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Engineering advanced

THE FUTURE OF PROCESS OPTIMIZATION IS HERE

CHEMCAD NXT delivers fast single and multiple objective function optimization based on rigorous first principles simulation

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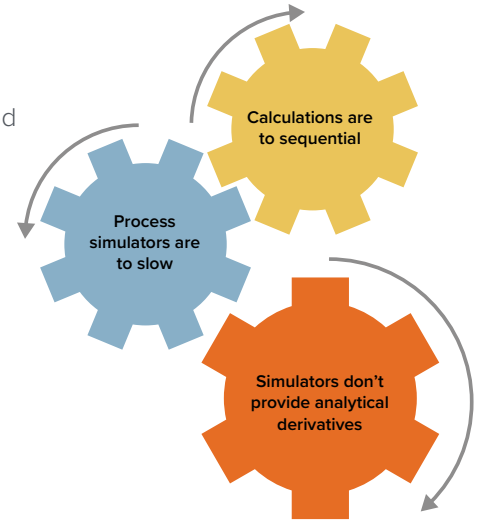
CHEMCAD NXT

→ CUSTOMERS

Since 1988, Chemstations has been a recognized leader in chemical process simulation software, and the company has continuously improved CHEMCAD on both the software architecture and chemical engineering functionality levels.

→ BACKGROUND

Hiding in every chemical process is money, as is improved efficiency and reduced environmental impact. To date, however, optimizing even well-known processes is a daunting task. Using rigorous models, reaching an optimum could take months or more of calculation time, so companies often cut back the number of variables in an optimization, chose to use a non-rigorous model, or turned to custom written, fast executing code. This means the tradeoffs are either (1) having no idea whether a global optimum is found, or (2) spending large sums of time and money to build custom optimizations.



→ WHAT'S CHANGED

Computing power has increased (Moore's Law) significantly since the early days of process simulation. However, CPU clock speed isn't the driving factor anymore; it's number of cores. The ability to parallelize calculations to all the available CPU cores, as CHEMCAD NXT can, is the key to running orders of magnitude faster than before.

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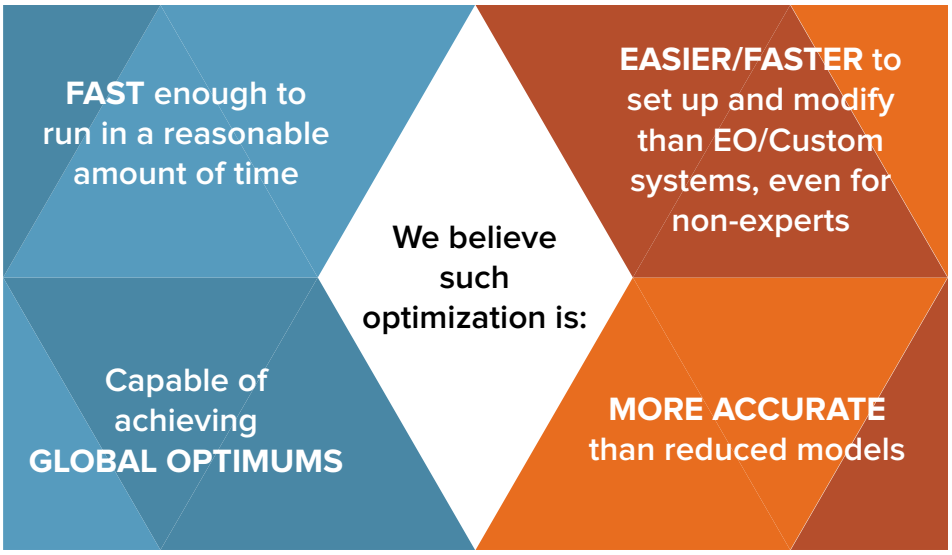
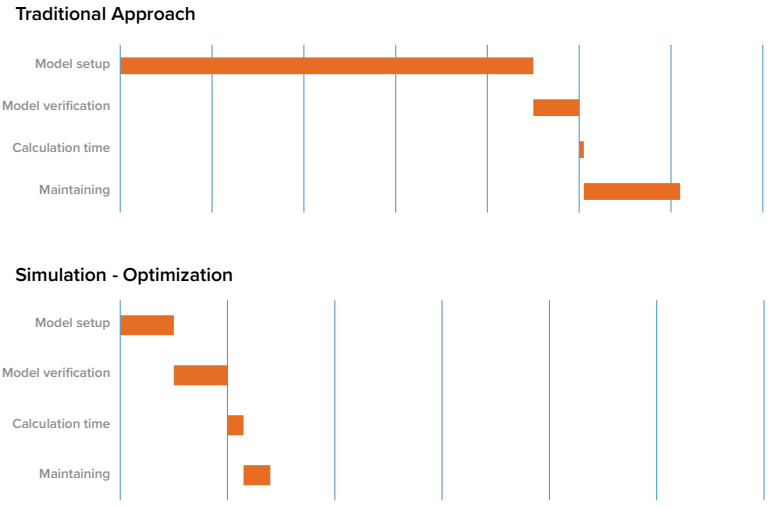


ADVANTAGES

Using CHEMCAD NXT's Simultaneous Modular SQP Optimizer (which includes mixed integer variables), companies can build optimizations right into simulations they are already using for their work. Most chemical engineers are familiar with flowsheeting in a simulator, and most also understand the principles of optimization. This makes setting up an optimization incredibly fast and easy for any engineer.



TRADITIONAL VS. RIGOROUS SIMULATION BASED OPTIMIZATION

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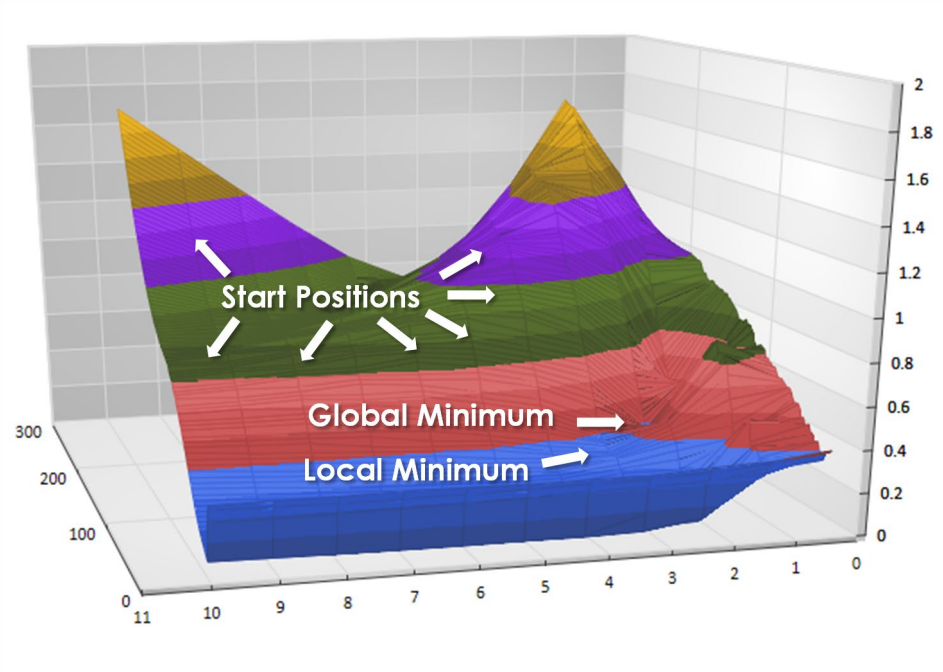
Engineers also need confidence that the optimum found by the model is the global optimum. CHEMCAD NXT handles this by parallelizing a large number of starting positions. Those starting positions are referred to as “restarts.” Multiple restarts are performed until several solutions converge within set tolerances. Therefore, CHEMCAD NXT’s calculation speed increases the odds of finding the global optimum because multiple restarts can be performed in a reasonable amount of time and each simulation run is extremely fast.



NOTE THAT OPTIMIZATIONS CAN GET “STUCK” IN LOCAL MINIMA

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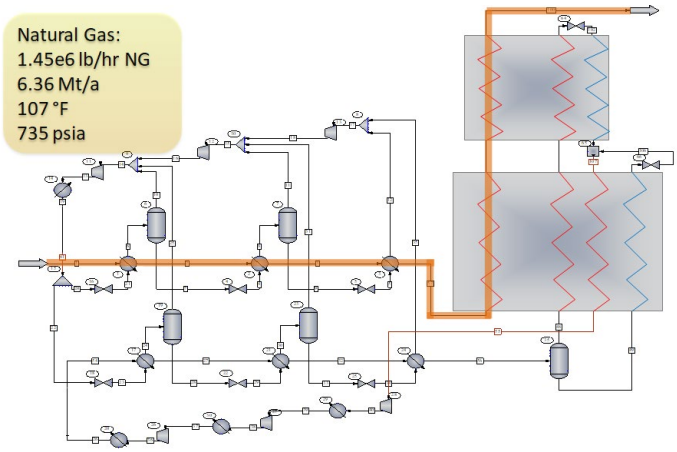
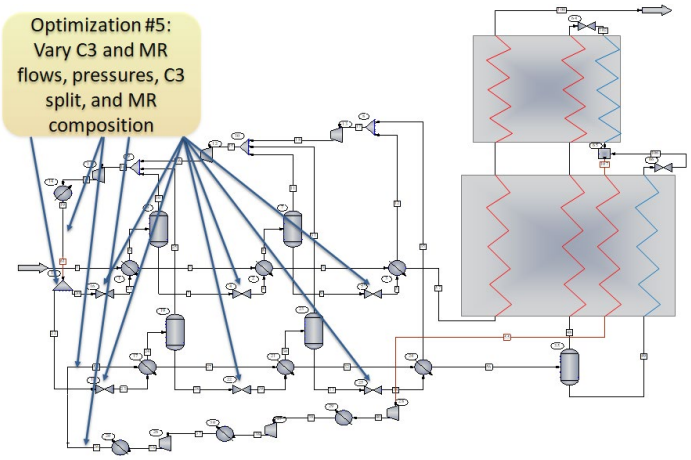
➔ EXAMPLE

Chemstations recently searched the literature for a commonly optimized process and chose a C3MR-LNG facility.



C3MR LNG PROCESS

Rather than limit the optimization to the few variables chosen by previous works, Chemstations chose to minimize compressor work by varying refrigerant flows, refrigerant pressures, refrigerant splits, and even refrigerant composition.



FULL ARRAY OF OPTIMIZED VARIABLES

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Minimization of compressor work, as a proxy for operating cost, is the “objective function” referenced in the results table following.

Name	Opt #1	Opt #2	Opt #3	Opt #4
Objective Function	859.273	814.1273	808.1582	754.5825
C3 Flow (lb/hr)	1307.5	134870.9	134345	128253.5
MR flow (lb/hr)	146184.5	144393.1	144448.7	132324.1
Valve #16 P (psia)	110	110.1497	110	110
Valve #4 P (psia)	40	40	40	40
Valve #5 P (psia)	15	15	15.00011	15
Valve #18 P (psia)	62.5	70.13029	70.12135	70.24414
Valve #22 P (psia)	19.5	25.6605	25.43986	25.74541
Valve #25 P (psia)	5	5.282272	5.63412	6.045956
C3 split ratio	0.15	0.15	0.185427	0.196982

COMPARISON OF OPTIMIZED VARIABLES ACROSS OPTIMIZATION SCENARIOS

→ RESULTS

While optimized results cannot be compared to a base case in our example, what can be analyzed is the improvement over a reduced-scale optimization. “Opt #1” in the table, with a minimum of variables (similar to what can be done with existing tools) can be improved over 12% by simply increasing the number of optimized variables, as can be seen in “Opt #4.” Keep in mind, Opt #4 can be set up and run in a reasonable amount of time by even an optimization novice, and most importantly, can be maintained, modified, and re-run easily. Finally, note that as seen in the graph following, the global optimum is likely attained with 128 restarts. These results were so encouraging that in later work, not covered by the scope of this paper, the optimization was expanded to multiple objectives: minimizing compressor work and minimizing heat exchange area, thereby also minimizing capital cost.

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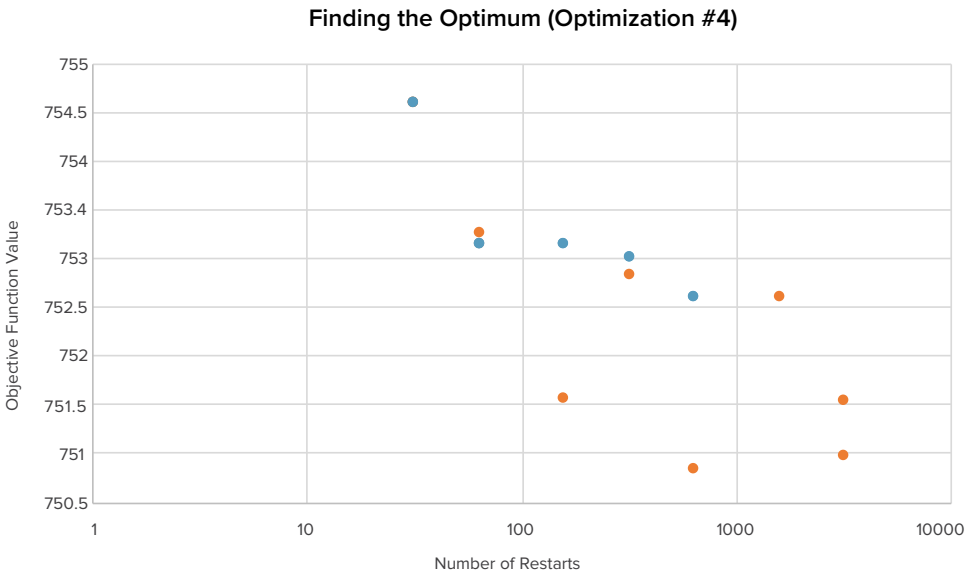
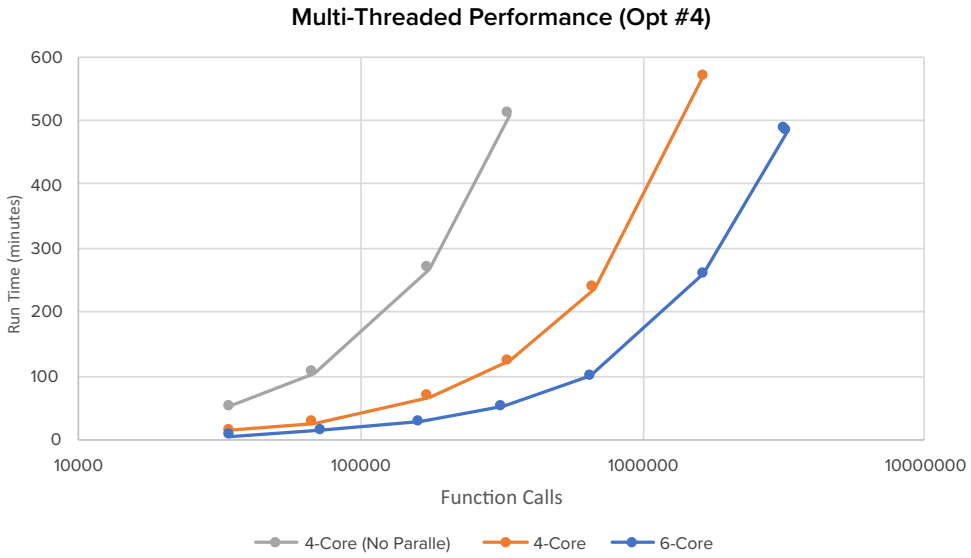


NOTE THAT GLOBAL OPTIMUM IS LIKELY FOUND HERE WITH 128 RESTARTS



RUN TIME VS # OF FUNCTION CALLS/SIMULATION RUNS

→ CONCLUSIONS

As can be seen in the graph, the improvement in run-time for a complex optimization is on the order of 7X-10X faster from single threaded to 6-core calculation. Machines with more cores will give relatively similar performance increases, depending on simulation complexity (less complex simulations will reach a plateau in performance).

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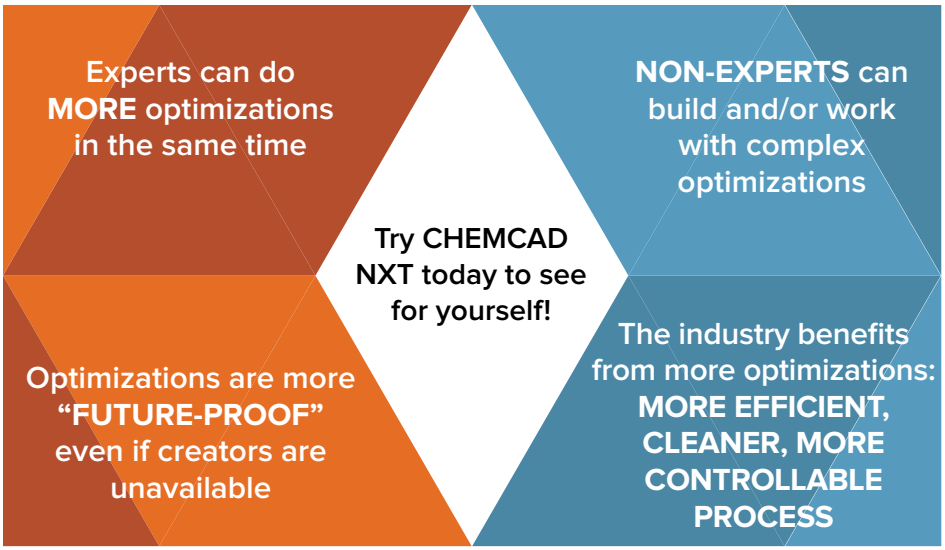
The CHEMCAD NXT team is working with customers on new and exciting applications at all process scales, and the early feedback is that (1) experts in process optimizations will be able to take on more projects in a given time frame, and, possibly more importantly, (2) even non-experts can tackle optimizations and feel comfortable that the results are accurate and actionable.



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