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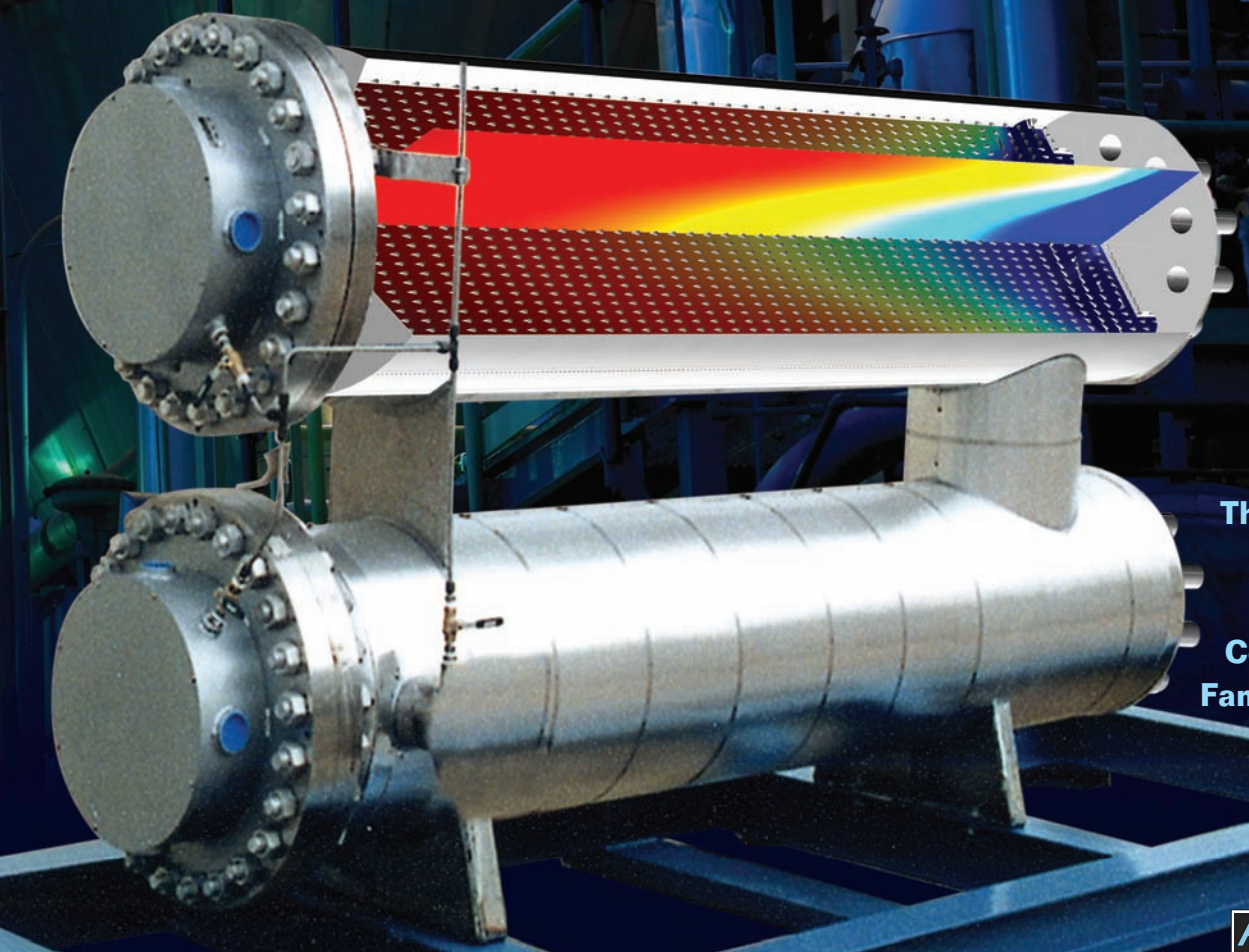

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Process Modeling Moves Center-Stage

A model solution for the CPI: reducing risk while increasing profit

Mark Matzopoulos
Process Systems Enterprise Ltd.

Process modeling has progressed from the "molecule accounting" of steady-state flowsheeting packages to become a central platform for capturing and deploying chemical process industries' (CPI) intellectual property (IP). Systematic modeling has moved center stage to help companies differentiate themselves from their competitors while also providing a set of tools with which it is possible to adapt rapidly to changing market conditions.

The traditional approach

Until recently, process modeling usually meant "process simulation", and simulation typically meant either performing flowsheeting studies using a commercial program, running an in-house Fortran model of a reactor, or performing a computational fluid dynamics (CFD) analysis of the fluid flows inside a stirred tank.

Each of these activities still has a valid place in the panoply of techniques deployed within the CPI to generate information for design and operational decisions. Indeed, each has unique advantages: process flowsheeting tools are easy to use and generate heat and material balances and basic equipment-design information quickly; in-house programmed models embody valuable corporate knowledge collected over many years; CFD tools can model individual units to a very high level of mechanical detail for detailed equipment design.

However, besides the fact that each of the approaches outlined above is usually pursued largely independently with little overlap between either the software or the groups of people doing the work, each has its own limitations. Flowsheeting is effectively a "molecule accounting" exercise that uses standard off-the-shelf (and "black-box") models that are not able to reflect the complexity of many common processes, particularly in industries other than the traditional oil-and-gas and petroleum-refining base. In-house programmed models are often inflexible and difficult to maintain, and have the added disadvantage that the knowledge of the code and the assumptions inherent in the model typically reside in one or two individuals; they also tend to be limited to single units and cannot deal with the surrounding flowsheet. CFD models generate high accuracy information on fluid flow and mixing, but are not ideally suited to handling complex chemical phenomena such as crystallization and polymerization occurring within the fluids — information that is of critical importance to the process designer or reaction engineer.

In addition, none of these traditional approaches deals effectively with process dynamics, meaning that it is not possible to design for transient conditions. This is the chemical engineering equivalent of architects being restricted to designing in two dimensions, and it limits or eliminates application in the whole area of batch processing.

Notwithstanding the drawbacks of the traditional approaches, in recent years modeling as a whole has taken on a much-more-elevated and central role within the CPI, from the mainstream chemical manufacturers in Japan and Korea to catalytic technologies providers such as Süd-Chemie, fuel cell companies such as UTC Power and Toyota and food manufacturers such as Friesland Foods.

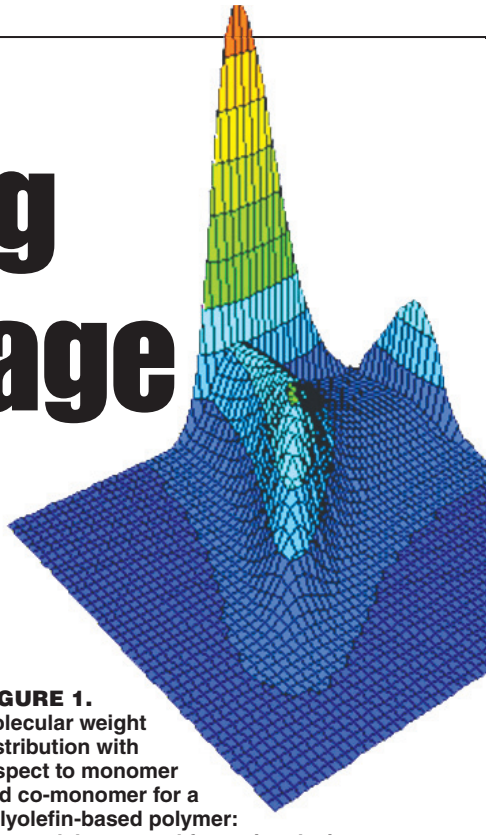

FIGURE 1. Molecular weight distribution with respect to monomer and co-monomer for a polyolefin-based polymer: The model was used for recipe design for production of a new grade of polymer

What has brought about this change? Well, for a start, modeling tools and methodologies have matured significantly. Concerted research, investment in software implementation and successful application to large-scale systems have gone a long way to overcome the limitations described above. The net effect is that it is now possible to model complex chemical processes to a high degree of predictive accuracy, to the point where models provide reliable quantification for support of many key design and operating decisions and — crucially — for management of the IP and the risk associated with innovation.

Secondly, new methodologies have been devised, refined and proven. Current tools allow the incorporation of experimental data — laboratory, pilot and plant — into models in order to ensure that they reflect observed reality. If performed correctly, this can provide models with a predictive capability that is virtually scale invariant.

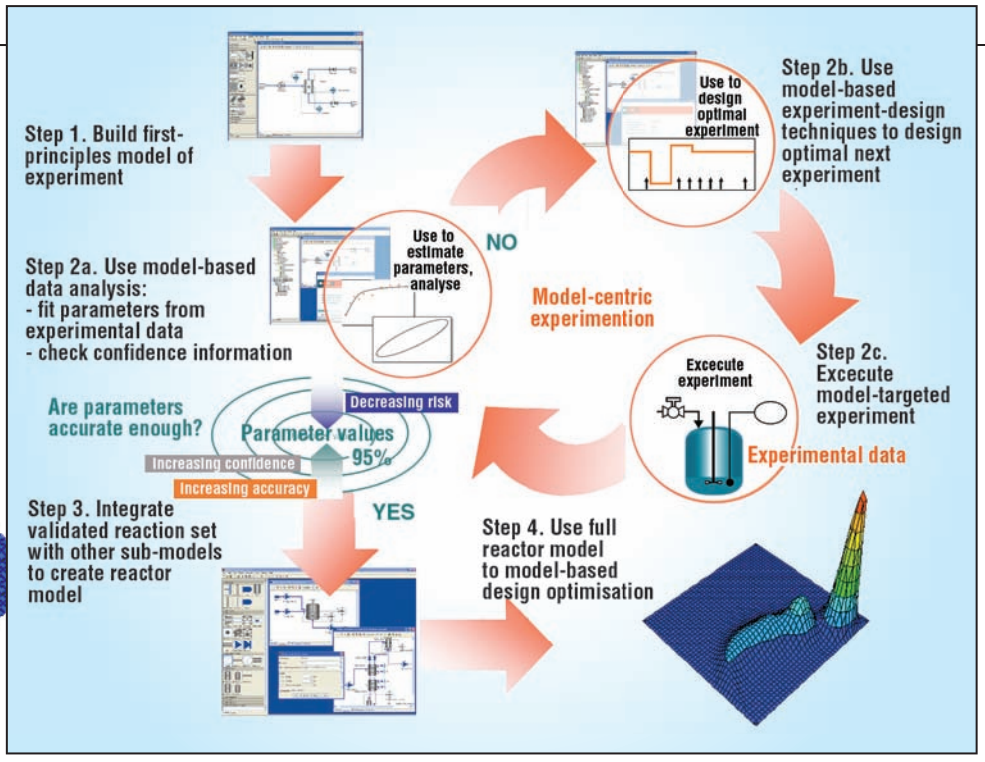

FIGURE 2. Shown here are the key steps in constructing a validated first-principles model with a good predictive capability over a range of scales

Similarly, the ability to couple CFD hydrodynamic models with models of chemical phenomena, now well established, means that complex mixing effects and chemical reactions can be considered simultaneously. The combination of these factors means that activities such as crystallizer scaleup or the design of multitubular reactors, once black arts, are now routine applications of modeling.

Models can now provide accurate quantification in support of most areas of design or operation within a single framework — from highly detailed models of individual equipment to plant-wide flowsheets; from start-up to shutdown as well as the steady-state operation in between; across the "process lifecycle" from experimentation by research chemists to day-to-day operation by plant operators, and across all sectors of the CPI.

Modeling has, in fact, reached the stage where models have enough predictive accuracy to replace physical testing in many cases. Model-based innovation technologies apply high-accuracy models to rapidly explore the design space for new reactors, fuel cell design or new catalyst formulations, with only the most promising candidates going to physical testing.

Perhaps as important as the technological advances is a change in perception by management. "Modeling-aware" managers increasingly realize the potential of modeling to capture IP, and use this not only to accelerate innovation and develop unique commercial advantages, but to drive down development costs and make their organizations more efficient. Equally important, there is an increasing body of qualified people schooled in process systems engineering, many who used state-of-the-art modeling tools for their Ph.D. research, and there is an increasing body of "off-the-shelf" models discussed in literature and available commercially.

All of this means that the companies deploying such techniques are gaining a rapid innovation advantage over their slower peers. This will be particularly true in the future for IP-based organizations, such as process technology companies and process licensors.

Capturing IP

So how does a company go about capturing its IP in a model?

The model. First it is worth defining what a process model is. Whether written in Fortran or a modern modeling language, a model is essentially a collection of physics, chemistry, engineering and operating knowledge in equation form, coupled in some way with empirically determined data. When executed for a given set of inputs (for example feed flowrates and conditions and fixed unit parameters), it will calculate outputs (for example, product flowrates and other values). It should by definition have a predictive capability so that, given a new set of feed or reactor operating conditions, it calculates accurate revised rates for the product streams. At its best, a model is capable of predicting actual behavior with accuracy over a wide range of conditions, making it possible to explore the design or operational space comprehensively and be confident in the results.

Past practice has combined models — the relationships describing a process — with their mathematical solutions, often with data thrown into the mix in the form of hard-coded values or empirical functions with limited ranges of applicability. The resulting models — often black-box models, where users were unable to modify or even see the underlying relationships — were limited in scope, inflexible, difficult to maintain and often lacked robustness. The coarse assumptions in the generic models gave them limited predictive capability.

Modern "equation-based" techniques separate the engineering aspects from the mathematical solution using fourth-generation languages or graphical representations. They also separate model and data. This means that a complex unit can be now described in tens of lines of physical and chemical relationships rather than thousands of lines of code, with significant implications for development time, quality assurance, ease of understanding and maintenance, and of course, lifecycle cost. This fact alone has removed a significant hurdle from the development and application of models.

Modeling across the corporation and process lifecycle. Perhaps the main advantage is that equation-based systems provide the ability to customize models to include valuable corporate knowledge and reflect exact process configurations. This significantly improves their ability to be used for innovation and genera-

tion of competitive advantages.

Modern modeling environments provide this capability in the most natural and accessible way. In equation-based, "open model" systems the model is essentially an executable document — in effect, a blueprint for the process — that captures the fundamental structures of the physics and chemistry without requiring the authors to concern themselves with the details of the mathematical solution.

Once such a blueprint is available, it becomes a place where different groups within the organization can deposit their corporate knowledge in a way that can readily be utilized by other groups. For example, reaction specialists can work with R&D chemists to create a reaction set, which is then used by reaction systems engineers to design a reactor, which is deployed within a flowsheet by chemical engineers, and so on. Once seen as a management dream, this type of workflow is becoming more commonplace in companies adopting a systematic modeling approach.

Combining first principles models and data. Models are typically a combination of the theoretical and the empirical. Current best practice is to fix everything that can reliably be known from theory. There is no point in attempting to infer a mass balance by analyzing data when the equation can simply be written down. This drives models toward "first-principles," which are usually the chemical engineer's definition of first principles — multicomponent diffusion, reaction kinetics, and so on — rather than a more rigorous definition involving molecular or quantum physics.

When all the "known knowns" (to paraphrase Donald Rumsfeld) are listed — typically heat- and material-balance relationships, reaction kinetics, hydraulic relationships, geometry, and so on — it is time to address the "known unknowns". These are typically the parameters — well known to engineers and chemists — within these equations: heat transfer coefficients and reaction kinetic constants, for example. Generic values for these can often be found in the literature or in corporate knowledge for the process, which sometimes is sufficient. However as can be seen below, there is often significant advantage to be gained in determining more accurate or appropriate values from real data — experimental, pilot or operating data.

This approach brings the best of both worlds, combining as it does well known theory with actual observed values. But how does it work in practice?

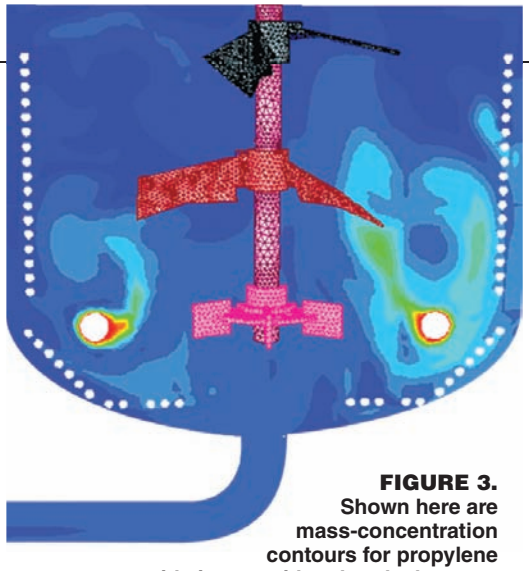

FIGURE 3. Shown here are mass-concentration contours for propylene oxide in a semi-batch polyol reactor

A 'how to' summary

The key steps in constructing a validated first-principles model with a good predictive capability over a range of scales are as follows:

Step 1. Construct the first-principles model. This is probably perceived as the most daunting step by people not familiar with the art. However, it need not be as onerous as it sounds. If starting from scratch, many of the relationships you would implement have been known for generations: conservation of mass, conservation of momentum, conservation of energy and pressure-flow relationships are standard tools of the trade for chemical engineers. Thermophysical properties are widely available in the form of physical properties packages, either commercially or in-house. The challenge lies mostly in selecting the appropriate level of fidelity for your requirements and availability of data.

However, most people don't start from scratch. There is an increasing body of first-principles models of many types of processes available from university research, in equation form in the literature, or as commercially supplied libraries. In fact, as models increasingly become constructed from faithful representations of fundamental phenomena, such as multicomponent mass transfer and reaction kinetics, they become more universally applicable to diverse processes.

Step 2. Estimate the model parameters from data. Having constructed the first principles model of a unit or a process, it will often — and almost always when dealing with reaction, for example — be necessary to estimate some parameters from data. This can be simpler or more challenging than it sounds, depending on the quality of data available. Usually initial values are taken from literature or corporate information sources. Then, in order to ensure a high degree of predictive ability across the design or operational space these values are adjusted by applying mathematical optimization-based, parameter-estimation (PE) techniques to the experimental (laboratory or pilot plant) or operating data using the information contained in the model. Thus the model parameters are "tuned" to reflect the observed behavior as closely as possible.

If performed correctly, with data gathered under suitably defined and controlled conditions, parameter estimation can generate scale-invariant sets of parameters, which has enormous implications for predictive modeling. It means that, for instance, the reaction kinetic parameters determined from an experimental apparatus at a scale of cubic centimeters can accurately predict performance in a reactor several orders of magnitude larger.

Modern parameter-estimation techniques are capable of estimating multiple parameters in complex models involving tens or hundreds of thousands of nonlinear equations using data from dozens of experiments. In addition, the ability to use dynamic as well as steady-state experiments means that it is now possible to design experiments that generate far greater information content than previously possible.

Step 3. Analyze the experimental data. Parameter estimation has an important additional benefit: model-based data analysis. The estimation process produces quantitative mea-

UTC Power Corporation

FIGURE 4. UTC Power systematically applies modeling to reduce the cost of physical testing during fuel cell development

sures of the degree of confidence associated with each estimated parameter value, as well as estimates of the error behavior of the measurement instruments.

Often this analysis exposes inadequacies in the data — for example certain reaction-kinetic constants in which there is a poor degree of confidence, or which are closely correlated with other parameters. It is usually easy to identify the parameters of most concern and devise additional experiments that will significantly enhance the accuracy of, and confidence in, subsequent designs.

Step 4. Design additional experiments, if necessary. Frequently this is done in an intuitive way, for example, by designing an experiment that maximizes production of an impurity rather than the main product, in order to better characterize the kinetics of the side reaction. For more complex situations, model-based techniques for the design of experiments — a major recent development — make it possible to design experiments that maximize the information generated, thereby minimizing the uncertainty, for the target parameters.

Optimal experiment design is achieved by determining the optimal values for key aspects of experimental procedure, such as the temperature profile to be followed over the duration of the experiment, the initial charges and temperature, and the times at which measurements (for example, samples for analysis) should be taken. In addition to maximizing parameter accuracy, the approach typically results in significantly reduced experimentation time and cost.

Step 5. Repeat Steps 2 to 4 until parameter values are within acceptable accuracy. Determining acceptable accuracy in this context means evaluating the effects of possible values of parameters on key design criteria (for example, the conversion of a key component in a reactor), as part of a formal or informal risk assessment. This can be done using the model itself.

It is the combination of the first-principles model and suitably refined data that provides the uniquely predictive capability of such so-called advanced process models over a wide range of conditions.

Once suitable model accuracy has been achieved, the model can be used to optimize many different aspects of design and operation. It is possible to determine optimal size and configuration of reactors; to minimize process energy costs; to optimize recipes and operating policy in order to reduce batch times and maximize product quality; to scale up crystallizers with confidence that they will actually produce crystals of the right size and shape; to determine the likely temperature gradients in a fuel cell on load change; to rank catalyst alternatives and select the optimal catalyst type; to determine catalyst loading regimes; to determine optimal operating conditions for given plant constraints; to determine optimal operating policies for changes in feedstock or other upsets or events; to troubleshoot poor operation; to generate linearized models for model-predictive control within the automation framework; and so on.

The benefits to this approach

The procedures outlined above are all readily achievable and are being applied in many different areas of the CPI.

For companies designing new processes or catalyst formulations, for example, models of sufficient accuracy reduce the need for physical (for example, pilot plant) testing by restricting this to the one or two examples identified by a comprehensive preliminary exploration of the design space.

What this means in broad terms for the process corporation is that it is now possible to do the following:

- Design process, equipment and operations to an unprecedented level of accuracy, and apply formal optimization techniques to determine key parameters rather than rely on trial-and-error simulation. This alone can bring about percentage improvements in "already optimized" processes, translating to significant profits for products in competitive markets
- Represent very complex processes — for example, crystallization and polymerization, or the complex physics, chemistry and electrochemistry of fuel cells — in a way that was simply not possible in the past. This facilitates and accelerates the design of new processes, enables reliable scaleup, and provides a quantitative basis for managing the risk inherent in any innovation.
- Integrate R&D experimentation and engineering, as well as use models as a medium of transfer for the activities of various departments within those divisions.

The ability to create models that can be used in a number of contexts within the organization means that it is possible to recover any investment in developing models many times over. For example, models are increasingly embedded in customized interfaces and supplied to end users such as operations or purchasing personnel, who benefit from the use of the model's power in providing advice for complex decisions without having to know anything about modeling.

What is in the pipeline?

There are still well-known cases where different tools perform different jobs better. For example, fluid dynamics is better handled by CFD packages than by the advanced process-modeling approach described above, which is better for dealing with complex chemical phenomena. Increasingly it is possible to combine the two approaches to get the best of both worlds. For example, it is now possible to reduce the modeling of a full-3D fuel-cell stack from a CFD model that would involve many millions of calculations to a hybrid model that contains only a few hundred thousand. Similar considerations apply to multitubular reactors, which may contain as many as 20,000 catalyst-filled tubes — all with different temperature profiles — within a liquid-filled shell. The computation is still challenging, but results can be achieved in hours rather than days or weeks and without any significant compromise on accuracy.

More exciting developments are on the way. Advances in the related fields of global sensitivity analysis (GSA) and global optimization will have significant implications for process design in the future. Global sensitivity analysis can be used to map the uncertainty — in the form of probability distributions — in various process parameters onto the probability distribution for various plant key-performance indicators (KPIs). Thus, the uncertainty in a particular reaction-kinetic constant can be translated into the likelihood of making a product that represents less-than-optimal profit — or indeed zero profit. The resulting analysis can be used to direct research dollars into the study of the parameters that have the greatest effect on, say, profitability, raising the possibility of quantitatively justified R&D spending.

Similarly, global optimization coupled with robust numerical-solution techniques will make it possible to search much-wider design spaces than are currently possible. New developments in modeling of thermophysical properties such as the SAFT (statistical associating fluid theory) equation of state — an advanced thermodynamics platform that is revolutionizing physical property calculation for complex or "difficult" materials such as associating fluids, polymers and electrolytes — make it possible to predict accurate, pure component and mixture properties from a minimum of data. In the near future it will be possible to model, for example, the power station CO_2 post-combustion clean-up and include the design of the solvent as an optimization variable.

Jack be nimble, Jack be quick

This may well be the motto of the CPI in the future (or indeed at present) as supply and demand positions change daily, with significant financial consequences.

Innovation by its nature always involves a degree of risk arising from uncertainties and gaps in available knowledge. To make rational — and in many cases rapid — decisions on complex matters requires accurate quantification of the options available.

The availability of powerful general-purpose models means that this is now possible. The companies that adopt such techniques wisely will benefit in competitive advantage in the future. ■

Edited by Gerald Ondrey

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