Chemical Plant Simulation on Cray Research Supercomputers: An Industrial Success Story

Stephen E. Zitney, Cray Research, Inc., Eagan, MN, USA

ABSTRACT: *With the goal of demonstrating the advantages of supercomputer simulations for process design and operations, Bayer AG recently teamed up with Cray Research to perform plantwide dynamic simulations of an entire Bayer production facility in Leverkusen. This paper presents project results and benefits from both a computational standpoint and a Bayer company perspective. Regarding computational aspects, special attention is focused on the performance of the process simulation software (SPEEDUP from Aspen Technology). SPEEDUP on Cray Research systems features new sparse matrix technology, vectorized residual calculations, and parallel asynchronous data transfer for exploiting the full capabilities of supercomputer architectures. From Bayer's perspective, the collaboration clearly demonstrated that plantwide dynamic simulation using SPEEDUP on a supercomputer provides a powerful and valuable extension to traditional process engineering activities, and most importantly, delivers tangible financial benefits to the bottom line.*

Introduction

The future success of a chemical company depends on its ability to design and operate processes that achieve the highest possible output of the best quality using the smallest possible amount of raw materials and energy and generating as little waste as possible—and all of this with the highest possible safety for employees and environment. To meet these challenges, Bayer critically analyzes its production processes using state-of-the-art dynamic simulation technology, namely the SPEEDUP package from Aspen Technology (1993).

SPEEDUP is a dynamic modeling and optimization system which lets engineers analyze chemical process dynamics and their influence on process performance. Process industry applications include designing process control strategies, meeting safety requirements in the event of equipment failure, troubleshooting operations during upsets and during start up and shutdown, and training operators on how best to respond to a full range of operating conditions. SPEEDUP may be used off-line or on-line, in the latter case either as a guide to plant operators, directly to provide set points to a distributed control system, or in other model-based control schemes.

In Bayer's most extensive SPEEDUP project to date, the Systems Process Technology Department developed a rigorous plantwide dynamic model for eight coupled distillation columns (nearly 1200 trays) representing one of the largest separation systems ever built in Europe. With some of the columns measuring four meters in diameter and towering to a height of nearly 80 meters, the heat-integrated plant distills eight high-value products from more than 40 components. Plant operation is characterized by a very large total holdup (more than 500 m3) and time-varying feed conditions. Depending on the yield in the upstream reaction, the composition of the feed changes by a considerable amount (changes of up to 100 percent in some components). Moreover, the plant has nearly no buffering between the single distillation columns, which leads to an unsteady continuous process. The incentives for Bayer to model this specific plant were to study process control problems and to look for ways to increase plant capacity, while at the same time improving quality and reducing the energy requirements.

SPEEDUP Case Studies and Performance

Over a period of about one year, a detailed mathematical model of the entire distillation plant was developed with SPEEDUP using process flowsheet information and actual plant data. The model includes standard mass and energy balances, tray hydraulic equations, and vapor-liquid equilibrium relations (Wilson equation). Off-line steady-state and dynamic simulations of the individual distillation columns and the whole plant were performed on a CRAY C90 supercomputer. Dynamic simulation of the eight coupled distillation columns required the repeated solution of a differential-algebraic system that contains more than 75,000 equations, making it the largest known industrial SPEEDUP application in production use in the world.

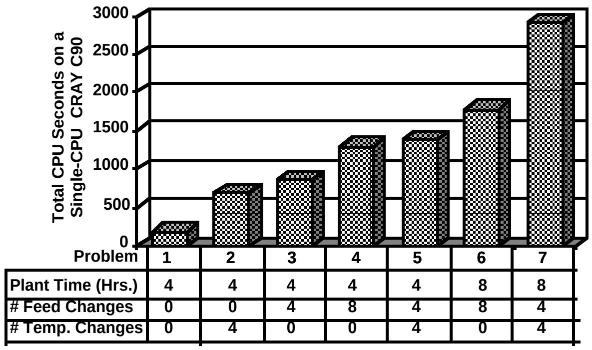

Figure 1: CRAY C90 single-CPU times for seven Bayer SPEEDUP case studies.

Figure 1 presents the CRAY C90 single-CPU times for seven Bayer case studies differing in the length of plant operation time simulated (four or eight hours) and the type (feed flowrate and/or temperature) and number of process disturbances. The results show that the solution time not only depends on the plant operation time being simulated, but is also strongly correlated to the number and type of external perturbations affecting the chemical process during the simulation. Since the relaxation times of several components in the Bayer process are relatively long, plant operation times of several days with many external perturbations must be simulated to obtain a realistic picture. As discussed below, the Cray Research version of SPEEDUP offers enhanced capabilities to make such simulations tractable.

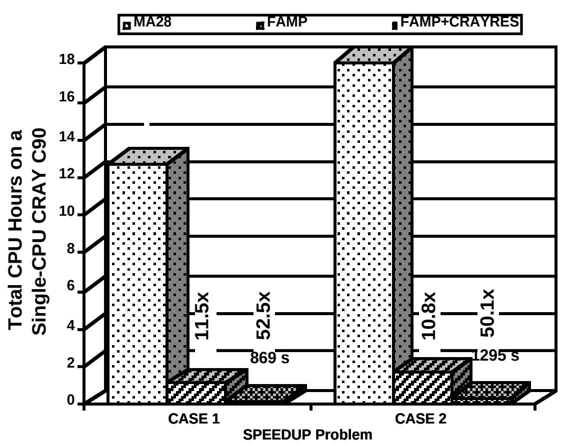

Figure 2: Performance improvements from using CRAY-optimized version of SPEEDUP on a single-CPU CRAY C90 supercomputer.

Figure 2 presents the results for two case studies simulating four hours of plant production time, with one (CASE 1) and two (CASE 2) disturbance(s) per hour in total feed flowrate. For each case, the bar on the left represents the CRAY C90 simulation using the standard version of SPEEDUP available on other computer platforms. The other two simulations for each case represent the value of using the CRAY optimized version of SPEEDUP which contains improved algorithms for sparse linear equation solving (FAMP) and residual evaluation (CRAYRES).

Compared to SPEEDUP's conventional sparse matrix techniques (e.g., Harwell's MA28), an improved out-of-core frontal solver, FAMP (Zitney and Stadtherr, 1993; Zitney et al., 1994), provides substantial savings in overall problem solution time, more than an order of magnitude for the Bayer simulations in Fig. 2. By relying on efficient dense matrix kernels, the frontal method factors a sparse matrix with a series of dense frontal matrices, each of which corresponds to one or more steps of the overall LU factorization. The frontal process avoids the problem of indirect addressing, which degrades the vector performance of conventional sparse matrix methods. Table 1 shows that FAMP is well over 250 times faster than the MA28 routine when solving a single linear system from the Bayer problem on a single-CPU C90 system. The middle bar for each case study in Fig. 2 shows the effect of this new solver on overall SPEEDUP performance. Performance gains of 11.5x and 10.8x are achieved using FAMP since slightly over 90 percent of the SPEEDUP solution time for each case is spent in the linear solver when using MA28.

Table 1. Single-CPU C90 Time Comparison of Sparse Matrix Solvers on a Single Sparse Linear System from the Bayer Problem.

			CPU Time (Sec.)	
Order	Nonzeros	% Sparsity	MA28	FAMP
75724	349716	99.994	854.8	3.2

After rethinking the sparse matrix methods used in SPEEDUP, a performance analysis shows that a substantial amount of computation time is spent in residual calculations. By invoking the CRAYRES command in SPEEDUP, a post-processor automatically modifies the SPEEDUP residual FORTRAN to generate DO loops and vectorized code, thereby improving vector performance when running dynamic simulations using either the DAE or SUPERDAE integrators. Figure 2 shows that the optimized residual calculations give nearly a factor of five performance increase on the Bayer simulations.

As model size and the length of simulation time increases, SPEEDUP stores more and more data to its database file for use in run-time and post-run plotting. Therefore, it becomes more important to perform as many input/output (I/O) operations as efficiently as possible. The Cray Research version of SPEEDUP provides an easy-to-use flexible file I/O library for parallel asynchronous data transfer to and from the SPEEDUP database. For the Bayer application, overlapping I/O and arithmetic computations in this way reduces the I/O wait time by more than an order of magnitude. This uses supercomputer resources efficiently, and lets large-memory SPEEDUP jobs complete and exit the system more quickly.

Providing more than a 50-fold increase in overall SPEEDUP performance in some cases, the software enhancements described above coupled with the fast I/O and CPU performance of the CRAY C90 hardware let Bayer and Cray Research engineers perform plantwide dynamic simulations that were previously intractable for mainframes and workstations. For example, simulating four hours of plant production time in CASE 2 now takes only 21 CPU minutes instead of the 18 CPU hours required with the standard version of SPEEDUP. As a result, Bayer engineers can run this plantwide simulation many more times per day and can even consider it for on-line use where real-time simulations are required.

Project Results and Benefits

Steady-state simulations were done with SPEEDUP to optimize on the basis of different feed concentrations and loads. The result of these optimizations is the plant characteristic, which reveals how much of the plant needs to be revamped to achieve a given increase in plant capacity. The plant characteristic found with the simulations indicated that to double capacity requires revamping only half of the plant. As a result, Bayer aims to expand production capacity for the chemical plant considered here by more than twofold over the next few years.

Since plant characteristics only provide optimal operating points, a method must be developed to run the plant at these optimal operating conditions regardless of load changes and varying feed conditions. Such a process control strategy requires dynamic simulation of the plant. The SPEEDUP dynamic simulations had the following objectives:

- Perform sensitivity studies to define the necessary process measurements (temperature, pressure, analyzers) for control purposes.
- Perform sensitivity analyses to define the control structure, i.e., which variable should be controlled by which manipulated variable. Determine if a conventional PID (proportional integral derivative) control can be used or if a more advanced control is required.
- Test the designed process control by simulation of load and setpoint changes of the complete plant, including controllers.

Figure 3 shows part of the sensitivity analysis for an increase of reboiler duty in a heat-integrated distillation column. Figures 3a and 3b show temperature profiles along the column and concentration profiles of the main component in this column. The profiles are moving from the operating point (lower curve) upward. The time difference for the profiles is four hours, which provides excellent insight into the dynamics within this unit. From these sensitivity studies for all the manipulated variables (approximately 30) in the plant, the necessary process control measurements can be defined (Fig. 3c). The chief result was that one-third of the existing analyzers on the plant were no longer necessary.

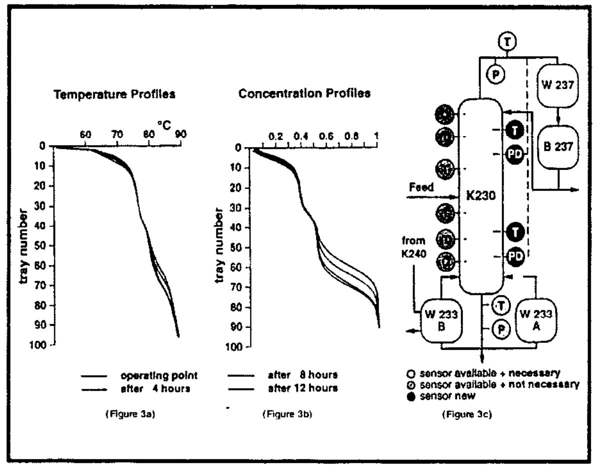

Figure 3: Sensitivity analysis and measurement selection.

On the basis of the newly defined process control measurements, Bayer engineers developed a completely new control strategy for the plant, which has shown potential for energy savings of three to five percent. The controllers and plant models are then simulated together to check the controller performance. The major points of interest in this case are disturbance rejection (e.g., the ability to handle changing feed conditions) and decoupling (reducing the influence of one control loop on another one).

Being able to test all the controllers before implementing them on the plant saves much troubleshooting and leads to a faster and more successful startup of the new controllers. Moreover, the well-defined experiments, which can be done in simulation but which are virtually impossible in the real plant, lead to a much better understanding of the process and may also yield decisive directions for further optimization and, ultimately, a competitive advantage.

The enormous time constants of several days or more within the plant are another interesting outcome of the simulation experiments with the complete plant model. Keeping in mind that plant operators usually make setpoint changes and perform some manual operations during their shifts, it became apparent that these operators never see the result of their manipulations, but a later shift does. As a result, it was concluded that plant operators should leave their process in automatic operation for as long as possible. This will require the operators to change their basic approach to work. Again, simulation can be helpful by showing possible reactions of the plant controllers to disturbances, thereby leading to a faster acceptance of the process controller as a member of the team.

Conclusions

The results described in this paper confirm that total plant simulation offers great potential for reducing operating and capital costs, leading to the optimization of chemical plant processes, such as Bayer's, and ultimately to a competitive advantage in quality, flexibility, and costs. The results of the joint project demonstrated to Bayer the effectiveness of dynamic simulation made possible by the high performance of supercomputers. To continue these efforts, Bayer AG has installed a CRAY C92 system at its Leverkusen facility. Bayer, Cray Research, and Aspen Technology plan to carry out further improvements in the capabilities and the performance of dynamic process simulation software on supercomputers.

Acknowledgments

The author wishes to thank Ludger Bruell and Lothar Lang of Bayer AG and Robert Zeller of Cray Research for their collaborative efforts throughout the course of this project. Special thanks also go to James Goom, Phil Mahoney, and Peter Ward of Aspen Technology, Inc. for their responsiveness and support in using SPEEDUP. Finally, the author wishes to express appreciation to the Benchmarking and Corporate Computing and Networking groups at Cray Research for providing generous amounts of assistance and computer time on the supercomputer systems in Eagan, Minnesota and Chippewa Falls, Wisconsin.

References

Aspen Technology (1993). SPEEDUP User Manual, Vols. I and II, Version 5.4, Cambridge, Massachusetts.

Zitney, S. E. and M. A. Stadtherr (1993). Frontal algorithms for equation-based chemical process flowsheeting on vector and parallel computers. Computers chem. Engng., 17(4), 319-338.

Zitney S. E., K. V. Camarda and M. A. Stadtherr (1994). Impact of supercomputing in simulation and optimization of process operations. Proc. Second International Conference on Foundations of Computer-Aided Process Operations. (FOCAPO-II, Mt. Crested Butte, Colorado, July 18-23, 1993; D. W. T. Rippin, J. C. Hale, and J. F. Davis, Eds.), CACHE, Austin, TX, pp. 463-468.