are thus implemented within WellNet for standalone simulation of manifolds: in the first case, Eqs. (1) and (2) from Table 3 are solved to determine the inlet pressure and enthalpy and then the thermodynamic state. In a second case, the flowrate becomes an unknown, whereas the outlet pressure is given. Critical flowrate is also flagged on when it appears.

In the overall simulation, one or several wells are interconnected with one or several manifolds. The mixture effect at inlet point of manifolds given by Eqs. (17a) and (17b) must be incorporated here. Inclusions of these equations allow calculation of those variables related to the inlet thermodynamic state in manifolds. These variables correspond to those that were given during the standalone simulation. Besides equations related to thermodynamic states, the system is considered to generate two equations, and hence two degrees of freedom, per each conceptual unit.

Calculation of critical flow and its effect becomes an important issue for the overall simulation. An option to model this effect is by introducing auxiliary variables in Eqs. (14) and (18) to extend their applicability to critical flow and to allow that their residuals be nil in those cases where the outlet pressure is lower than the calculated value when using critical flow. However, it was observed that Knitro allows solving non-linear equations with dynamic bounds on the variables. Thus, the maximum flowrate, calculated with (10), was incorporated in WellNet as a bound for the variable. Then, a simple conditional was programmed to make the residuals in Eqs. (14) and (18) nil when the flow is critical and the real outlet pressure is lower than the one calculated with these equations. Section 5 contains examples where some simulation situations are analyzed.

### 4.2. The optimization problem

The optimization problem attached to the operational problem can be formulated in several forms. In general terms, the objective function consists of maximizing profits, minimizing costs, or a combination of these purposes. For instance, when oil production comes from different reservoirs and coming from another platform. Mass and energy balances are also required in mixing points. The equations related to these constraints have been already described in the simulation problem and they are directly extracted in WellNet from the declared conceptual units and their interconnectivity.

In addition, gas and oil production in the world is regulated by international laws and agreements. Hence, the production must always satisfy a given demand so that the imposed constraint must be an equality equation:

$$f_W = d, \quad \forall u \in W$$

where $d$ is the given demand. Molar flowrate is again considered here but volumetric flow could easily be used instead.

It can be observed that flowrates are the most natural variables for the optimization problem. Since valve apertures are used to control flowrates in the model proposed here, valve apertures are used as the optimization variables. In principle, this choice is consistent with the real system since valves associated to wells are physical means to flow control. Valve apertures clearly contain specific bounds [0, 1], which can be enforced to satisfy throughout the optimization process within Knitro.

The optimization problem consists then in using the objective function, Eq. (20), to satisfy a given demand (Eq. (21)) subject to the equations of the model for wells and manifolds (Tables 2 and 3), where aperture of valves for wells are the unknown variables. Any standalone optimization for wells would then produce information on the possibility of satisfying the given demand but there is no standalone simulation for manifolds in WellNet.

The overall optimization problem contains the following equations: the objective function (Eq. (20)); demand constraint (Eq. (21)); two equations and the $T_{\text{State}}$ code for each well (Eqs. (14) and (15)); ($c + 3$) equations and the $T_{\text{State}}$ code for each manifold (Eqs. (17a), (17b), (18), and (19)). The result is an...
objective function that is certainly linear and a set of constraints that are highly non-linear. If the cheapest resource could satisfy the demand then the solution is rather trivial since the optimum value would obviously be to keep production with just one well. However, when several interconnected wells are needed to satisfy the demand the answer is not so simple because of interconnectivity effects. There have been real cases of study where one well may even attempt to inject into another one. In other words, the maximum production of a group of interconnected wells is not equivalent to the sum of the maximum production of each individual well. This mistake in the model occurs very often during multiperiod planning where interconnectivities are not included in the model. Next section contains a description of some real cases of study where the proposed model has been applied.

5. Illustrative examples

As indicated above, a prototype called WellNet has been programmed using C++ Microsoft Visual Studio 6.0 in order to test our approach. It allows incorporation of all conceptual wells and manifolds having the system memory as the limitation. Knitro was incorporated into the Visual Studio project via a conventional library. The code has not been optimized and may take too much time to solve a given problem because of a continuous memory verification that has been programmed. However, it has been sufficient for our research purposes. The main user interface in Knitro is shown in Fig. 4.

Several examples have been solved to highlight the scope of the proposed approach. Some of them are presented below to show not only convergence properties but also feasibility of the model. All examples were calculated in a 700 MHz PC with 390 kB RAM. Though several cubic equations of state could be selected in our prototype for thermodynamic properties estimation, the Peng–Robinson equation has been used in most examples given below.

5.1. Case of study I

The first case of study corresponds to a single Mexican well called CHUC 62. Table 4 shows the reported molar fraction for the mixture in this well. Experimental production flowrate and outlet conditions are also known. Other thermodynamic experimental values have been omitted but Peng–Robinson and Soave cubic equations of state seem to predict well those properties. To detect the accuracy and robustness of the proposed formulation, it was decided to simulate the well in WellNet for the known flowrate to compare the outlet pressure with the experimental value.

The numerical evidence indicates that, for the given well production, the error in the outlet pressure estimation compared to experimental data was within 15%. The pressure profile obtained in WellNet, when thermodynamic properties were estimated with Peng–Robinson and Soave, is shown in Fig. 5. It is convenient to show these results in a P–T graph to detect the two-phase zone.

Fig. 6 shows the predicted P–T thermodynamic behavior for this mixture using Peng–Robinson and the estimated pressure profile. It is observed that the error increases when the mixture separates into two phases in equilibrium. This separation occurs at around 3000 m deep.

Table 4
Molar composition in well CHUC 62

<table>
<thead>
<tr>
<th>Species</th>
<th>Mol%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methane</td>
<td>34.029</td>
</tr>
<tr>
<td>Ethane</td>
<td>11.138</td>
</tr>
<tr>
<td>Propane</td>
<td>7.565</td>
</tr>
<tr>
<td>n-Butane</td>
<td>3.756</td>
</tr>
<tr>
<td>Isobutane</td>
<td>1.313</td>
</tr>
<tr>
<td>n-Pentane</td>
<td>1.326</td>
</tr>
<tr>
<td>Isopentane</td>
<td>1.838</td>
</tr>
<tr>
<td>n-Hexane</td>
<td>3.010</td>
</tr>
<tr>
<td>C7+</td>
<td>32.456</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>0.230</td>
</tr>
<tr>
<td>Carbon dioxide</td>
<td>2.446</td>
</tr>
<tr>
<td>H2S</td>
<td>0.893</td>
</tr>
</tbody>
</table>

Fig. 5. Pressure profile in well CHUC 62.

Fig. 6. P–T and pressure profile in well CHUC 62.
5.2. Case of study II

An 800 m deep vertical well connected to a 50 m length manifold is considered as a second case of study. Fig. 7 shows this system that is a real case situated in the north area of Mexico and the well is named Cañas 2. The system was modeled assuming that conditions of 95 bar and 340 K remains constant at wellbore. The pipe diameter is 0.073 m and composition of the mixture is given in Table 5. The numerical experiment purpose in this case of study was to test the model capability to include reverse flow calculation. The outlet pressure at the manifold was then modified and flowrate was calculated in each simulation. Convergence was indeed achieved in all cases in less than 10 iterations and 30 evaluations of the residuals. However, it was observed that convergence around the nil flow took too much time to achieve the solution. The difficulty was in solving the differential set of Eqs. (6) and (7) where the integration step tends to be too small. The solution taken to avoid this numerical situation was to introduce a disjunctive equation where the flowrate is enforced to be nil when, in any iteration, the suggested flow is \([-0.5, 0.5]\) in mole. Thus, Fig. 8 shows the final results where it can be seen that reverse flow may occur when outlet pressure is greater than 100 bar. Optimization of this system is allowed in WellNet but the problem is too small. The result however is consistent and provides the aperture of the valve to satisfy a given demand.

Table 5
Molar composition in well Cañas 2

<table>
<thead>
<tr>
<th>Species</th>
<th>mol%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methane</td>
<td>65.33</td>
</tr>
<tr>
<td>Ethane</td>
<td>5.66</td>
</tr>
<tr>
<td>Propane</td>
<td>6.61</td>
</tr>
<tr>
<td>n-Butane</td>
<td>2.08</td>
</tr>
<tr>
<td>Isobutane</td>
<td>0.41</td>
</tr>
<tr>
<td>n-Pentane</td>
<td>0.38</td>
</tr>
<tr>
<td>n-Hexane</td>
<td>0.02</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>18.34</td>
</tr>
<tr>
<td>Carbon dioxide</td>
<td>1.15</td>
</tr>
</tbody>
</table>

5.3. Case of study III

The third case of study consists of a gas field having four vertical wells with natural flow and one manifold (Fig. 9). Since all of them are producing from the same field, then the overall composition of the mixture is the same (Table 6). Each pipe in the well has a diameter of 0.073 m, and lengths of 1355, 1800, 1700, and 1390 m, respectively. The manifold is 2000 m length and 0.073 m diameter and the outlet pressure is 40 bar. The process simulation indicates that the gas production would be 2315, 3632, 3853, and 2007 MSCF/day, respectively. It took 8 iterations and 56 residual evaluations in WellNet.

Table 6
Molar composition in case of study III

<table>
<thead>
<tr>
<th>Species</th>
<th>mol%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methane</td>
<td>86.74</td>
</tr>
<tr>
<td>Ethane</td>
<td>10.56</td>
</tr>
<tr>
<td>Propane</td>
<td>1.19</td>
</tr>
<tr>
<td>n-Butane</td>
<td>0.17</td>
</tr>
<tr>
<td>Isobutane</td>
<td>0.12</td>
</tr>
<tr>
<td>n-Pentane</td>
<td>0.08</td>
</tr>
<tr>
<td>n-Hexane</td>
<td>0.03</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>1.03</td>
</tr>
<tr>
<td>Carbon dioxide</td>
<td>0.08</td>
</tr>
</tbody>
</table>
Considering the same topology, it was decided to modify the outlet pressure at the manifold to verify the possibility of reverse flow. When the outlet pressure in the manifold is considered 50 bar, the gas production is $-463, 5360, 5589,$ and $-405$ MScf/day. These results indicate that two wells would stop producing and possible would receive mass injected from the two other wells. In this case, it took 7 iterations and 49 evaluations to achieve the solution.

The same topology is considered to show the optimization capability. A demand of 11520 MScf/day was established and the cost of production associated to wells was 11.4, 12.6, 12.3, and 11.4 expressed in Mexican pesos per MScf, respectively. The optimal results indicate that valves in wells 1, 3, and 4 should be totally open, whereas the valve in well 2 should be 85% open. In this case, it took 16 iterations and 114 evaluations to achieve the solution. This result is as expected since it goes well with the logical analysis of producing first with the cheapest resource, then with next cheapest resource until the demand is achieved.

It indicates that the production system was not badly designed. However, it should also be clear from above that increasing the outlet pressure might produce reverse flow in which case the optimization answer is not so simple.

To continue with testing the accuracy and robustness of the model and numerical approach, several numerical experiments were carried out. Number of iterations, gradient and function evaluations, and time of convergence were registered. Same mixture composition used in the above three cases of study were used with up to 20 wells and 5 manifolds in different topologies and different conditions to force reverse flow. It was observed that same conclusions could be obtained from these experiments or from the already discussed cases of study. The main disadvantage observed in the proposed model is that, when production in one of the wells becomes nil or reverse, the time required for convergence may take more than a day, which is obviously unacceptable.

6. Conclusions

An innovative model has been proposed in this paper for simulation and optimization of gas and oil production systems. The proposed approach integrates the whole process from reservoirs to surface facilities where all units are rigorously modeled. Several features such as reverse flow and detection of critical flow have been incorporated in the model. In principle, the resulting model represents a very difficult set of differential-algebraic equations. However, separating thermodynamic state calculations yields great results in terms of iterations and time of convergence. Results obtained in several cases where this algorithm has been applied demonstrate the robustness of this approach. However, numerical evidence indicates that solving the set of differential algebraic equations may be impractical though they do not generate multiple solutions.

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