



EXPERIENCE WITH GDS –

A FIRST PRINCIPLES INFERENTIAL MODEL FOR

DISTILLATION COLUMNS

By:

Y. Zak Friedman, PhD
Petrocontrol, New York, NY
pertocontrol@earthlink.net

Gwilym T. Reedy
Texaco, Pembroke, Wales

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INTRODUCTION

Advanced process control (APC) makes money by maximizing a key process variable (usually throughput), pushing plant equipment to limits within safety parameters, while at the same time maintaining product quality targets. That second requirement – maintain product quality targets – cannot be overlooked. As illustrated in figure 1, pushing equipment to its limits, within safety parameters, without controlling product qualities can be counter productive and lose money. There are tools on the market to achieve the maximization part of APC but quality control is more problematic. To achieve product quality control we must be able to measure quality in real time, which is difficult. Traditionally APC relied on on-stream analyzer measurements, but being very slow, analyzers are not useful for synchronizing quality with fast acting constraint controllers. They are only useful for long-term steady state correction at constant throughput. There are also issues of cost and reliability that impede the use of analyzers in closed loop control.

In recent years Industry has started to develop methods for treating the equipment itself as an “on-stream analyzer”, measuring process variables around the equipment of interest and passing them through a mathematical inference model to produce an estimate of product quality. This concept is illustrated in figure 2. Most of the models in current use are empirical, based on regression analysis, either via statistical tools or neural network software. Such models do not make use of our chemical engineering knowledge, and while being better than nothing, are generally inferior to first principles models.

There is a great need for better first principles inferential control models. In particular that need is obvious regarding prediction of distillation product purities. Most units culminate with a series of distillation columns where products are cut, and more often than not, product specifications are given in terms of purity or other distillation related properties. Furthermore, regression models of distillation equipment cannot cope well with distillation columns. Gaussian theory requires all input variables to be independent, whereas on a typical distillation column all temperatures move up and down together, and are dependent in some way. Appendix A elaborates on this and a number of other problems faced by empirical distillation models.

And there is a wealth of distillation knowledge, which makes first principle models possible.

This paper deals with a class of first principle inferential control models for distillation. The modeling approach involves a short cut simulation of a section of the column, typically a bottom half of the stripping section or a top half of the rectifying section as shown in figures 3. Hence the name of the model: GDS (General distillation shortcut). GDS works by fitting a bottom (or top, when the model covers the top section) column composition that would best agree with column measurements. That is fairly easy to accomplish with binary distillation, and the novelty of GDS is that by looking at a number of tray temperatures it is equipped to address multi-component distillation.

GDS first calculates separation parameters for the section of interest based on process measurements and column configuration. Those parameters are complex and nonlinear with respect to temperature, pressure and vapor-liquid traffic. Then, once separation parameters are produced, the model for inferring top or bottom composition can be expressed as a linear set of simple equations, and once through calculations with no convergence issues. That makes the GDS model very suitable for on-line closed loop work.

The GDS theory has been published several years ago [1], and since that time we have implemented a large number of GDS inferences. It is time now to take stock and report the performance of these models. This paper discusses a group of models implemented at the Texaco Pembroke refinery in Wales, UK, what they were set up to do and why, and how they perform in a closed loop control environment.

PROJECT DESCRIPTION

The Pembroke refinery has initiated a project in early 2000, to install advanced control applications in its FCC complex, which comprise three units: FCC, gas concentration and alkylation. The project was executed by a team of engineers from Texaco, Petrocontrol and Honeywell.

The main FCC equipment is shown in figure 5. It includes a Texaco side-by-side reactor with a main fractionator and gas concentration section. The main fractionator separates out naphtha, two sidestreams and bottom slurry. The gas plant has three columns: deethanizer, debutanizer and naphtha splitter.

The alkylation unit is of a Phillips HF design, taking olefinic LPG (butylene and propylene) and reacting them with isobutane in high stoichiometric excess. The main alkylation equipment is shown in figure 6, including olefin feed preparation section, alkylation reactor riser-settler, and separation section. The IC4 feed preparation section (not shown in the figure) has a stabilizer and deisobutanizer (DIB) to produce 96% pure isobutane feed. Reaction products are separated in a depropanizer and isostripper. The depropanizer separates out inert propane and some of the excess isobutane. The isostripper separates out the remaining isobutane at the top, inert normal butane as a vapor sidestream and alkylate at the bottom. Excess isobutane is returned to the reactor.

By and large, the APC makes money by maximizing FCC severity and alkylate production. To accomplish this maximization the APC applications make substantial hour-to-hour changes in manipulated variables of all three units. To permit tight product quality control through these process changes we applied many inferential calculations, as listed below.

Pembroke has a large number of onstream analyzers, and has been generally successful in maintaining the analyzers and getting reasonable service factors.

When this project started we were ready to acknowledge the superiority of well-maintained analyzers, and reset inference models to agree with analyzer signals. But even the most reliable analyzers have exhibited three failure patterns:

- “Freeze” -- when the analyzer signal stays for a long time without changing.
- “Jump” -- when the analyzer signal changes abruptly.
- “Dive” -- when the signal abruptly changes to zero and stays there.

To detect analyzer failure we apply a validation procedure, testing for the common failures above.

Once the analyzer signal passes the three tests it is deemed reliable. A dynamic predictor then corrects for the slow analyzer dynamics, reconciling model versus analyzer reading by gradually resetting a bias in the inferential prediction. We started out this project with an assumption that analyzer readings are more accurate than inferential indications, however we are no longer of the opinion that that is a universal truth, and presently the decision of biasing the inference is left to the operator.

LIST OF INFERENCE MODELS

While this paper is about distillation GDS models, for completeness we list in this section all inferential models incorporated in the project. The model supplier is noted in parenthesis.

- **FCC Reactor severity model (Hi-Spec)**
This model was supplied by Honeywell Hi-Spec and is out of the scope of this paper.
- **FCC Fractionator GCC model (Petrocontrol)**
Petrocontrol’s GCC model was used. This model has been described in several references [2, 3] and will not be dealt with in this paper.
- **FCC Deethanizer GDS model (Petrocontrol)**
 - Inference of bottom LPG content
 - Inference of bottom C2 expressed as % C2 in LPG. An analyzer measuring C2 in debutanizer LPG product, one column downstream, also exists.
- **FCC Debutanizer GDS model (Petrocontrol)**
 - Inference of C5 in LPG. An analyzer measuring C5 in LPG also exists.
 - Inference of C4 in naphtha.
- **FCC Naphtha Splitter GCC model (Petrocontrol)**
Petrocontrol’s GCC model was used and will not be discussed further here.
- **Alky feed Stabilizer GDS model (Petrocontrol)**
 - Inference of IC4 loss with stabilizer off gas. An analyzer measuring IC4 in off gas also exists but is not always reliable.

- Inference of bottom composition: NC4 versus IC4. An analyzer measuring bottom IC4 content also exists.
 - Inference of vapor and liquid traffic, not covered by this paper.
- **Alky feed DIB GDS model (Petrocontrol)**
 - Inference of top NC4 content. An analyzer measuring NC4 in IC4 impurity exists but is not always reliable.
 - Inference of IC4 content in sidestream NC4 product. An analyzer measuring IC4 in the NC4 product exists but is not always reliable.
 - Inference of bottom composition: NC4 versus C5. An analyzer measuring bottom C5 content also exists.
 - Inference of vapor and liquid traffic, not covered by this paper.
- **Alky olefins Deethanizer GDS model (Petrocontrol)**
 - Inference of C2 content in alkylation reactor feed
 - Inference of vapor and liquid traffic, not covered by this paper.
- **Alky Reactor stoichiometric model (Petrocontrol)**
A stoichiometric model based on analyzer readings and downstream GDS inferences. It is out of the scope of this paper.
- **Alky Depropanizer GDS model (Petrocontrol)**
 - Inference of IC4 loss with the top propane product. An analyzer measuring IC4 in the propane product also exists.
 - Inference of NC4 content in depropanizer IC4 sidestream. An analyzer exists but its reliability is questionable.
 - Inference of C3 content in depropanizer IC4 sidestream. An analyzer exists but its reliability is questionable.
 - Inference of vapor and liquid traffic, not covered by this paper.
- **Alky Isostripper mixed technology model (Petrocontrol)**
 - Inference of NC4 content in isostripper top IC4 stream. An analyzer also exists.
 - Inference of C3 content in isostripper top IC4 stream. An analyzer also exists.
 - Inference of IC4 loss with the isostripper NC4 sidestream. An analyzer exists but it is not always reliable.
 - Inference of NC4 content in alkylate.
 - Degree of sub-cooling of the top IC4 stream after condensation. This is an inference of condenser constraint.
 - Inference of vapor and liquid traffic, not covered by this paper.

This column is a special inference case. The column does not have enough temperature points to support GDS models and we had to use knowledge and measurement of reactor effluent composition to help create these inferences. Since this paper deals primarily with the GDS model, we will not discuss the mixed technology models any further.

EXAMPLE GS MODEL

Figure 4 shows an example of how the GDS model works. Consider a debutanizer problem where the light key component is C4 and the heavy key is C5. The off key light components are C2 and C3 in varying amounts. There are four unknown distillate component compositions, and hence we need four equations to solve the inference problem. The column is equipped with a temperature point on tray 7 (from the top), and the example shows how this tray temperature is used in the model.

In this example there is no off gas and the overhead accumulator contains liquid at bubble point equilibrium conditions. The first equation reflects a bubble point condition, where X_{Di} is the distillate composition and K_{Di} is the volatility of component i at accumulator pressure and temperature.

The column top composition is the same as the distillate composition, but here this material is vapor at dew point equilibrium condition. The second equation reflects dew point condition, where K_{Oi} is the volatility of component i at column top pressure and temperature.

The third equation simulates the distillation process of the top 7 trays. The model assumes constant volatility throughout the section, and in that case there is a constant ratio between top and tray 7 liquid composition. This ratio is a function of component volatility and L/V . The formula of this equation was developed by Colburn [4].

Lastly, the bottom equation of figure 4 simply states that the sum of all concentration is one.

There are three issues of interest in this example:

- Tray 7 temperature is sensitive to the content of C5 on tray 7, however it cannot be used for C5 inference because it is also sensitive to the light off keys, mostly to C3.
- The separation in the top section must also be corrected for L/V as being done in the Colburn equation.
- The K and R values of figure 4 involve nonlinear thermodynamic calculations, but once these coefficients are found – the resulting set of equations is linear and there are no convergence problems.

GDS MODEL PERFORMANCE

This chapter explains the column configurations in more detail, indicating the GDS model input measurements, and then going on to show trends of model predictions versus analyzer readings. At the time this data was taken many of the APC applications were not yet in closed loop. That gives us the opportunity to observe the inferential model performances through wide movements in the operation. After

closing the APC loops most of the product qualities lined out and our trends became somewhat “boring”.

FCC deethanizer

The FCC deethanizer incorporates absorber-deethanizer configuration as shown in Figure 7. The object of this column is to separate out C2 and lighter material from FCC LPG without losing much C3 to fuel gas. FCC olefinic LPG is fed to the alkylation unit where C2 contamination would be problematic. On the other hand, stripping of C2 from LPG must be accomplished without substantial loss of C3 in the off gas, because of the value of propylene as alkylation ingredient. These two purity requirements dictated a fairly complex absorption and reflux arrangement.

To control this column well we need inferences of both top and bottom purities. Considering the complexity of rectifying in this column however, a GDS inference of how much propylene is lost to fuel gas is not practical. We have therefore taken the approach of inferring bottom C2 content, and configured two control variables: bottom C2 and LV. The premise being that when the bottom C2 content is at target, a reasonable column loading would minimize propylene losses. As opposed to the rectifying section, the stripping section is simple, well instrumented and can support a GDS model for calculating bottom C2.

Figure 8 shows a trend of model prediction versus analyzer reading of C2 in LPG. The analyzer is located one column downstream of the deethanizer and a dead time of four hours can be observed. GDS first predicts bottom composition, including C2 and LPG, but since the entire bottom C2 ends up in LPG, it is of interest to express the bottom C2 content as LPG contaminant. To achieve that we must find out how much LPG is in the bottom, and then calculate C2 in LPG assuming all of the LPG is recovered. The inferred bottom LPG content is also plotted in figure 8. The steady state fit of model C2 in LPG versus analyzer reading is good, except during a three-day period. At this time we do not have a proven explanation for the temporary deviation. It is possible that butane was lost to the naphtha, and then the LPG product flow would be lower and C2 concentration higher than normal. There could also be a drift of the analyzer signal. Such a suspicion is not out of the question on ground that the trend does expose an analyzer reliability issue: The signal was inactive for some time. Considering the validity issue and the long delay between inference and analyzer it is questionable whether analyzer feedback would be useful at all, though for now we did incorporate a feedback bias resetting action based on the analyzer reading.

FCC debutanizer

The FCC debutanizer diagram is shown in Figure 9. The object of this column is to separate out essentially all of the LPG without much C5 contamination and without losing C4 to the bottom. Minimizing losses of C4 to naphtha is an economic driving force because of the value of butylene as alkylation ingredient. The debutanizer

column is sufficiently well instrumented to support a GDS model in both the top and bottom sections of the column. The top section model provides an inference of the amount of C5 contamination in LPG whilst the bottom section model provides a model of the amount of C4 loss to naphtha. In order to prevent conflict between the two temperature based models only one model is closed loop within the advanced control application at any time. Currently the C5 in LPG model is configured as the working model.

Figure 10 shows a one-month trend of model prediction of top and bottom composition, compared against analyzer measurement of top C5 %. While this model was calibrated against the analyzer, it gives results that are in many respects better than the analyzer. The analyzer is slower, exhibiting a dead time of about two hours and it occasionally jumps or freezes. Still, we configured this analyzer with a validation routine and predictive feedback feature to bias the inference. Our validation procedure is able to detect all of the obvious analyzer failures seen on figure 10.

Alky feed Stabilizer

The alky feed “stabilizer” is essentially a stripper as shown in Figure 11. The main task of this column is to strip light products from the saturated butanes alky unit feed. If penetrated into the alkylation unit, these light contaminants could cause severe problems. In addition to the removal of light material, the control objective is to minimize losses of IC4 to off gas. Ideally we would need inferences of both top and bottom impurities to accomplish the control objectives.

The top section of this column is instrumented enough to support a GDS model, although this model must be equipped to deal with a difficulty of varying light component tail gas composition, which affects the interpretation of temperatures. As discussed in the model description literature [1], GDS deals with such situations by adding equations for known conditions, and in this case a flash calculation in the overhead drum is sensitive to the composition of lights in tail gas.

On the other hand, the stabilizer bottom section is not instrumented enough for an inference model. Given this situation we resorted to the use of two control variables for this column: IC4 in off gas and column loading -- L/V in the stripping section. With the loss of IC4 at the top being under control, we guarantee effective stripping of the lights by loading the column to a reasonable L/V.

Figure 12 shows a two months trend of the IC4 in off gas inferential calculation against analyzer reading. It can be seen that during one of these months the analyzer was not working at all, while during the other month it gave a reasonable signal. The correlation between inference and analyzer is not brilliant, though it is not clear whether or not the analyzer is reliable. We will continue to monitor the inference and analyzer and perhaps run lab tests before making a decision on the use of analyzer and/or inference for this case.

Alky feed Deisobutanizer column

The DIB is a complex column with three feeds and a sidestream as shown in Figure 13. The column feed comes from three sources with different flows and compositions. IC4 is separated out at the top and taken to the alkylation unit. Normal C4 is drawn out as a vapor sidestream from tray 11. The bottom stream is small, containing whatever C5 enters the column plus some normal C4, as needed for MOGAS blending in the refinery. Economically it is best to minimize IC4 contamination in the NC4 sidestream, and at the same time also minimize NC4 in alkylation unit feed. The content of C5 in the bottom is not terribly important, though a very high C5 concentration can cause reboiling constraints.

We have implemented two GDS models on the DIB column; one on the rectifying section, predicting top IC4 product purity; the other on the stripping section, inferring sidestream purity and bottom C5 content. This column is well instrumented with tray temperature measurements in good locations, and we have been able to achieve good agreement between models and analyzers. Figures 14, 15 and 16 show the DIB inference fidelities for the bottom C5, top NC4 and side IC4 respectively. The excellent fit of these models against analyzer readings is obvious in all three cases.

Considering analyzer problems, does it make sense to connect these analyzers in closed loop? For now we decided to continue with this approach, but every inference bias loop can be switched off.

Alky Deethanizer

Alkylation begins with selective hydrogenation of di-olefins, and following the selective hydrogenation reactor is a deethanizer column for removing hydrogen and light by-products from the treated olefins. The deethanizer is shown in figure 17. Alkylation unit considerations dictate removal of essentially all C2 and lighter material. At the same time the APC has to minimize losses of propylene to off gas.

Ideally the control scheme for this column would rely on inferences of both top and bottom contamination, but that is not possible. Figure 17 shows that the stripping section of this column is instrumented enough to support a GDS model, but the rectifying section is not. We have therefore taken the same approach here as in several other columns: Control the bottom C2 contamination, and minimize the loss of propylene in off gas by loading the column to a reasonable L/V.

Figure 18 shows a one-month trend of bottom C2 inference against analyzer reading. In the latter half of this month the agreement between the two signals is good, whereas during the first half it is not brilliant. During the first week the analyzer did not work at all. Then it began to trend with the inference but at a lower level. Finally, after two weeks the two have reached agreement. We will continue to monitor inference and analyzer, and perhaps run lab tests before making a decision on the use of analyzer and/or inference for this case.

Alky Depropanizer

Figure 19 shows the alky depropanizer. This column takes about half of the reactor effluent stream and it removes propane as the top product. In addition, the column separates most of the excess IC4 in its feed into a sidestream and returns it to the reactor. Alkylate, normal butane and leftover IC4 make the bottom product, which goes to the isostripper. Propane is an inert in the alkylation reaction, and economic considerations call for minimizing the sidestream C3 content. At the same time IC4 losses to propane are to be avoided. Normal butane is also an inert component, and economics call for maximization of the sidestream IC4 as long as it does not contain much NC4.

A look at figure 19 reveals that the rectifying section of this column has sufficient instrumentation to support a GDS model, and we make use of such a model for predicting IC4 in propane and propane in IC4. There is no good solution for inferring NC4 contamination in the sidestream, and we ended up simply controlling the column to have a reasonable section L/V plus bottom yield. This control policy leaves some IC4 in the depropanizer bottoms, to be recovered in the isostripper.

Figure 20 trends the inference of IC4 loss with the top propane against analyzer measurement. The agreement is not bad when the analyzer works. Even during periods of instability the two measurements trend well together. At times there seem to be small disagreements, and we intend to monitor the two indications and make a judgement regarding analyzer feedback.

CONCLUSIONS

We have shown an inferential modeling technique for distillation, based on fundamental physical principles. The GDS method makes use of available column measurements to create simple models for predicting the product contamination by light or heavy key component. Such a technique is crucial, if one is to achieve precise distillation control. Having published the theory of inferring distillation product purities, we have now demonstrated that GDS works well, particularly when there are temperature measurements on key trays in the column.

LITERATURE CITED

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2. Friedman, Y. Z., "Control of Crude Fractionator Product Qualities During Feedstock Changes by Use of a Simplified Heat Balance". American Control Conference, 1985.
3. Friedman, Y. Z., "Crude Unit Advanced Control Experience". Hydrocarbon processing Journal, February 1994.
4. Colburn, A. P., Ind. Eng. Chem. 33, 459, 1941

APPENDIX A. EMPIRICAL VERSUS FIRST PRINCIPLES MODELS

A) Empirical models require large volumes of lab data.

The vast amounts of data needed to develop a statistical correlation cannot come from high quality test run data, and the regression engine must input every-day lab data. A fair percentage of daily lab data is biased, and then there is no possibility that the resulting correlation would be reliable.

B) Much of the time units work to a fixed product quality.

Normal day-to-day operation often does not provide enough movement in the data to give meaningful information. The development of regression inferential models without deterministic tests is in conflict with factorial experiment design theory. When data movement is too small -- the regression simply models noise patterns.

C) There is no replacement for process engineering.

The measurements set ought to "have the inferential information in them". GDS requires the use of a meaningful set of inputs, and if those are not available there is no possibility of developing a model. The regression model on the other hand, does not provide a method for analyzing the information content of a set of inputs.

D) Regression requires independent inputs.

The regression (Gaussian) theory requires all inputs to be independent. That is not possible with normally measured process data. Temperature measurements on a distillation column tend to all go up or down together. While all of the temperatures data contain information of product purities, they are also dependent of each other in some ways, and hence cannot yield a reasonable regression model.

E) GDS provides the means for checking instrument errors.

Identifying erroneous input data is most important during model calibration time. In the GDS case, from the input data GDS computes engineering parameters such as tray efficiencies, liquid – vapor traffic, components K's (Y/X values), anchored in thermodynamics and column geometry. Should a set of bad data come in, the GDS model is equipped to identify such an event.

F) Ability to survive process modifications.

Any inferential model would need to be re-calibrated upon modifications of the column equipment, but in the case of GDS, previous knowledge of tray efficiency and thermodynamic parameters makes re-calibration easy. In the case of an empirical model, it would be turned off for a period of several months until a meaningful set of lab data is accumulated and the model re-developed from scratch.

Figure 1

Why apply inferential control?

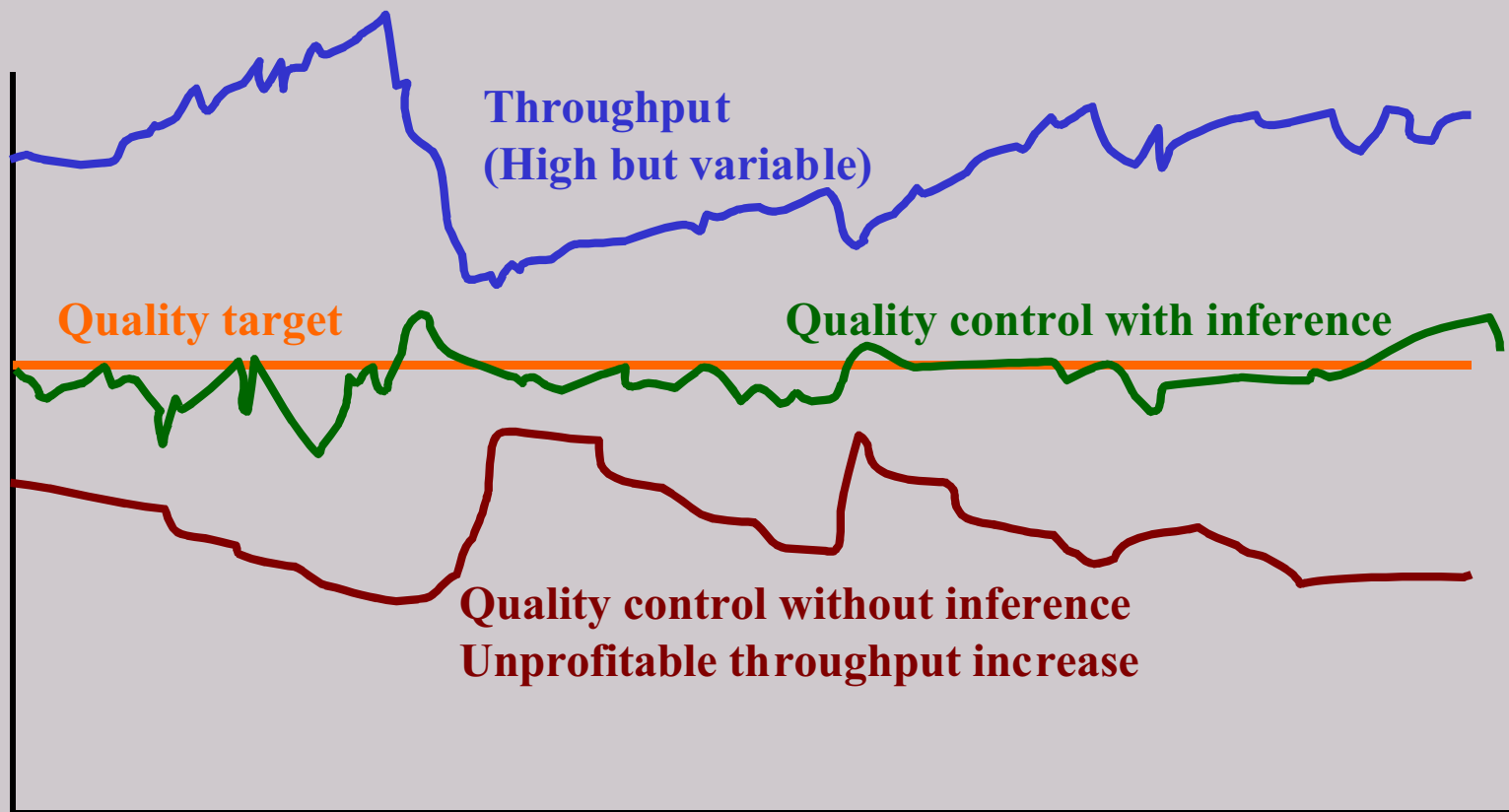


Figure 2

Inferential control concept

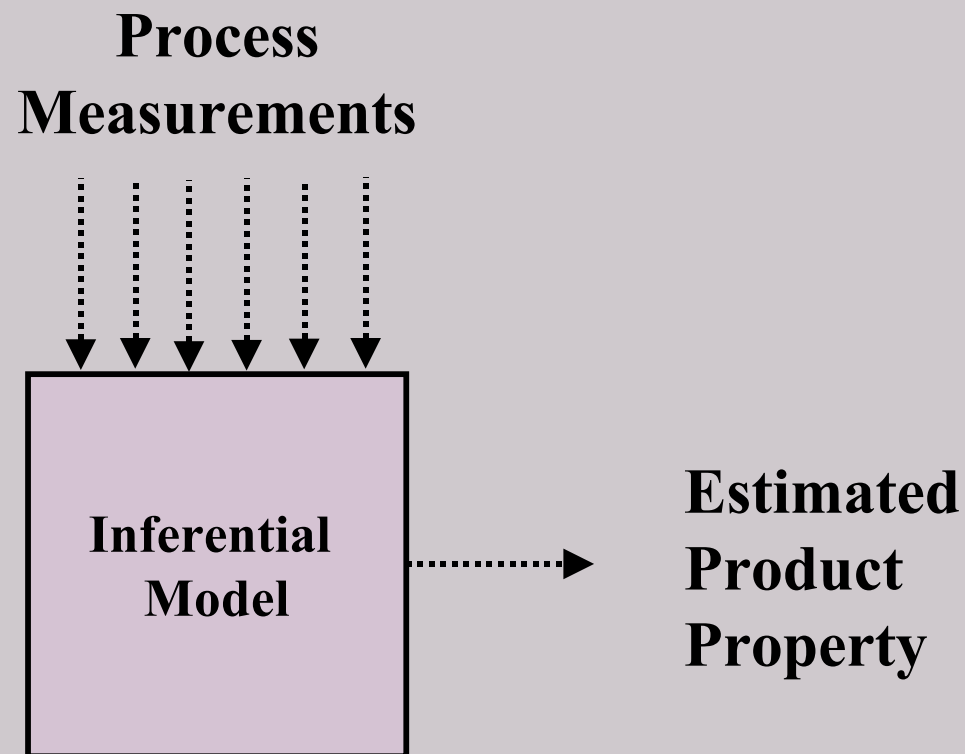


Figure 3. Typical GDS configurations

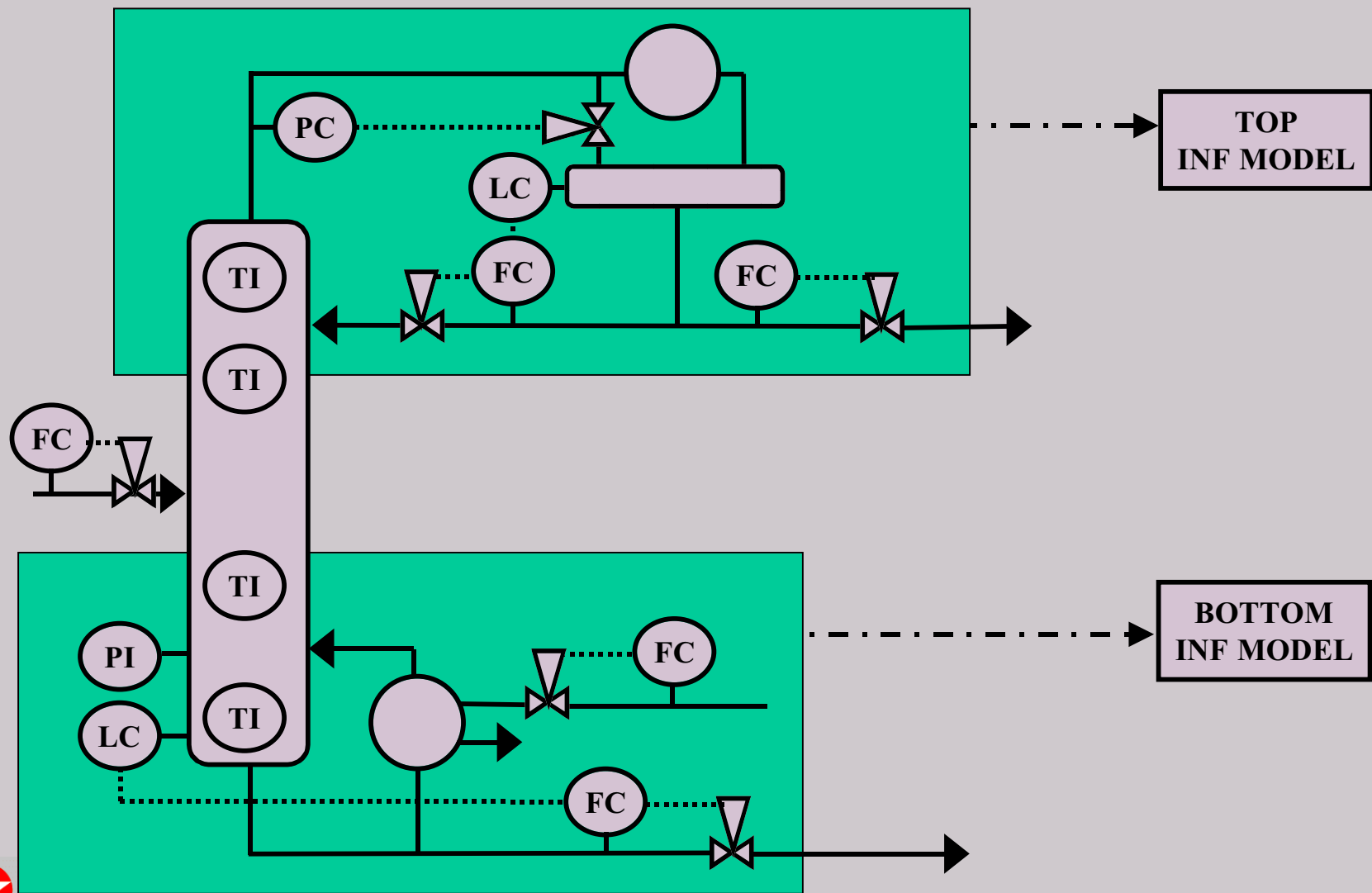


Figure 4. Example Top section model

Four unknowns: C2, C3, C4, C5.

Four linear equations

- **Equation 1. Drum bubble point equation**
$$\Sigma (K_{Di} * X_{Di}) = 1$$
$$K_{Di} = Y_i/X_i \text{ drum conditions}$$
- **Equation 2. Top dew point equation**
$$\Sigma (X_{Di} / K_{Oi}) = 1$$
$$K_{Oi} = Y_i/X_i \text{ top conditions}$$
- **Equation 3. Section separation (Colburn equation)**
$$\Sigma (R_i * X_{Di}) = 1$$
$$R_i = X_{Ti}/X_{Di} \quad T = \text{tray 7}$$
$$= F(\text{Tray 7 } T, P, L/V)$$
- **Equation 4. Mass balance equation**
$$\Sigma (X_{Di}) = 1$$



Figure 5. FCC Simplified Diagram

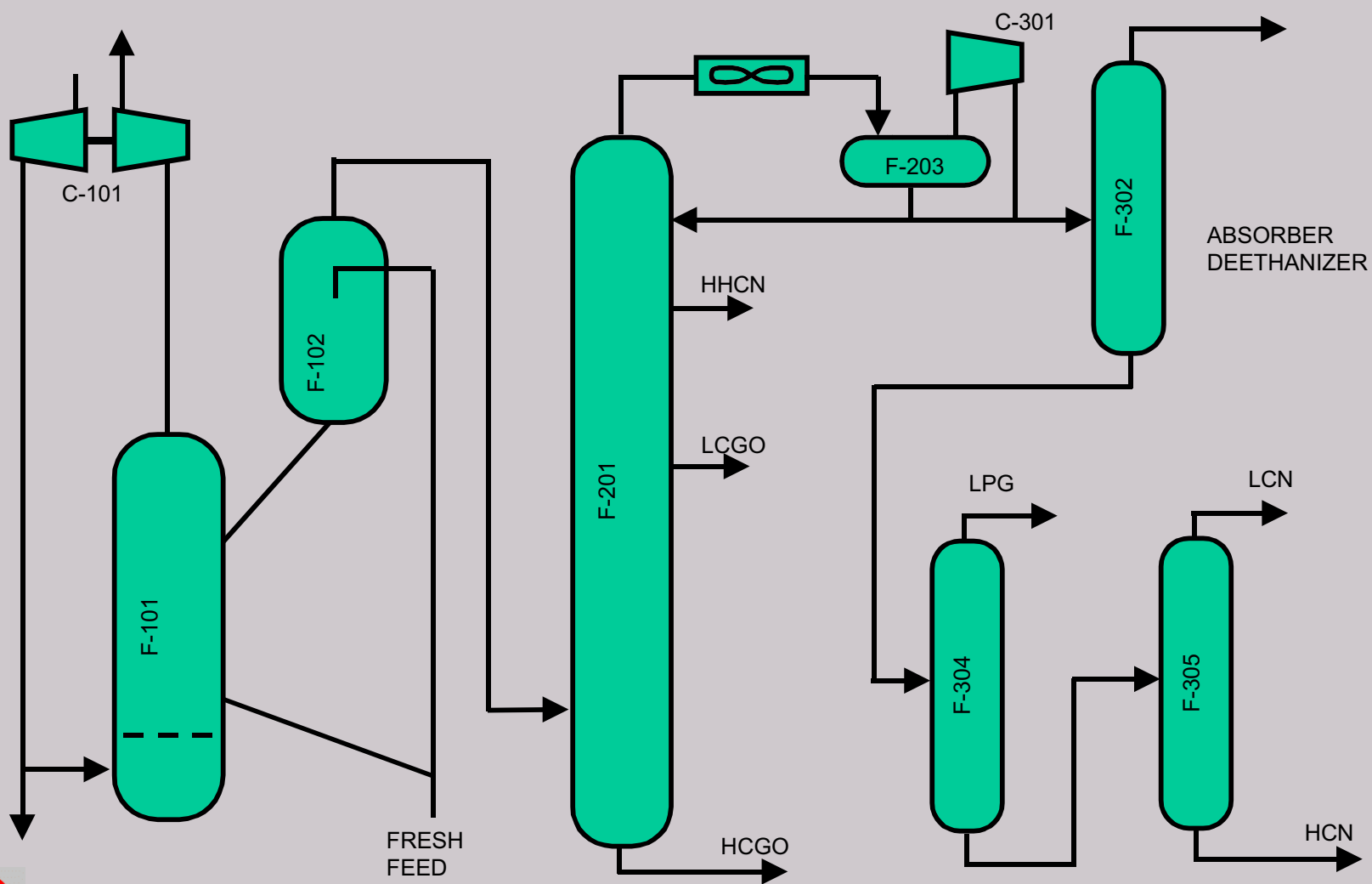


Figure 6. Alkylation Simplified Diagram

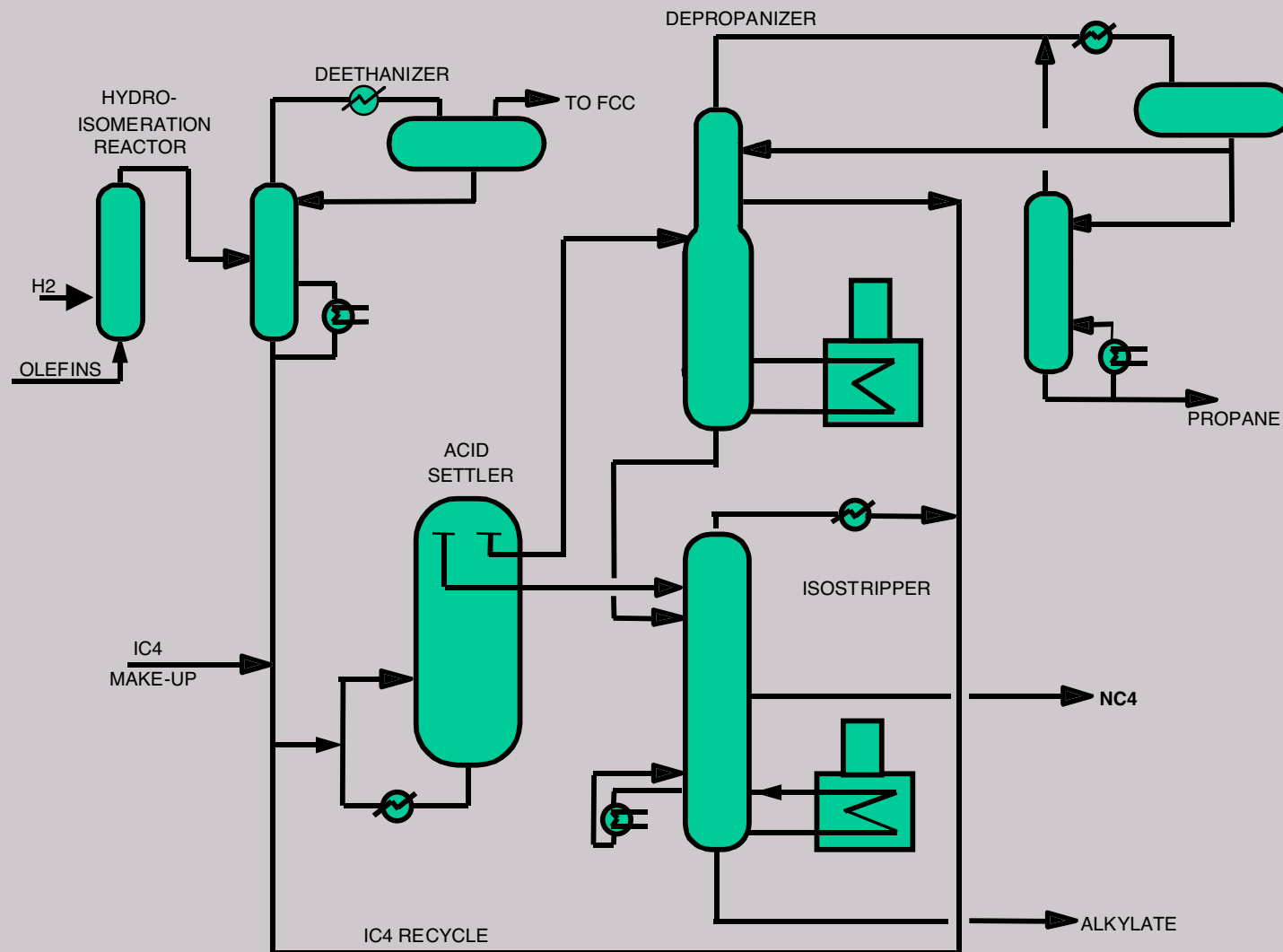


Figure 7. FCC Deethanizer

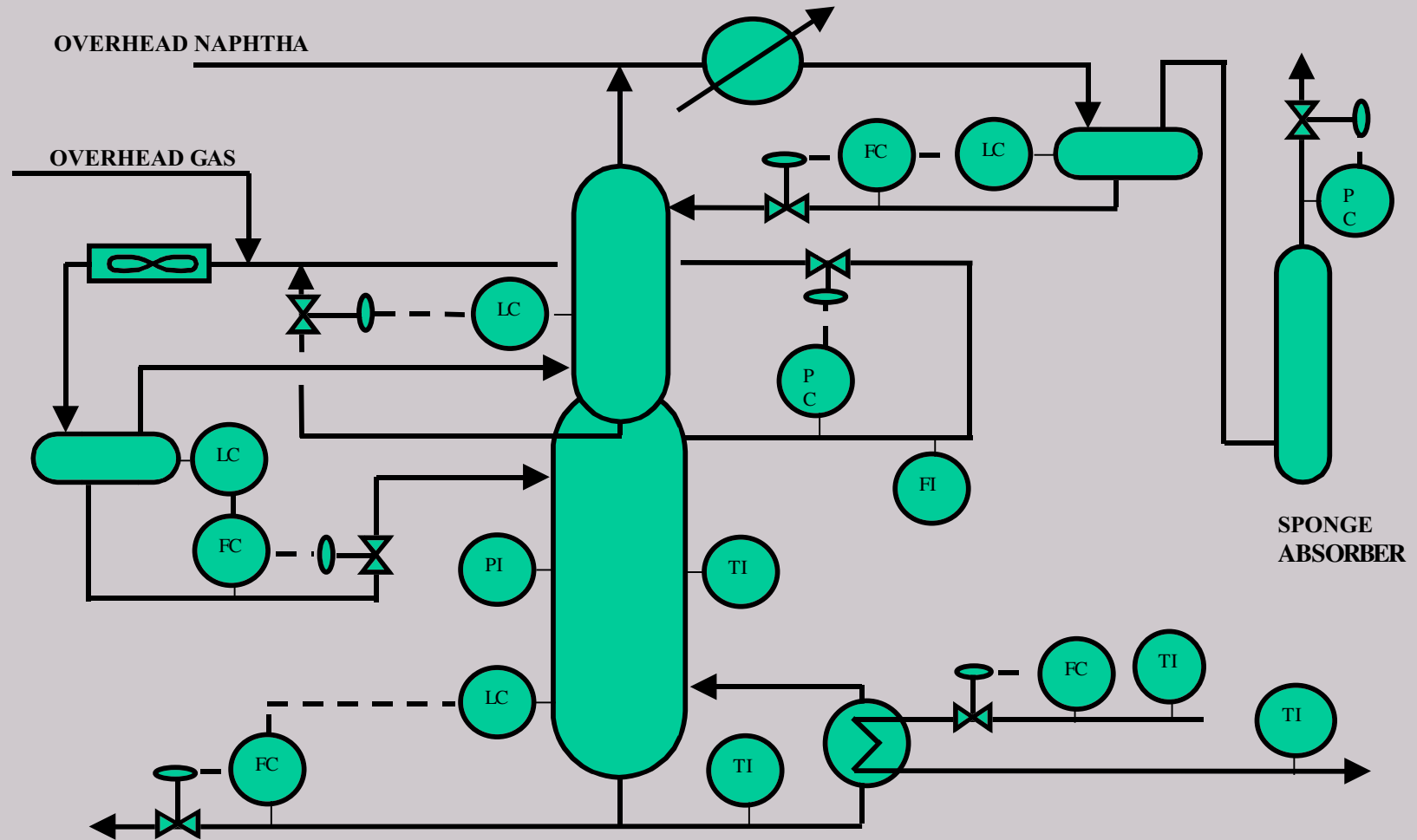


Figure 8. FCC DeC2 Inferences

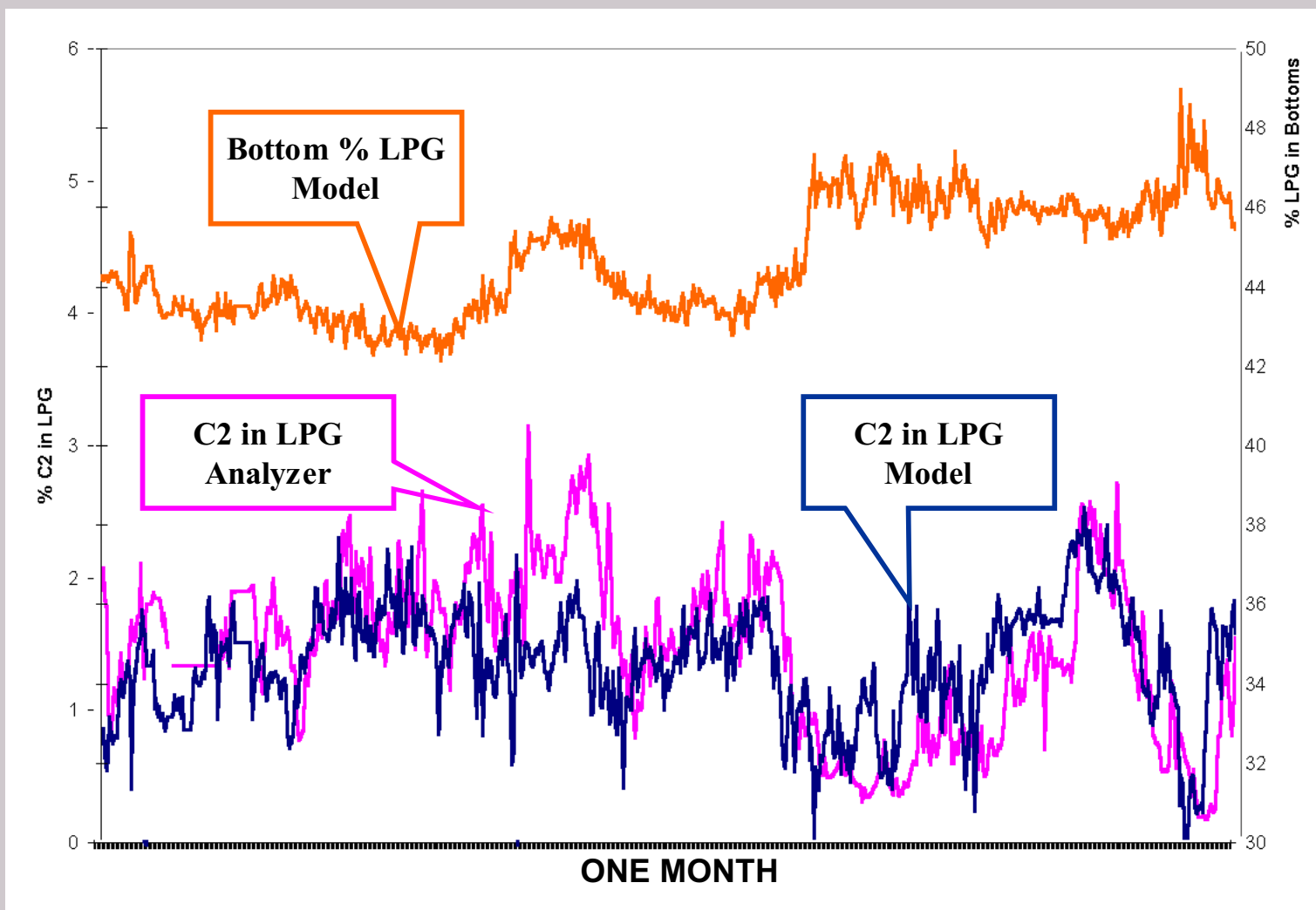


Figure 9. FCC Debutanizer

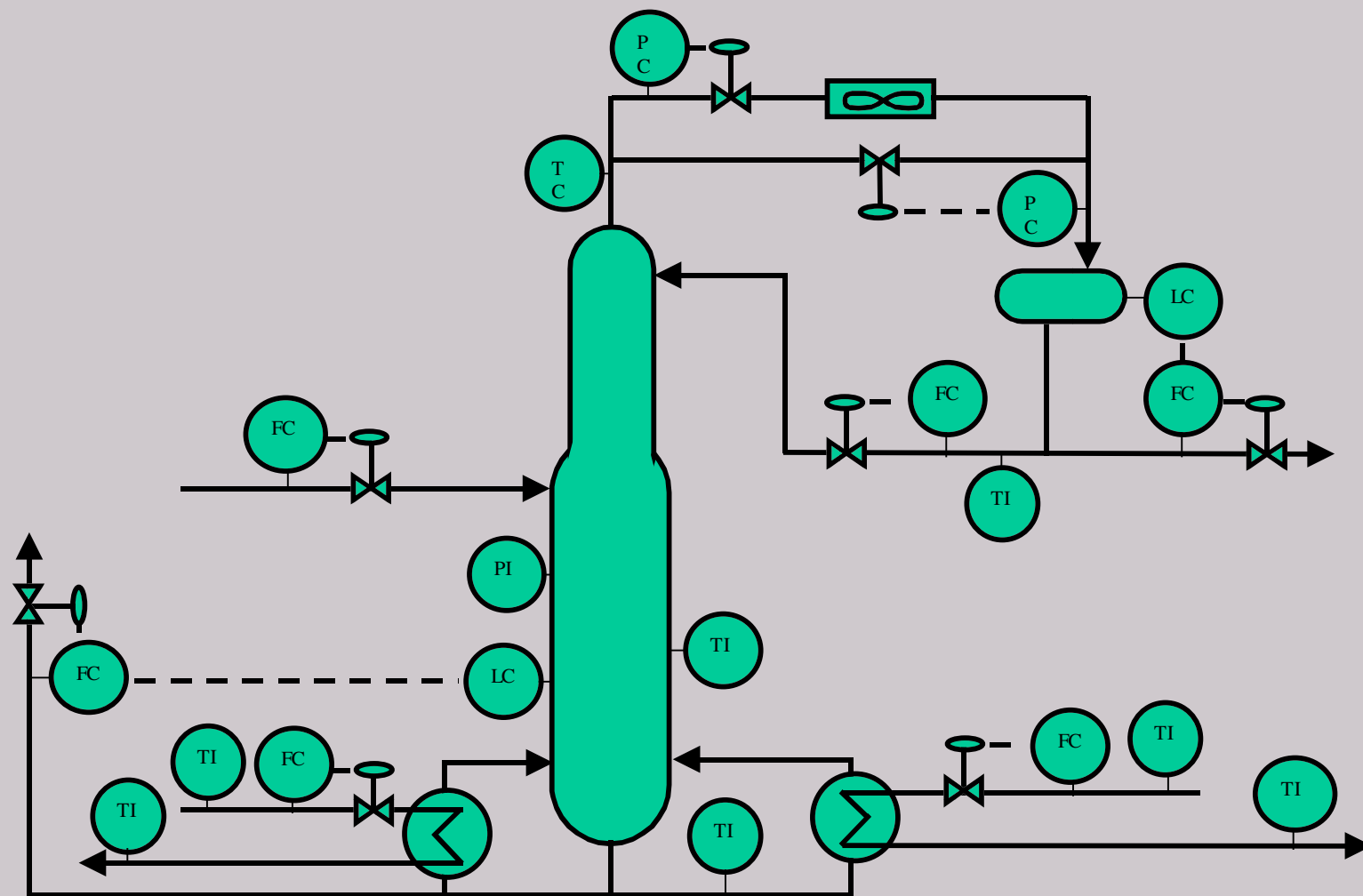


Figure 10. FCC DeC4 Inferences

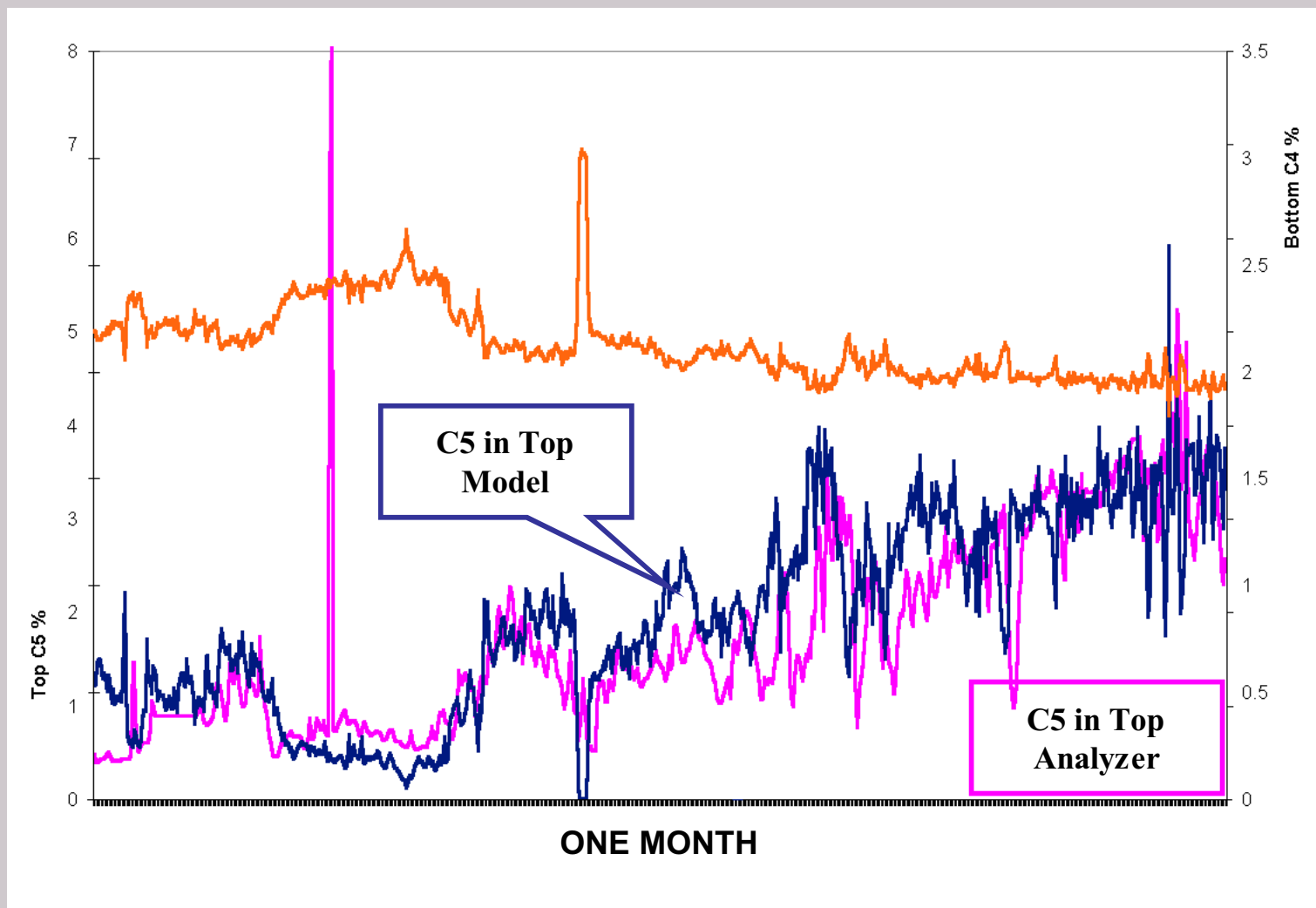


Figure 11. Alky Feed Stabilizer

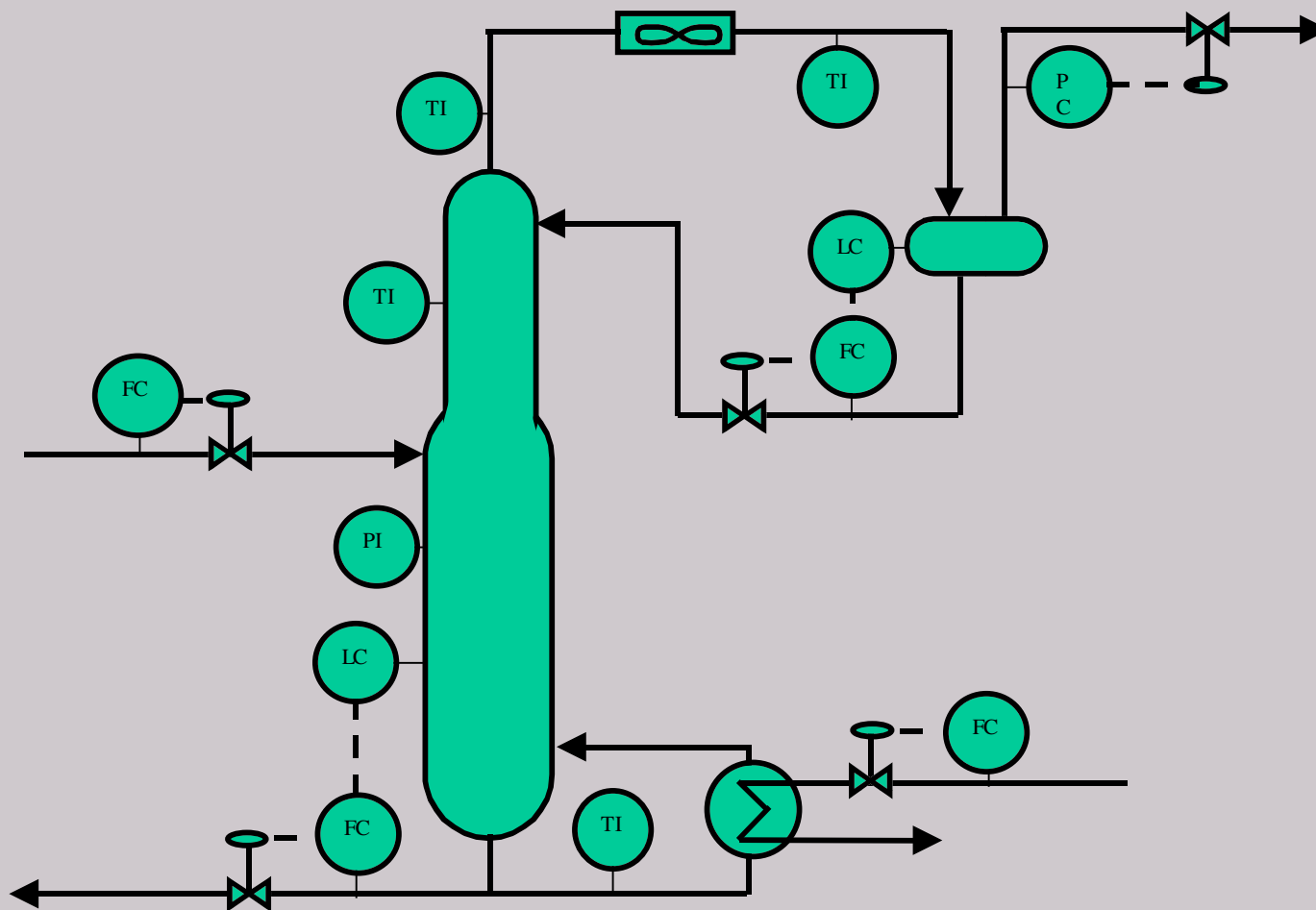


Figure 12. Alky Stabilizer Inference

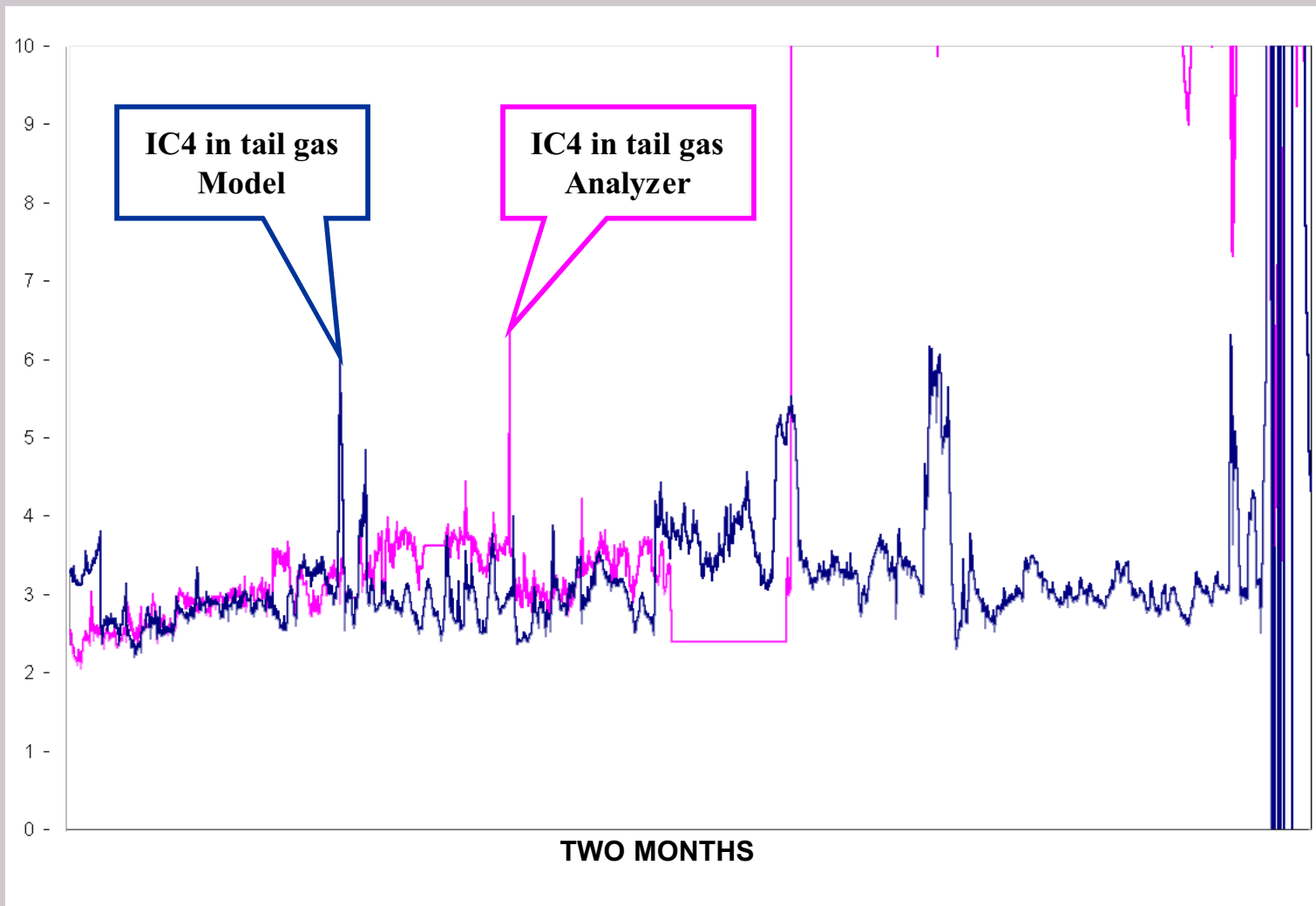


Figure 13. Alky Feed Deisobutanizer

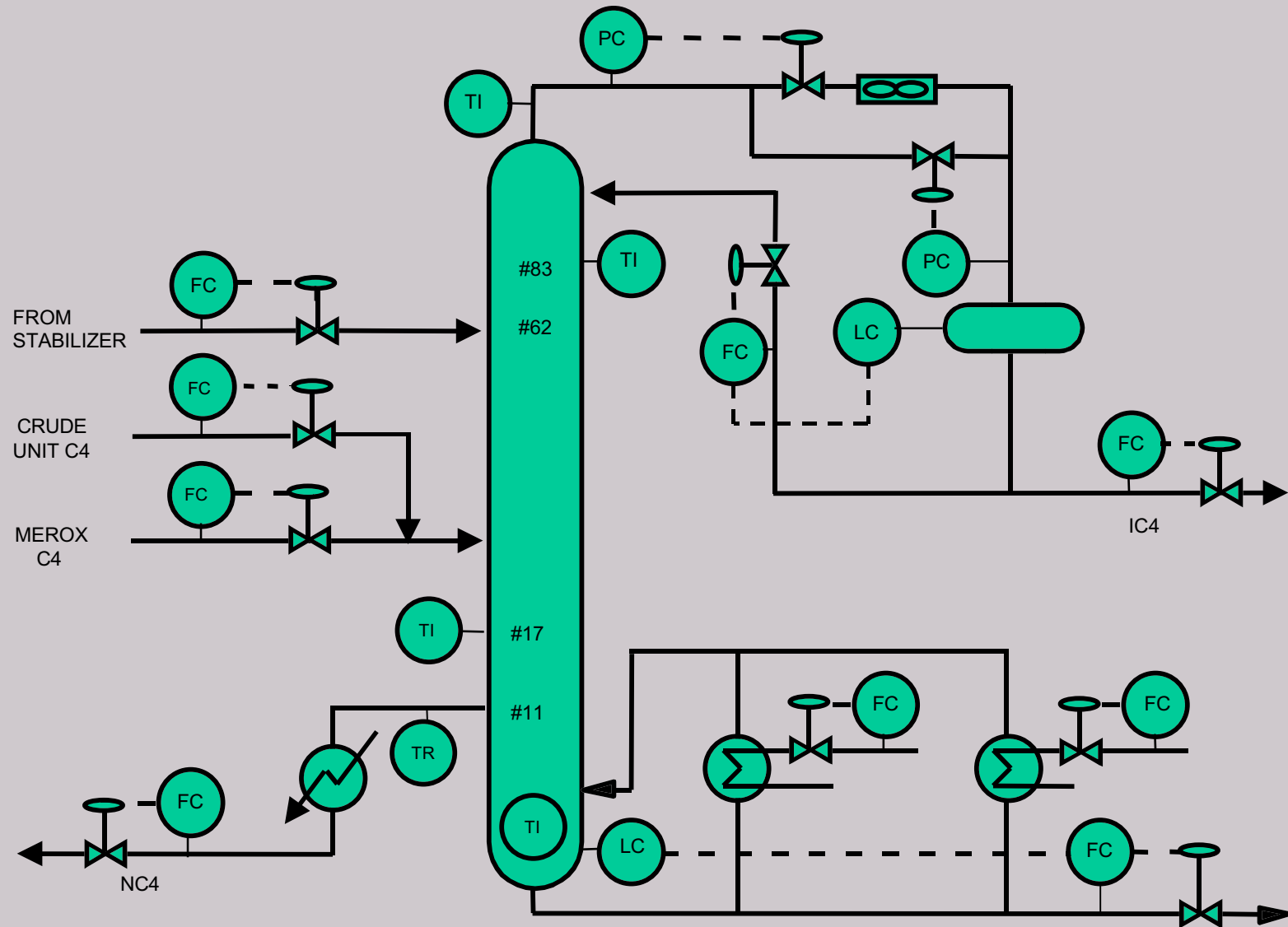


Figure 14. DIB bottom C5 inference

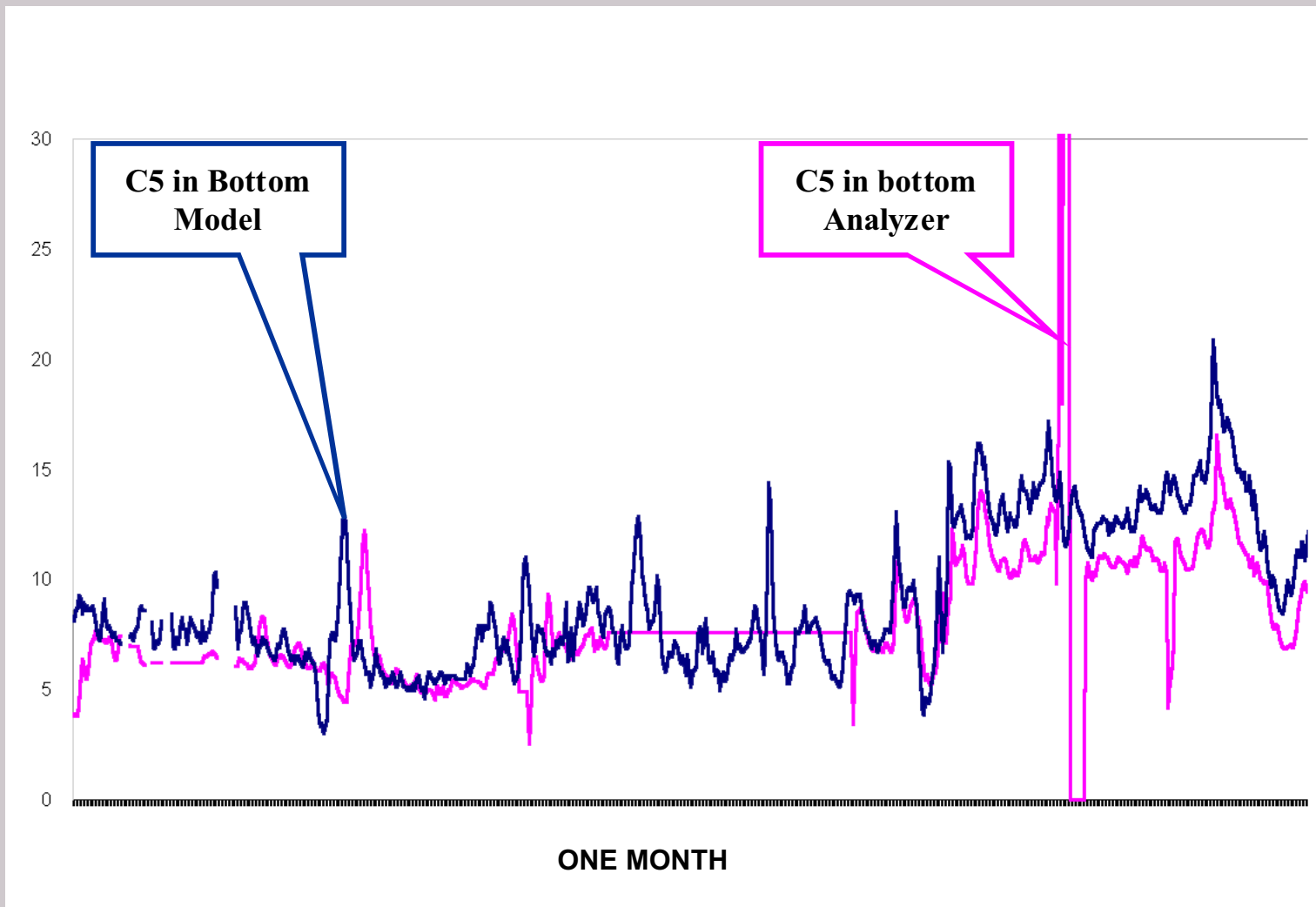


Figure 15. DIB top NC4 inference

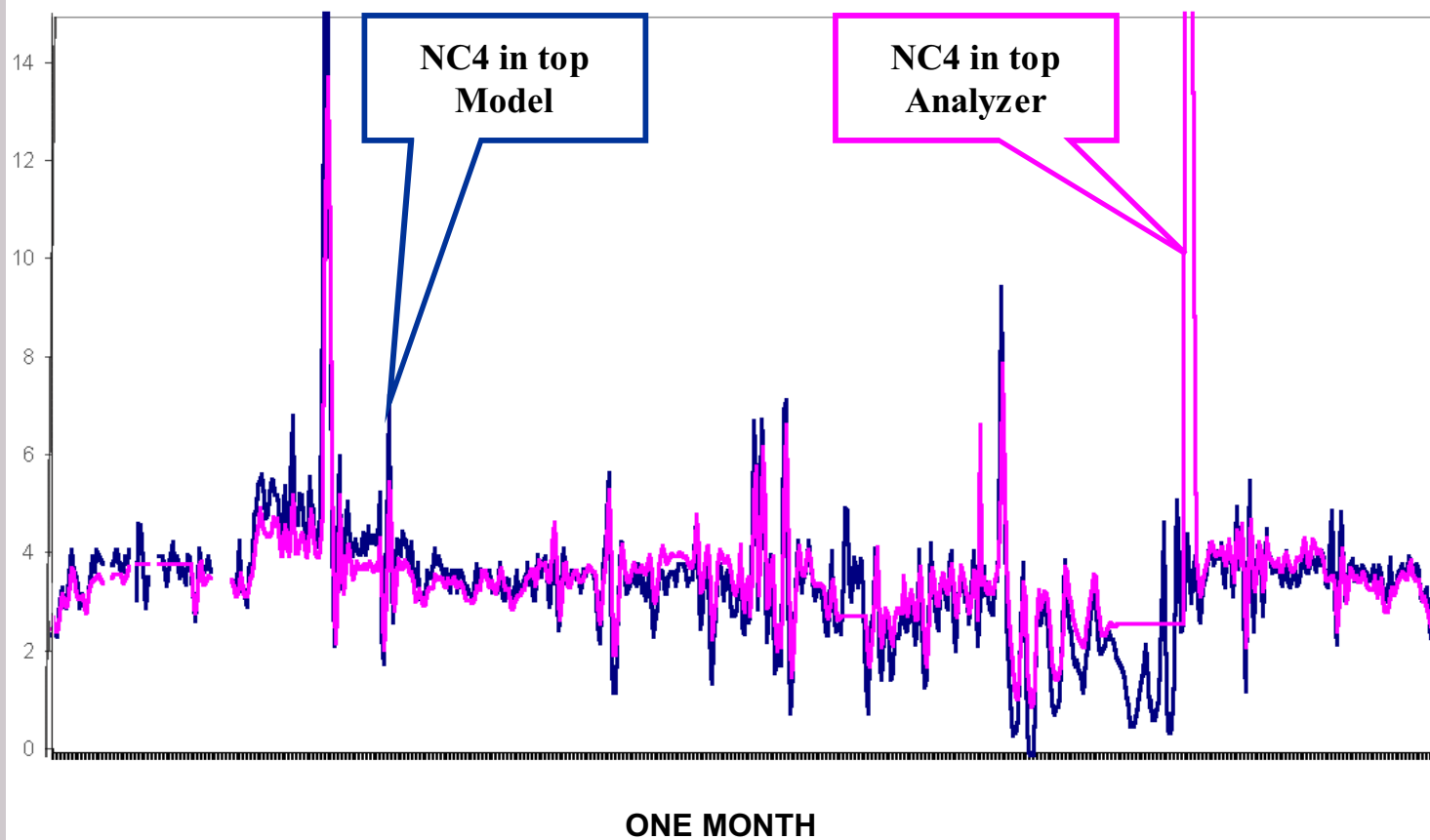


Figure 16. DIB SS IC4 inference

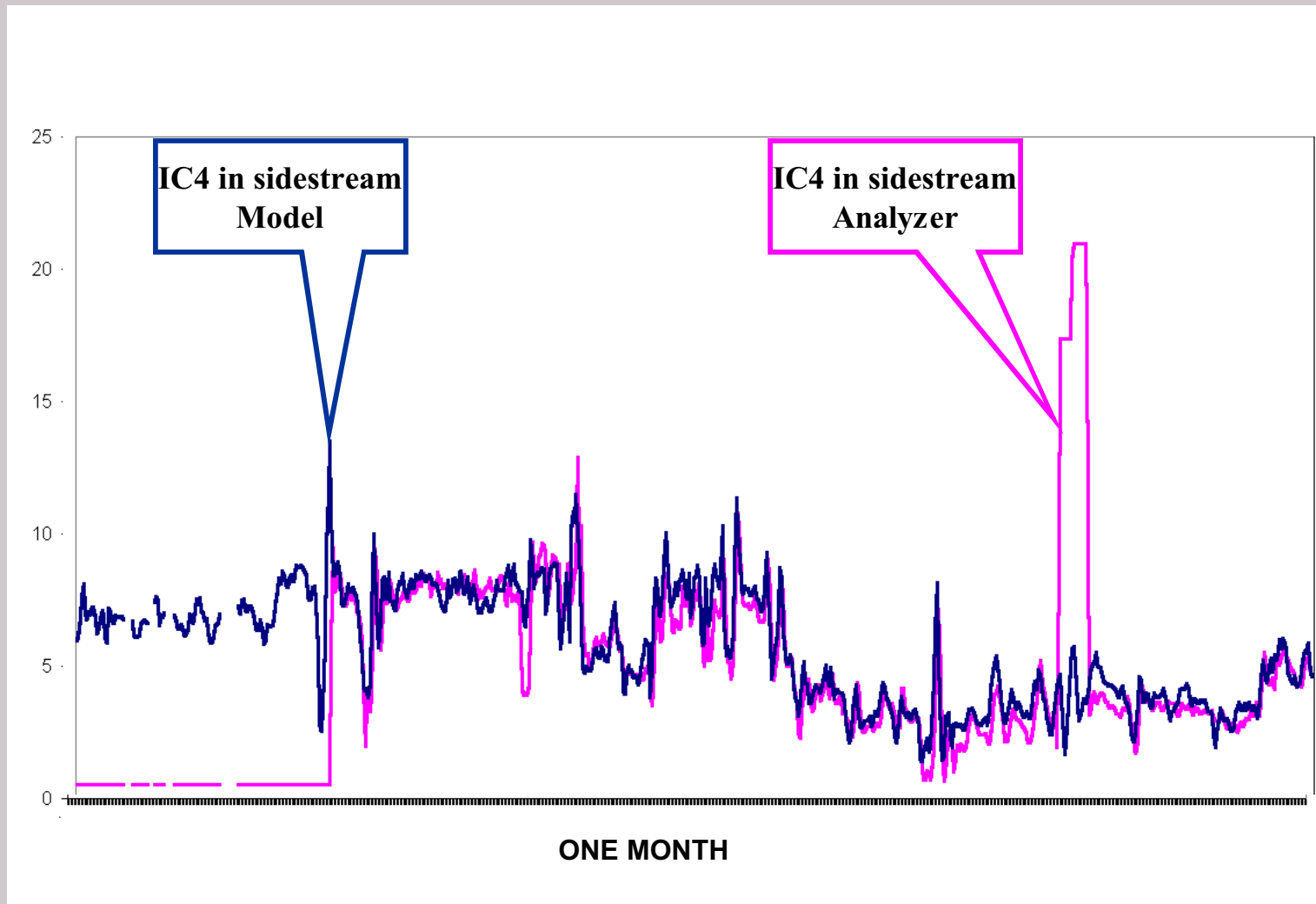


Figure 17. Alky Deethanizer

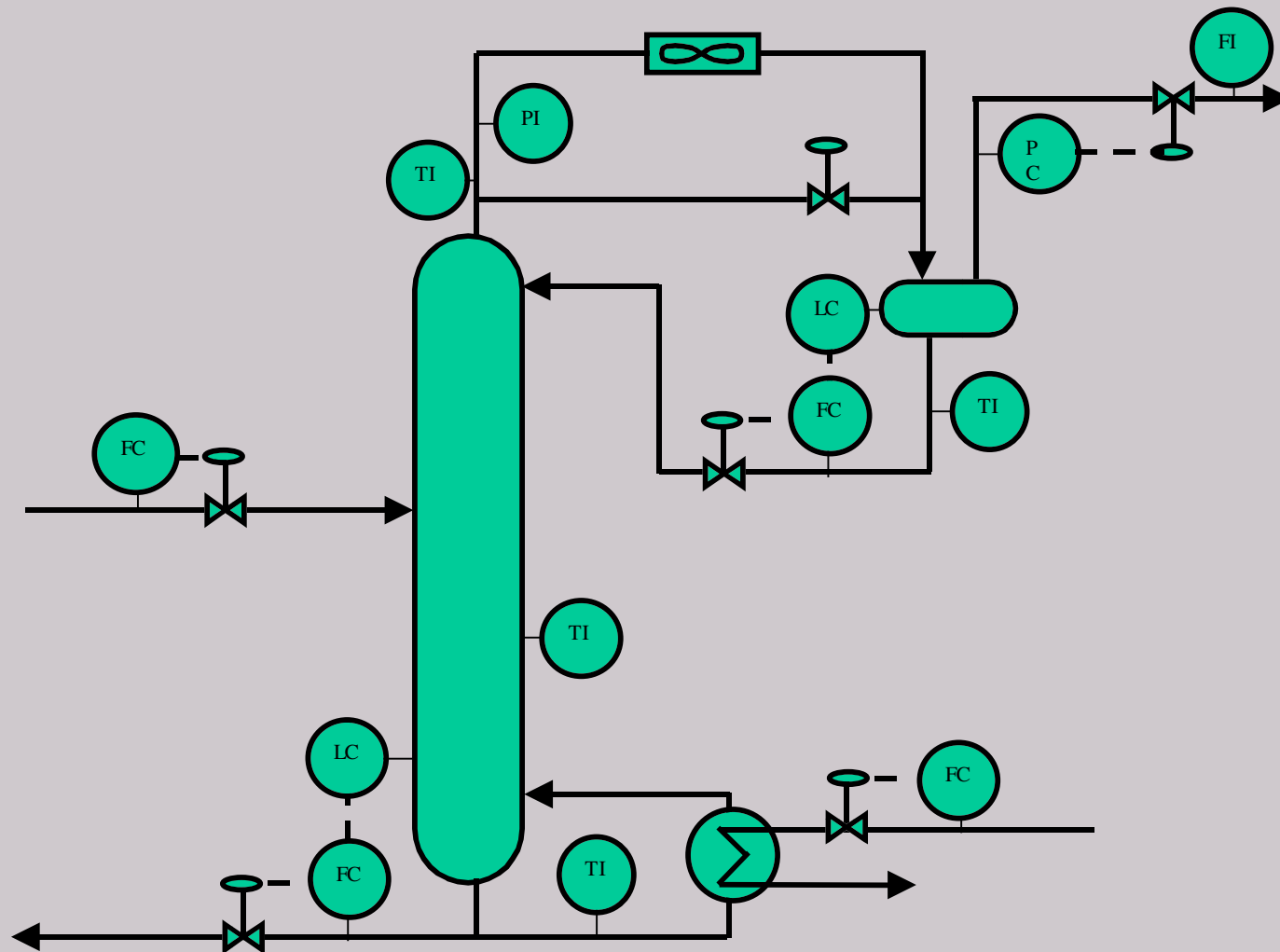


Figure 18. Alky Deethanizer Inference

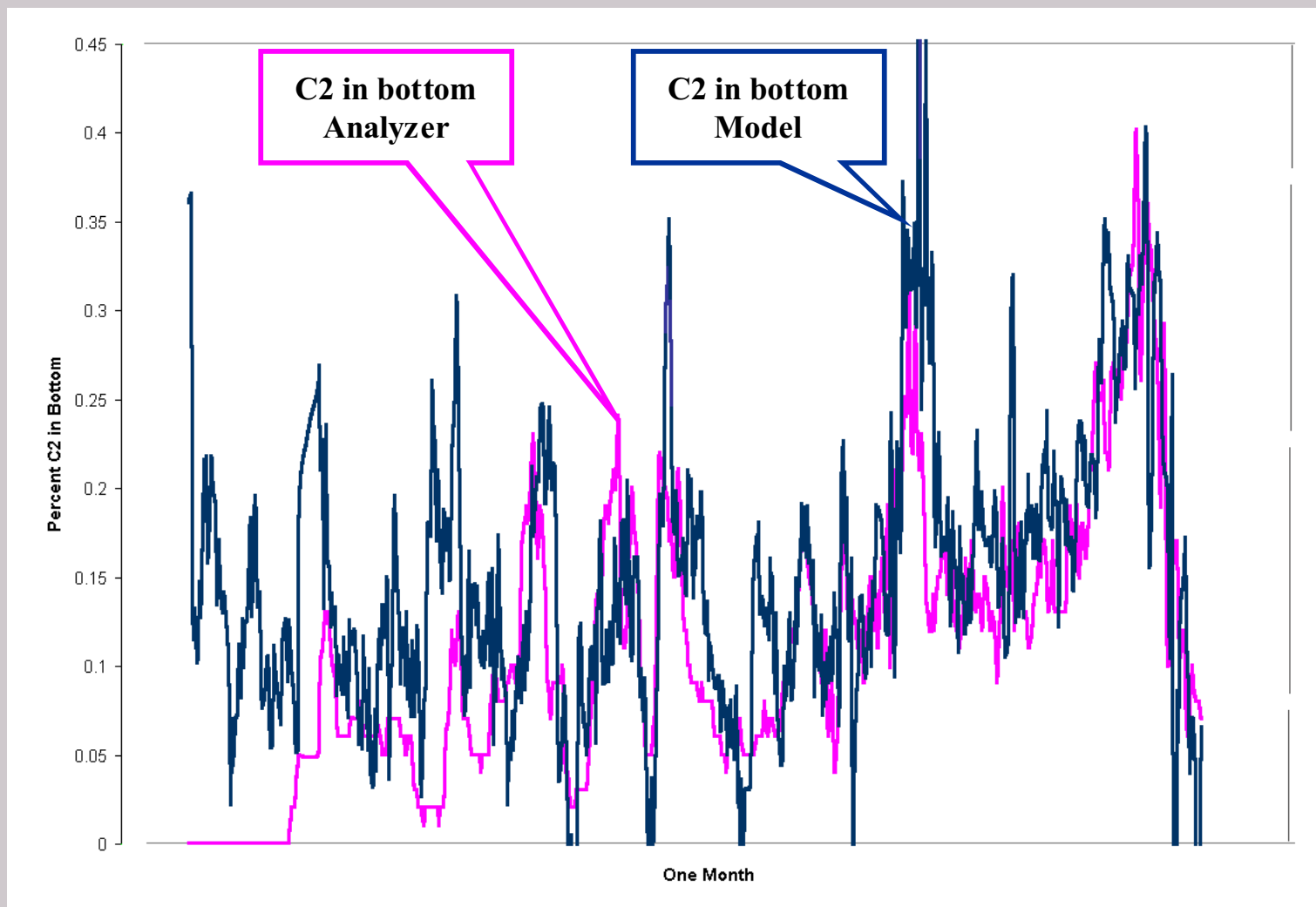


Figure 19. Alky Depropanizer

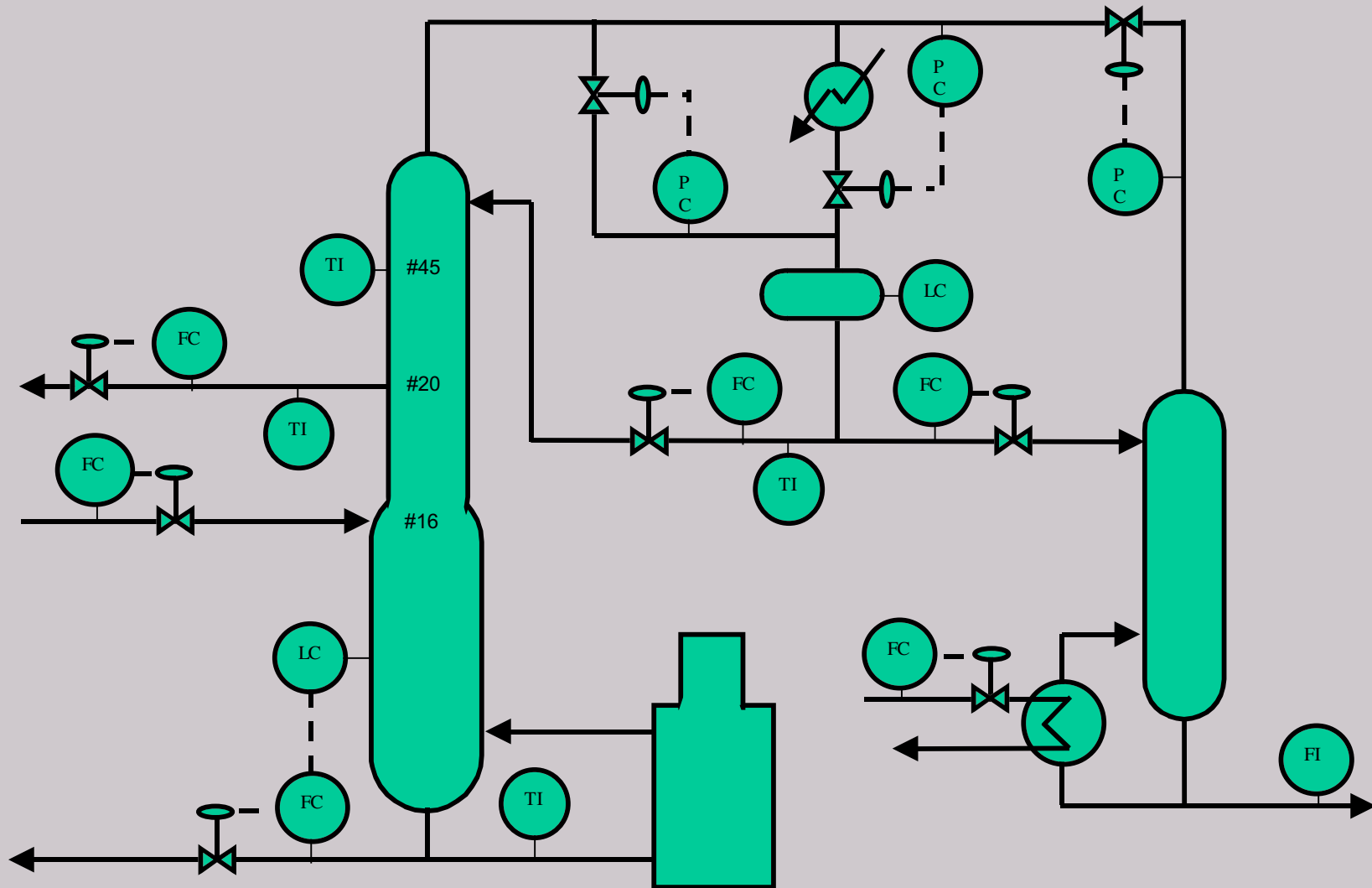


Figure 20. Alky DeC3 Top Inference

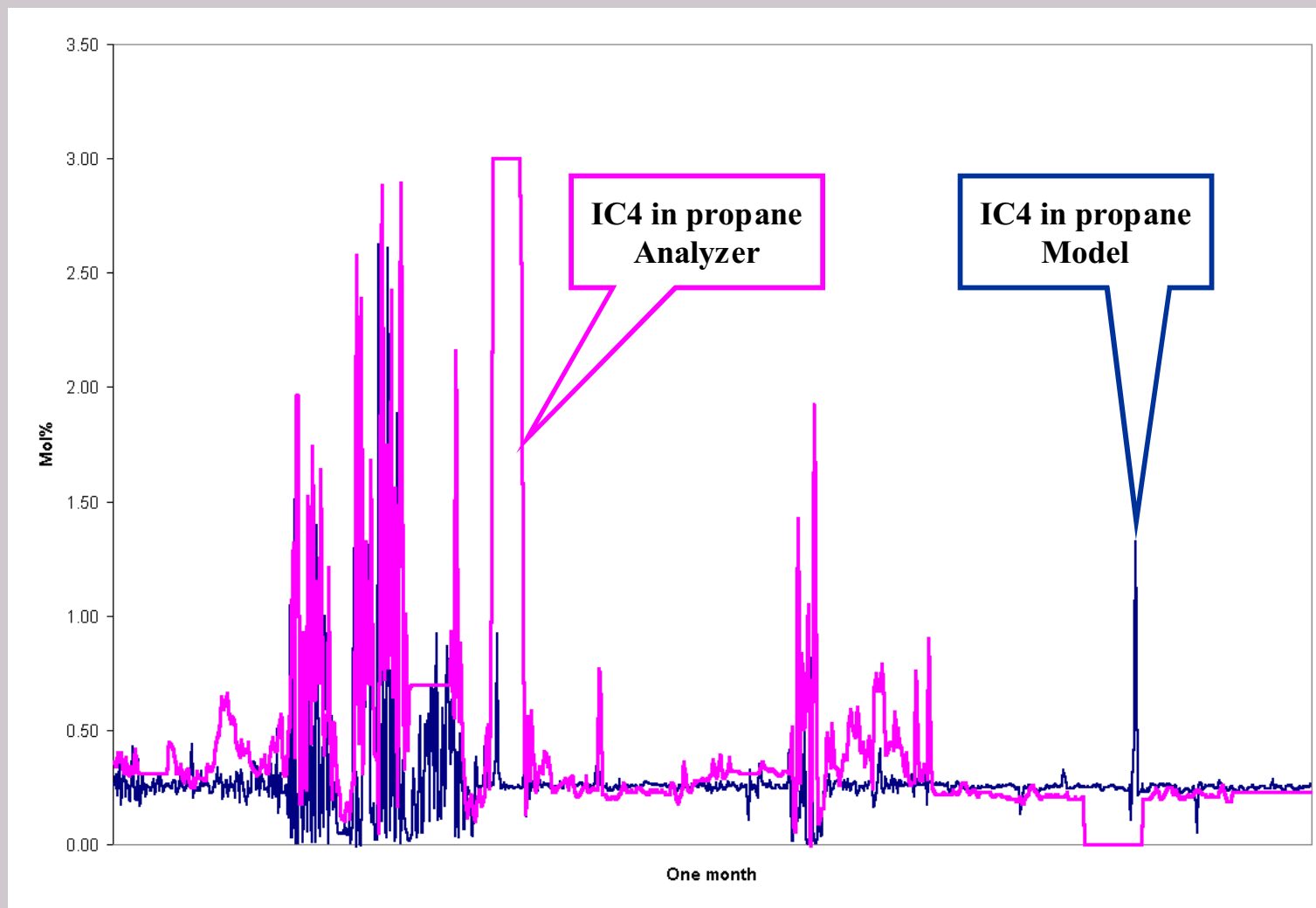


Figure 21. Conclusion

First principle distillation inference models are the facilitator for maximization applications

