

First-principles inference model improves deisobutanizer column control

When the input data are clean, model fidelity is better than that of onstream analyzers

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A generalized distillation shortcut (GDS) model was implemented on an alkylation unit deisobutanizer (DIB) column. GDS employs first-principles models by way of a short-cut simulation of a column section, hence the name of the model. GDS works by fitting a bottom (or top) column composition that would best agree with the column temperature profile. The advantage: this approach correctly accounts for the very nonlinear effects of temperature, pressure and vapor-liquid ratio.

The DIB column separates alkylation reactor effluent as shown in Fig. 1; alkylate (C_8) at the bottom, normal butane (nC_4) as a sidestream and isobutane (iC_4) at the top. As a valuable reactant, iC_4 is circulated back to the reactor, whereas nC_4 is an inert to be removed from the process. Given the close proximity of boiling points, nC_4 would necessarily carry with it some iC_4 , and the main advanced process control (APC) objective is to minimize those iC_4 losses. On the other hand, the APC should not be too

aggressive in eliminating iC_4 loss because that would suppress nC_4 removal, causing a buildup of nC_4 in the reactor and ensuing octane and yield losses.

To assess the APC benefit of controlling a DIB tower, consider a 30,000 bpsd unit, where it is possible to cut iC_4 loss by 200 bpsd (1% of the iC_4 feed). This improvement of the iC_4 balance amounts to \$0.8 million annually. In addition, avoiding the octane and yield loss associated with nC_4 buildups are typically worth another \$0.4 million.

United Refining Company (URC) purchases isobutane from Midwestern locations, where it is separated from mixed butane streams. Therefore, the price difference between iC_4 and nC_4 bears the price of transporting isobutane to the site and transporting unrecovered isobutane back. The DIB tower at URC is smaller and the benefit identified for just eliminating iC_4 losses is approximately \$0.2 million annually.

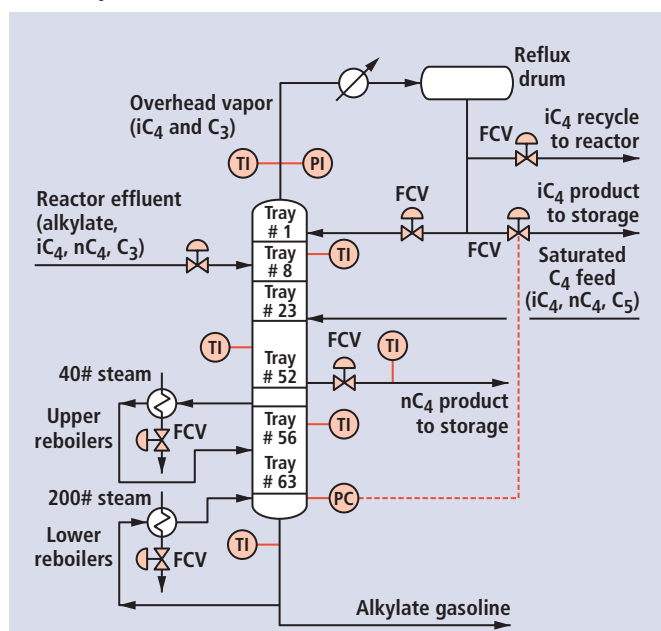


FIG. 1. The DIB column separates alkylation reactor effluent.

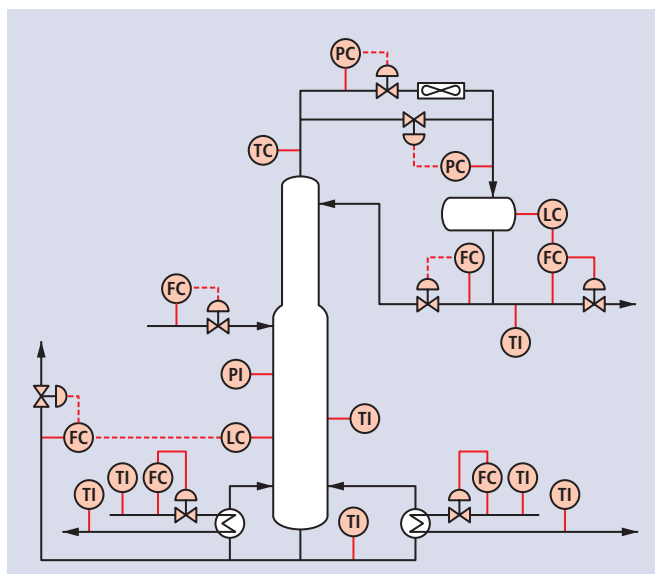


FIG. 2. Measurements available on the FCC debutanizer.

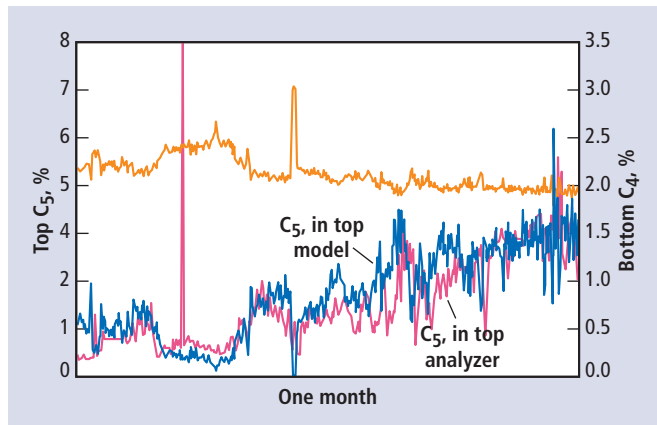


FIG. 3. This trend of the top and bottom impurities shows several problems with the analyzer.

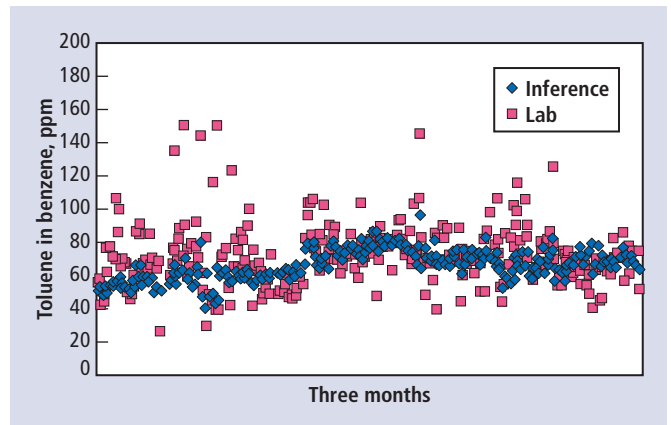


FIG. 4. Lab results for toluene in benzene varied almost randomly between 20 and 160 ppm.

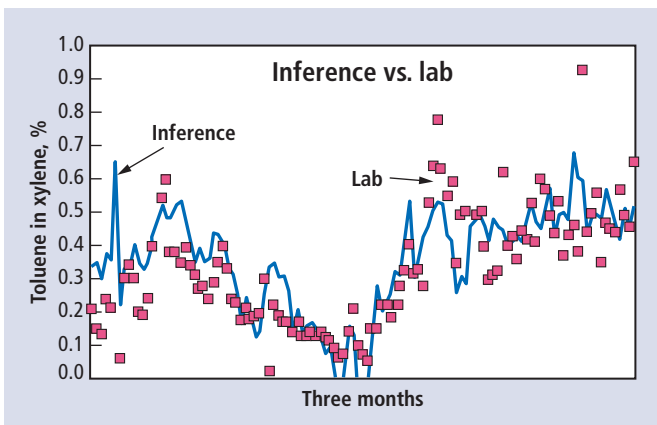


FIG. 5. The model and most lab data are in agreement.

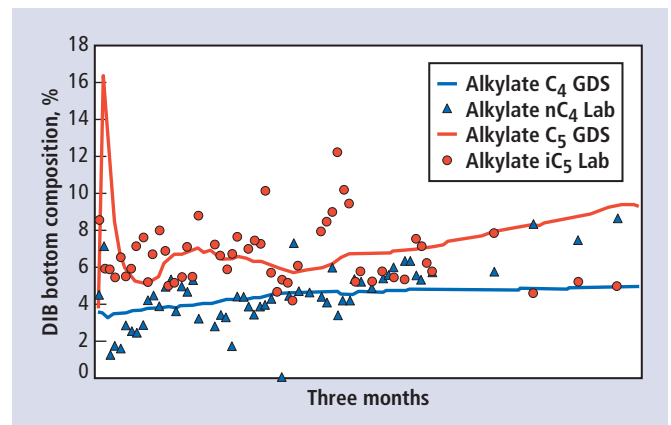


FIG. 6. While the lab values exhibit high variability and some improbable numbers, the fit is reasonable.

GDS experience. GDS employs distillation purity inferential control models that make use of chemical engineering principles. We published the model principles in 1995,¹ though at that time data to judge prediction performance was not yet available. Since then, about 40 models have been implemented. Such a large number of applications has permitted a thorough evaluation of the GDS prediction fidelity. The first evaluation was published in 2001.² That article compares model prediction versus analyzer readings on several distillation columns at the Texaco Pembroke refinery.

Figs. 2 and 3 show one simple example from the Pembroke article, addressing a debutanizer column. Fig. 2 is a diagram of the column, highlighting the available measurements. GDS modeled both top and bottom purities on the debutanizer. Fig. 3 trends the top and bottom purities and shows the agreement between the top analyzer (C_5 in LPG) and model. The agreement is not perfect, and it is difficult to judge which signal is more correct. There clearly are several problems with the analyzer:

- Occasional periods of a frozen signal
- Occasional unexplained jumps
- Periods where the analyzer reading is very sluggish, lagging several hours behind the inference.

In the end, Pembroke decided that the model results were better than the analyzer. This inference has since been working in closed loop.

The main conclusion from the Pembroke article was that

where key model input measurements existed, the inference models are excellent. Whereas when input data are imprecise and we are forced to make assumptions—the models might not be exact—though they could still be useful for closed-loop control.

Following the Pembroke experience, we worked on a benzene, toluene, xylene (BTX) unit at the Petrobras RPBC refinery, where we tackled two intricate problems. The first application involved a benzene superfractionator whose benzene purity specification is 200 ppm. Inference at that impurity level has never been tried before, not only because the ppm level prediction is difficult, but also because it is challenging to calibrate, given that the lab test repeatability is about 50 ppm. The second BTX application dealt with separating toluene from xylene, done by two parallel but different columns, with insufficient set of measurements and a common lab sample point.

We reported the benzene superfractionator experiment in another article.³ Fig. 4 illustrates the lab repeatability problem. Lab results for toluene in benzene varied almost randomly between 20 and 160 ppm, whereas the GDS inference model showed that in reality there was little change in unit conditions. The unit operators were not oblivious of the lab repeatability issues and they responded to lab results with much caution, because incorrect actions could drive either toluene or benzene off spec. Usually the lab result would indicate that product contamination is within specification, and no further action would be

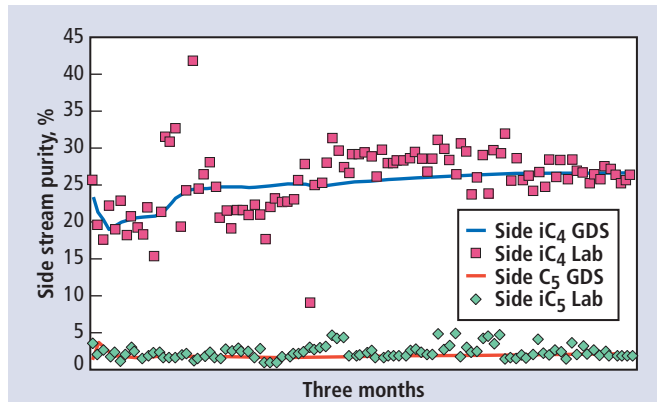


FIG. 7. Considering that taking a butane lab sample is complicated, variability of the lab samples should not be surprising.

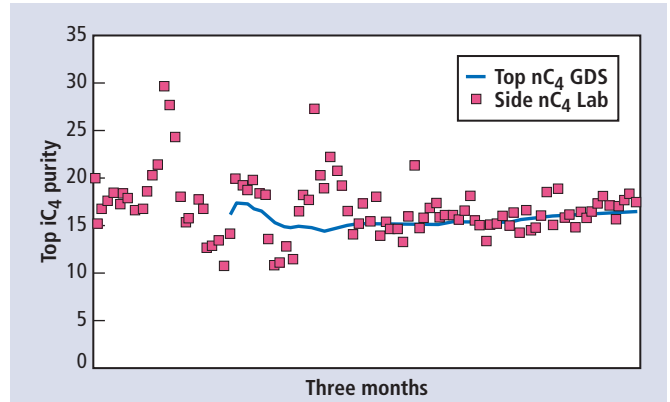


FIG. 8. In spite of the unusual temperature measurement solution, modality fidelity is reasonable.

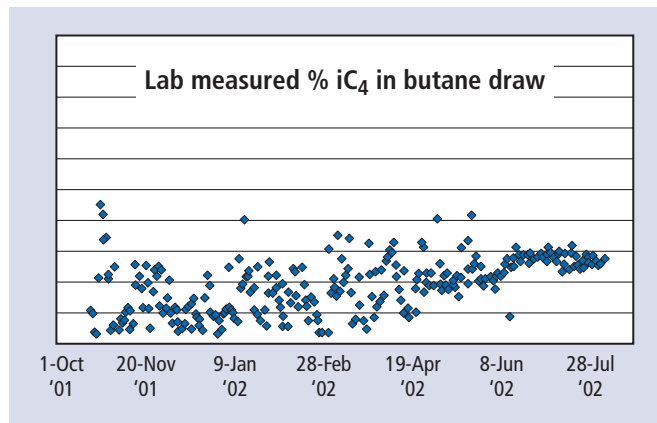


FIG. 9. Control performance improved dramatically in June 2002.

taken. Occasionally the result would come off spec, and then the operator would order another sample before acting. What had been overlooked was that while the specification is 200 ppm the column was producing benzene at about 80 ppm, and RPBC was paying a high energy and capacity penalty for the purity giveaway.

The toluene-xylene separation problem was reported at the 2002 ERTC Computer Conference.⁴ Incomplete input measurements and common lab samples for the two columns have forced us to make assumptions. Such assumptions degrade the quality of inference, but eventually workable models were obtained. Fig. 5 shows one of these models as an example. The model and most lab data are in agreement, and the inference is now working in a closed-loop service.

Our conclusion from the RPBC project is that when dealing with an incomplete set of inputs, it is possible to make certain assumptions and obtain workable closed-loop models. However, such models would need a higher level of lab support.

URC DIB column. URC had a problem keeping the alkylation unit steady. The alkylation reactor effluent contains about 15% alkylate (C₈), 70% isobutane (iC₄), 10% normal butane (nC₄) and 5% C₃ and C₅ impurities, to be separated in the DIB column. In addition to reactor effluent, the column receives a second feed stream of mixed butanes with variable amounts of C₅ impurities. The column (Fig. 1) separates the two feed streams, taking iC₄ and

C₃ at the top, nC₄ as a tray 52 vapor sidestream and alkylate plus C₅ impurities at the bottom. Given the close proximity in boiling points, separation of iC₄ and nC₄ would necessarily be incomplete, even with a 63-tray column. Normal operating practice is to permit the top iC₄ to contain about 10% nC₄ and minimize iC₄ loss to the sidestream. Further, the desire is to take essentially all of the C₅ at the bottom, plus some C₄, subject to Rvp constraint.

Operators try to reduce the nC₄ purge sidestream to cut iC₄ losses. That is a good idea as long as the nC₄ entering the unit is adequately purged. If not purged, nC₄ would build up, causing incorrect reactor operation—with associated product octane and yield loss. Prior to GDS implementation, URC took lab samples only once each day, which was not often enough for early identification of nC₄ buildups. When buildup did occur, the operator would start drawing a large amount of sidestream, regardless of how much iC₄ is lost. The alkylation unit thus ended up cycling between octane and yield loss and iC₄ loss.

Varying amounts of C₅ contamination in the butane feed presented another problem. The bulk of C₅ must leave the column as liquid with the bottom alkylate product. When more C₅ comes into the column, the operator must reduce the bottom temperature to permit absorption of liquid C₅ in alkylate, or else C₅ would accumulate and flood the bottom section. However, the operator is not aware of C₅ contamination until the column is already flooded.

Bottom inference model. We deal with the bottom C₅ and C₄ control problem by predicting their bottom content and controlling C₄ to a 5% target in summer or 2% in winter. The column section between trays 59 and 63 lends itself to a GDS model solving for three components: nC₄, C₅ and alkylate C₈. Having implemented that control logic, we quickly found that we needed to add an Rvp constraint because when the bottom C₅ content was high, C₄ content must be reduced to avoid gasoline blending Rvp difficulties.

Fig. 6 shows performance of this model compared with lab values. While the lab values exhibit high variability and some improbable numbers, the fit is reasonable; most predictions lie within two standard deviations of the lab tests. Judgment of the inference model validity should take into account known lab accuracy problems. First, the bottom lab sample is taken in a corked bottle, which tends to lose light components over time. Second, certain lab results are not consistent with column thermodynamics.

Thermodynamic considerations dictate that the C₅ concentration in the side draw is about one-third of the C₅ bottom concentration, whereas that is not always the case with the lab tests. We

conclude that while possibly not completely accurate, the model prediction appears to be more helpful to the operator than lab tests, because it is not subjected to the large random error of the lab. Our bottom C_5 model does predict a C_5 buildup correctly. The controller does purge the C_5 with the bottoms, alleviating the flooding problems, while keeping the Rvp within specification.

Sidestream inference model. Having dealt with alkylate Rvp and C_5 purge control, we next tackled the nC_4 purge and iC_4 loss problem by predicting sidestream composition and controlling it to a constant target. Our hope was to limit iC_4 loss to about 1% of the iC_4 feed, which translates to about 5% iC_4 in the sidestream. Once the sidestream composition is under control, setting internal reflux ratio to a reasonable target would guard against buildup of nC_4 at the top. We initially chose that approach because the tower did not have a temperature measurement near the top to support a top GDS model.

The middle section between trays 37 and 52 handles four components: iC_4 , nC_4 , C_5 and C_8 . The model first simplifies the problem, estimating the heavy C_8 concentration on both trays 37 and 52 by a mass balance against the bottoms, making use of the fact that C_8 is not volatile at middle section conditions. As a second step, the model estimates C_5 content in the section.

C_5 requires a more elaborate model because it is somewhat volatile on tray 52 and some of it leaves with the sidestream. However, knowledge of the thermodynamic ratio between the sidestream (tray 52) vapor C_5 concentration and tray 52 liquid C_5 concentration makes it possible to calculate the concentration of tray 52, as well as tray 37, again with the help of mass balance against the bottom composition. Following the calculation of C_5 and C_8 , the GDS model for this section has only two unknowns: iC_4 and nC_4 .

Fig. 7 exhibits trends of the sidestream C_5 and iC_4 predictions versus lab values over a three-month period. Considering that taking a butane lab sample is complicated, variability of the lab values should not be surprising, and we would judge the fit as reasonable on that basis. The C_5 fit is actually better than that of the bottom model.

At that point we started controlling the side iC_4 content to about 5%, a target that column should be able to satisfy without building up nC_4 in the reactor. The column control was working well in the sense that it was keeping the sidestream composition at target, but to our surprise the column was unable to purge all the C_4 at those conditions. We had to go to nearly 30% iC_4 in the sidestream to avoid a buildup of nC_4 . An analysis of the data showed that the column had lost performance and its tray efficiency is below 50%. URC then conducted a nuclear liquid profile test on the column, which confirmed moderate-to-severe entrainment throughout the column. The entrainment is likely due to tray fouling caused by tray corrosion and acid ester deposition.

Top inference model. With the tower being blocked, the feasible sidestream target became dependent on throughput. We had to continue to rely on frequent lab analyses of the top stream to ensure that the reactor nC_4 content is acceptable. We, therefore, decided to try a model for the top nC_4 content. Even a very approximate model should be able to show a buildup trend, alarming the operator to take a lab sample quickly. Such a feature would be useful until the column can be shut down for cleaning.

The top stream is mostly iC_4 with C_3 and nC_4 contaminants. If not for the C_3 , a simple top temperature measurement would suffice to detect the nC_4 concentration, but that was not an option, since C_3 comes with the feed in unknown quantities. It was also impos-

sible to make use of the accumulator to estimate the C_3 because the accumulator is flooded and subcooled. The only way to construct a reasonable GDS model at the top section of this column was to install a temperature measurement on a tray near the top.

At the suggestion of the instrument department, they installed a "tray-4 temperature measurement" by placing a thermocouple underneath the column insulation. A second couple was inserted under the insulation in the proximity of the top temperature measurement to estimate the measurement error. The delta top temperature error was added to the external measurement on tray 4, and that signal was used in our top GDS model. In any other respect it was a standard GDS model as described in our previous article.

Fig. 8 shows performance of our approximate top nC_4 inference model against lab tests. The inference curve starts about one month later than the other models because, as previously explained, we did not initially intend to have a top model. In spite of the unusual temperature measurement solution, model fidelity is reasonable. As opposed to the bottom and side models, which are not recalibrated often, we do permit frequent recalibration of the top model. However, the recalibration option was not overused and the trend of Fig. 8 had a constant calibration through the two-month model activity period.

Control performance. It would be of interest to have another look at Figs. 6, 7 and 8. These figures cover the same three-month period. At the outset of this period, models were being introduced to operators. After an initial open-loop test, the models were either placed in closed-loop service or the operators had learned to manually close the loop.

After a first month of fairly unstable operation with lab results badly scattered, the operation began to stabilize in the second month. In the third month, it became very stable with almost no lab scatter. Fig. 6 shows more scatter, indicating that the feed C_5 contamination continued to vary. Then during the third month, the C_5 in feed became more stable. We believe that since any feed C_5 contamination quickly shows up in the bottom C_5 inference, it is possible for the operator to detect and eliminate problems in upstream columns.

Fig. 9 is taken from the refinery post project audit report. It shows a trend of the sidestream lab analysis over an eight-month period. For comparison, the period of Figs. 6, 7 and 8 is toward the end of that of Fig. 9, though Fig. 9 continues for several more weeks. This figure demonstrates how control performance improved dramatically in June 2002. A look "between the lines" of Fig. 9 shows how the reality of column tray blockage gradually sank in.

At the beginning of the period, operators would try to lower the iC_4 loss, only to encounter reactor nC_4 buildup and loss of octane and yield. They would then go into a quick purge mode with high iC_4 loss, and the unit would oscillate that way about once every two days. Following our better understanding and better control, we are able to keep the column at steady targets, which are the best that this equipment can achieve. In several months, the column is to be cleaned and our targets will then be adjusted to maximum column performance. **HP**

LITERATURE CITED

- 1 Friedman, Y. Z., "Simulation Based Inferential Control," AIChE spring meeting, 1995.
- 2 Friedman, Y. Z. and G. T. Reedy, "Experience With GDS—A First-principles Inferential Model for Distillation Columns," *Petroleum Technology Quarterly*, fall 2001.

³ Friedman, Y. Z., E. A. Neto, C. R. Porfirio, "First-Principles Distillation Inference Models For Product Quality Prediction," *Hydrocarbon Processing*, February 2002.

⁴ Friedman, Y. Z., E. A. Neto, C. R. Porfirio, "First-Principles Distillation Inference Models For Controlling A Toluene-Xylene Splitter," ERTC Computer Conference, June 2002.



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