

The Use of Process Simulation Models in Hydrocarbon Allocation Systems

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1 INTRODUCTION

This paper discusses the use of process simulation models in allocation systems associated with upstream and midstream hydrocarbon processing facilities - typically these include both offshore installations and onshore gas plants and oil terminals. It is concerned specifically with steady state simulation models and hence does not include a discussion of dynamic models.

The main purpose of simulation models used within hydrocarbon allocation systems is to provide information regarding how hydrocarbons are behaving in a process plant. The use of simulation models ranges from the prediction of physical properties and calculation of shrinkage factors, to full integration of the model, (using cloned components) within the allocation process itself.

The paper describes the appropriate construction of a simulation model for allocation purposes and incorporation of available measured plant data. It also discusses the commonly available commercial simulation packages and talks about issues such as stability, reproducibility, licensing and maintenance associated with such models.

A novel alternative approach to constructing process models (using chemical engineering calculations) outwith a commercial package is described. This alternative approach has been implemented in a number of North Sea allocation systems and provides the advantages of: direct integration into software, robustness and transparency.

Finally the paper concludes with a discussion regarding the necessity of a process simulation model and whether the allocation results can be replicated without recourse to a model at all.

First a consideration of what a process simulation comprises is discussed.

2 WHAT IS A PROCESS SIMULATION MODEL?

In the context of allocation systems, process simulation models are normally associated with models constructed in commercial simulation packages such as Aspentech's HYSYS, Honeywell's UniSim and Simsci-Esscor's PRO/II.

In essence though, process simulations are examples of the general class of models, which can be defined as a broad collection of methods used to study and analyse the behaviour and performance of actual or theoretical systems.

Any model involves the solution of equations that describe the system being studied in order to derive information about that system. Typically in process simulators, equations are constructed that describe the following types of relationships:

- Heat balances
- Mass balances
- Vapour liquid equilibria
- Equipment performance (e.g. compressor duties)
- Etc.

Hence, commercial process simulators could be described basically as equation solvers. This may sound a simplistic description but in practice the problem the software is dealing with is often complex involving large numbers of equations (linear and non-linear) solved using

relatively sophisticated techniques. The software also has to be easily configurable so that it can model a wide range of chemical processes. Generally such software includes a number of other features to facilitate model building for the user, for example:

- A graphical user interface or keyword input file to allow the model to be defined easily, including the process topology, (i.e. how the various pieces of equipment are connected together), equipment performance parameters, etc.
- A large physical property database for a wide range of compounds
- Thermodynamic methods to predict the behaviour of components
- Reporting and data transfer features
- Etc.

Though such software makes the modelling of chemical processes easier it does place demands on the user to ensure that sufficient equipment data, stream flows, compositions and process operating conditions are supplied to render the model (i.e. the equations) solvable.

Before considering in more depth the data the user needs to supply to a process model, it is worth considering what such a model can provide for allocation purposes.

3 WHAT CAN A MODEL TELL US?

The main purpose of simulation models within hydrocarbon allocation systems is to provide information relating to the behaviour of hydrocarbons in a process plant. The use of simulation models ranges from the generation of process information to full integration of the model within the allocation process itself. For example typical uses in allocation systems include:

- Calculation of “shrinkage” or “expansion” factors
- Calculation of component recovery factors
- Direct allocation of hydrocarbons
- Calculation of physical properties
- Estimation of unmeasured streams (e.g. wellstreams, flare, etc.)

Each of these is discussed more fully below.

3.1 Calculation of Shrinkage and Expansion factors

Consider an offshore platform topsides process such as that presented in Fig.1 below:

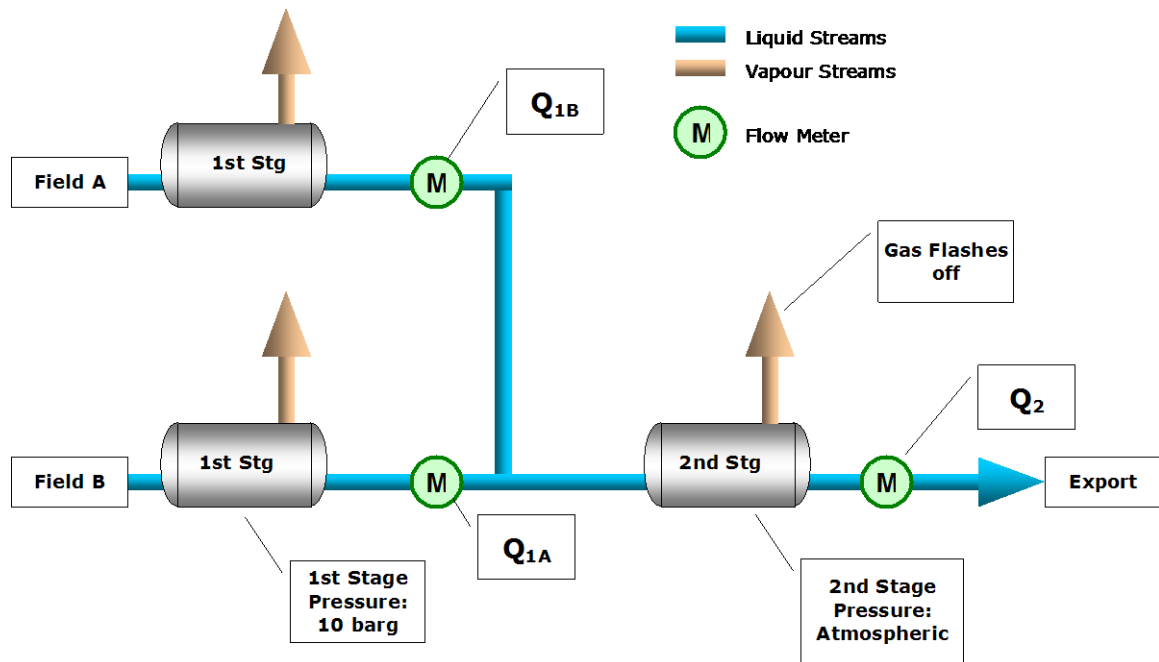


Fig. 1 – Schematic of Two-Stage Separation Process

The commingled metered export oil is to be allocated between Fields A and B based on their respective 1st Stage Separator metered rates. The 1st Stage Separators are operating at 10 barg but the fluids are flashed down to atmospheric conditions in the 2nd Stage where some hydrocarbons are vapourised. Hence, the exported metered quantities, on a mass basis, will be less than the sum of the 1st Stage metered quantities (ignoring the impact of any meter uncertainties). To allocate equitably it is necessary to understand how much material is flashed from each Field's fluids in the 2nd Stage Separator.

A factor may be applied to each Field's metered quantity to estimate how much product oil remains after gas is flashed off in the 2nd Stage. This factor is commonly referred to as a shrinkage factor and for Field A may be defined as:

$$S_A = \frac{Q_{2,A}}{Q_{1,A}} \quad (1)$$

The problem is that the quantity $Q_{2,A}$ is not directly available from any plant measurements. However, a process simulation would predict $Q_{2,A}$, by modelling Field A's fluids as though they were being processed alone. Fig.2 illustrates the results from such a two-stage process generated in a HYSYS simulation:

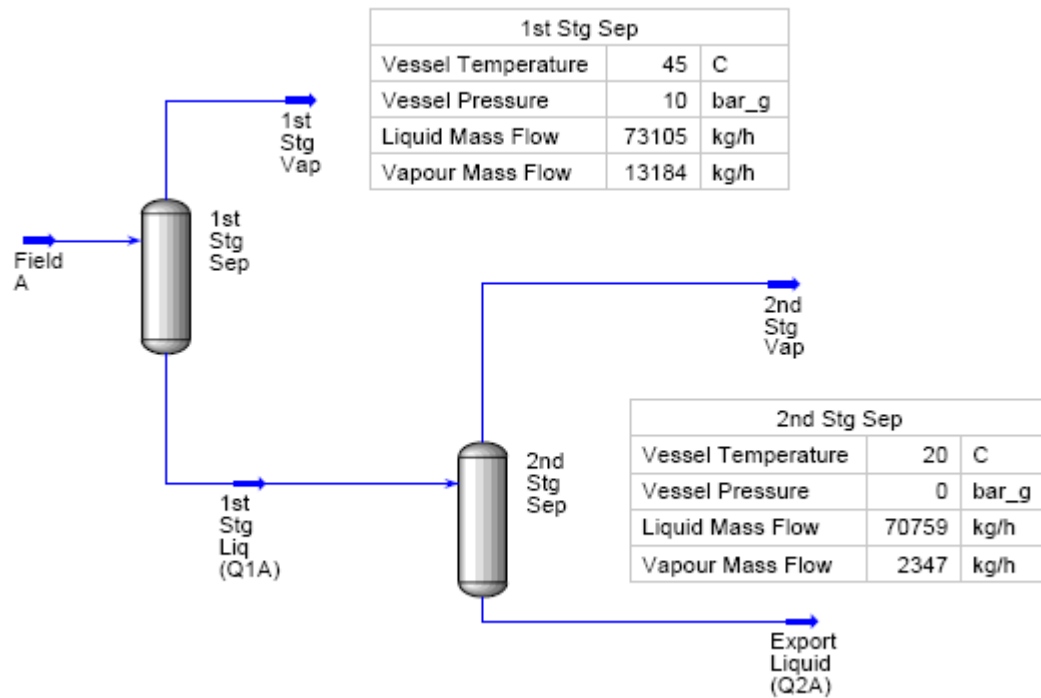


Fig. 2 – HYSYS Simulation of Two-Stage Process Illustrating Shrinkage

The stream flow rates are summarised in the tables. The shrinkage factor is calculated, on a mass basis, from:

$$S_A = \frac{70759}{73105} = 0.9769 \quad (2)$$

Similarly Field B's shrinkage factor can be calculated; this may be different, as Field B may be a more or less lively crude, or it may experience a different temperature or pressure in its first stage separator.

The first-stage metered quantities can then be multiplied by the respective Field's shrinkage factors to obtain an estimate of their individual export oil quantities and the actual metered export oil then allocated proportionately.

Such factors may be expressed on a mass, or indeed a volume basis (not generally recommended since volumes tend not to be additive and their value is dependent on the conditions they are quoted at, e.g. standard versus actual conditions).

As already indicated, shrinkages are affected by fluid composition and process conditions such as vessel temperatures and pressures. A range of shrinkage factors can be calculated for each Field at various conditions and applied appropriately.

Gas expansion factors may be calculated analogously. Consider the 2 Stage Separation process now with a compression train as presented schematically in Fig 3:

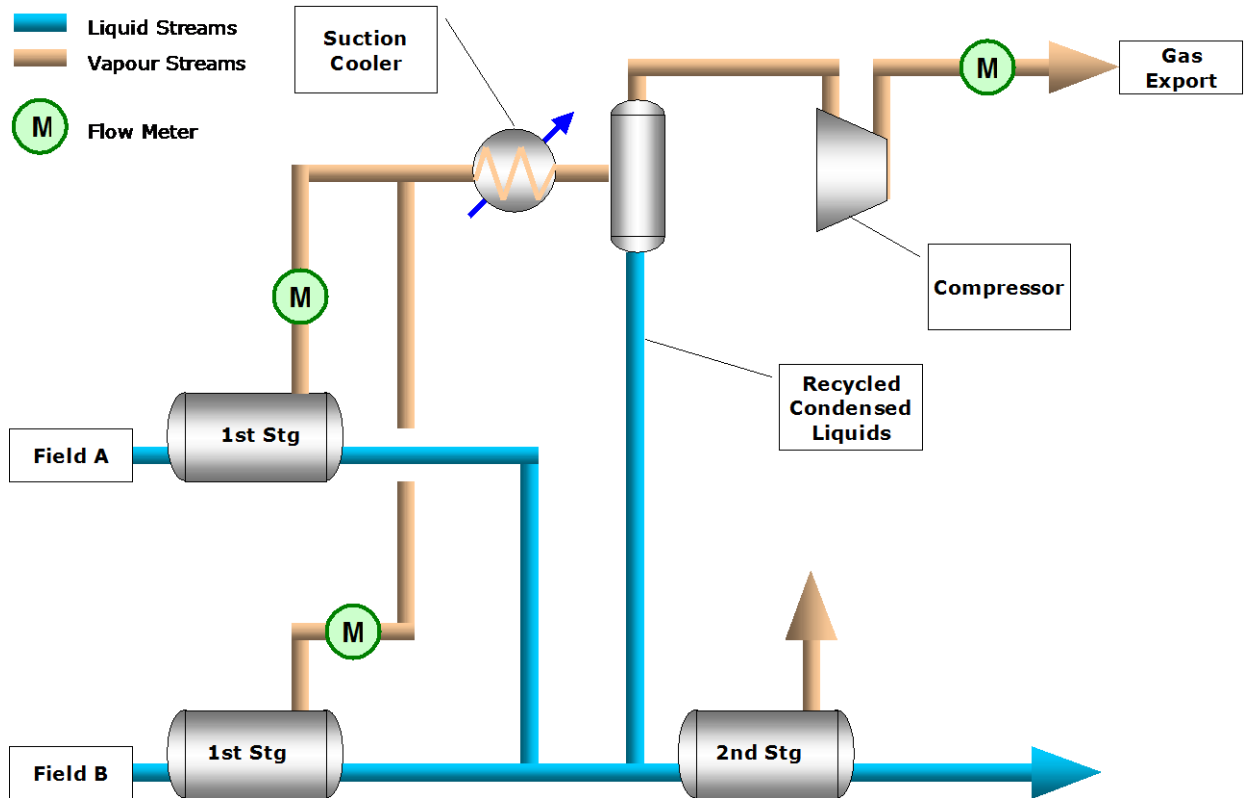


Fig. 3 – Schematic of Two-Stage Separation Process with Compression

The gas expansion factor is the ratio of a Field's export gas to its 1st Stage Separator metered gas and this would be calculated for each Field individually using a process simulation model in a similar manner to that described above for the oil shrinkage.

The terms "shrinkage" and "expansion" factors can be confusing terms. For example even on a mass basis it is possible for liquid shrinkage factors to be greater than one. This is particularly likely when a hot, light condensate fluid is processed and due to cooling of the 1st stage gas in the compression trains, liquid is removed and combined with the product oil thereby generating more liquid than was measured at 1st stage conditions. Conversely gas expansion factors may be less than one. A further paradox associated with the word shrinkage is that the larger the shrinkage the smaller the factor.

It is also acknowledged that the terms are interchangeable, for example shrinkage may be applied to gas streams.

This use of such factors can be extended to estimate the production from individual wells based on well test rates. In addition to the flashing effects and condensate recycles in a multistage separation process, the factors have to represent the effects of temperature variation which may be considerably different in the well test when compared with the commingled production.

3.2 Calculation of Recovery Factors

An extension of the calculation of shrinkage or expansion factors, which apply to whole stream rates, is to calculate recovery factors for each component in a stream. The term recovery factor is simply defined as the fraction of a component recovered in the exported liquid or gas stream (depending on how the factor is defined) from a measured feed stream. This requires the composition of the feed stream to be measured or determined (possibly using simulation).

This approach, though slightly more involved, does tend to improve the accuracy of the estimated production in comparison with the use of shrinkage (or expansion) factors.

3.3 Calculation Approaches

Stand-Alone Approach

Whether shrinkage, expansion or recovery factors are used, there are various methods available to calculate them using a process simulation. The actual method may be dictated by the allocation rules themselves – for example it may be stipulated that the factors are calculated on a “stand-alone” basis, i.e. as though the individual Field was being processed through the plant on its own and not commingled with other Fields’ hydrocarbons.

The example in Fig 2 illustrated the concept of calculating factors using the “stand-alone” approach. The estimated production from each field is then summed and allocated against the actual metered quantity. It should be noted that the sum of the individual production from each Field will not generally be exactly equal to the simulated production from the combined Field throughputs. This is sometimes referred to as the “effect of commingling”. Indeed the more dissimilar the Field compositions the larger the effect of commingled production on the factors.

By-Difference Approach

A lean condensate field will behave quite differently when commingled with heavier fluids in a process than when processed on its own. To account for this, an alternative approach is to simulate production with all Fields flowing, then simulate with all Fields except the Field of interest. The contribution from the Field of interest is calculated by difference between the two sets of results. This concept is illustrated in Figs 4 and 5.

Consider Field A now to be a lean condensate field: Fig 4 shows the output from a HYSYS simulation of Field A, commingled with other heavier Fields (which represent the bulk of the production). Fig 5 shows the same process with Field A removed (process conditions held constant). Field A’s production is obtained as the difference in the two Export Oil rates and equals 27,204 kg/h.

This can be compared with Field A on a stand-alone basis, which according to Fig.6 is estimated to produce 22,429 kg/h. The difference in estimated production is over 20%. In terms of estimating the contribution of Field A to the total export oil it can be argued that the by-difference method is more representative than the “stand-alone” approach but as mentioned above, this is subject to what is stipulated contractually.

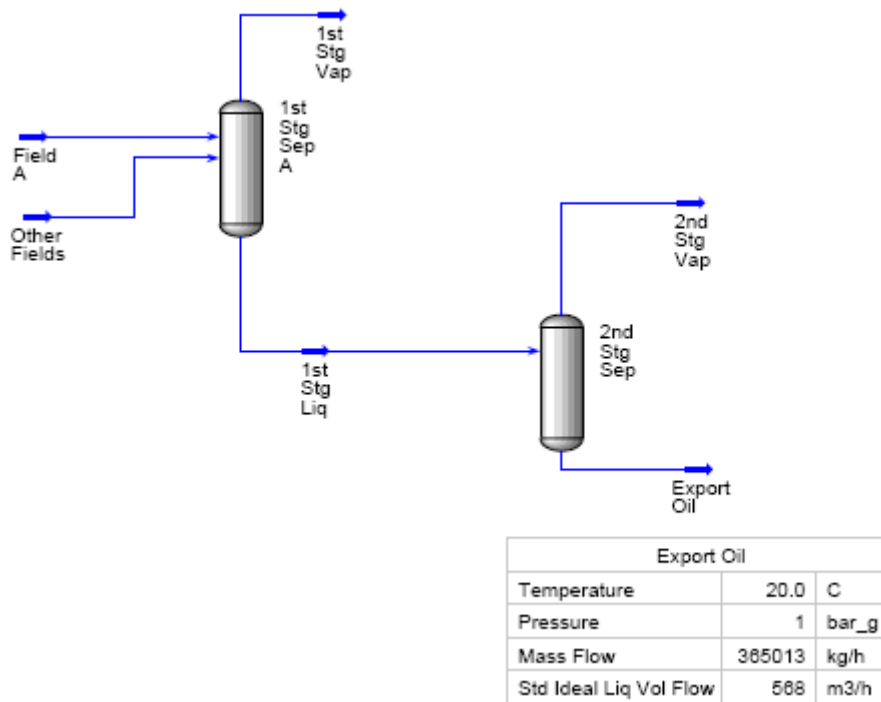


Fig. 4 – HYSYS Simulation of Two-Stage Process
 Commingled Production

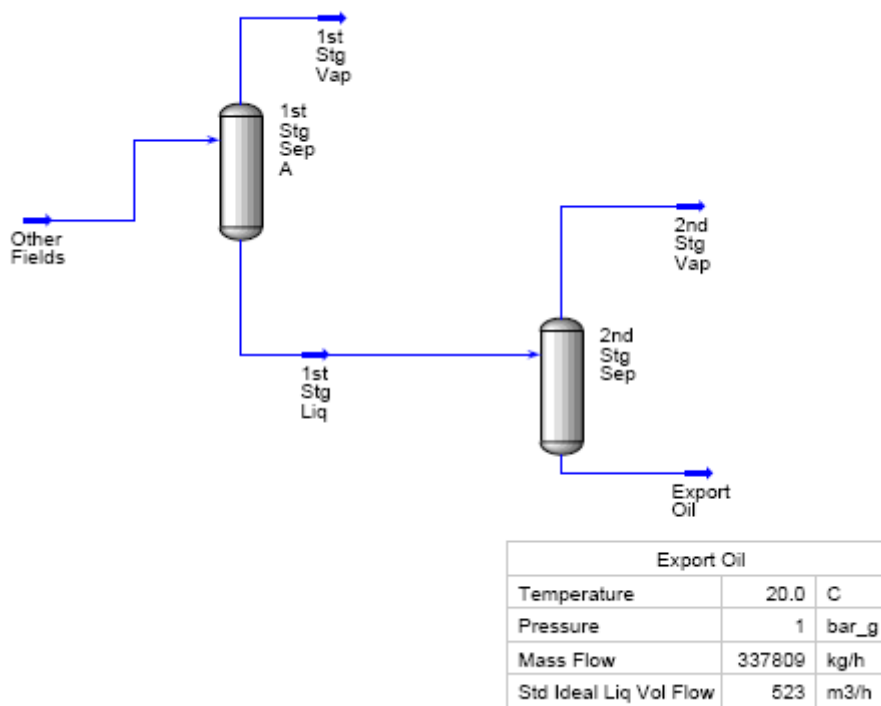


Fig. 5 – HYSYS Simulation of Two-Stage Process
 Field A Removed

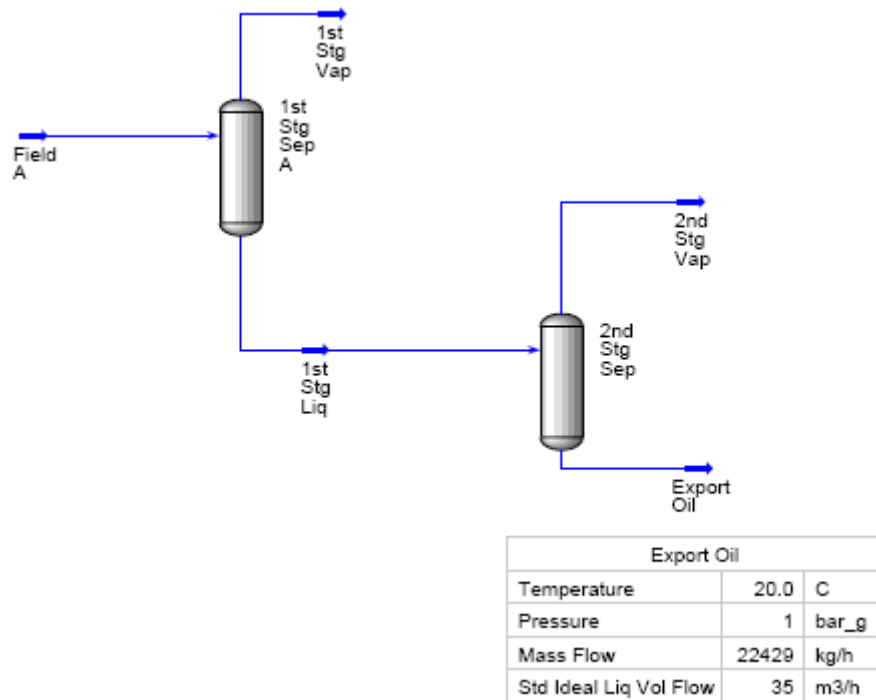


Fig. 6 – HYSYS Simulation of Two-Stage Field A Only

This approach can be extended so that the individual Field contributions to the export oil are obtained directly from a single simulation with all Fields flowing. This is achieved by utilising cloned components. In fact the simulation can be used to allocate products directly.

3.4 Allocation Using Cloned Components

Cloned components are, as the name indicates, copies of components. For example methane may be cloned to generate a new component that possesses identical properties to methane except the molecules are tagged so that they can be identified as being distinct from normal methane. This distinction is not real but is possible in the world of process simulations. It is as though collections of methane molecules are labelled as belonging to a certain Field. A real world analogy is a radioisotope of a compound, which exhibits identical chemical properties and behaviour to its non-radioactive counterpart but can be identified using a Geiger Counter.

Fig. 7 illustrates the results of a simulation of two Fields (A and B) with cloned components.

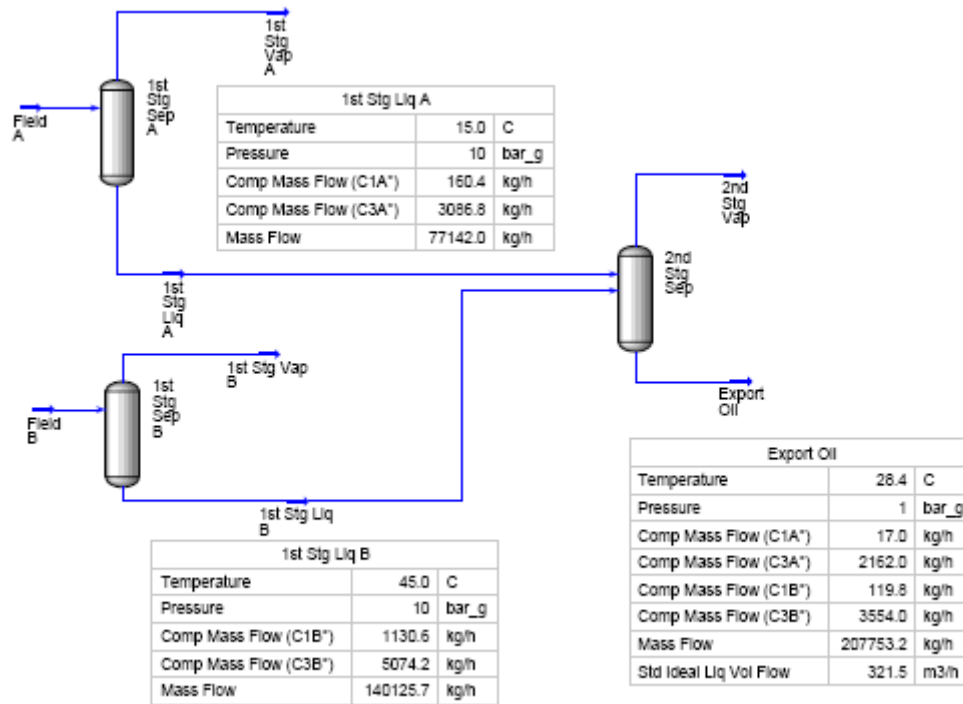


Fig. 7 – HYSYS Simulation of Two-Stage Process with Cloned Components

The C1 (methane) and C3 (propane) contents of the first stage liquid streams are presented and tagged as “belonging” to Field A and B (the remaining components are similarly identifiable in the model but only two components are presented for clarity). When commingled in the second stage separator the individual Field component flows can be identified in the final export oil. This approach can be extended to the rest of a plant and the individual Field component flows identified for any stream.

However, a word of caution when constructing such simulation based allocation systems as unanticipated consequences may result. The inclusion of recycle streams such as lift gas distributes all Fields’ components throughout all the process, and hence product streams that at first sight might be expected to be allocated to a single Field include components from other Fields – Fig 8. illustrates the point:

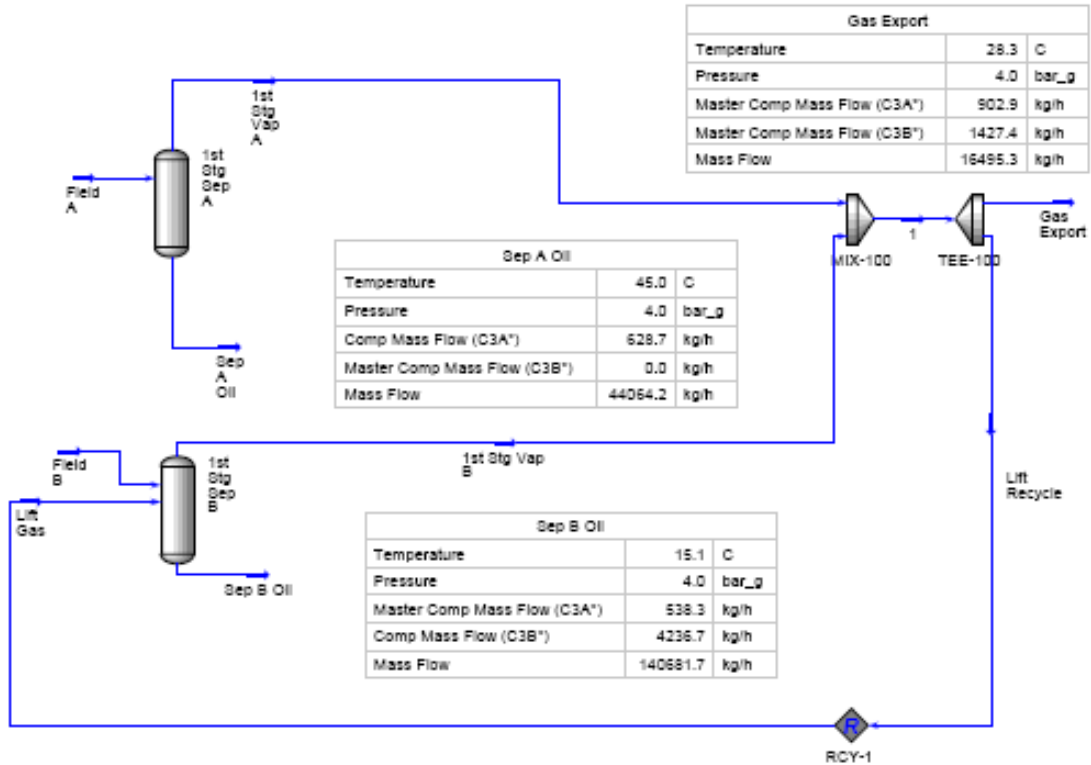


Fig. 8 – HYSYS Simulation Lift Gas Recycle with Cloned Components

The two Fields (A and B) produce liquids from dedicated separators with their produced gas being commingled. However, the lift gas stream is a mixture of all Fields' hydrocarbons and therefore Field A's hydrocarbons find their way into the lifted Field B's separator and hence produced liquid oil – this may not be a desirable allocation result.

3.5 Calculation of Unmeasured Streams

Simulations may be used to estimate the flow rate of unmeasured streams. For example flare stream rates may not be directly available and these can be inferred using a simulation.

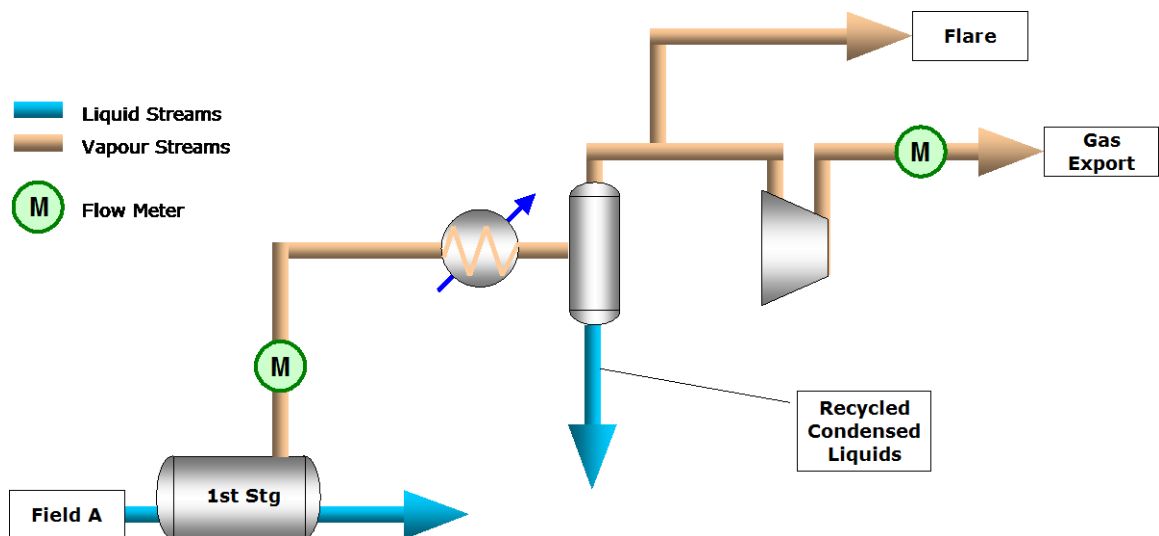


Fig. 9 – Schematic of Compression Train with Flaring and Condensate Knock Out

In Fig. 9 above, the stream entering the compression train is metered as is the export stream but there are two unmeasured flows: the flare and condensed liquid from the scrubber. The sum of the two unknown stream rates can be simply calculated by difference between the metered rates. However, a simulation may be used to estimate these unknown flows individually, though caution is warranted as these streams will often represent the difference between two large metered quantities. Judicious tuning of compositions or process conditions may further improve estimates from the simulation.

Also simulations, replicating well tests may be used to estimate wellstream compositions without recourse to extensive routine sampling and analysis.

3.6 Physical Properties

Simulation packages contain an extensive database of physical property information available for both individual compounds and also multi-component mixtures at any conditions that might be encountered in the majority of upstream processes. This data can be extracted for use in allocation calculations, for example liquid densities, gas calorific values, etc.

4 MODEL CONSTRUCTION

4.1 Introduction

This section describes the construction of process simulation models specifically with allocation purposes in mind. In order to construct a model of a process using a commercial simulation package the user has to input the following:

- Process flow diagram, i.e. how are all the pieces of equipment are connected together. This is normally entered using a graphical user interface that represents the process pictorially or a via keyword input file.
- Process equipment data, e.g. compressor performance curves or efficiency, etc
- Components to be used
- Thermodynamic package, e.g. Soave Redlich Kwong (SRK), Peng Robinson (PR), etc.
- Process input data, i.e. flows, compositions and process operating conditions
- Control functions and product specifications

Each of these is discussed below.

4.2 Process Flow Diagram and Equipment Data

Process simulations are used routinely by process engineers to model processes for design purposes. Such models can be complex and include such items as control valves, pumps, compressors, heat exchangers, etc. At first sight, the use of such design simulations for allocation purposes has apparent appeal, in that a common model is used to represent the same process throughout an organisation, the model probably being maintained and updated by the process engineering department which is more likely to be aware of any changes or modifications to a process. However, such simulations may not be sufficiently stable for allocation purposes, especially if there are recycle streams, compressor curves, anti-surge, etc. included. Such simulations may frequently require intervention by a process engineer to ensure they solve.

For allocation purposes model stability is very important. Frequent intervention by a process engineer is undesirable and it is better if the simulation runs robustly and quickly when required. To aid speed and stability it is better to construct such models with the least equipment possible whilst adequately modelling the process. Generally in an allocation system, the simulation is only used to determine how hydrocarbons entering the process are distributed between the various liquid and gas products exiting the process; stream enthalpies, equipment performances, etc. are not of interest. The only important unit operations in the flow scheme are those where material streams are combined or separated. Therefore, the allocation simulation can be constructed simply as a series of flashes, mixers and splitters

providing the operating conditions in the flashes are known or specified. The fact that there may be a number of equipment items between the flashes does not affect the vapour-liquid equilibria in the vessels, which are determined by the operating conditions therein. The results from these simplified schemes are identical to those generated by the more complex “full-blown” simulations, with the advantage of improved speed and reliability of solution.

The following process simulation, which compares a simplified scheme (top), with a more complex representation of a compression train illustrates this:

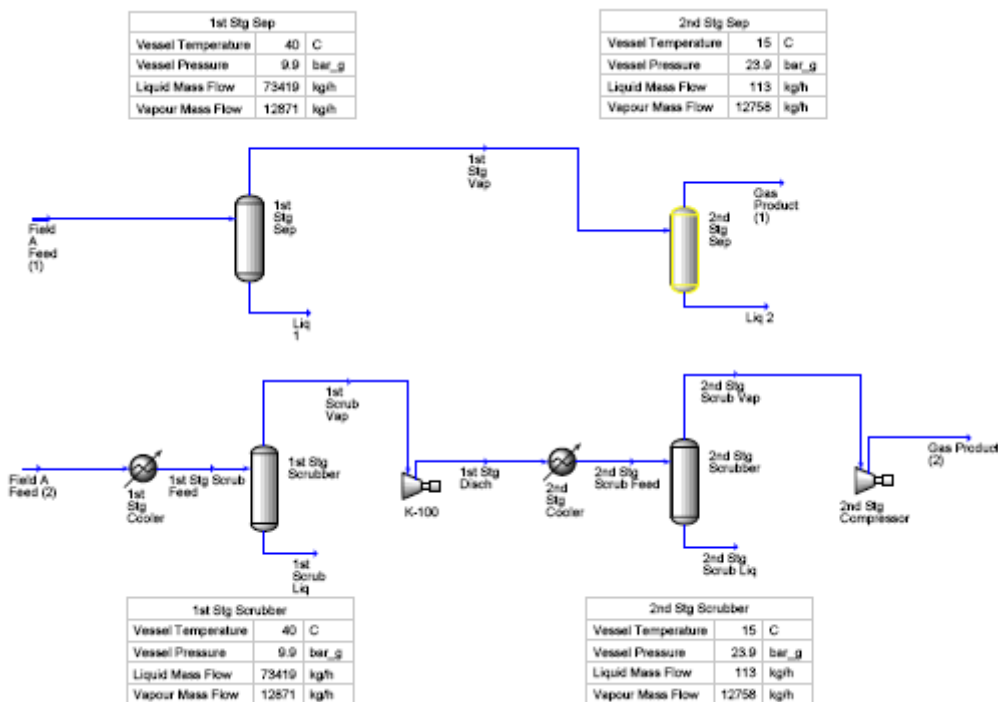


Fig. 10 – Two Methods of Simulating a Compression Train

As can be seen in Fig. 10, for both simulations of the compressor train, the flow rates in the discharge streams of the two scrubbers are identical. The conditions the stream experiences in the compressor and heat exchanger are irrelevant if the conditions in the scrubber vessels are known. For allocation purposes the simpler scheme is preferred.

4.3 Component Data

The user selects the range of components to be used in the simulation. This will normally draw on a range of library components, such as methane, propane, carbon dioxide, water, etc.

In addition, the heavier components in oil systems are best represented by hypothetical components, which represent a mixture of similar hydrocarbons and are analogous to boiling point fractions obtained from a distillation. Characterisation of these hypothetical components (or pseudo-components) is important. Even in gas systems the heaviest component (e.g. octane plus) has a great effect on the dewpoint of a gaseous mixture of hydrocarbons. These hypothetical components are normally defined by supplying molecular weights, boiling points and densities – the simulation package then predicts other properties based on this input data.

4.4 Thermodynamic Packages

There are a number of thermodynamic packages available in commercial simulators, which incorporate various equations of state. Equations of state describe how a fluid will behave thermodynamically and much experimental research has been deployed to measure the

parameters used in such equations for a wide range of components. Such equations of state provide an accurate reflection of the behaviour of streams. With so many available, which is the best or most appropriate one to choose?

Oil and gas systems consist of mainly of well-understood hydrocarbons, which are relatively non-polar, and are as such “well behaved”. The two most commonly encountered equations of state are the Peng Robinson (PR) and Soave Redlich Kwong (SRK). These equations are based on the ideal gas equation but have additional parameters included to account for deviations from ideality. For most simulations either of these methods is perfectly adequate. These equations are instrumental in generating component K-factors (see Section 5) used in calculating vapour liquid equilibria in vessels.

To provide an idea of how accurate such equations of state are, the following data (taken from Campbell [1]) compares predicted vapour liquid split of a hydrocarbon mixture at various temperatures and pressures generated using the Peng Robinson equation of state with experimental data:

Table 1 – Comparison of Predicted vs Experimental Condensation Fractions

Temperature (°C)	Pressure (bara)	Weight % Total Fluid Condensed		
		Experimental	Peng Robinson	Difference
-51	69	17.1	18.7	1.6
-57	62	19.0	19.7	0.7
-73	69	33.8	31.0	-2.8
-51	34	23.2	24.9	1.7

On an individual component level the agreement is slightly worse. This provides some insight into how faithfully simulations as a whole represent reality.

4.5 Process Input Data

Typical process input data usually comprises:

- Metered flows
- Measured compositions (e.g. from chromatographs and/or distillations)
- Vessel temperatures and pressures

It is preferable to obtain mass based metered values since mass balances across the all parts of a process is an essential feature of simulations.

It is possible to have too much data for the simulation, i.e. it can be over-specified, and the data may need to be reconciled before being entered into the model. For example if all the component flows entering and leaving a process are measured, one set must be discarded. The simulation model cannot match both simultaneously since it is unlikely that its thermodynamic calculations would result in precisely the same products as those measured.

4.6 Control Functions

Simulations also provide functions that allow one stream rate or a vessel temperature or pressure, etc. to be varied in order to meet some desired output rate, e.g. a final metered oil export value. Similarly the plant can be controlled to meet product specifications such as liquid True Vapour Pressure (TVP), Reid Vapour Pressure (RVP) or gas Gross Calorific Value (GCV).

5 ALTERNATIVE SIMPLIFIED MODELLING APPROACHES

5.1 Simplified Modelling Basis

As described in Section 4.2, since a process model can be reduced to a series of relatively simple splitters, mixers and flashes the calculations associated with these unit operations can

readily be performed outwith a commercial simulation package. Mixer and splitter calculations are determined using mass balance relations and those associated with the flashes determined using K factors and the Rachford-Rice equation.

5.2 K Factors

For a hydrocarbon two-phase mixture in equilibrium, the K factor is the ratio of the mole fraction of a component in the vapour phase with its mole fraction in the liquid phase.

$$K_i = \frac{y_i}{x_i} \quad (3)$$

K factors can be expressed as correlations, which are functions only of temperature and pressure. The K factors are weakly dependent on composition, which means that one set of K factors is appropriate for use with a wide range of compositions and the K factor correlations do not have to be revised or continually updated for new fluids.

The K factor correlations are derived using data generated by a commercial simulation to model the behaviour of each component at any conditions within a given range of temperatures and pressures. This allows the prediction of compositions and flowrates of both vapour and liquid streams from any flash separation where the feed composition and operating conditions are known. Over a limited range of temperature and pressure, K can be expressed using a relatively simple equation as a function of temperature and pressure, for example:

$$\log(K_i) = \frac{A}{T} + B \cdot \log(P) + C \quad (4)$$

Where P is pressure, T is temperature and A, B, and C are constants.

5.3 Flash Calculation Methodology

The Rachford-Rice equation for a 2-phase equilibrium flash is:

$$\sum_i \frac{z_i}{(1 + (V/F) \cdot (K_i - 1))} = 1 \quad (5)$$

Where z_i is the feed mole fraction of component i , K_i is the K factor, V is the vapour molar rate and F is the feed molar rate. This equation may be solved iteratively for V/F using, for example, Newton's method. The equation can be extended to account for water as a second immiscible liquid phase.

5.4 The Complete Model

The above approach basically involves solving a complete material balance for the plant incorporating phase equilibria relationships. It is also possible to extend the approach to incorporate heat balances, utilising component heat capacities and latent heats of vapourisation. This extension allows calculation of temperature drops between vessels assuming an adiabatic process. Coupled with the fact that:

- standard liquid and gas densities, calorific values, can readily be calculated based on composition
- methods are available to calculate liquid TVPs and RVPs and gas dewpoints

the approach can be extended to relatively complex processes including recycle streams and even simple columns such as stabilisers. Hence it is possible to build a simplified process

simulation in place of the “full blown” simulation. All these calculations can be embedded directly into the allocation system, on a spreadsheet for example, or as a section of code.

The advantages of such models over commercial simulation packages are:

- Ease of software integration within allocation systems
- No requirement to periodically update software versions
- Transparency of calculations
- Reproducibility of calculations
- Improved robustness
- Improved speed
- Reduced costs.

These factors need to be weighed against the fact that commercial simulations are:

- more accurate (though the improvements may be considered negligible in comparison with deviations from reality – see Table 1 in Section 4.4),
- are more generally applicable and configurable for a host of processes
- the fact that at some point too much complexity may be introduced into the simplified models, making recourse to a commercial simulator more appropriate.

However, as shown in Section 5.5, the simplified models can reproduce commercial simulation results accurately.

5.5 Comparison with Commercial Simulation Results

An oil stabilisation plant was modelled both in HYSYS and a simplified model – this is illustrated schematically in Fig.11.

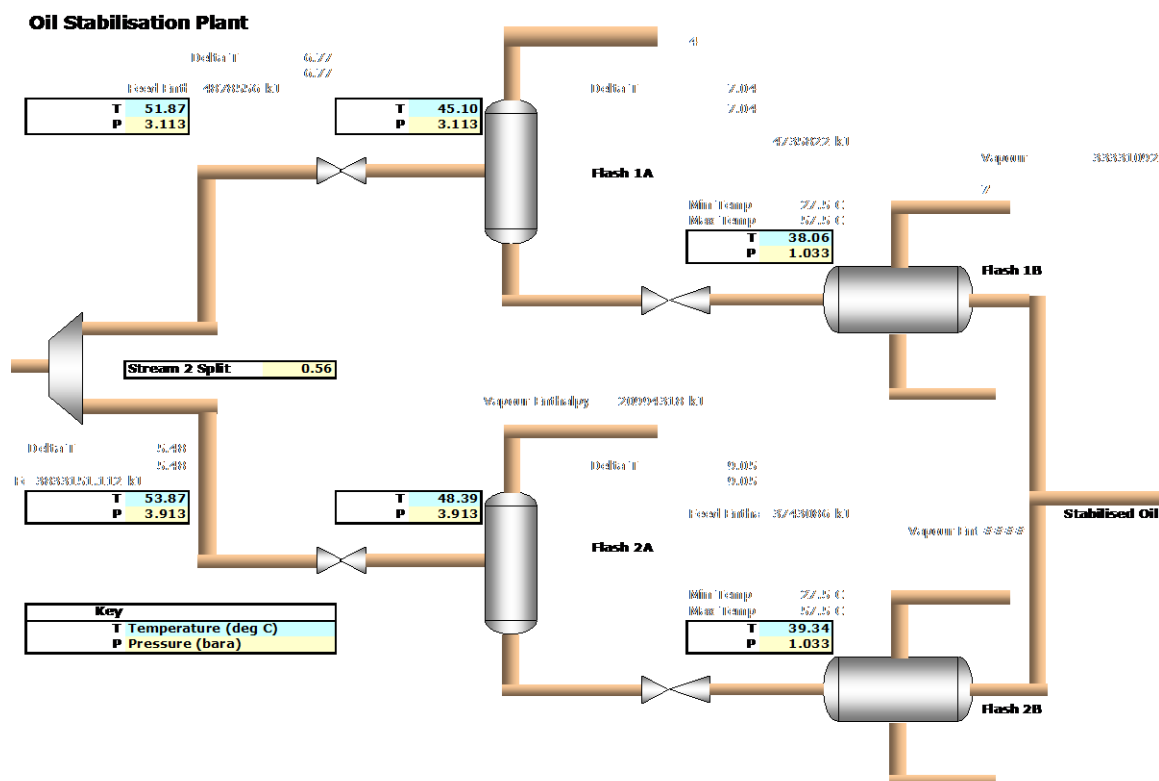


Fig. 11 – Schematic of Oil Stabilisation Plant

The only inputs to the models were the feed composition, vessel pressures and the requirement for the Stabilised Oil to achieve an RVP specification. The simplified model varied the feed temperatures to achieve the specification and calculated all other vessel temperatures and stream component flows using K factor correlations, flash algorithms, adiabatic process calculations and RVP calculations. A comparison of the resultant stabilised oil flows is presented in Table 2:

Table 2 – Comparison of Simplified Model versus HYSYS Results

	Simplified Model	HYSYS	Difference
	kg/h	kg/h	
Nitrogen	0.04	0.04	-0.06%
CO2	90	90	0.24%
Methane	18	18	0.23%
Ethane	2,142	2,146	0.18%
Propane	36,307	36,278	-0.08%
i-Butane	26,082	26,038	-0.17%
n-Butane	83,580	83,439	-0.17%
Pentanes+	3,807,137	3,806,725	-0.01%
Total	3,955,356	3,954,734	-0.02%

These differences illustrate that the results generated by simplified models can be in extremely good agreement with those from commercial simulation software especially when considering the differences with reality – see Table 1 in Section 4.4.

6 IS A MODEL NECESSARY AT ALL?

Returning to the model using cloned components described in Section 3.4, it might be argued that this is the most appropriate model to provide an understanding of how a particular Field is behaving in the commingled process.

Clones of a component behave identically and at the same temperature and pressure have exactly the same K factor. Hence when commingled in a vessel the normal components (e.g. methane, propane, hexane, nitrogen, etc) for each Field will have the same K factor. If it is assumed that this is extended to the heavier hypothetical components then it can be proved that the ratio of each Field's cloned component in the vapour and liquid product streams is directly proportional to their ratio in the feed stream. Indeed this can be extended to a series of vessels and include recycle streams. Therefore across a whole process if the final product streams are allocated in proportion to the inlet rates of each Field's components, this will produce identical results to a full-blown simulation using cloned components. For example, consider the simulation results of the hypothetical process presented in Fig 12:

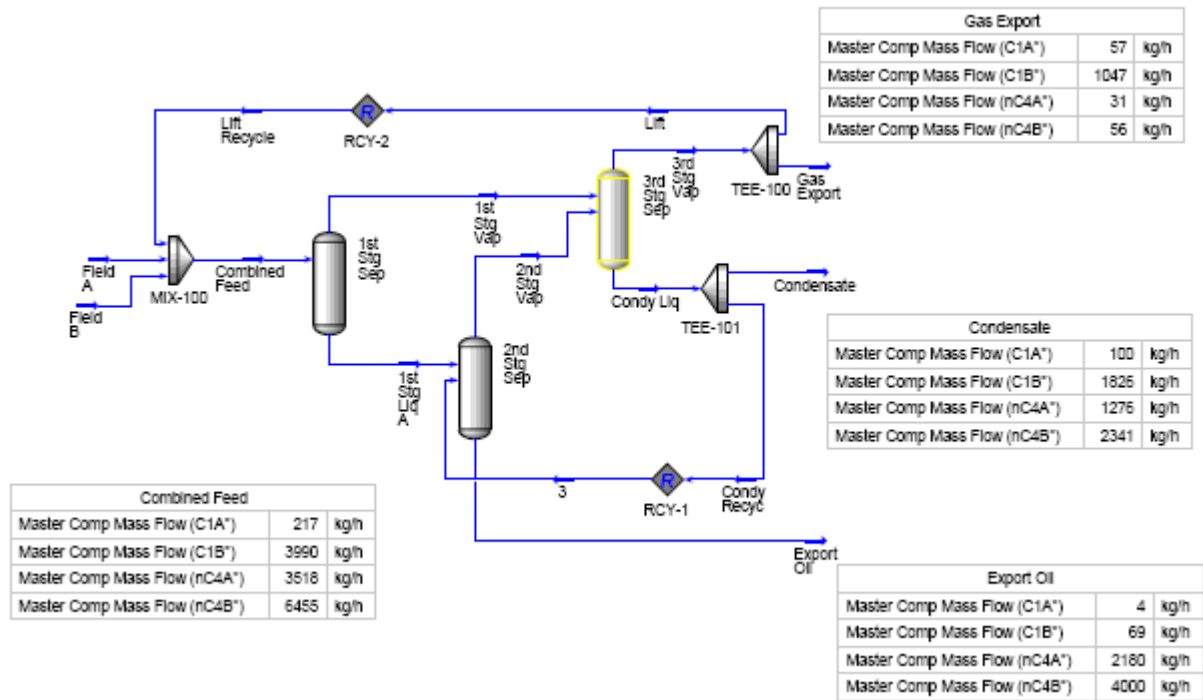


Fig. 12 – HYSYS Simulation of Multi Stage Process Incorporating Recycles with Cloned Components

The results are summarised in Table 3, for normal-butane (nC4):

Table 3 –Percentage Share of Fields' nC4 in Feed and Product Streams

	Field A	Percentage of Stream	Field B	Percentage of Stream
	kg/h		kg/h	
Feed	3,518	35.3%	6,455	64.7%
Gas Export	30.6	35.3%	56.1	64.7%
Condensate	1,276	35.3%	2,341	64.7%
Export Oil	2,180	35.3%	4,000	64.7%

A similar result is obtained for methane (C1) where the split is 5.2% (Field A) and 94.8 % (Field B) in all streams.

For certain allocation systems, this result begs the question is a simulation required at all?

7 NOTATION

A	Constant coefficient	S_A	Field A shrinkage factor
B	Constant coefficient	V	Vapour molar rate
C	Constant coefficient	x_i	Liquid mole fraction of component i
F	Feed molar rate	y_i	Vapour Liquid mole fraction of component i
K_i	K Factor for component I	z_i	Feed mole fraction of component i
P	Pressure		
$Q_{1,A}$	Flow of Field A (1 st Stage Separator)		
$Q_{1,B}$	Flow of Field B (1 st Stage Separator)		
$Q_{2,A}$	Flow of Field A (2 nd Stage Separator)		
T	Temperature		

8 REFERENCES

- [1] John M. Campbell. Gas Conditioning and Processing, Volume 1: The Basic Principles, Table 5.2, July 1992.