EXPLOITING THE USE OF EQUATION-ORIENTED MODELING FOR DESIGN-TYPE PROBLEMS

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Abstract

The BP Chemicals para-xylene (PX) group has successfully used equation-oriented (EO) modeling technology for traditional process engineering modeling tasks, such as design, debottlenecking, troubleshooting, etc. Historically, primarily specialists have used EO technology for on-line optimization and dynamic simulation process engineering activities. The PX group is placing EO technology in the hands of normal process engineers to solve their process design problems. The PX process requires the use of EO technology because the process is tightly heat integrated and has an extremely large number of recycles and design specifications. Equation oriented technology is well suited to handle these types of problems robustly and efficiently. Aspen+ EO technology has proven to be an enabling technology for the PX group, allowing problems of an order of magnitude greater complexity and detail to be routinely solved. Closed loop, cascaded refrigeration systems and process sections that involve parallel trains with recycles have been modeled. Full rigor for unit operations and physical properties are used. No shortcuts have been taken. Our implementation procedure and plans to further exploit this technology will be discussed.

Keywords

FOCAPD 2004, equation-oriented, sequential modular, ASPEN+.

Background

Although they were both conceived in the 1960s, sequential modular (SM) modeling has gained a much wider industrial and commercial usage and acceptance than equation-oriented (EO) modeling. This was due to a variety of hardware and software limitations and historical reasons.

EO modeling is welled suited to solve large complex problems but requires a reasonable starting point to be able to solve. SM modeling requires minimal input data and it is able to solve from a sparsely defined starting point. SM modeling performance and robustness degrades with large complex problems, i.e. numerous recycles, significant heat integration.

EO simulation was initially utilized for some of the more challenging and specialized applications such as real-time optimization (RTO) and dynamic simulation. Since the EO modeling community was primarily expert users, technical functionality (such as how to solve bigger problems faster and more robustly) was the focus and user interfaces and usability were an afterthought. Hardware always limited the size of the problem that could be solved. SM simulation tended to focus on smaller problems. Ease of use and user interfaces became a focus

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of the commercial SM simulation tools. A majority of process engineers gravitated to the SM modeling techniques since they were easier to use, primarily due to the fact that all commercial process simulators employed only SM technology.

By 2003, EO simulation had finally addressed a number of the usability features and the user interface issues that the SM simulation environments had addressed earlier making EO modeling a more practical process modeling tool. Until this time, the key limitation to complex and large scale modeling problems was the SM method itself. It just could not solve large and/or complex problems. There is now an enormous potential that can be gained if EO models are utilized for process engineering studies. This then makes optimization a reality with complex flowsheets. Today, EO models of more than 200K equations are solved in minutes running on a personal computer.

With the release of Aspen Technology's Release 11.1 of Aspen+, EO modeling can now become a mainstream modeling technology for process engineers. This release combined both SM and EO technology in a single environment. It is now possible to take advantage of the strengths of both the SM and EO modeling techniques in a single environment and to be able to switch between the techniques easily. The range and size of problems that the process engineer can solve is increased dramatically with this ability.

The para-xylene (PX) group in BP Chemicals has begun to exploit the EO technology to solve flowsheets of greater complexity than ever before. The PX technology group became involved with EO technology starting in 2000 for on-line optimization projects. Because of fortunate coincidental timing, they were early implementers of on-line optimization using Release 11.1 of Aspen+ w/ RTOpt. The BP PX RTO team was also part of the process design group. This allowed them to more easily roll out EO design tools to other process engineers in the group for several real debottlenecking project studies.

It is important to describe the characteristics of design-type models and compare these to their on-line counterparts since EO methods came into Aspen+ from their on-line optimization group. This is summarized in Table 1. Note that a debottlenecking project model can have aspects of both a design model and an online model.

Table 1 Design Models vs. On-line Model Differences

Design	**Online**
Driven via unit-op specifications	Driven by MEASUREMENTS
Symmetric trains of equipment	Symmetry not required
All equipment is "on"	Equipment can be on or off
Control issues not considered	Control issues critically important
Developed by process engineers	Developed by on-line opt engineers
Consider many flowsheet changes	Flowsheet static

Aspen Technology Implementation Methodology

Aspen Technology has added EO capabilities as a core-modeling component to their process simulator Aspen+ Release 11.1. It keeps the strong points of SM modeling and added EO as a convergence option. The process engineers define their model using a flowsheet graphic and graphical user interface (GUI) in a unit-operation-centric manner. This is consistent with how engineers (not mathematicians) think. Aspen+ then has an option to "synchronize" the model for EO where the unit operations, specifications, and streams are converted into a huge matrix for EO solution. This matrix is populated with the values from the SM run as initial guesses, which does NOT have to be (and usually isn't) from a converged run. The user then has the ability to "swap" specifications that are not allowed in SM, but degrees of freedom must of course be maintained. Then, the matrix can be solved. Also, fixed values can be changed directly in the EO formulation and the matrix is re-solved in a fraction of the time it initially took.

In other words, SM is used to define the basic problem and provide initial guesses while EO is used to solve the fully mass and heat integrated process model with the ability to overcome the specification limitation in the SM environment.

para-Xylene Process and "why EO?"

The BP para-xylene (PX) process is extremely complex. Figure 1 represents an extremely simplified process flow diagram of the major sections of the process. Although this diagram is simple, the Crystallization box can contain 100s of unit operations, 10-20 tear streams, 10-20 design specifications, and a cascaded refrigeration system. In past Aspen+ simulations, BP modeled this as a single simple component separator (SPE2) block and had a separate stand-alone tool to model the crystallization section, which assumed "symmetry", considered only a single process train, and had many other simplifications to permit convergence. Our crystallization process utilizes parallel trains of equipment, which may not be of the same type.

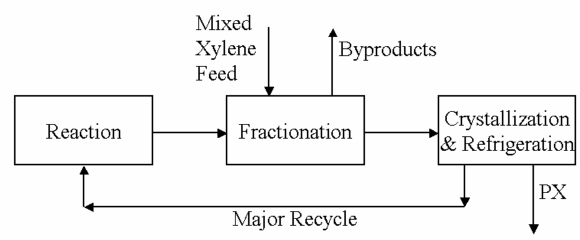

Figure 1. Simplified para-Xylene Process Flow Diagram

The previous technique of modeling the PX process using the Aspen+ SM model and a stand-alone tool involved sequential runs of both tools and manual data transfer meant that in 2 days the engineer had an "almost closed" heat and material balance. In addition, the SM model, after years of refinement, still was extremely problematic to converge for large process changes and often took over 50 iterations and several hours to converge.

Because of the large number of tear streams and design specifications, the crystallization section (crystallization plus refrigeration) was essentially impossible to converge using SM techniques. However utilizing EO methods, it solves fast and robustly over a wide range of conditions. Utilizing EO methods, BP's crystallization section models now include ALL unit operations and have no simplifications.

Design-Type Problems Solved

In early 2003, two simultaneous events took place. First, the real-time optimization projects were wrapping up and second, two debottlenecking projects became active. It was determined for these debottleneck projects that it would be required to handle ALL the equipment because of non-symmetric equipment issues. The PX RTO team developed offline versions of the RTO on-line models, which already contained all the equipment. The on-line features (MEASUREMENTS, validity check, etc) were removed which made the resulting offline models about 50% as complicated, more robust, and faster than the online models. These models were then turned over to three process design engineers, who were given some basic EO training specific to these models. These engineers were very familiar with and competent users of Aspen+ SM but had never used EO modeling. The RTO team continued to provide support, develop custom reports, and make complex model changes. About 5 formulations of the models were required to get the models into the final form that the engineers found most usable. The resulting simulations used 3 different physical property options and contained all the unit operations that were in the plants. These models were the most complete and rigorous process engineering design models BP had ever developed for the PX process.

Case 1, as described in Table 2, just considered the crystallization and refrigeration section of a BP plant. This was converged using EO. The SM model provided the initial guesses and was not converged (MAXIT=3).

Table 2 Case 1 Design Model Summary

Entire Simulation EO	**Crystallization + Refrigeration**
# Blocks	95
# Streams	152
Min Tear Set #	11 Material + 4 Heat
# Spec Groups	21
CPU Times	10 sec SM 1 Iteration 8 sec EO 1st Full Solution 3 sec EO "edit" Solution
# equations	8500
# non-zero	35000

Case 2 modeled the entire PX process of a different plant. It actually started from a previous Aspen+ design model that had a SEP2 crystallization block. This SEP2 block was replaced by a hierarchy for the crystallization and refrigeration sections that were based on the rigorous crystallization and refrigeration section from an on-line model. The "mixed mode" convergence option in Aspen+ was used, where only the crystallization hierarchy was modeled as EO, as part of an overall SM model. The mixed mode approach was used because several important features used in the original SM model were not supported in the EO formulation and the project timeline did not permit re-defining the simulation so that a full EO model could be developed.

Table 3 Case 2 Design Model Summary

Mixed Mode Simulation	**Full PX Process**
# Blocks	170
# Streams	269
Min Tear Set #	14 Material + 4 Heat
# Spec Groups	7
CPU Times	37 sec SM portion 1 Iteration 10 sec EO portion 1st Time 2 sec EO portion 2nd+ Time 218 sec Total Convergence Time
# equations in EO hierarchy	11000
# non-zeros in EO hierarchy	46000

Findings & Usage Recommendations.

From a technical perspective, EO methods can solve design-type problems but this is really no surprise since EO modeling is used for on-line optimization models which are much more complex.

From a process engineer's perspective, these EO models proved to be extremely useful. Compared to previous models used, these new models were an order of magnitude more complete/complex, more flexible in terms of changing the flowsheet and specifications, faster (minutes vs. days), and more robust. All three process engineers that used these models agreed that EO design-models should be developed for all of our units and more complete EO training should be provided to all design engineers.

However, the process design engineers did not find everything easy and intuitive. Listed below are some issues they identified:

- There are too many ways (at least 8) to specify data and specifications (#1 issue with the engineers).
- SM specifications were made to insure there were no simulation errors from the SM run and to insure the partially converged model was in a feasible region. These specifications were then changed to the desired specifications as part of the EO formulation.
- The EO-only and SM-only options add new items to the GUI which can be confusing.
- While the mixed mode solution option proved useful, current requirements for Aspen+ to switch from using SM to initialize the hierarchy to using EO for solution was problematic. This is being addressed by Aspen Technology.
- Debugging failed EO cases was much harder (compared to the SM method) for the process engineers. This has always been a major deficiency of the EO method compared to the SM method. The RTO team handled this for the engineers. This is an area where further development and research is needed.

To utilize EO technology at this time, a reasonable amount of EO expertise is normally needed. At this point (Release 11.1 of Aspen+), most SM models will NOT automatically convert to EO without any issues and converge. Some things to consider changing in your SM model include:

- Have no zero flow streams.
- For closed loop systems (refrigeration, steam, cooling water), do not close the loop in SM but do this in EO using "connections" (a really great trick!). This technique can also be applied to solving different sections of a flowsheet separately in SM but then connecting them in EO.
- For SM, define tear streams, give initial guesses, and set MAXIT=3. This increases likelihood of EO convergence.
- Use no design specifications (i.e., DESIGN-SPECS) in SM since they can be defined in the EO formulation easily.
- To improve robustness, use special options to reduce matrix size and non-zeros: component mapping, vapor- or liquid-only flashes, and packing of components (i.e., COMP-GROUP).

Conclusions

BP has found that EO modeling is ready for prime time but that it takes significant expertise and effort to convert models to utilize EO methods. It is harder to use and more confusing but it is much faster, more robust, and more flexible than SM. Process models that are an order of magnitude more complex can routinely be solved.

EO is truly an enabling modeling technology. BP is developing, and PX process engineers are utilizing, EO models that could not be solved using only SM techniques.

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