CHEMCAD: meeting the expanding needs of chemical engineers

MCA talks to Noelle Garza, a chemical engineer and Technical Specialist for CHEMCAD – distributed and supported in South Africa by Chempute Software – about CHEMCAD NXT, an advanced chemical process simulation software suite for process design, optimisation and reporting.

CHEMCAD was initially developed in the 1960s at the University of Houston, as part of a US government-sponsored project to develop process simulation software for synthetic fuels. It was commercialised in 1988 and has since become a flagship product in the Datacor Engineering Software Suite.

Over the years, CHEMCAD has continually evolved into the comprehensive simulation suite it is today. Batch process simulation and detailed heat exchanger design were added in 1992, followed by full integration of dynamic simulation by 2000. "With the unveiling of CHEMCAD NXT in 2021, which has a modern interface and advanced tools such as parallelisation and multi-objective optimisation, we have continued to prioritise the user experience," begins CHEMCAD Technical Specialist, Noelle Garza, adding that joining Datacor has enhanced the available resources and strategic alignment, allowing more ambitious development goals for CHEMCAD.

Datacor is a leading global provider of software solutions for process manufacturers and chemical distributors. Datacor solutions support over 15 diverse sectors, including oil & gas, mining, food & beverage, nutrition, packaged gas, pet food and pharmaceuticals. Together, Datacor and CHEMCAD support engineers with tools that enhance productivity, data-driven decision-making and promote smarter business growth.

Noelle Garza: engineer, data analyst and marketing specialist

Noelle Garza found her way into chemical engineering through science, mathematics, a love for problem-solving and a deep curiosity about how the world works. "What resonates with me is the idea that chemical engineers make sense of complex systems to help drive meaningful progress.

"Our CHEMCAD team likes to use the phrase 'ChEs are Heroes' because it reflects how the work of chemical engineers can improve lives, support innovation and solve some of society's biggest challenges. Our customers engineer products that bring food, energy, medicine and clean drinking water to people, among many other living essentials," she says.

Chempute's journey with Datacor

Chempute has a long history as a partner of Datacor in both Chemical Process and Pipe Flow, having first introduced CHEMCAD into South Africa in 1986, making it one of the earliest international dealers to purchase and distribute the software. Some of the company's first clients included leading South African manufacturers, engineering firms and chemical producers who adopted CHEMCAD to modernise their process design and optimise plant performance. Over the years, Chempute has steadily grown its customer base, supporting organisations across a wide range of industries – from petrochemicals and mining to food processing and pharmaceuticals.

Early global successes for CHEMCAD included its adoption by engineering firms, operators, and OEMs looking for a flexible, user-friendly simulation tool that could support all stages of chemical process design. Notable global users include companies such as BASF, Chevron, and Pfizer, who have utilised CHEMCAD for process design and optimisation.

Key features and uses

CHEMCAD helps chemical engineers simulate complex processes through steady-state and dynamic modelling, equipment sizing, thermodynamic analysis, sensitivity studies and optimisation tools.

"CHEMCAD helps engineers to save time and money by enabling them to test ideas virtually before making costly real-world changes. It supports innovation, reduces trial-and-error, shortens design cycles, improves process reliability and supports better decision-making. Ultimately, this leads to higher product yields, lower energy use and fewer operational surprises," says Garza.

"One everyday use for our software is evaluating the performance of piping or equipment. Consider a liquid-liquid absorber column used to recover acetone from a mixture with benzene, for example, a scenario typical of a mixed solvent waste stream from a speciality chemical plant, or a byproduct separation in a petrochemical facility," she says.

In this setup, as shown in Figure 1, acetone and benzene enter the extractor from the bottom, while water enters from the top. "Because acetone is partially miscible with water, it selectively transfers into the aqueous phase, while benzene remains in the organic phase. This simulation is used to determine the optimal conditions for a 99.96% recovery of acetone in the extract," Garza explains. The results from a sensitivity study simulation are shown in Figure 2.

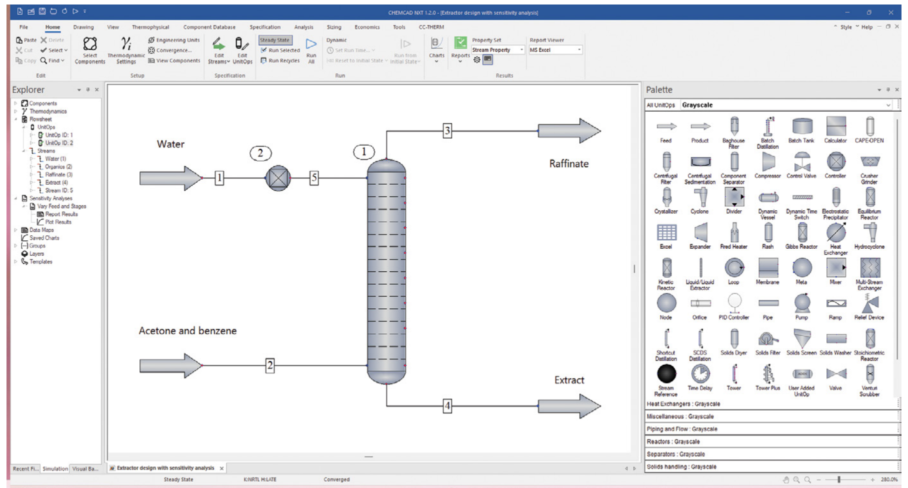

Figure 1: CHEMCAD allows engineers to go beyond static modelling by analysing what-if scenarios using steady-state or dynamic simulation. In this case, a sensitivity analysis is used to test multiple scenarios with varying numbers of stages, ranging from 2 to 7, and water flow rates from 5 to 95 kmol/h, to simulate the mole rate of acetone in the extract stream [4].

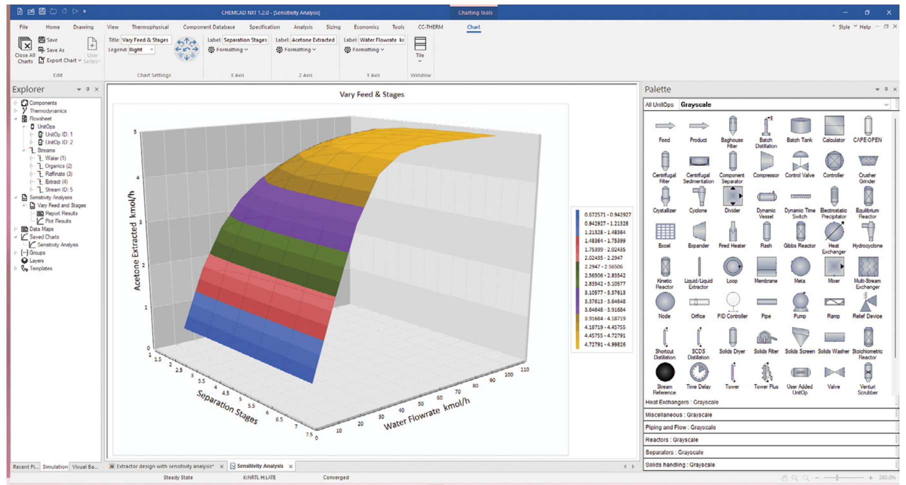

Figure 2: Sensitivity study simulation results for the scenario shown in Figure 1, which shows how the mole rate of acetone in the extract stream [4] varies with the number of stages and the water flow rate (5 to 95 kmol/h).

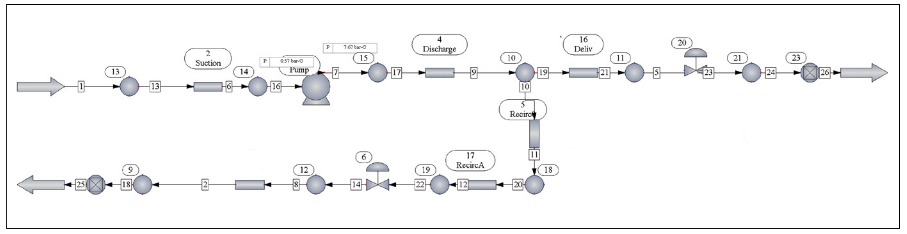

Figure 3: For a fuel blending system upgrade, CHEMCAD was used to evaluate whether an existing ethanol-gasoline blending system could handle increased ethanol content. This flowsheet was built using piping layouts from isometric drawings and pump performance was modelled from manufacturer curves to verify capacity.

This example also shows how CHEMCAD can enable engineers to go beyond static modelling by analysing 'what-if' scenarios using steady-state or dynamic simulation models.

"This may be for a new design or to help troubleshoot existing equipment, especially when issues arise in the plant. Engineers can use CHEMCAD as a virtual twin of the equipment or process being assessed, to determine whether the facility can handle anticipated operational conditions or process changes before making any physical modifications," she explains.

A great example comes from Fluid Quip Technologies (FQT), a leader in biotech engineering. "FQT used CHEMCAD to optimise a biofuel production facility. Starting with process data and equipment drawings, FQT built a steady-state simulation in CHEMCAD to evaluate performance, identify bottlenecks and improve energy efficiency. They used CHEMCAD's distillation modelling tools to test tray configurations and match site specifications. CHEMCAD's advanced heat exchanger modelling tools were used to size exchangers for better heat integration.

"This optimisation resulted in significant energy savings without requiring additional capital investment. This project shows how CHEMCAD can be used to improve performance, reduce operating costs, and support sustainability goals in large, complex processes," Garza notes.

CHEMCAD is especially useful for smaller-scale projects where engineers need to make decisions quickly. Noelle Garza cites a fuel blending system upgrade in the UK, where engineering firm P&I Design used CHEMCAD to evaluate whether an existing ethanol-gasoline blending system could handle increased ethanol content [Figure 3]. "Using steady-state and dynamic modelling, P&I identified limitations in the current infrastructure and developed a cost-effective strategy to meet the new blending requirements.

"Here, CHEMCAD was used to simulate control responses, pressure behaviour, and to test short-term fixes before implementing long-term upgrades. This is a perfect example of how CHEMCAD supports troubleshooting and incremental improvements while saving time, reducing risk and avoiding unnecessary spending, all without disrupting ongoing operations," she tells *MCA*.

CHEMCAD is also making it easier for engineers to run cleaner, more efficient processes. "Whether they are designing alternative energy systems, carbon capture solutions or optimising traditional hydrocarbon and chemical processes to meet sustainability and energy reduction goals, engineers are using CHEMCAD to find energy-saving opportunities.

"Many companies have used CHEMCAD to improve energy usage and incorporate heat integration to cut utility costs and reduce waste. It's a powerful tool for developing control strategies that reduce or prevent emissions at source. If emissions do occur, however, CHEMCAD can also help quantify their composition and volumes," says Garza.

On the cost-effectiveness of its use, she says CHEMCAD delivers a strong ROI by helping engineers make smarter decisions when simulating process changes, testing breaking points, and evaluating operating conditions. "Unexpected shutdowns can cost thousands per hour, and CHEMCAD reduces that risk by allowing engineers to explore 'what-if' scenarios, such as feedstock changes or equipment swaps, before real-world testing. This saves time, energy, avoids wasted materials and improves reliability.

"By optimising reaction conditions, separation efficiency and energy use, CHEMCAD boosts product yields and helps engineers get more out of existing assets. That means lower operating costs (OPEX) and more informed capital investment decisions (CAPEX), especially in resource-constrained environments," concludes Noelle Garza.

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