APPLICATION OF CHEMICAL ENGINEERING METHODS TO INTEGRATED PRODUCTION MODELLING

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ABSTRACT

The main objective was to apply advanced methods, first developed for the solution of chemical engineering processes, to petroleum engineering problems; specifically the modelling of hydrocarbon flows from underground reservoirs, through wells, flowlines, risers and processing equipment. This is, essentially, a pressure bounded problem where the reservoir pressure and the reception facilities pressure are fixed, at a given instant in time, and the production rate adjusts accordingly. The *equation oriented* approach was used as the basis of the numerical algorithms. The entire process, from reservoir to end-user, can be viewed as a *digraph* where the physical equipment items form the *nodes* and *edges*, collectively referred to as *objects.* Each object is described by a set of equations – founded on the conservation principles – with variables shared between object equations depending on the connectivity of the digraph. The algorithms assemble the entire set of equations into a large *sparse matrix* which is then reduced to *block triangular* form for solution. The paper gives an overview of this methodology. The results of two integrated production modelling (IPM) case studies are summarised, highlighting the important predictions and describing how these are used to resolve key techno-economic decisions in oil and gas design. It is concluded that the application of these methods, first developed for the solution of chemical processes, provides an efficient approach for the solution of petroleum engineering problems, in this case IPM, resulting in highly accurate and physically representative predictions generated in practical engineering timeframes.

INTRODUCTION

The simulation of chemical engineering processes has advanced considerably over the last three decades, as computer hardware has improved, and new methods have been developed. This trend looks set to continue as parallel processing techniques are exploited in conjunction with affordable multi-processor machines.

At present, commercial process simulation software can be separated into either of two classifications: *sequential modular* or *equation oriented*. The first commercially available simulators were based on the sequential modular approach. For this method, individual modules are developed for each *unit operation* (UO) in the flowsheet. These modules 'operate' on their input streams to produce their output streams. The separate modules are then solved in a sequence determined by the topology of the flowsheet to form the solution of the entire flowsheet. Where recycle streams appear, as is often the case, iteration is required to converge the solution for the flowsheet.

The equation oriented approach is quite different from the sequential modular method. To our understanding, the approach was first proposed in the 1960s (Westerberg and Sargent, 1964) as a general method by which transient chemical processes may be simulated. However, it was not until the 1980s that the first commercial process simulator became available (Pantelides, 1988). For this approach, each unit operation is viewed as being defined by a set of equations, explicitly known to the algorithms, that relate the variables in the output streams to those in the inputs streams. The entire flowsheet is then described by a large set of non-linear equations with adjacent unit operations sharing variables in connecting streams. The algorithms then solve the system of equations simultaneously by one means or another.

This paper describes the application of the equation oriented method to the solution of petroleum engineering problems, specifically the modelling of hydrocarbon flows in production systems and processing equipment. The equation oriented method is very general in its formulation, and while this makes it very versatile in application, different physical problems have their own nuances which must be accounted for if the solution algorithms are to be robust. This paper also tries to highlight some of the particular difficulties that necessitate a degree of specialisation for the solution of these problems.

METHODOLOGY

Mathematical Modelling of Networks

In mathematical terms, petroleum production systems, comprising of wells, flowlines, risers and processing facilities, form *digraphs* of nodes connected together by branches or edges (Wilson and Watkins, 1990). Figure 1 shows an example digraph formed by a four well subsea production system together with separation and recompression processing facilities.

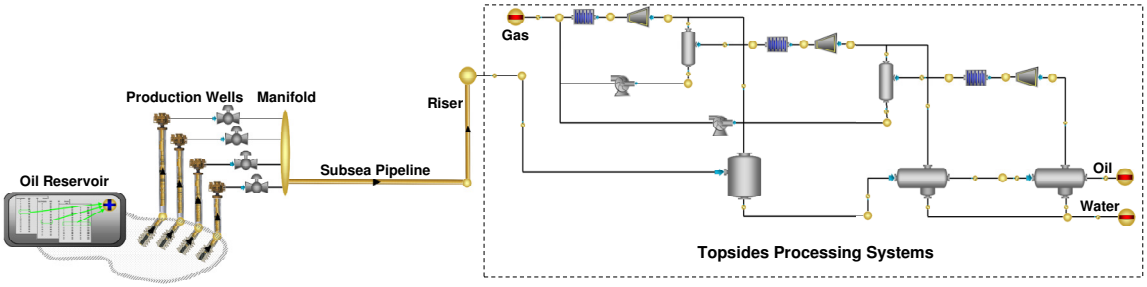


Fig. 1: Subsea Production System with Processing Facilities

In this analysis, all single input / single output equipment items are defined as branches with all other equipment items defined as nodes. Therefore, pipelines and risers are defined as branches together with other equipment items such as chokes, pumps or compressors. Equipment items with the potential for multiple inputs or multiple outputs, for example manifolds or separators, are defined as nodes in this analysis.

To solve network problems, such as the one shown in Figure 1, it is necessary to balance the pressures and flows throughout the system, together with conserving mass and energy across the network. To balance the pressures and flows, functional relationships are required for all branches allowing their pressure drop / flowrate

behaviour to be quantified. Introducing these functional relationships, represents the first significant departure from conventional process simulation, which is usually restricted to the solution of only mass and energy balances across unit operations. For this analysis then, pressure drop / flowrate equations were introduced for all branch-like unit operations. For pipe flows, these equations were based on the momentum conservation equation.

Compared to the sequential modular method, the equation oriented approach is significantly more general and consequently has much greater flexibility when posing the problem. In view of this, it is able to solve a much wider class of problems. The first step in the application of the method, is to formulate the entire set of equations describing the behaviour of a particular problem. Each unit operation contributes its own equations and variables. However, the topology or connectivity of the network implies that adjacent unit operations share variables. In general, the system of equations formulated is non-linear and can be rearranged to take the form:

$$\underline{F}(\underline{x}) = \underline{0} \tag{1}$$

$$\underline{F} = (F_1, F_2, \cdots, F_i, \cdots, F_{N-1}, F_N)^T \tag{2}$$

$$\underline{x} = (x_1, x_2, \cdots, x_j, \cdots, x_{M-1}, x_M)^T \tag{3}$$

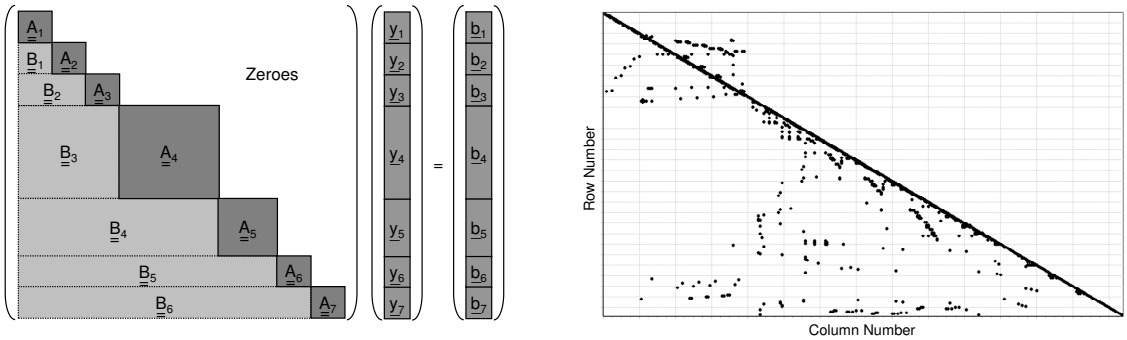
Initially, M > N and the system of equations contains more unknowns than equations. Before solution, M – N specifications are required to reduce the degrees of freedom to zero. To achieve this, it is usual to specify boundary conditions for the network, such as the reservoir pressures and delivery pressures, and model parameters, such as pipeline diameters and pump duties. An advantage of the equation oriented approach is that any set of specifications is permitted, provided the resulting system of equations forms a mathematically well-posed problem. This offers significant benefits over traditional solution methods, because problems can be solved more flexibly. After the imposition of specifications, the equations form the N × N system:

$$\underline{F}(\underline{y}) = \underline{0} \tag{4}$$

$$\underline{y} = (y_1, y_2, \cdots, y_j, \cdots, y_{N-1}, y_N)^T \tag{5}$$

The nature of most production system networks (of practical size) is that they are represented by hundreds, or even thousands, of equations originating from the individual unit operations. However, each equation usually only depends on a small number of variables in the solution vector. Therefore, these systems naturally form very large *sparse matrices* (i.e. containing a high proportion of zero elements). For such systems, there is considerable benefit to be gained by analysing the system of equations to identify the most efficient strategy. To do this, the equation system is first represented by its *incidence matrix* and then row and column manipulations are used to convert the system to block triangular form (Duff *et al*, 1986). An example of a simplified block triangular system is given schematically in Figure 2a. The system is reduced to a set of much smaller blocks that may be solved separately from top to bottom. Figure 2b shows the block triangularised matrix describing the model given in Figure 1. The topology of this model, coupled with its specifications, yields one block

for the wells and subsea systems and the rest of the system is lower triangular. Figure 2b also emphasises the natural sparsity of the problem.



(a) Simplified Schematic *(b) Triangularised Matrix*

Fig. 2: Example of Block Triangularity

The block triangularised form is closely related to the topology of the problem and its particular specifications. If a flowsheet is structured such that it is possible to solve the unit operations sequentially, arriving at the product stream in a single pass, then the block triangularised form will be close to lower triangular with only small blocks for each unit operation. However, if recycles are added, that link unit operations in one location to those elsewhere in the flowsheet, then larger blocks are created.

In general, the blocks emanating from the block triangularisation are multidimensional and an appropriate method is required to solve each individual block. This analysis uses a globally convergent variant of Newton's method (Burden and Faires, 2001). If the sub-system of equations represented by the block is:

$$\underline{G}(\underline{z}) = \underline{0} \tag{6}$$

Then the iterative map defined by Newton's method is given by:

$$\underline{z}^{k+1} = \underline{z}^{k} - \left[\underline{\underline{J}}^{k}\right]^{-1}\underline{G}^{k} \tag{7}$$

Where $\underline{z}$ is a subset of the variable set $\underline{y}$ and $\underline{G}$ is a subset of the equation set $\underline{F}$. The superscripts k and k+1 refer to the old and new iterates respectively. The matrix $\underline{\underline{J}}$ is the Jacobian matrix whose elements are defined as:

$$J_{i,j} = \frac{\partial G_i}{\partial z_j} \tag{8}$$

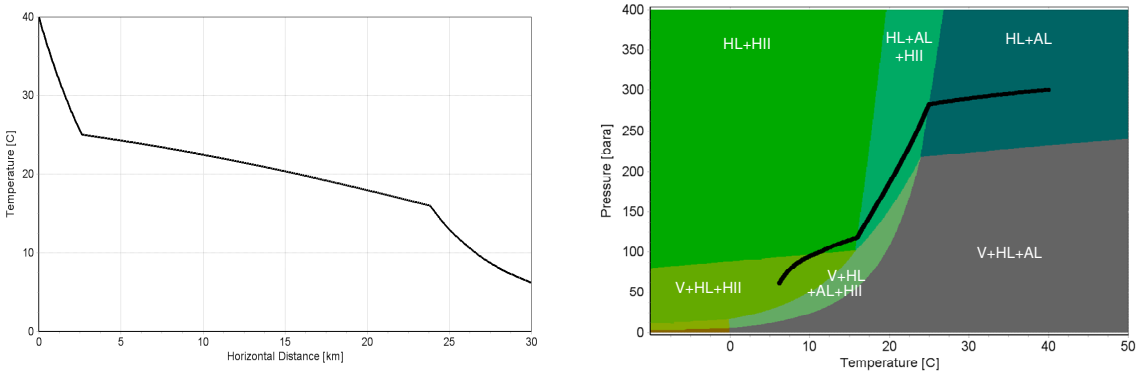
For this analysis, the Jacobian matrix was initialised with analytic derivatives where possible, and finite difference estimates when analytic differentiation was not possible. Computing the Jacobian can be computationally expensive and it is often unnecessary to calculate it exactly at each iteration. For this work, a hybrid method was implemented based on Broyden's least-change secant update (Broyden, 1965) coupled with analytic updates for those elements that are available cheaply. This hybrid method is computationally efficient and avoids the problem of 'fill in' where zero elements receive non-zero values at subsequent updates.

Using the iterative map represented in Equation (7), it is possible to solve the block of equations $\underline{G}$ before moving on to the next block. Once all the blocks have been solved, then the entire network solution has been achieved.

Physical Models for Unit Operations

The unit operations required to simulate hydrocarbon production systems include reservoirs, wells, trees, manifolds, flowlines and risers, together with other equipment items, such as pumps, compressors, expanders, separators, heaters, coolers, chokes, valves and non-return valves. The physical models for these are quite diverse and it is impractical to attempt to describe them all here. Hence, this discussion is confined to tubings, flowlines and risers. These are all examples of diabatic multiphase flows in cylindrical tubes, albeit with typically different diameters and inclinations. The modelling of these is based on the spatial integration of the steady state conservation equations for mass, momentum and energy. Since the flows are generally multiphase, appropriate closure models are required to quantify the holdups of the phases and the frictional losses. Various published models have been incorporated, for example Hagedorn and Brown (1965), Beggs and Brill (1973, 1991), Taitel and Dukler (1976), Ansari *et al* (1994) or Fan *et al* (2007).

To guarantee accuracy and efficiency of spatial integration, a high-order adaptive method was used based on a Cash-Karp Runge-Kutta scheme (Cash and Karp, 1990). Thus, accurate integrations are usually assured, even if the equations being integrated undergo steep gradient changes, because the integration step length is modified to resolve these changes. Figure 3 presents the results of integration along an uninsulated subsea pipeline in which hydrate formation occurs. The pipeline temperature profile (Figure 3a) shows two gradient discontinuities which have been resolved by the integrator. Reference to the corresponding pressure-temperature profile on the phase diagram (Figure 3b) shows that these discontinuities occur when phase boundaries are crossed. In the region where hydrate is forming the heat of formation helps to maintain the fluid temperature, which gives rise the flatter region on the temperature profile plot.



(a) Temperature Profile *(b) Phase Diagram*

Fig. 3: Flow in Uninsulated Subsea Pipeline

For integration along pipes, it is important that discontinuities, such as phase boundaries or flow regime transitions, are resolved accurately. Failure not to do so introduces 'noise' which can prevent solution convergence. This is a problem that arises

frequently in network solvers that use fixed pipe segment lengths; where it is observed that alternating flow regime transitions, in one or more segments, can prevent convergence.

Particular Difficulties

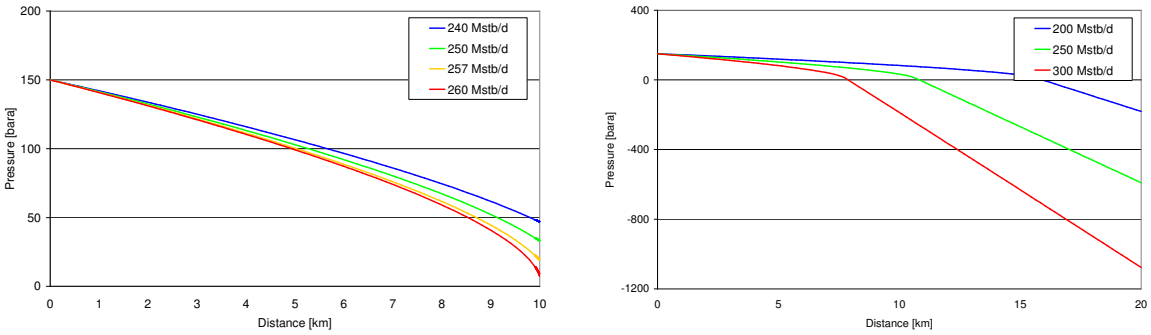
As with chemical engineering processes, the solution of hydrocarbon production systems also encounters several difficulties. Leaving aside the problems in common, such as mathematical ill-posedness, arising from under-specification, over-specification or structural singularity perhaps, there are several problems that are particular to systems of this kind. Three important examples are:

Flow Reversal. As the branch pressure drop / flowrate characteristics are solved in conjunction with the mass and energy equations, it is quite common for flow reversals to occur, either momentarily at a particular iterate, or in the final solution. To account for this, the equations describing each unit operation must be formulated to permit negative flows, even if the behaviour itself would not be observed in practice. In some cases, the solution achieved may not be physical because of the modelling assumptions made about reverse flow behaviour in some unit operations. However, it is still useful to have the solution because this then informs the engineer of potential problems with the physical posing of the problem. The possibility of flow reversals, and the need to handle these satisfactorily, represents another significant difference between the modelling of conventional chemical processes and hydrocarbon production systems.

Ill-Conditionedness. The mathematical models describing several of the unit operations in hydrocarbon production systems can exhibit ill-conditioned behaviour, with the solutions displaying 'elevated' sensitivity to their specifications. Most notable of these are pipelines operated at high flow rates where the outlet pressure approaches atmospheric. The ill-conditionedness arises because of the expansion of the fluid at low pressures, leading to higher velocities and rapidly increasing frictional pressure losses. Figure 4a shows pressure profile results for a 10 km pipeline carrying a multiphase oil-gas-water mixture. The graph shows that increasing the flowrate from 240 to 260 Mstb/d causes the outlet pressure to reduce from 47 to 7 bara. At the lowest flowrate, the pressure gradient is almost linear. However, as the flowrate increases the gradient becomes increasingly non-linear towards the outlet. As a result, the behaviour of the outlet pressure becomes very sensitive to comparatively small variations in the flowrate.

'Negative' Pressures. The equations describing the pressure drop / flowrate behaviour of branches in the network are usually posed in a simplified form that can permit the calculated pressure drop to exceed the inlet pressure, for certain unphysical specifications. For example, for a given inlet pressure, if the flowrate into a pipeline is increased, a critical value of flowrate is reached where the pressure at the outlet is reduced to zero. For all flowrates greater than this critical value, the outlet pressure is always zero. Hence, above the critical flowrate, the equation describing the pressure drop / flowrate behaviour becomes indeterminate on flowrate. Now this indeterminacy presents difficulties during solution because the equations provide no information about which direction to proceed in order to balance pressures in the network. For this analysis, this problem has been resolved by introducing negative pressures. This is done by fixing physical properties calculations at some lower bound positive pressure,

but allowing the equations themselves to predict negative pressures. Figure 4b shows the integrated pressure profile along a 20 km pipeline for three different flowrates. While the solutions shown are unphysical, the fact that the dependency on flowrate is maintained means that the solution algorithms know which way to return to a physically sensible domain. This greatly improves the performance of the algorithms.



(a) Ill-Conditionedness *(b) Negative Pressures*

Fig. 4: Pipeline Pressure Profile Results

RESULTS AND DISCUSSION

The results of two integrated production modelling (IPM) case studies are summarised, highlighting important predictions, and describing how these are used to resolve key techno-economic decisions in oil and gas design.

Case 1: Oil Field Development

Figure 5 presents an example that is typical of the incremental developments that occur in mature regions, such as the North Sea, where new smaller fields are 'tied back' to existing infrastructure with spare capacity. Initially, Platform 1 was built to process oil from the large oil field, Field A. However, as Field A was depleted, the production rates reduced, and spare processing capacity became available on Platform 1. This made it economically viable to develop smaller fields in the region by connecting these to Platform 1. The first incremental addition was Field B. After this, Fields C and D (located 10 km from Platform 1) were also included, but this time via the minimal processing facilities on Platform 2. Finally, Fields E and F were developed through a multiphase pipeline to Platform 2. Fields developed after Field A helped to support the production through Platform 1, keeping the facility going and delaying ultimate abandonment.

The model pictured in Figure 5 includes reservoirs, subsea production systems, processing facilities and export pipelines. In the design of new 'green field' developments, it is not usually necessary to model the processing facilities in detail as part of the IPM exercise because there is still latitude in the specification of these facilities. However, for incremental 'brown field' developments, the existing facilities are already operational and, hence, new incremental production must be accommodated within the prevailing constraints. This then necessitates more detailed representations of the processing facilities. In this case, the processing facilities were included in order

to incorporate constraints arising from product specifications and installed compression power.

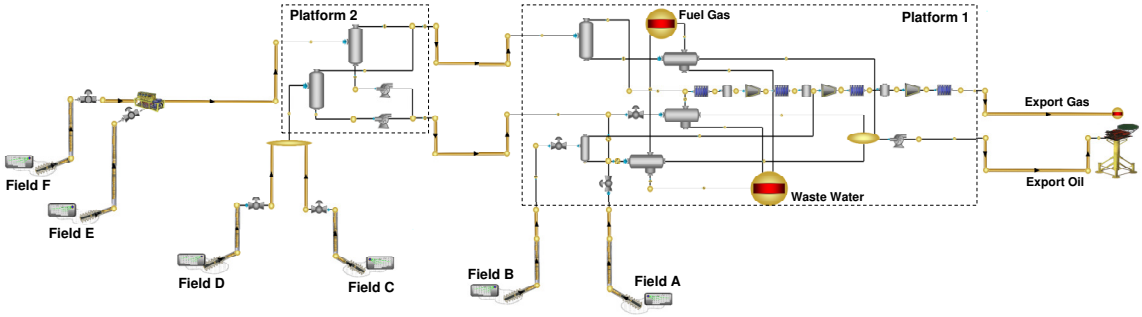
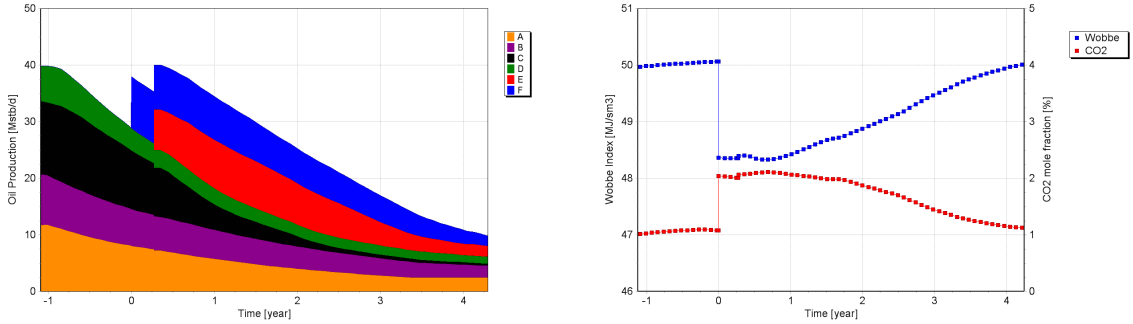


Fig. 5: Case 1 – Oil Field Development

Figure 6a shows the predicted oil production rates, before and after the commencement of production from Fields E and F. The results show that production from E and F helps to fill the gap in declining production from A, B, C and D. The simulations were performed using fully compositional descriptions of the reservoir fluids, allowing the prediction of compositional variations with time. For example, Figure 6b shows the forecast of Wobbe Index (a measure of the heating value of a gas) and CO_2 mole fraction in the export gas. These parameters are important in determining whether the gas meets sales contract specifications. The graph shows that the higher CO_2 concentrations in Field F lead to a doubling of the CO_2 mole fraction and a commensurate reduction in the Wobbe Index. These predictions of oil production rates and product specifications are central to the techno-economic decision making regarding the development of new fields. IPM predictions of this kind are only possible using a fully compositional analysis, and while this is a standard methodology in the modelling of chemical process systems, it is not commonplace in IPM simulation.



(a) Oil Production *(b) Gas Specification*

Fig. 6: Case 1 – Production Forecast Results

Case 2: Gas Field Development

The model for the second case study is pictured in Figure 7; it consists of two separate fields, each comprising of two reservoirs. The reservoirs were modelled using compressible gas tanks. While the reservoirs comprising Field B are isolated, the reservoirs comprising Field A are expected to communicate with each other and with an underlying aquifer. The gases flow from five production wells via short pipelines to a central manifold were they are mixed. Thereafter, the gas either flows directly to the

export pipeline via a subsea choke valve or via a compression platform. The model includes two different export pipelines because two alternative routes to shore were under consideration. The gas is eventually delivered to a shore-based gas plant.

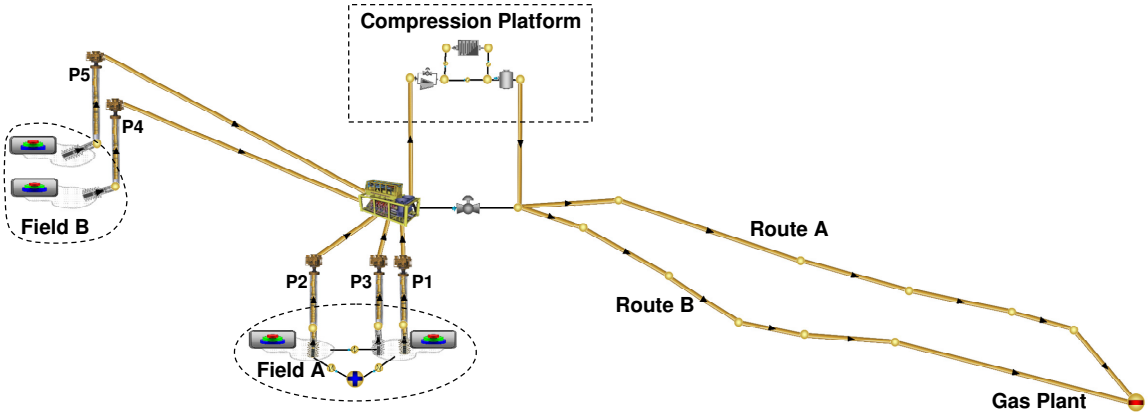
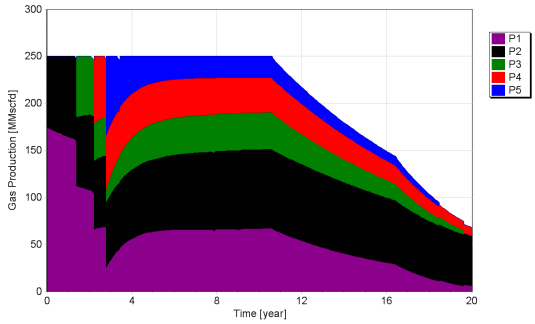
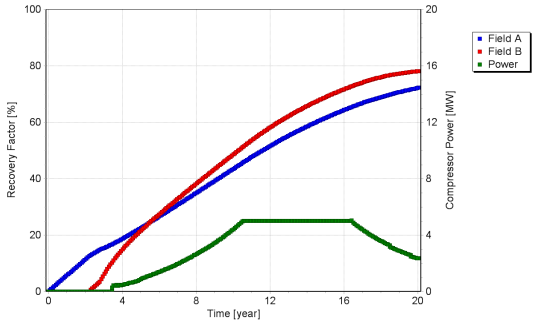


Fig. 7: Case 2 – Gas Field Development

Figure 8a shows the predicted production rates; the target rate was 250 MMscfd. Initially, this can be met with just two wells (P1 and P2) flowing via the subsea choke valve. However, after about 1.4 years another well is needed to meet the target and P3 is brought onstream. This is then followed by wells P4 and P5 at 2.2 and 2.8 years respectively. With five production wells flowing, production is then sustained until about 3.4 years. After this, the gas is routed via the compression platform to maintain the production rate. The compressor power is then increased steadily until it reaches its maximum constraint of 5 MW at about 10.6 years when the production then slips into decline. Figure 8b shows the variations in the recovery factors (i.e. cumulative production as a fraction of initial reserves) and the compressor power. The information predicted regarding the timing of new wells, and the installation of the compression platform, allows the designer to establish the capital expenditure profile. These predictions are key to the economic evaluation of the proposed gas field development.



(a) Gas Production



(b) Gas Recoveries

Fig. 8: Case 2 – Production Forecast Results

CONCLUSIONS

The methods described were applied to two case studies and predictions of product flows and qualities, suitable for techno-economic evaluations, were generated as functions of time. From these studies (and numerous others), it was concluded that the

equation oriented approach, first developed by chemical engineers for the solution of chemical process systems, provides an efficient method for the analysis of hydrocarbon production problems. However, while the generality of the method certainly offers great flexibility, reliable solutions still require a degree of specialisation to the problem in hand. For example, the issues of flow reversal, ill-conditionedness in pipelines, and the possibility of unphysical negative pressures should be addressed. This can be done, conveniently, during model formulation.

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