Originally appeared in HYDROCARBON PROCESSING® February 2005, pg 17-18. Posted with permission.

Y. ZAK FRIEDMAN, CONTRIBUTING EDITOR

Zak@petrocontrol.com

More about inferential control models

My friend and colleague, Myke King, wrote an article[1] proposing rules for dealing with inferential control models. For the most part, I agree with the arguments, and especially enjoyed the funny illustration of how a supposedly high-fidelity inferential model failed to predict stock disasters. However, I have issues with two of Myke's points: how to assess inferential model performance and the benefit of engineering models vs. regression models.

Plotting preferences. Advice 3 in the article argues that trending an inference model against lab results tricks the eye into believing that an inference is performing well, whereas an X-Y scatter plot of the model against lab results would reveal a much larger scatter. Nevertheless there are arguments in favor of simple trending as follows:

1. **Time interpretations of inference and lab are different.** Inference models read current process measurements directly placed on the equipment of interest, whereas lab samples are taken downstream of process equipment and heat exchangers from a sample point that is reached long after the product has left the main process equipment. Two hours for many units is not a bad estimate.

Thus, comparison of a three o'clock lab result against a single inference reading at three o'clock is not an "apples to apples" comparison. The trend plot is much more telling because one can train the eye to take the time delay into account in the lab vs. inference comparison.

2. **The inference would likely lead even more because of its predictive nature.** Inferences are by and large steady-state models, and, to avoid control problems, slow inputs to an inference model—such as temperatures—must be corrected dynamically. The need to correct the dynamics of inferential model inputs is noted in Myke's advice 7, and such dynamic prediction makes the inference also predictive. Following dynamic correction, the inference model calculates not the property of current product, but rather what the property would come to—should all manipulated variables stay put. Predictive techniques easily add an hour or more to the inferential lead.

3. **Monitoring lab sample times is not easy.** Advice 13, to keep track of the precise lab sampling time is easier said than done. Lab technicians are busy enough taking a large number of samples over a span of two hours, and if they are forced to also keep the time of each sample, they quickly slip into a habit of marking the same time every day.

4. **Lack of steady state.** Further, the unit is often not at steady state, particularly when driven by advanced process control (APC) against constraints. Comparisons of one inference point at a certain time, even if we can assess that precise time against a single lab point, is meaningless. The trend advantage is that it lets us view the inference hours before and after the official sample time and observe the unsteady-state behavior.

5. **Event identification.** Fig. 1 shows a recently developed model, which is obviously a decent inference trending well against the lab, but it has two periods of discrepancy. First, from mid-March to mid-April, the model is biased 5°C down; in May, June and July, it is biased 5°C up. Further investigation revealed that one flowmeter was suspect, and unit mass balance was off during March and April. Then, the meter was calibrated at the end of April, causing a mass balance error in the other direction. In practice, such events are unavoidable and are dealt with by inferential bias changes or by the operator shifting the targets, but we can identify such events only by trending. The high-fidelity inference of Fig. 1 would show poorly on an X-Y scatter plot.

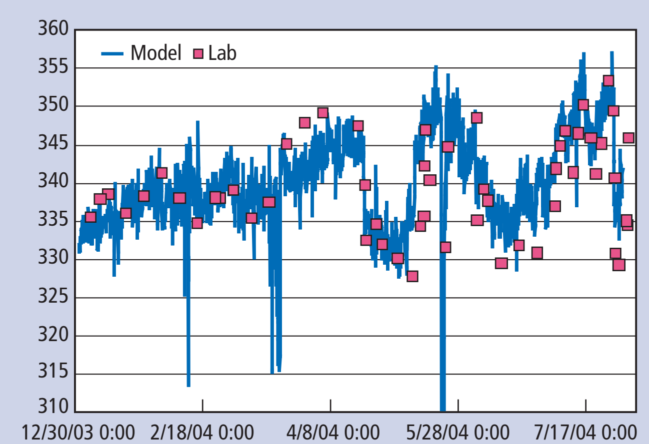

FIG. 1 This seven-month trend of inference vs. lab readings would show poorly on an X-Y scatter plot.

Myke recognizes that a good-looking X-Y plot is not necessarily a sign of high fidelity, and he illustrates a funny example of failing to predict stock disasters. The opposite is also valid: Poorly looking X-Y plots are not necessarily a sign of a bad model. One has to evaluate them in the time domain to discover more. The condition for valid model evaluation is real activity in the data: change of targets and operating conditions, of magnitude that is several times larger than the ranges of lab repeatability and process noise.

Engineering versus regression models. In a reference to one of my articles,[2] Myke acknowledges that engineering-based inferences have certain advantages, but he goes on to say that disadvantages are model and maintenance costs. Being an ardent supporter of the scientific approach to inferential modeling, and also being a supplier of such models, I would challenge that high cost statement. When the need for lab support is taken into account, cost and complexity of regression models skyrocket. The following points summarize the overwhelming advantages of engineering models and explain why the lab support requirements of regression models are high.

1. **Regression requires independent inputs.** Whereas Gaussian

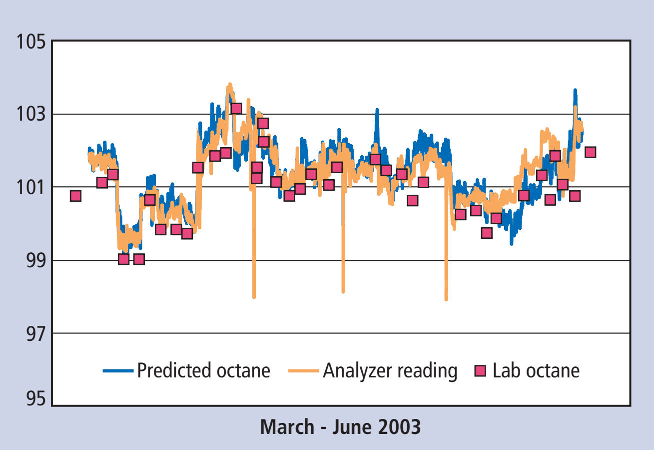

FIG. 2 After one year, the model has retained its original fidelity.

theory requires that regression inputs be independent, that is not achievable on our process equipment. Temperatures, pressures and flows are related in several ways: mass balances, heat balances and equilibrium equations. Ignoring these relations makes the modeling process theoretically incorrect, and such models would drift on changes in process conditions.

2. **Empirical models require large volumes of lab data.** Regression requires hundreds of laboratory data. This poses a problem. A fair percentage of daily lab data is biased, and reliable process data are obtainable only by test runs.

There is no hope that the quantity of lab data needed for regression would come from high-quality test runs, and empirical model developers have to rely on imprecise, everyday lab data: imprecise because it permits occasional spike contamination, sampling during process changes, inappropriate sampling procedures and long delays between sampling and testing. Myke's advice 12, to avoid use of daily lab data in developing an inference, is doable for first-principles models but infeasible for regression models.

3. **Empirical models must identify a large number of coefficients.** Scientific models incorporate model gains inherently, and the calibration procedure amounts to adjusting one or two parameters. One example is tray efficiency and weight in a weighted-average formula. The effect of signal-to-noise ratio on such a calibration procedure is minimal.

Empirical models, on the other hand, must identify 10 to 50 coefficients. That is a problem because normal day-to-day operation may not provide enough movement in the data to permit identifying many coefficients.

4. **First-principles models provide the means for checking instrument errors.** The sister problem of erroneous lab data is erroneous instrument data. Instrument errors occur due to poor calibration, partial plugging of orifice meters, improper installation, incorrect meter range and, finally, computer interface errors. First-principles models cannot hide such problems, as Fig. 1 demonstrates. In contrast, the large number of regression coefficients can hide almost any instrument problem and come up with a useless model.

5. **There is no replacement for process engineering.** And what if the measurements set is inadequate? A key measurement could be missing or in the wrong location. To obtain a good model, the set of measurements ought to "have the inferential information in them." A first-principles modeler would identify an insufficient set of inputs at the outset by a simple sensitivity study. The empirical modeler would go through model development, and the problem would only be found at the time of model validation.

6. **Ability to survive process modifications.** During turnarounds, units are often modified by replacing trays, cleaning heat exchangers, etc. Any inferential model would need to be recalibrated upon equipment modifications. First-principles models might require equation coefficient changes, but empirical models would be turned off for several months until a meaningful set of lab data is accumulated and the model redeveloped from scratch.

As a further illustration of first-principles modeling fidelity, consider Fig. 2. This is a three-month trend of an inference model, predicting reformer octane on a CCR unit against octane NIR analyzer and lab readings. Usually, people publish inferential comparisons from the time of evaluating the inferential model immediately before or after installation. Fig. 2, however, is taken one year after the model was accepted and paid for by the client. It can be seen that the model has retained its original fidelity. It tracks well, having no bias with respect to the analyzer and a small bias of 0.3 octane numbers against the lab.

I come now to Myke's most important argument: Black-box models do not work. I agree with that assessment whole heartedly. There ought to be a person onsite who understands the model and is in charge of maintenance. In my opinion, that requirement is not unique to first-principles models. Advice 5, to avoid developing a regression model without a thorough understanding of the unit, leads to a similar conclusion.

Inferential models are developed via the use of process knowledge, and, if such knowledge is only partially available at the site, it would be productive to retain the services of the original model developer. Having said that, I know sites that manage to keep first-principles models running for many years with support of a local APC engineer and minimal outsourcing. Whereas, if no one is assigned locally for APC maintenance, no model is long lived.

Modified advice. In summary, modified advice on inferential modeling is in order: Where the knowledge exists, try to develop inferential models based on chemical engineering principles. If complete knowledge is not available and you must employ regression, go for engineering inputs rather than simple measurements. For example, prefer use of heat duties over input of flows and temperatures, use pressure-compensated temperatures, etc. The more you use chemical engineering, the better the model. If you purchase a first-principles model, avoid black boxes and train the APC engineer to support the model. If possible, test the model long before you use it in closed loop. **HP**

LITERATURE CITED

1 King, M. J., "How to lose money with inferential properties," *Hydrocarbon Processing,* October 2004.
2 Neto, E. A., C. R. Porfirio and Y. Z. Friedman, "First-principles distillation inference models for product quality prediction," *Hydrocarbon Processing,* February 2002.

Y. Zak Friedman is a principal consultant in advanced process control and online optimization with Petrocontrol. He specializes in the use of first-principles models for inferential process control and has developed a number of distillation and reactor models. Dr. Friedman's experience spans over 30 years in the hydrocarbon industry, working with Exxon Research and Engineering, KBC Advanced Technology and in the past 12 years with Petrocontrol. He holds a BS degree from the Israel Institute of Technology (Technion) and a PhD degree from Purdue University.