DIGITALLY TRANSFORMING REFINERIES

Peter Blaser and Rajat Barua, CPFD Software, USA, explore the significant impact of digital transformation on the refining industry.

While reading this article it is quite likely that a smartphone is within easy reach, close enough to be checked if necessary. *Necessary? What is so critical about a phone that it needs to be nearby?* The answer to that question is surprisingly important to this discussion.

This article is about digital transformation of refineries and the role simulation plays. Before discussing the specifics of refineries and simulation, and a case study resulting in drastic emissions reductions, the term 'digital transformation' needs to be explored, using the mobile phone as a starting point.

The mobile phone began as a wireless replacement for an existing technology, namely the landline. Over time, additional functionality was added, including SMS messaging, email and web browsing. But these were really stepping stones for more generic applications, or apps. Today, many use their phone as a calendar, to listen to music, to arrange travel, to connect with their social groups, for entertainment, and even to replace their wallet. For most people it is probably safe to say that the digital technology of the mobile phone has transformed the way we live our lives.

Before delving into the digital transformation of refineries, it is helpful to consider several terms commonly used today, namely digitisation, digitalisation and digital transformation. These terms are used in different ways in different contexts, but for this article they mean the following:

- Digitisation – this is the change from an analogue to digital form. Consider a healthcare business with paper records. Digitisation involves an after-the-fact data entry, so the patient records are no longer only on paper, but now exist in digital form.
- Digitalisation – this takes the concept of digitisation one step further, by using the digital information in the process itself. This is akin to a business doing away with paper records altogether. The business processes remain similar, but the record creation and storage is now done on an electronic device, rather than transcribed to a digital form after the fact. Storing a boarding pass for a flight on a smartphone, rather than printing out a physical copy, is an example of digitalisation.
- Digital transformation – this is when the processes themselves are changed through the use of digital technologies. The record-keeping efficiency is increased. Patient data is pre-loaded so that only new data needs to be entered. Past history is readily accessible. The forms can adapt based on symptoms presented. Prescriptions integrate directly with the pharmacy, and so on.

Returning to the smartphone example via this framework, modern mobile phones certainly represent digitisation; wired analogue signals are now transmitted wirelessly and digitally. Even a decade ago it would be safe to say the mobile phone also represented digitalisation. Existing processes, such as voice calls, messaging, email, and browsing web sites could all be done on the new digital platform of the phone. However, more recently the smartphone was central to a digital transformation; peoples' lives have been altered by the technology.

Digital transformation of refineries

Refineries and other downstream industries are rapidly adopting digitalisation technologies and strategies. As with the smartphone, the level of disruption caused by the technologies ranges from minor to significant. Some technologies, such as digital data acquisition, a historian for archival purposes, distributed control systems, and even predictive maintenance have been in use for decades.

Other technologies and concepts are much newer. Terms like Internet of Things (IoT)/Industrial Internet of Things (IIoT), advanced process control, predictive analytics, remote monitoring, big data, artificial intelligence (AI), cloud computing, digital twin, and virtual/augmented reality are now regularly heard at conferences the world over. Many of these technologies are already being applied while others seem to be more of an idea under exploration. And that is the norm and to be expected. Digital transformation is not about arriving at a destination – if it were, a new status quo would be reached. Rather, digital transformation is best understood in terms of an ever-fluid and evolving timeline: how things used to be, how things are now as enabled by digital technologies, and the ongoing pursuit of a better future in which both the technologies and the processes themselves might change.

That is a lot to consider. However, this article will neither speculate on the future digital transformation of refineries nor predict how the smartphone (or maybe a replacement technology) will be used in a decade. Instead, the remainder of this article looks at the role of simulation and its evolution from digitalisation to digital transformation.

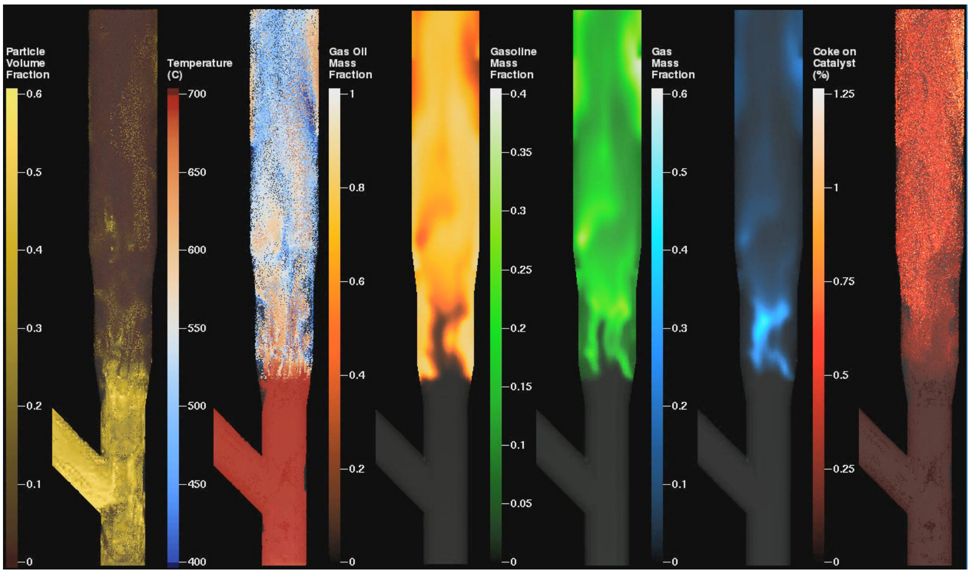

Figure 1. Multiphase, thermal, reacting CFD simulation of an FCCU riser.

Refinery simulations

Many types of simulations are used in the design and operation of refineries including structural analysis, heat transfer, process modelling (both steady state and dynamic) and computational fluid dynamics (CFD), to name a few. For consistency, the examples in this article are all taken from multiphase CFD simulations of fluidised catalytic cracking units (FCCUs), but the concepts are equally applicable to other types of simulation.

Figure 1 shows CFD simulation results for an FCCU riser.[1] The CFD model is based on first principles including the conservation of mass, momentum and energy. The equations solved by the CFD model are closed using empirical and numerical models such as gas-catalyst drag, heat transfer and reaction mechanisms. The simulation is based upon the 3D geometry of the unit and process conditions from the refinery.

Figure 1 demonstrates the computation of gas-catalyst hydrodynamics (left view), thermal behaviour (second to left view), gas phase chemistry (next three views) and solid phase chemistry (right view). This example utilises a simple four-lump kinetic model wherein the vaporised feed (VGO) reacts to make gasoline and other gases while depositing coke on the catalyst. Higher-order models are often used for refining and crude-to-chemicals applications.

Simulation and digitalisation

Digitalisation is a necessary first step toward digital transformation. Using the prior definitions as a framework, digitalisation means incorporating CFD simulations into existing workflows and processes surrounding the FCCU.

CFD simulation is used to complement the R&D processes used by technology licensors to develop intellectual property (IP). Traditionally, R&D processes utilise a combination of theoretical and experimental means for postulating and testing new ideas. CFD is a natural complement to these existing processes, moving some of the trial-and-error from costly experiments to the digital model, while also providing additional insights which may be difficult to obtain experimentally. Simulation not only replicates and/or replaces some of the iterations at the experimental scale (cold-flow, pilot unit, etc.) but can also be used for virtual testing of how the technology is expected to operate when deployed in a particular FCCU. CFD reduces both R&D and scale-up risks for new technologies.

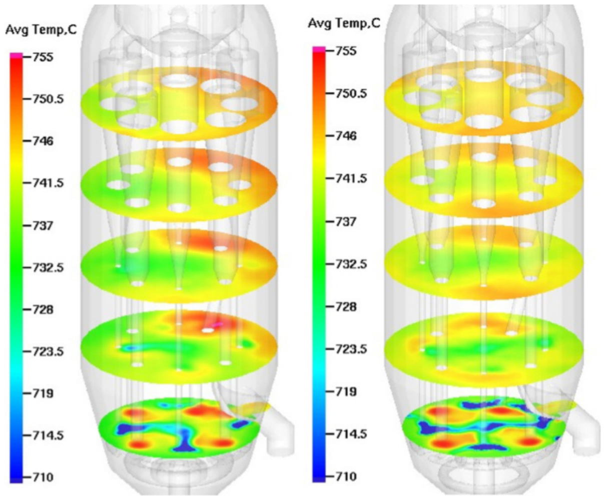

Figure 2. Simulation used for technology development and deployment.[2]

An example can be found in Figure 2 which illustrates how CFD simulation was used to optimise the performance of an FCC regenerator.[2] A baseline model (left view) was created and validated against refinery data. The model was subsequently used to recommend and test modifications to the refiner's configuration of the licensed technology which improved the gas-catalyst hydrodynamics, resulting in increased temperature uniformity (right view), ultimately reducing afterburn.

The above example can easily be extrapolated to other use cases already employed by refiners prior to the widespread use of the digital technology. CFD provides excellent insights in support of a post-audit analysis. Further, simulation is often used for unit trouble-shooting. In either case, identifying the root cause of underperformance through CFD complements other existing means of gathering insights, including instrumentation, catalyst testing, gamma scans or radioactive tracer tests.

Similarly, refiners already utilise many resources to minimise turnaround risk. Input is often sought from refinery engineers, central engineering groups, technology licensors, hardware vendors, catalyst suppliers, research organisations (e.g. PSRI) and others with specialty expertise, to name a few. CFD models, after being used for trouble-shooting and root cause analysis, can easily be extended to perform virtual testing of proposed turnaround changes. Using CFD within this workflow increases the likelihood of a successful turnaround while providing insights into additional opportunities for optimisation.

Simulation and digital transformation

The examples shown thus far illustrate the power of simulation, but do not yet meet the definition of digital transformation given earlier. These examples fit into the familiar processes and workflow already in use. Yet, as will be seen, digitalisation is often a precursor towards digital transformation, where the processes themselves change through technology.

The first step to most use cases involves the creation of a calibrated baseline model. Historically, these baseline models have been created within the existing workflows (technology development and deployment, post-audit analysis, trouble-shooting, turnaround planning, etc.). More recently, refiners are pro-actively creating baseline models of FCCU components and calibrating those models via operational data. These CFD digital twins (not to be confused with process model or life-cycle digital twins) enable rapid response in both traditional and non-traditional CFD use cases. By removing the model creation and calibration step from the urgency of traditional workflows, refiners also benefit by controlling costs.

The pro-active creation of calibrated baseline models is only one example of digital transformation, where the technology alters the very workflow in which it is used. Numerous other examples exist. CFD is altering R&D, scale-up, technology development, and is used to support patent applications. Simulation is also being used as a knowledge management tool. At a time when the industry is experiencing a disproportionate number of retirements of those with deep technical expertise, simulation is changing the way lessons learned are retained within an organisation and disseminated to all relevant parties.[3] Further, since high-quality data is a pre-requisite for high-quality simulation results, the instrumentation used in FCCUs is evolving as well, with some already using virtual instrumentation from simulation to augment physical instrumentation.

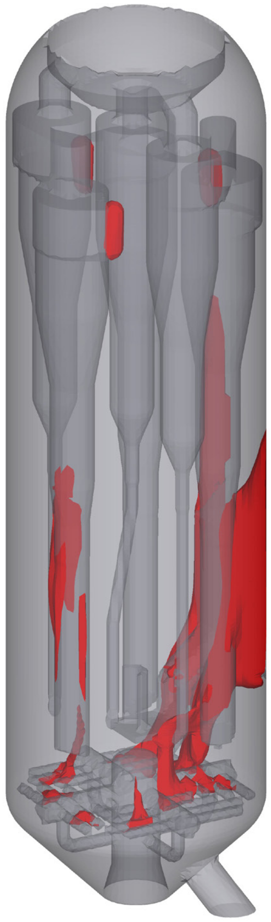

Figure 3. Combustion air channeling revealed in post-audit study.

Digitalisation and digital transformation case study

How this comes together can be observed via a case study taken from a North American refiner. In this example, nitrogen oxide (NO_X), carbon monoxide (CO), and particulate emissions from the regenerator increased significantly following the replacement of a combustion air distributor and cyclones during a turnaround. After startup, NO_X emissions exceeded the permitted 365 day rolling average by approximately 10% while CO emissions nearly doubled. Traditional trouble-shooting techniques, such as combustion promotor addition and air rate optimisation, were ineffective. A radioactive tracer study was performed which indicated the presence of severe air maldistribution deep in the dense bed. Air grid damage was suspected, and a shutdown was eventually scheduled to repair the damage. Yet, the question remained: what if nothing is broken?

A CFD study was undertaken which confirmed the presence of severe maldistribution, as shown in Figure 3. The red areas in the figure highlight regions with the highest gas velocities. However, the simulation showed the potential for this phenomenon without air grid damage. Did something happen to worsen maldistribution leading to the emissions problems?

Figure 4 shows the effect the hardware changes had on CO levels at the cyclone inlet elevation. The CFD simulation revealed that some maldistribution was always present, but the combination of hardware changes clearly exacerbated the problem.

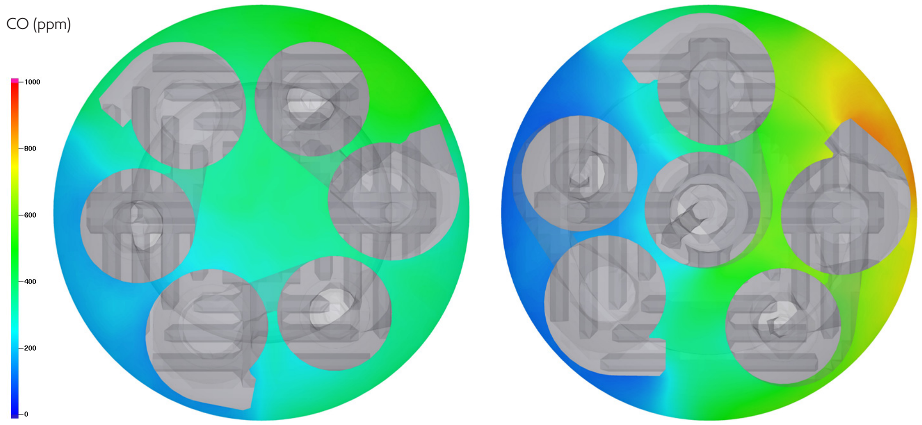

Figure 4. Increased CO maldistribution predicted (left – original, right – post-turnaround).

Thus far, this post-audit analysis case study represents digitalisation; the refiner is using the digital technology within the existing workflow of a post-audit analysis. While the insights obtained from CFD were powerful, what happened next was truly transformative.

Once it became clear that damage might not be the reason for increased emissions, the refiner urgently sought the means to mitigate the underlying maldistribution, using only simple modifications that could be completed within the upcoming shutdown. Simulation quickly took on a different role in this context. Systemic trial and error was not feasible in the mere weeks prior to the scheduled shutdown. Instead combinations of potential modifications were tested simultaneously in an effort to identify which configurations might minimise the underlying issue.

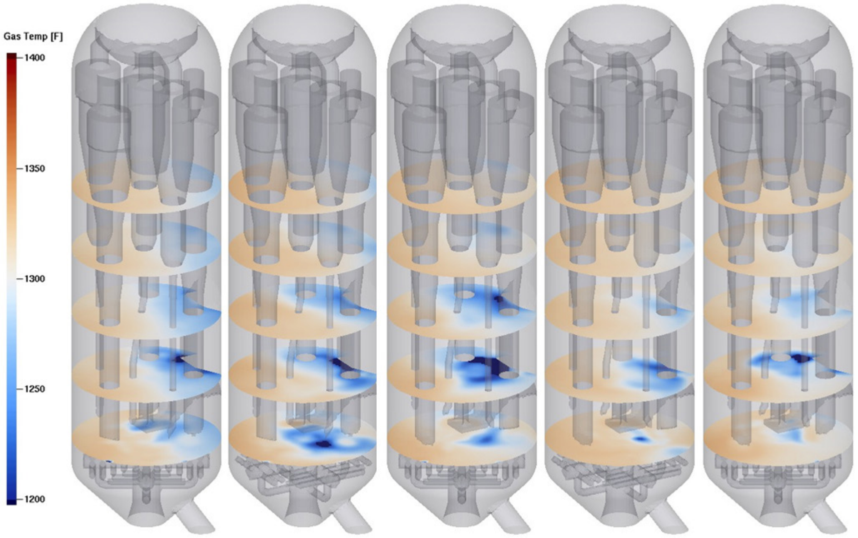

Figure 5. Simulation used to explore effects of potential modifications.

Figure 5 shows maldistribution of gas temperature for sample cases tested. Clearly, the severity of the maldistribution is not the same in all cases. Simulation changed the workflow of the refiner, identifying a practical yet counter-intuitive workaround. It was discovered that the maldistribution leading to the emissions issues could be drastically reduced via simple modifications to air grid and primary cyclone trickle valve orientations alone. The most promising cases were studied further in preparation for the shutdown.

During the shutdown, inspections revealed no air grid damage. This novel use of CFD gave the refiner confidence to implement a simple but non-obvious change. Following subsequent start-up, the new configuration responded to traditional optimisation, resulting in full regulatory compliance and elimination of the transient catalyst loss phenomenon.[4]

Experiencing digital transformation

Digital transformation has made a profound impact on many industries, with CFD becoming an essential element of the product design process.

In the refining industry, the impact of digital transformation is already being realised and the future possibilities are exciting. Models are more data-driven than ever before. Tighter integration with plant information systems is likely. Other concepts are being explored, such as self-calibrating models, neural network-like approaches to mapping out the unit response to specific variables, and combining the simulation with BIg Data type analysis of both the inputs and outputs.

With all the possibilities, it is easy to lose sight of the big picture; the technology is not the goal, it is an enabler. The technologies will change and processes will change, but the changes are only helpful if they support the things that do not change: safety, reliability, environmental responsibility and profitability.

So where to start? With new simulation technologies, perhaps start small. Keep in mind that since digital transformation affects both technology and people's workflow, this is as much of a sociological challenge as it is a technological one. Get quick wins and build confidence. Build on what works; discard what does not.

For more mature simulation technologies such as CFD for FCCUs, refiners should start with traditional uses supporting existing processes and use CFD to reduce turnaround risk or to trouble-shoot current operations. For those who have already attained digitalisation in this area, get ready to experience digital transformation. Prepare calibrated baseline models when not under strict time constraints, or roll out simulation-based knowledge management programmes. Allow the processes to change along with the technology and watch what happens.

References

1. All CFD results shown were created using Barracuda Virtual Reactor® from CPFD LLC.
2. Figure courtesy of TechnipFMC Process Technology. For additional details on the case, see SINGH, R. and GBORDZOE, E., 'Modeling FCC spent catalyst regeneration with computational fluid dynamics', Powder Technology, 316, pp. 560 - 568, (2017).
3. BLASER, P., CLARK, S., PENDERGRASS, J., and FLETCHER, R., 'Simulation as a tool for learning from historical FCCU operations', AFPM Cat Cracker Seminar, (2018), CAT-18-980.
4. FLETCHER, R., BLASER. P., PENDERGRASS, J., and PECCATIELLO, K., 'The experience of a team of experts to resolve severe FCC regenerator maldistribution', AFPM Cat Cracker Seminar (2016), CAT-16-17.

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