

The Case for Integrated Process Simulations in Allocation Systems

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1 INTRODUCTION

This paper discusses and makes the case for the use of integrated process simulation models in hydrocarbon allocation systems used by upstream and midstream hydrocarbon processing facilities such as offshore installations and onshore gas plants and oil terminals.

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 e.g. shrinkage factors, to full integration of the model within the allocation process itself. In the remainder of the paper the outputs from process simulations used in allocation systems have been generically termed “process factors”.

The simulation model is intended to reflect the changing operating conditions, flow rates and variations in composition experienced in the process, expressed in terms of the process factors.

The paper describes three main ways a simulation model can be used to provide the process factors:

- Offline intermittently run process model
- Correlations and look-up tables
- Fully integrated daily process model.

Ideally the full process simulation should be run each time the allocation is run, typically daily. Only the fully integrated process model option fulfils this ideal. However, in the authors’ experience this approach is not the normal practice in allocation systems, the other two methods generally being preferred. The paper discusses the issues surrounding why integrated process simulation is not the de facto standard approach and describes the limitations of the alternative methods employed to provide these process factors for allocation systems.

Finally, the paper concludes with a proposed solution to the issues of fully integrating simulation models into an allocation system and the advantages so accrued.

First, a brief description of the use of process simulations in allocation systems is presented in the next section.

2 PROCESS SIMULATION MODELS FOR ALLOCATION

Process simulation models can be used to determine how hydrocarbons entering the system are distributed between the various liquid and gas streams exiting the process. The simulation can provide information regarding the behaviour of hydrocarbons

within a process that would be otherwise difficult to obtain. 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.)

A fuller discussion of the use of process simulation models in allocation systems is provided in [1].

Traditionally, commercially available process simulation packages (e.g. HYSYS, PRO/II and UniSim) have been used to characterise these hydrocarbon behaviours. Though at first sight there may be an appeal to use such models there are a number of issues that militate against their use.

General purpose simulation packages are built to model a wide range of processes and are routinely used by process engineers for design purposes. Such models can be complex and include items such as control valves, pumps, compressors, heat exchangers, etc. which can make the models complex and unstable requiring the intervention of a process engineer, whose priority may not be allocation and hydrocarbon accounting, to ensure the models solve.

Also such relatively complex simulation software packages are not readily integrated with allocation system software.

The above issues can render the daily running of the process simulation model impractical from the Operator’s perspective.

To overcome these issues, the simulation model can be run independently of the allocation system on an intermittent basis. The process factors can then be updated periodically in the allocation system. The approach is discussed in the next section.

3 OFFLINE MODELLING

In order to overcome the practicability of running simulations on a daily basis, some Operators resort to running the simulation model independently of the allocation system on an intermittent basis. The process factors can then be updated periodically in the allocation system. This assumes the process remains relatively constant in the periods between the updates.

The reality is that often the models are not updated and even when they are, the update frequency is arbitrary when ideally the model should be used every day to capture changes in the process.

In order to analyse the impact of offline modelling and intermittent updating of process factors a simulation of a typical process was modelled. The process schematic is presented in Figure 1:

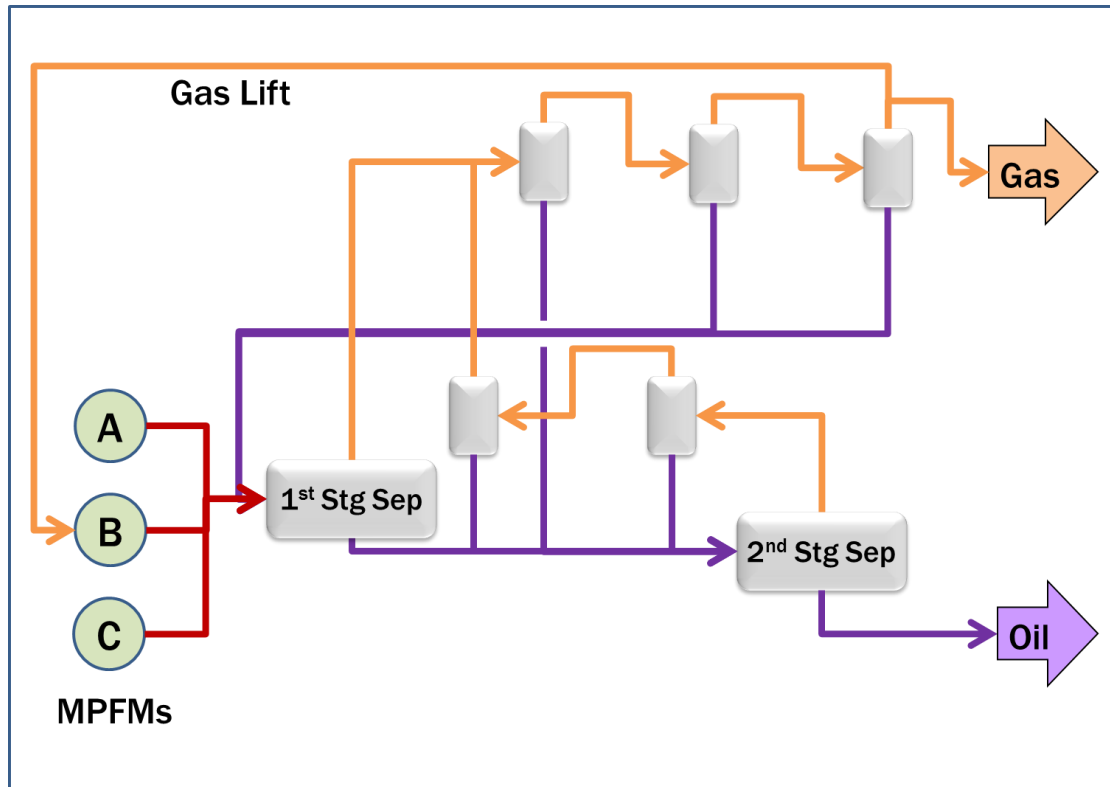


Figure 1 – Offshore Process Three Fields

Three fields (A, B and C) are being produced and their respective flows at the inlet to the process are measured using multi-phase flow meters (MPFMs). The three fields have different compositions and Field B is gas lifted.

1,000 days of relatively steady production were simulated. In order to emulate realistic, modest process variability the operating conditions in the vessels were randomly varied about nominal values:

- Pressures ± 0.5 bar
- Temperatures $\pm 3^{\circ}\text{C}$

Also, the field compositions were varied $\pm 10\%$ (relative) before being renormalized. Field flows were varied within $\pm 5\%$ and each field was assumed to have a 95% uptime which was also randomly sampled for, i.e. on average 1 in every 20 days a field would be producing zero.

Process factors for each field, in this case shrinkage factors, were calculated as the mass of each field's components in the export oil divided by the oil mass at the MPFM. These were calculated each day for each field. Field A's shrinkage factors are presented in Figure 2, indicated by the solid blue line:

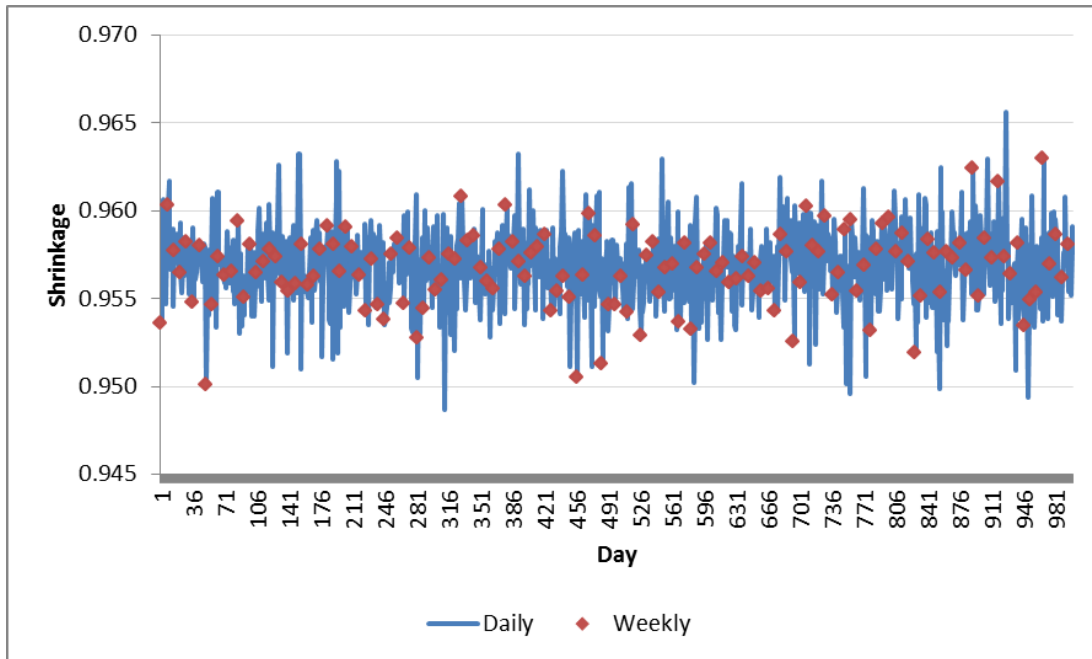


Figure 2 – Field A Daily and Weekly Shrinkage Factors

In order to assess the periodic calculation of shrinkage factors, the allocation was calculated using a fixed shrinkage factor for a period. For example if the simulation was run weekly the shrinkage factor from every 7th day (indicated by the red diamonds in Figure 2) was used to allocate the ensuing 7 days. This was compared against calculating the shrinkage daily and the results for Field A are presented in Figure 3:

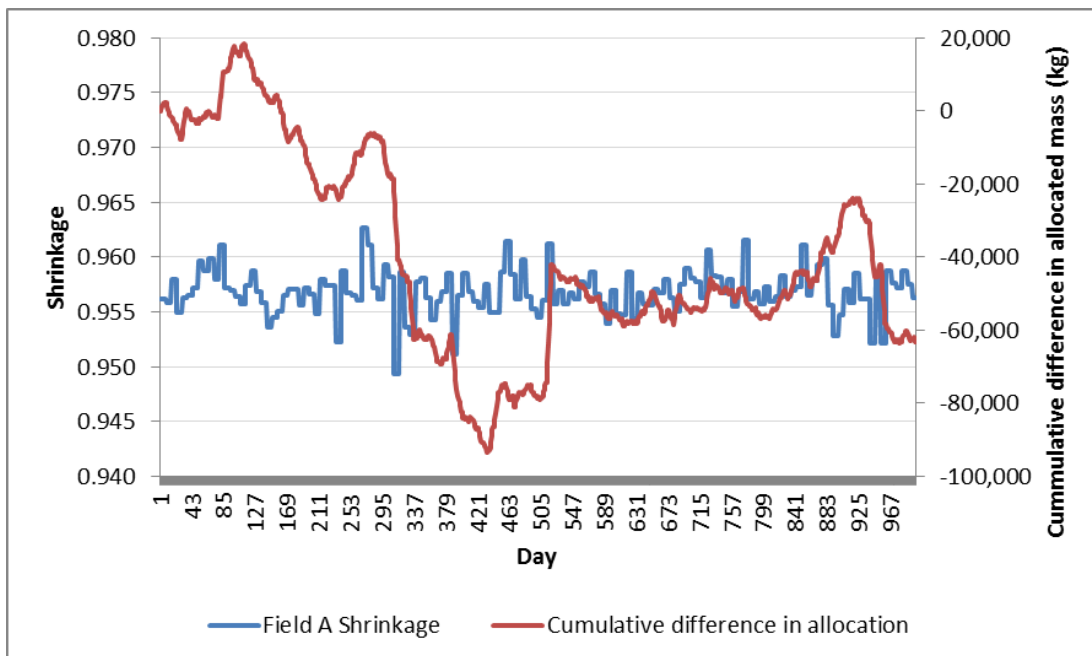


Figure 3 – Field A Allocation Weekly vs Daily Shrinkage Factors

The blue line (referenced to the left hand axis) is the weekly shrinkage factor for Field A.

The cumulative difference in the allocation between the weekly based and daily shrinkage factors is indicated by the red line (referenced to the right hand axis). Though it meanders randomly above and below zero, by chance it ends at a negative value after 1,000 days. This cumulative difference represents the impact on the allocation of the intermittently updated process factors.

Similar plots are observed for Fields B and C:

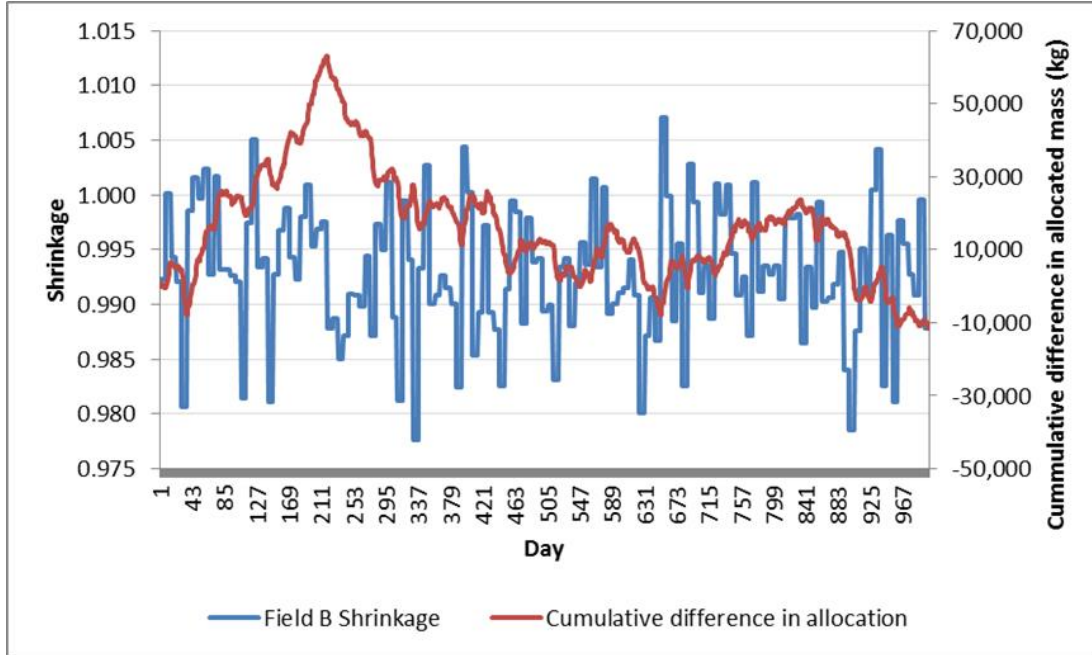


Figure 4 – Field B Allocation Weekly vs Daily Shrinkage Factors

The shrinkage can be above one for Field B because of the stripping effect of the lift gas in the MPFM.

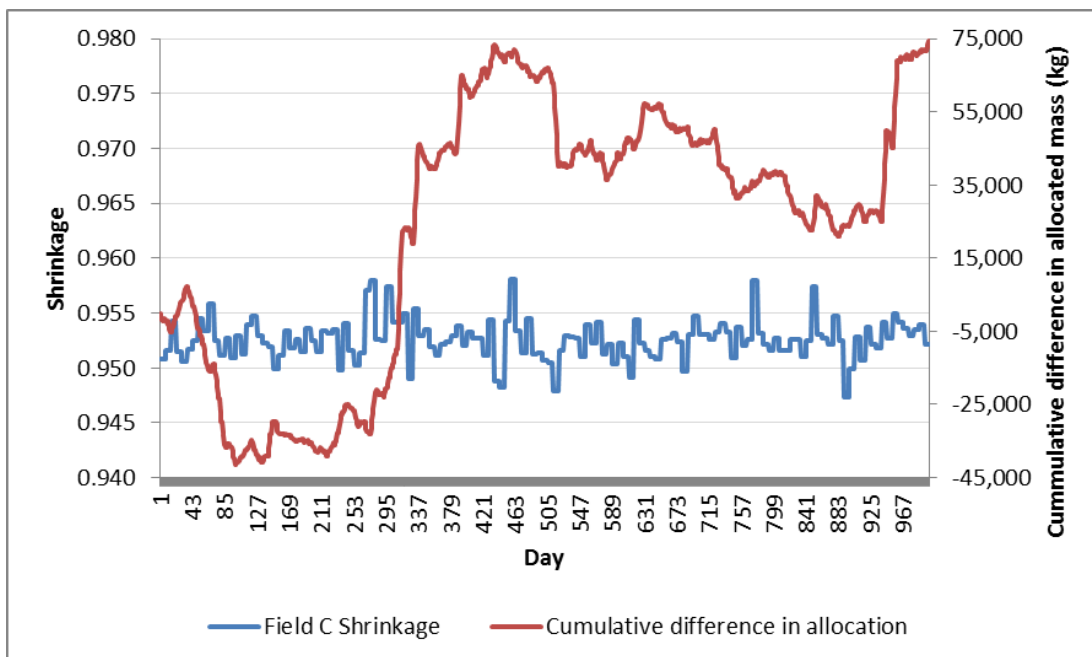


Figure 5 – Field C Allocation Weekly vs Daily Shrinkage Factors

Field B's shrinkage factors are more variable than A and Cs'. The cumulative differences in allocation between weekly based and daily based shrinkage factors do not appear to be biased to any one field. However there are differences and the weekly update does have an impact. The gains or losses experienced by the fields sum to zero exactly.

The update is not necessarily weekly, it could be monthly or quarterly (or even yearly). To examine how this affects the allocation the next plot, Figure 6 shows how the cumulative allocation difference at the end of the 1,000 days varies with period of the interval between update of shrinkage factors for Field B:

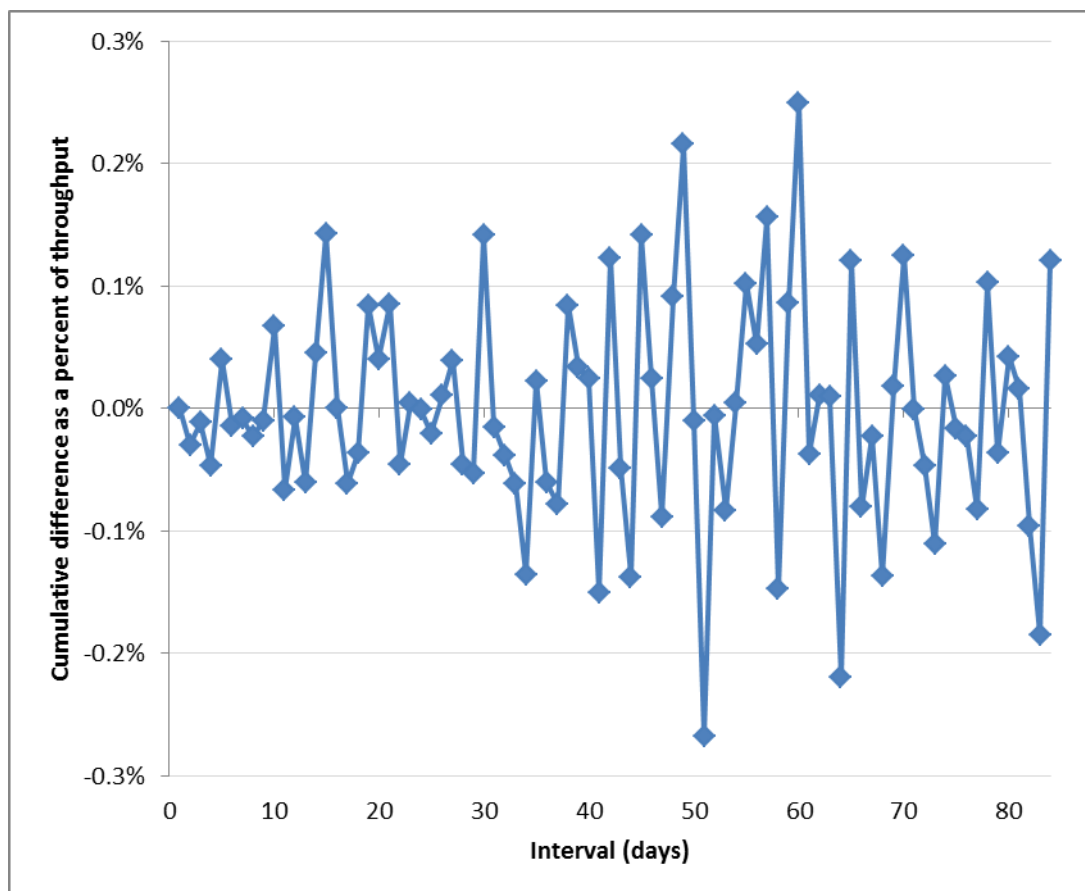


Figure 6 – Field B Cumulative Difference Allocation Weekly vs Daily Shrinkage Factors

The weekly cumulative difference was -0.0084% (of total mass throughput) but as can be seen it can vary randomly up to $\pm 0.25\%$ depending on the interval duration. This occurred even with a reasonably stable system.

To examine the impact of greater process variation a second set of simulations was performed in which the variability in Field B's flow alone was increased to $\pm 50\%$. The weekly shrinkage and associated cumulative difference becomes:

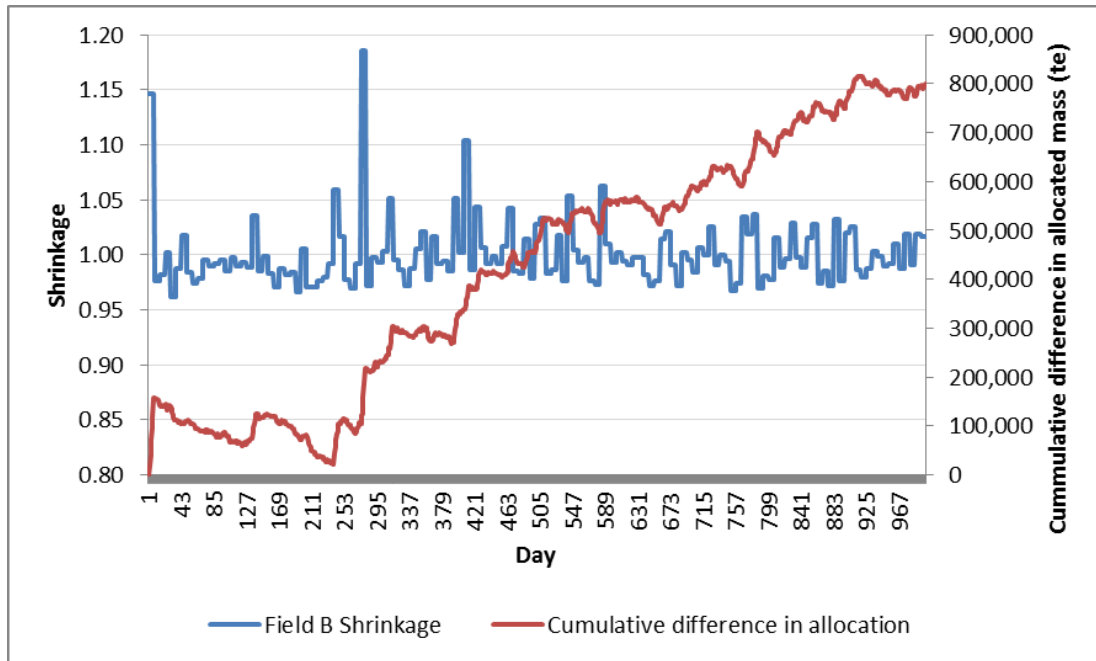


Figure 7 – Increased Variability Field B Allocation Weekly vs Daily Shrinkage Factors

Field B’s shrinkage factor is now not evenly distributed about a nominal value but skewed towards high values. This effect results in its cumulative difference becoming significantly positively biased and therefore Field A and C suffer losses.

The cumulative difference across the range of interval durations now becomes consistently positive for Field B, as can be seen in Figure 8, and there is bias in the system.

The reason Field B’s shrinkage is skewed is because occasionally its shrinkage factor can be anomalously high which occurs when its flow is very low compared to the other fields and the commingling effects are significant. So the shrinkage factor values are not equally distributed about a nominal average value but skewed to the high side. This was not observed with the more stable simulation because the variability did not produce such low Field B flows.

It could be argued that such unusual days could be avoided in an actual system but the potential is there within the system for a bias to occur.

In any case a system can exhibit much more process variability and as such demands the calculation of daily process factors. One way to accommodate this is to use correlations or lookup tables as discussed in the next section.

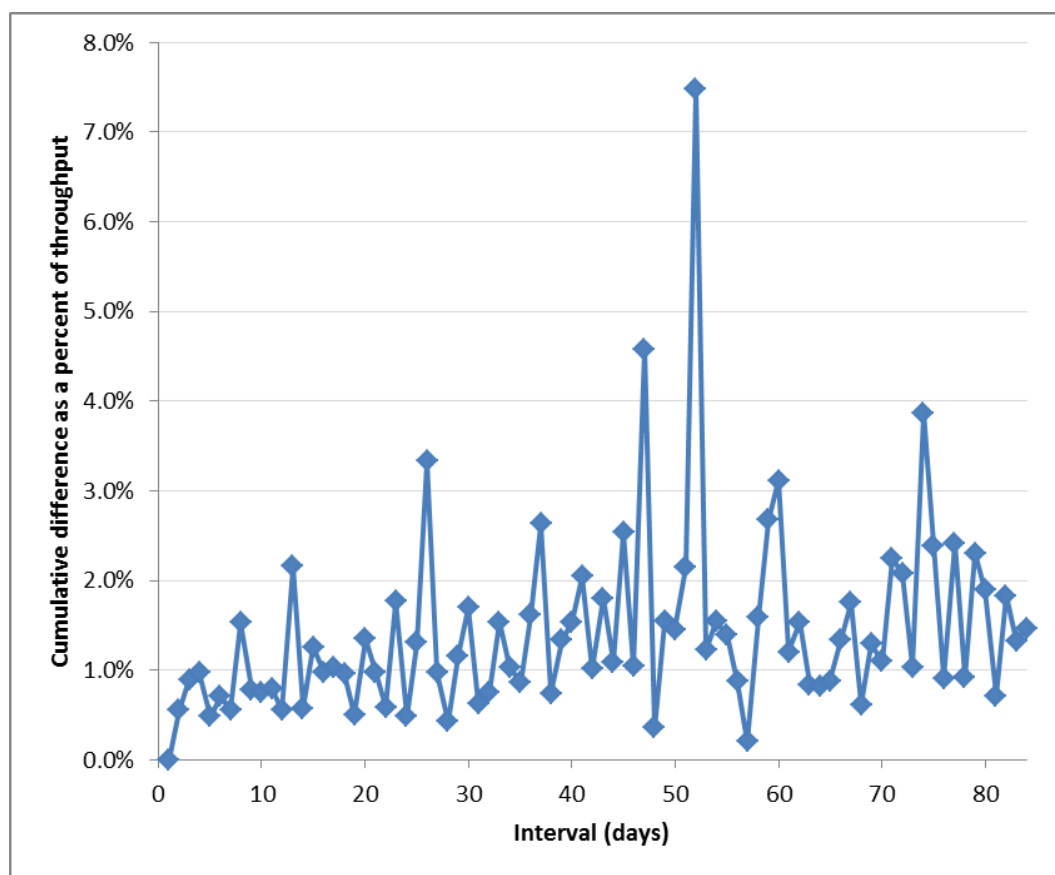


Figure 8 – Field B Cumulative Difference Allocation Weekly vs Daily Shrinkage Factors

4 CORRELATIONS AND LOOK-UP TABLES

A common approach is to curve fit empirical correlations to simulation data in an attempt to mimic the simulation results. This method does not require the running of the simulation model on a daily basis. However, such correlations are approximations of the simulation and can be poor if they are functions of multiple variables. In addition, because they have no underlying physical basis, they are only applicable over the range of conditions they are fitted, and if all production scenarios are not anticipated, will produce spurious results.

Figure 9, Figure 10 and Figure 11 below show attempts to curve fit a polynomial correlation (of increasing order) to simulation data in order to determine the recovery factor of a hydrocarbon component. The three figures demonstrate that none of the attempts to fit are particularly satisfactory.

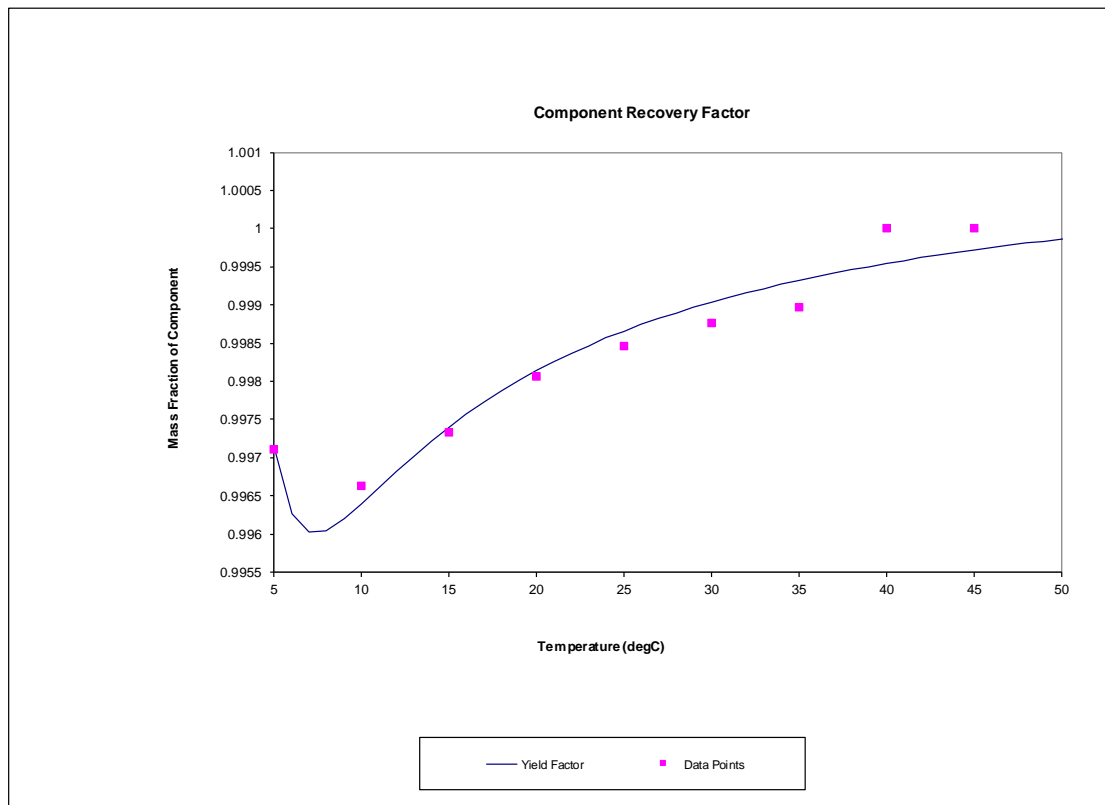


Figure 9- Quadratic Curve Fit

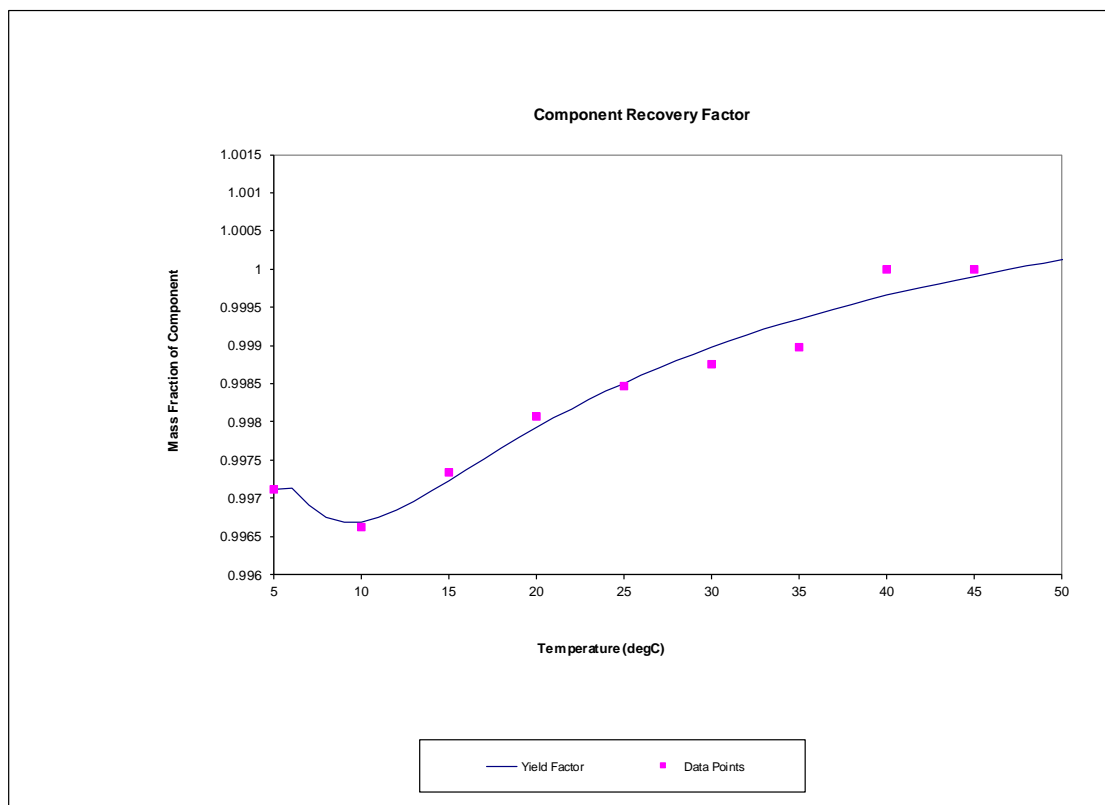


Figure 10 – Cubic Curve Fit

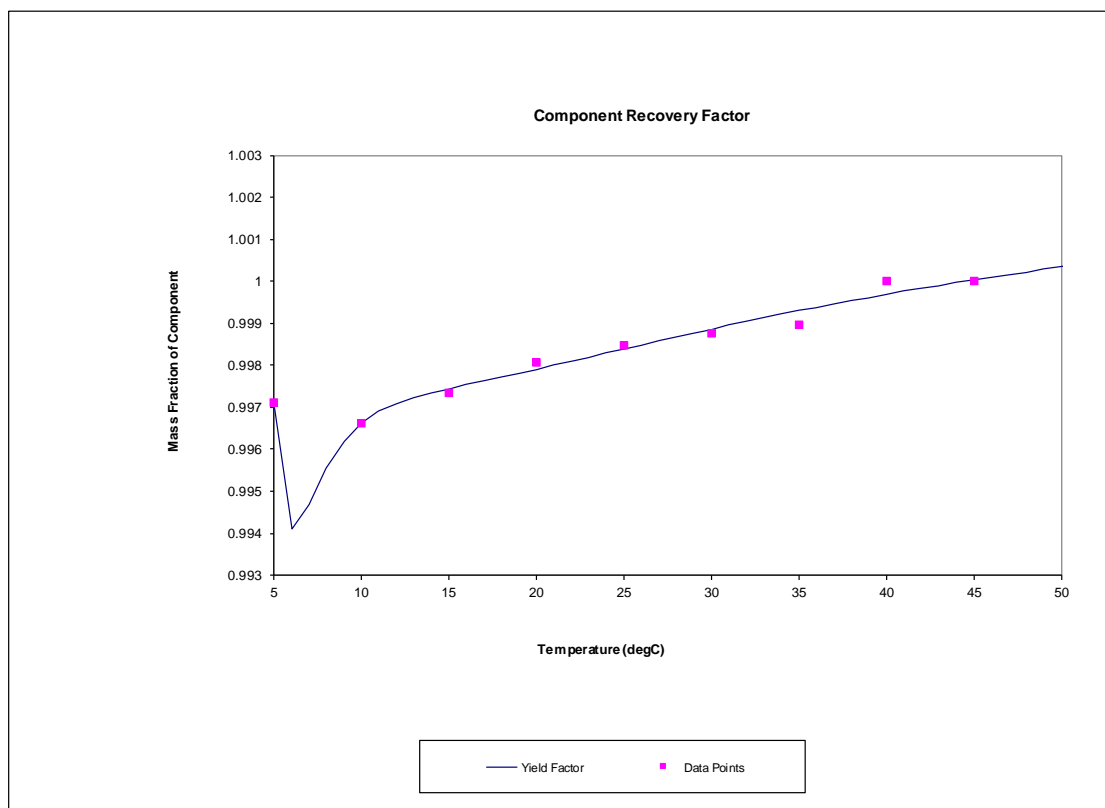


Figure 11 – Quartic Curve Fit

Figure 12 shows the importance of plotting the polynomial between the points it was fitted over. The blue diamonds are the results of the quartic equation from Figure 11 plotted only at the same temperatures as the purple data points.

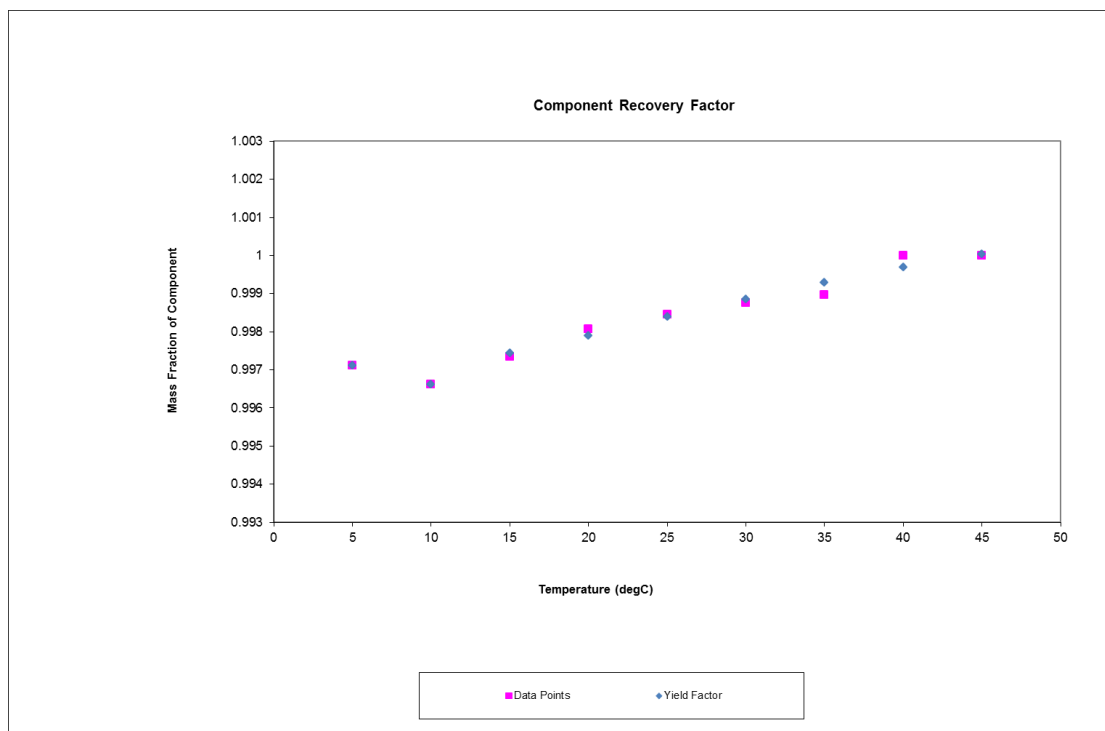


Figure 12 – Quartic Curve Fit – Fitted Points Only

The fit appears to be good and the erroneous minimum between 5°C and 10°C observed in Figure 11 is missed.

Extrapolating outside the range over which the curve was fitted can produce extremely erroneous values as demonstrated by extrapolating the quartic below 5°C, as illustrated in Figure 13.

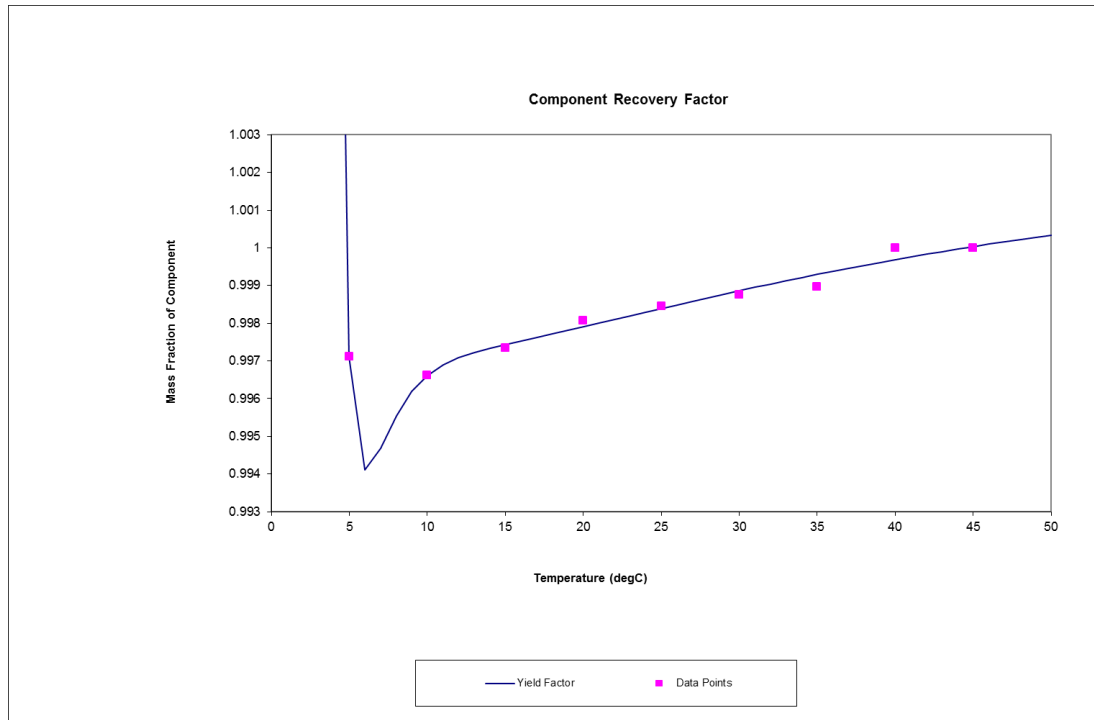


Figure 13 – Quartic Curve Fit Extrapolated

The predicted yield rises rapidly above one and is over 60 at 1°C.

The above yield factor was fitted as a function of only one variable. Often factors will be functions of multiple variables. For example, consider the simple process presented in Figure 14:

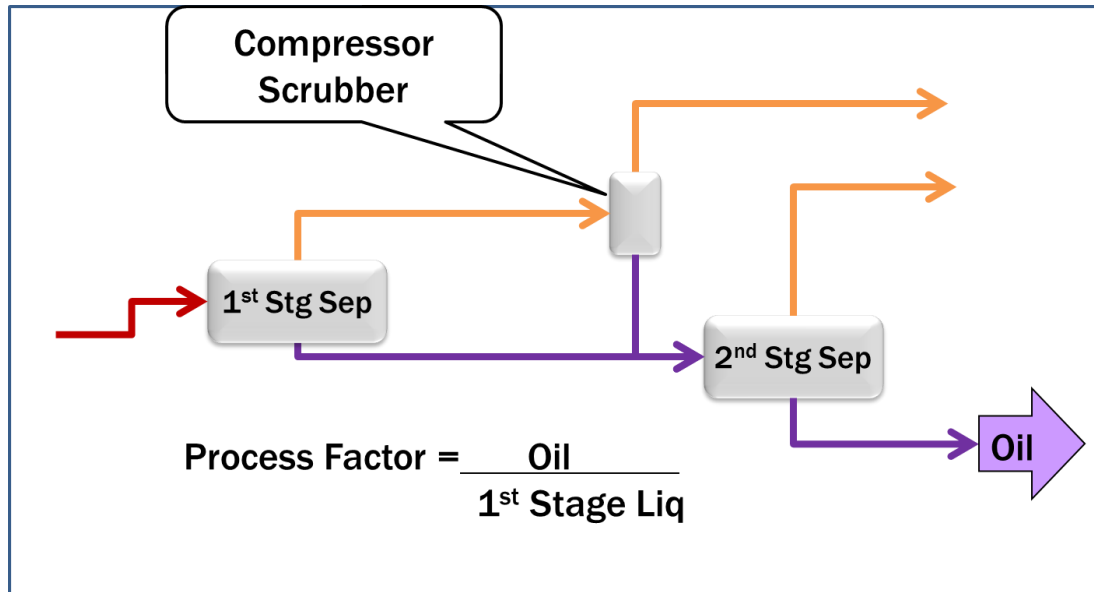


Figure 14 – Simple Process

A process factor (in this case a shrinkage from 1st Stage to 2nd Stage oil export conditions) for a lighter condensate type field was simulated over a range of 1st Stage Separator and Compressor Scrubber temperatures. The results are presented in Figure 15:

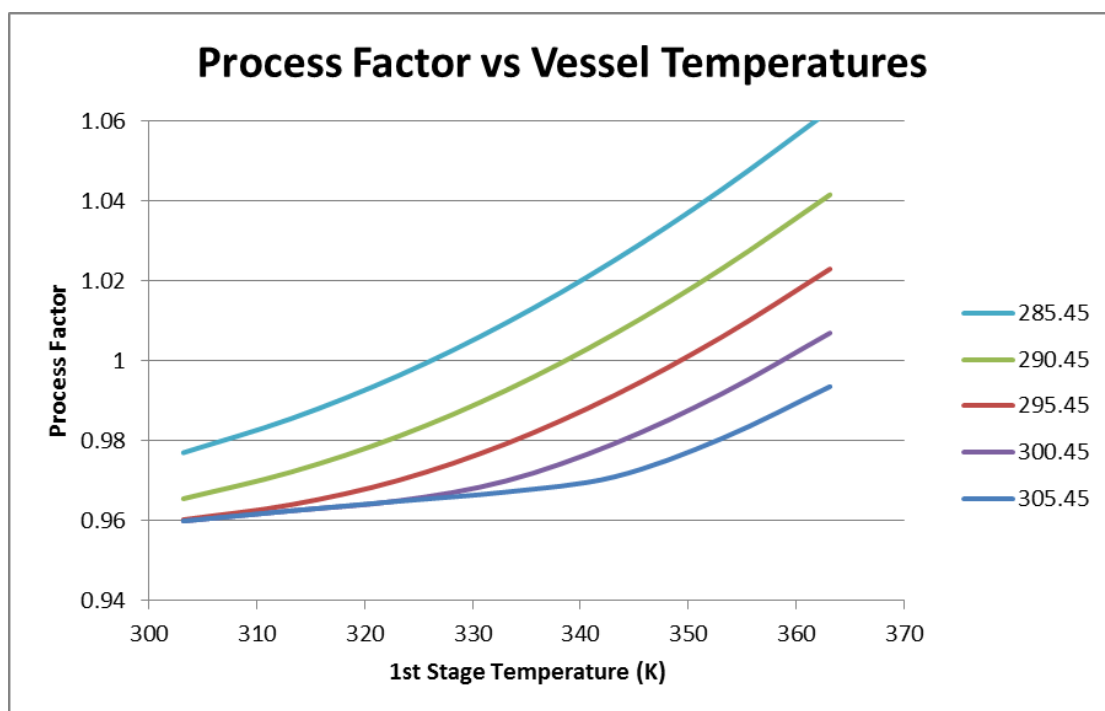


Figure 15 – Process Factor as Function of 1st Stage Separator and Compressor Scrubber Temperatures

The different coloured lines indicate the temperature of the Compressor Scrubber in Kelvin (K). The shrinkage factor can be greater than 1 as the Compressor Scrubber knocks out liquid from the 1st Stage Gas.

Attempting to model the process factor as a linear function of the two temperatures results in the following:

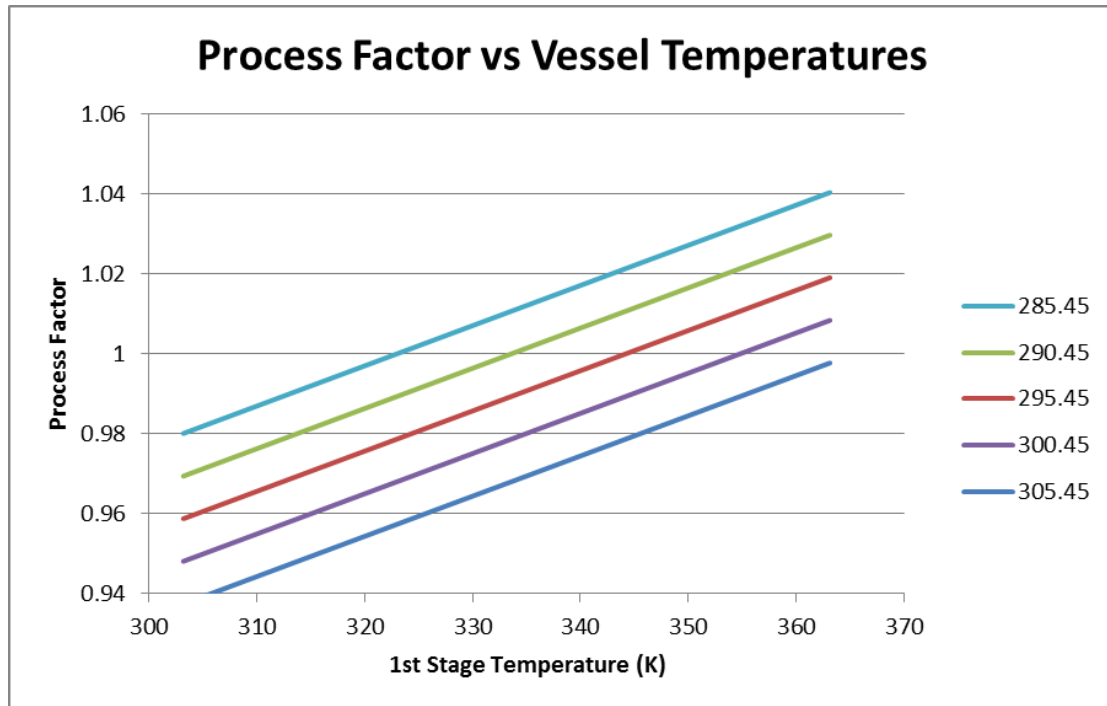


Figure 16 – Process Factor as a linear function of 1st Stage Separator and Compressor Scrubber Temperatures

Clearly not a good fit to the data. Going to quadratic in the two temperatures results in:

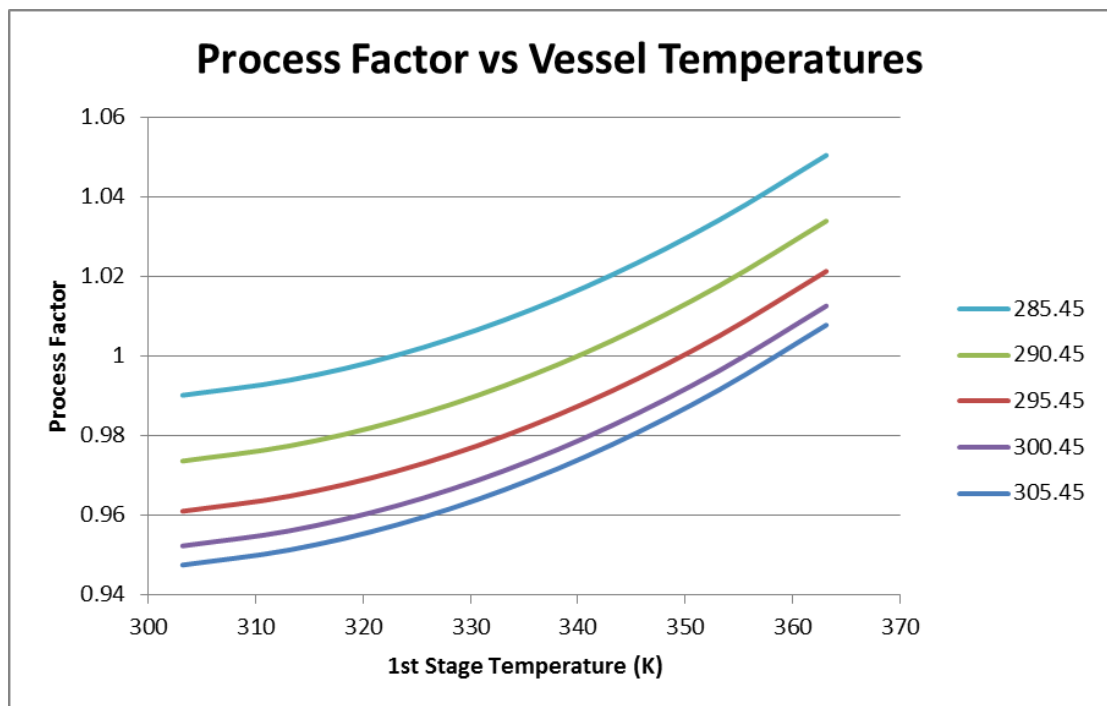


Figure 17 – Process Factor as a quadratic function of 1st Stage Separator and Compressor Scrubber Temperatures

The fit is only improved slightly. Going to higher orders may improve the fit further but the concurrent risk of the problems highlighted above for the quartic function may emerge. Also this is only a function of two of the vessel temperatures. Incorporating the 2nd Stage Separator temperature would exacerbate the problems.

Instead of producing correlations it is possible to store the process factors in look-up tables the values of which may be interpolated between. This potentially overcomes the maxima and minima problem observed above, but now the calculated factors exhibit discontinuities at each stored value. Also considerably more data point values need to be stored than with polynomial correlations where only the coefficients are required. This can become considerable if a process factor is dependent on a number of parameters. For example, if 10 data values are stored for a process factor as function of one variable, the incorporation of a second variable means 100 values are required, 1,000 for a third and so on.

In order to overcome the problems associated with empirical correlations an underlying physical model of the behaviour of the hydrocarbons can be introduced. This is the basis of the integrated modelling discussed in the next section.

5 INTEGRATED MODELLING

Integrating the process simulation model with the allocation system allows for the calculation of shrinkage factors, expansion factors and component recovery factors daily. The integration would also lead to the direct allocation of hydrocarbons and the estimation of unmeasured streams. If this is the case, why do Operators rarely use this approach?

Typically, neither commercial allocation software or simulation software packages are developed specifically to be integrated with each other. The effort required to facilitate the smooth communication between the two systems is often regarded as too difficult and hence such integrated systems are rare.

Even if an interface between allocation and simulation software is successfully implemented by an Operator, the software vendors will routinely update their software potentially rendering the interface between the two systems non-functional. Furthermore, even minor modifications to simulation software (e.g. changes to the solution algorithm) can result in small changes to allocation results; this is an undesirable feature of an allocation system where repeatability is important.

For allocation systems there is a need for accurate process simulations that can be seamlessly integrated within existing allocation software. This can be achieved by simplifying the model to only include the unit operations and equations necessary for allocation purposes. Often, using proprietary simulation software for allocation purposes is like using a sledgehammer to crack a nut.

Typically, a process simulation model, which has been created using general purpose simulation software, is far more complex than an allocation system requires. An allocation system is only concerned with unit operations where material streams are combined or separated. Therefore, the allocation simulation can be constructed simply

as a series of flashes¹, mixers and splitters providing the operating conditions of the flashes are known or specified. The fact that there may be a number of equipment items such as pumps, compressors and control valves between the flashes does not affect the vapour-liquid equilibria in the vessels, which are determined by the operating conditions therein. To quote from a commercial simulation vendor paper [3]:

“For example, if your real-life process shows a heat exchanger, a pump and a splitter, but the only thing that’s really necessary is that the temperature, pressure and separation are achieved properly, consider using a flash drum to accomplish all three functions instead of using a separate unit operation for each. The flash drum can set the temperature, the pressure and perform your separation all at once.”

Therefore, the process flow diagram in Figure 18 can be simplified to that shown in Figure 19.

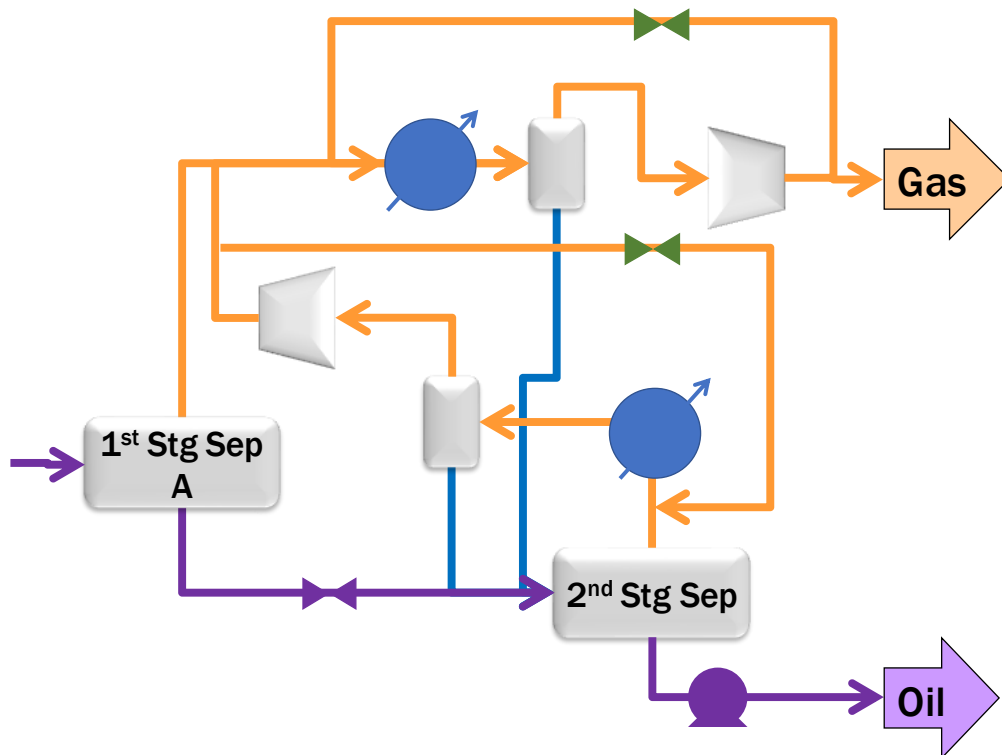


Figure 18 – Process Flow Diagram

¹ A “flash” is a term used to describe a unit operation that models a vessel, such as a separator or scrubber, where a stream separates into vapour and liquid phases. A part of the liquid “flashes” into vapour.

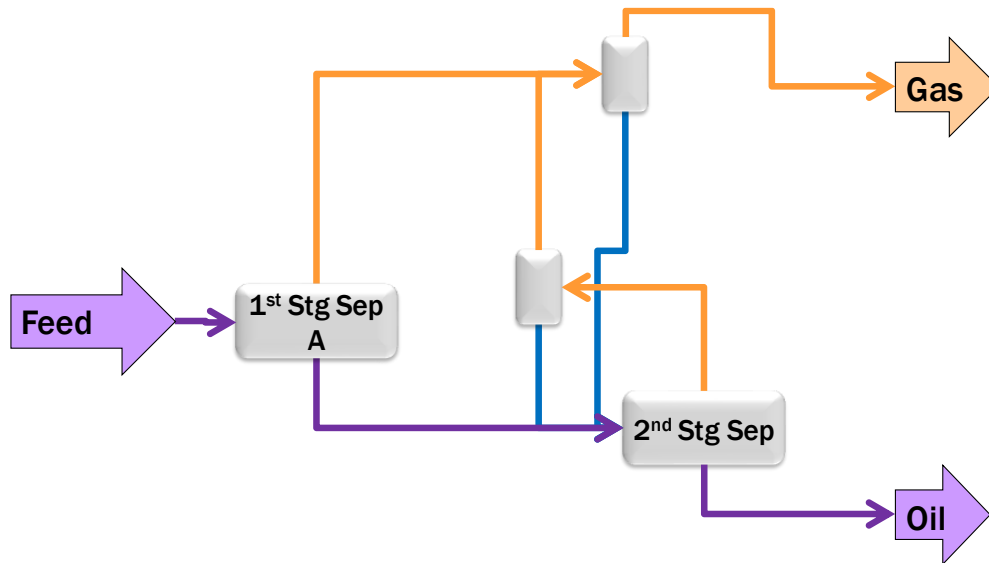


Figure 19 – Process Flow Diagram for Allocation Purposes

An allocation system only requires a process simulation to solve the equations necessary to determine how the hydrocarbons move through the process it is not concerned with steam enthalpies, equipment performances, etc. The Peng Robinson equation of state [2] is used extensively throughout the oil & gas industry to model vapour-liquid-equilibria in commercial simulation software packages, and in conjunction with the Rachford Rice equation [4], to solve the flash unit operation. The details of these calculations are available in the public domain.

As the simplified model will not be trying to solve as many equations as fully loaded simulation software it should be more stable and solve much faster. This makes the simplified model not only a realistic option for the running of daily allocations but should make a fully integrated model a possibility when running multiple days, weeks, months or even years of allocations.

Simplifying the model also means that it should be easier to code the model to integrate with an existing allocation system compared with using general purpose simulation software

6 DOES IT WORK?

A process model with three stages of separation, as shown in Figure 20, was created and solved using proprietary simulation software and also using a simplified model coded using component mass balances, the Peng-Robinson equation of state and the Rachford Rice equation.

The results from the two simulation models can be found in Table 1. It can be seen that there is good agreement between the full-loaded simulation software and Accord Energy Solution's simplified simulation meaning that for allocation purposes a simplified simulation model is more than adequate. The simplified model was able to solve in 0.03 seconds and was found to be repeatable.

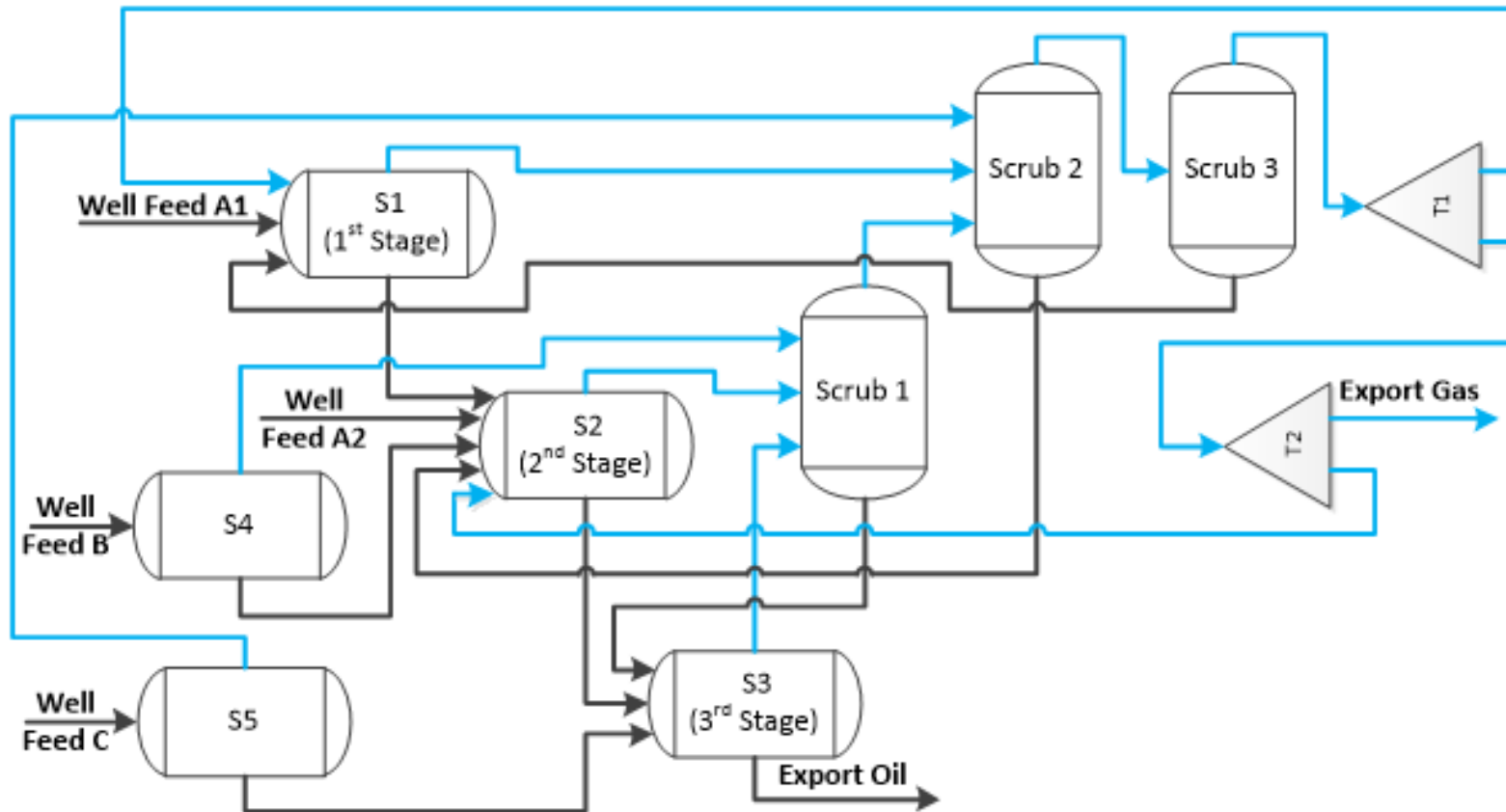


Figure 20 – Process Flow Diagram of Test Model

35th International North Sea Flow Measurement Workshop
24th– 26th October 2017

Table 1 – Allocation Results

Components	A1 (kg)	A2 (kg)	B (kg)	C (kg)	Proprietary Software		Simplified Simulation		Difference	
					Oil Export (kg)	Gas Export (kg)	Oil Export (kg)	Gas Export (kg)	Oil Export (%)	Gas Export (%)
Nitrogen	0.000	107.050	20.246	116.305	0.167	243.444	0.172	243.427	2.662%	-0.007%
CO2	0.000	403.632	76.639	954.205	24.125	1410.341	24.278	1410.174	0.637%	-0.012%
Methane	331.457	1937.294	1292.636	11688.314	64.080	15184.695	65.182	15184.387	1.721%	-0.002%
Ethane	155.316	1057.172	458.522	3467.905	187.299	4950.668	188.786	4949.967	0.794%	-0.014%
Propane	227.768	1247.000	409.815	3288.704	721.783	4449.373	725.128	4447.728	0.464%	-0.037%
i-Butane	0.000	222.117	112.755	804.400	374.272	764.674	375.526	763.572	0.335%	-0.144%
n-Butane	200.147	932.890	279.003	2243.382	1459.405	2192.427	1462.843	2191.885	0.236%	-0.025%
i-Pentane	124.224	441.152	146.476	1109.472	1251.796	567.647	1253.303	567.696	0.120%	0.009%
n-Pentane	124.224	772.016	230.456	1553.261	2069.322	608.544	2070.566	609.023	0.060%	0.079%
n-Hexane	148.374	1317.291	412.110	2319.038	4058.982	138.530	4058.123	138.629	-0.021%	0.072%
n-Heptane	345.050	2220.972	476.477	2003.119	5027.858	17.486	5028.064	17.524	0.004%	0.219%
n-Octane	393.352	2531.870	530.807	2441.611	5895.734	1.854	5895.761	1.856	0.000%	0.125%
n-Nonane	441.653	2156.583	460.588	2268.087	5326.670	0.201	5326.694	0.201	0.000%	0.048%
Mycyclopentan	0.000	0.000	0.000	465.899	454.529	11.384	454.456	11.438	-0.016%	0.471%
Benzene	0.000	0.000	64.839	264.243	320.793	8.388	320.614	8.465	-0.056%	0.916%
Cyclohexane	0.000	0.000	248.311	634.126	868.117	14.432	867.903	14.528	-0.025%	0.661%
Mycyclohexane	0.000	0.000	0.000	996.508	993.357	3.224	993.264	3.242	-0.009%	0.560%
Toluene	0.000	0.000	96.439	425.057	520.574	0.958	520.527	0.968	-0.009%	1.040%
E-Benzene	0.000	0.000	0.000	163.252	163.213	0.026	163.226	0.027	0.008%	1.258%
m-Xylene	0.000	0.000	0.000	489.757	489.648	0.058	489.698	0.059	0.010%	1.296%
o-Xylene	0.000	0.000	0.000	195.903	195.865	0.020	195.883	0.020	0.009%	1.431%
124-MBenzene	0.000	0.000	0.000	221.788	221.787	0.001	221.787	0.001	0.000%	1.403%
C10+*	6797.534	42012.549	8990.019	55819.599	113619.709	0.000	113619.700	0.000	0.000%	116.679%
Total Molar Rate (kgmole/h)	72.312	448.636	171.748	1344.461	714.688	1322.216	714.991	1322.116	0.042%	-0.008%
Total Mass Rate (kg/h)	9289.100	57359.586	14306.14	93933.933	144309.083	30568.374	144321.483	30564.816	0.009%	-0.012%

7 CONCLUSIONS

Out of the three methods for using simulation models with allocation systems discussed in this paper the ideal method is to fully integrate the simulation model with the allocation system.

There are a number of potential pitfalls when integrating simulation software with allocation systems. However, these pitfalls can be overcome by using a simplified model that only focuses on the unit operations and equations important to an allocation system.

The simplified model is more stable, faster repeatable than a traditional simulation model built using proprietary software without losing accuracy and can be coded to fully integrate with an allocation system.

In summary, the advantages of the simplified model include:

- Accuracy equivalent with existing commercial simulation software;
- Ease of integration with allocation software;
- Ease of configuration;
- Improved speed (does not need to resolve heat balances or calculate equipment performance, etc.);
- Improved robustness (uses specific solution routines that focus on solving the molar balances rather than expansive of matrix equations).

8 REFERENCES

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- [2] A New Two Constant Equation of State, Ding-Yu Peng and Donald B. Robinson, Industrial Engineering and Chemistry Fundamentals, Vol.15, No.1, 1976.
- [3] Most Common Pitfalls in Process Simulation Abstract ID# 302023, Authors: Richard Pelletier and Mike Donahue, Invensys Operations Management.
- [4] Rachford, H.H. and J.D. Rice, 1952, J. Petrol. Technol., 4 (10), Section 1, p. 19 and Section 2, p. 3.