A REAL-TIME OPTIMIZATION STRATEGY FOR PETROLEUM PROCESSES WITH SUCCESSIVE ADAPTIVE MODEL REFINEMENT

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Abstract

To enhance models for refinery processes it seems inevitable to increase the level of compositional detail to a much higher level than today. In previous work, we have developed a simulation technique for steady-state simulation, which pays respect to the particularities of this type of detailed composition models. With this new technique, it seems to be possible to significantly lower the computation time for obtaining high-resolution results. This work deals with the extension of our previous work to optimization problems. Using an adaptive composition representation in combination with a multigrid optimization strategy, the time span for the optimization of petroleum processes can significantly be lowered. The large potential of this approach for the implementation in real-time optimization schemes is illustrated by investigating a simple flash problem. It can be shown that the reduced dead time in which the process runs off the optimum operating points, yield a large economical potential.

Keywords

Adaptivity, Multigrid, Real-time optimization, Petroleum processes, Model reduction

Introduction

The huge number of single components in petroleum processes necessitates the use of a suitable model size reduction technique. Currently available methods are based on the idea to introduce a set of fictitious hypothetical pseudocomponents, which is usually set up based on heuristic rules (API, 1992). The quality of the model and consequently also the results of the real-time optimization largely depend on the number of pseudocomponents chosen. While low numbers result in a poor quality of the optimum and poor controller set points, large numbers lead to large computation times, especially if a refinery wide optimization is to be considered (Pedersen, 2000).
Since poor controller set points and therefore poor operation is unacceptable from an economic point of view, models with high compositional detail are highly desirable. To increase the detail by means of molecular information seem to be the most promising, if not inevitable way, to enhance the performance of all refinery processes (Katzer, et al. 2000). Briesen and Marquardt (2002a, 2002b) presented a new solution strategy for petroleum processes to overcome the limitations of currently employed pseudocomponent techniques. This technique seems to be superior to pseudocomponent methods with respect to accuracy, calculation time demands and robustness. This work aims to extend this approach to optimization problems and to show the possible benefits in connection with real-time optimization schemes.

Multigrid optimization

Algorithmic overview

The method uses a continuous distribution function for composition representation. Though this representation is not implementable in a straightforward way on a computer, it brings large flexibility with respect to the model reduction procedure. With the continuous representation

the model reduction problem can be considered as a discretization problem, for which many techniques are available in numerical mathematics. In the approach presented a method of weighted residuals has been chosen. The use of wavelet functions (Haar-wavelets) for function approximation and projection results in a Wavelet-Galerkin discretization.

With the possibility of using different grids for discretization, the main prerequisite for the use of multigrid concepts (Briggs et al., 2000) is given. Starting with an initial guess the optimization problem is solved on a quite coarse level of compositional detail (this step compares to an optimization with a low number of pseudocomponents). With this coarse approximation a residual error is calculated. The residuals are calculated on the full grid (high detail discretization). Using a norm of the residual error vector, we have a measure for the accuracy of the current iterate. If the model fidelity is lower than a prescribed value another iteration is initiated. The high detail in the residual evaluation allows us to localize the basis function, which presumably contributes most to the improvement within the next iteration. By this localization we can determine the detail in composition representation, which needs to be added to improve the model fidelity. Therefore, we have an adaptive selection of the composition representation paying respect to the current problem and physical state. Before the next iteration is performed the low detailed solution is, in the terminology of multigrid methods, *prolongated* to the fine grid. The choice of the prolongation techniques is a degree of freedom of the particular multigrid method. In this work the detailed grid approximation is constructed by a linearization of the full detailed nonlinear model equations at the reduced approximation. In the following iteration the problem does not have to be solved from scratch. In the sense of multigrid methods only a correction to the previous approximation has to be determined, which strongly reduces calculation time. This iterative procedure is looped until the bound for the residual error is met.

This multigrid procedure is particularly beneficial in a real-time optimization scheme. In a first step, only a coarse model is solved, which provides the controllers almost immediately with new, however inexact, set points. In subsequent iterations the set points are corrected until they attain the correct values. The application of the adaptive optimization strategy in a real-time optimization setting will be discussed in detail in the following sections.

Example problem

As a simple example problem, this work considers a flash operation to separate a feed stream given by a detailed analysis of a commercial gasoline consisting of 128 identifiable components. The optimization should find a point of operation for a certain separation quality, for which the cost is minimized. The objective function includes the cost for lowering the pressure below ambient pressure and the cost for heating in order to increase the temperature. By reducing the pressure of an operation point, we only need a lowered temperature to achieve a certain separation. However, decreasing the pressure to very low values the cost for this pressure lowering will become very high. So we can expect a certain optimal operation point for which the summed cost of pressure lowering and heating is minimal. To specify the desired degree of separation a simple quality constraint is used. This simple criterion states that $\kappa \cdot 100\%$ of the lighter half of the components given in the feed stream should be removed with the liquid flow.

Optimization results

In the optimization studies two different strategies have been investigated: First, a direct optimization considering all 128 components right from the start in a detailed model, and second, an adaptive multigrid solution of the optimization problem. The complexity of the model is initially equivalent to 8 pseudocomponents and is refined to satisfy a given accuracy constraint.

Table 1 reveals that the calculation time for a full detailed direct optimization with all 128 components takes almost 1000 seconds. For the adaptive calculation we have a first value for the optimal point of operation after 30 seconds. However, the results with the first coarse composition representation still show significant deviation from the true optimum values. A virtually exact solution is obtained with the second iteration after 118 seconds. So with the adaptive calculation we have cut down the optimization time roughly by a factor of 8.

Table 1. Error in the optimized variables with respect to the detailed model versus the time needed to obtain the results for an adaptive and a direct high-resolution optimization.

	Calculation time [s]	Relative error in T^{opt} [%]	Relative error in p^{opt} [%]
Direct optimization	993	0	0
Adaptive optimization 1st iteration	30	0.36	3.22
Adaptive optimization 2nd iteration	118	0.0025	0.0269

It is clear that a smaller model size compared to the full model optimization would have been sufficient in order to obtain reasonable temperature and pressure set points in this simple example. However, it should be pointed out that the formulation of the optimization

problem in industrially relevant cases may also involve quality constraints for certain molecular species. In this case a high resolution model is inevitable.

Real-time optimization strategy

Algorithm

Particular potential of this adaptive optimization approach lies in the application within a real-time scheme as it is frequently employed in petroleum plants.

A frequent problem in petroleum plant operation is for example the change in feed composition. During a dead time, in which the optimizer computes the new optimal controller set points, the process is not only away from the optimum, but the optimum is not even known. When the new set points finally have been calculated, the controllers of the plant are updated. The controllers then drive the process to the new optimum. After updating the controller set points, the problem is a standard set point control problem to change the operation point. For the loss of profit after the controller updates, therefore, only the performance of the controllers is important. But the profit loss before the controller update must fully be contributed to the ignorance of the optimal operation condition. So the quicker these updates can be provided, the smaller is the profit loss after a feed change.

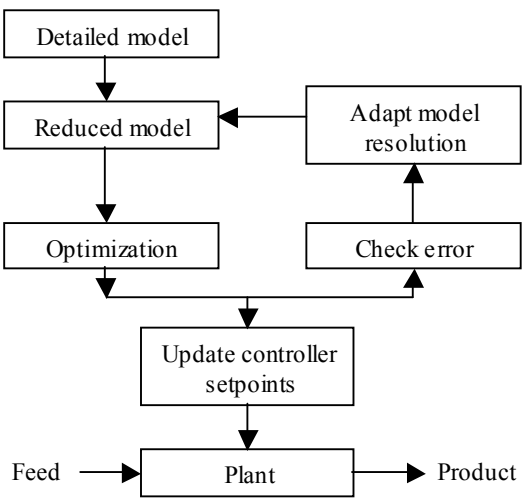

Figure 1. Adaptive multigrid real-time optimization strategy.

Besides a model, which reflects the plant behavior in reasonable detail, the success of the method therefore crucially depends on the computation time the optimization takes. Today, the optimization cycles for petroleum processes take about 1-2 h. Even if perpetually increasing computer speed can lower this time span, one has to keep in mind that the actually optimized models are still far away from a refinery-wide and molecular based point of view. For a refinery-wide view with detailed compositional description, the complexity, and therefore the calculation time, would increase significantly.

As seen above, the adaptive strategy has lowered the computation time by almost an order of magnitude. But not only the time needed to reach the "exact" optimum is important. As depicted in Figure 1 the controller set points can already be updated after the first initial step. Since the controllers need some time anyway to drive the process to the new optimum, they do not necessarily have to know the "final" optimal controller set points right from the start. The initial approximation is more a direction in which the process has to be moved instead of a final operation point. Most likely, the next iterated set point will be available before the steady-state for these intermediate set points will be reached. For more complex optimization problems this may involve a whole series of controller updates, which are subsequently generated for more and more detailed model formulations. Though this is not necessarily true, it is reasonable to assume that with more detailed models also the quality of the set points increases with each iteration.

Example problem

To use the above outlined optimization strategy in anreal-time optimization framework, the plant in Figure 1 has been replaced by a dynamic simulation of the flash. In the beginning the flash is fed with a stream of given composition, for which the optimum operation point for a separation quality constraint of $\kappa = 0.4$ has been determined off-line. After the first 60 minutes the feed composition is changed. With this feed change a new optimization is initiated considering the feed change and a change in the separation quality constraint to $\kappa = 0.6$. Due to the simplicity of the optimization problem, the calculation times are quite low. To have a more realistic setting the calculation times for the full grid direct optimization is scaled to 1 hour, which is a reasonable time for the optimization of a more complex technically relevant process. The calculation times for the adaptive calculation loops have been scaled accordingly.

Real-time optimization results

As shown in Figure 2, the first 60 minutes are used to take the process to the given optimal point of operation for the initial feed specification. At 60 minutes the process shows only weak reaction to the feed change if the optimization is performed directly with the full scale model accounting for all 128 components. In ignorance of any new set points, the process is operated at the old set points for the full hour of dead time. This not only leads to an increased cost function but also results in a violation of the separation quality constraint during the dead time period. After the 60 minutes of dead time, the new set points are finally provided to the process controllers. The controllers then become active and drive the process to the new optimum.

In the adaptive optimization scheme the controllers are provided virtually instantly with a first approximation of the real set points causing the process to react almost without any dead time to the feed and specification change. After the set points have been updated, the controller behavior is similar to the full grid case, only that it happens much earlier. So the process reaches the new, less expensive optimum much quicker. Also the time span in which the process is operated off specification is significantly shorter.

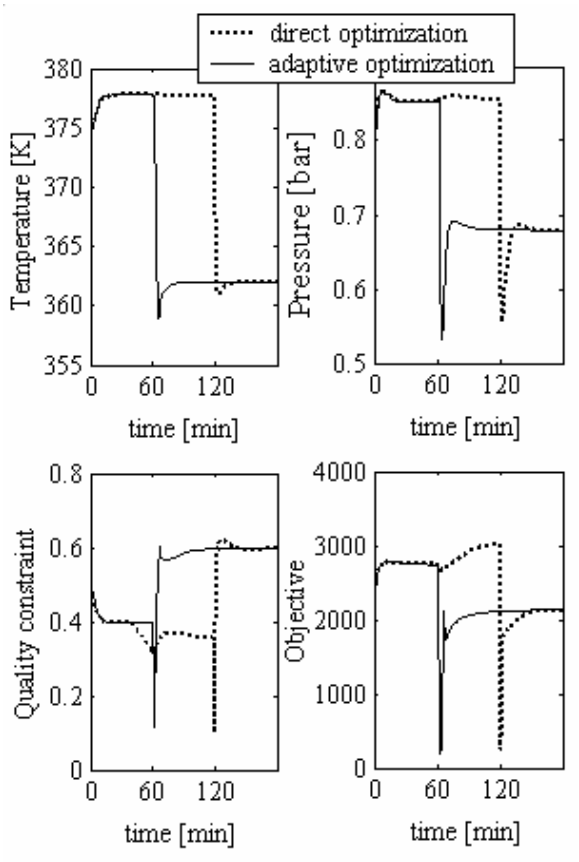

Figure 2. Dynamic flash simulation with a change in the feed composition at t = 60 min coupled with a real-time optimization scheme.

Conclusions and future perspectives

This work presents an adaptive model refinement strategy for real-time optimization of refinery processes. The strategy is based on a continuous problem formulation for which adaptive multigrid discretization techniques can be employed. With these techniques, the model can be formulated easily in various degrees of detail. An initial optimization giving only a coarse result for the optimum operation point can be obtained quite quickly with a coarse model formulation. After providing these initial coarse results to the plant control system, another iteration is initiated to refine the model and therefore refine the accuracy of the optimum operation point. Applying this strategy to a simple flash problem reveals that the profit loss for example after a feed composition change can significantly be lowered.

Note that the optimizer (NPSOL, Gill et al., 1986) is used as a black box in the example presented. Therefore, though the optimization strategy can easaily be implemented with available software, significant potential for improvement is present if optimization and refinement algorithms are integrated.

It should be pointed out that the simple academic example provided here can only serve to illustrate the potential use of the approach. The next steps of our research consitutes the set up of realistic benchmarks. These benchmarks should comprise the complexity of industrial settings.

References

API (2002). *Technical Data Book – Petroleum Refining*. American Petroleum Institute, Washington D.C..

Briesen, H. and W. Marquardt (2002a). An adaptive multigrid method for the steady-state simulation of petroleum mixture thermal separation processes. *In preparation for Ind.Eng.Chem. Res.*

Briesen, H. and W. Marquardt (2002b). A new approach to refinery process simulation with adaptive composition representation. *In preparation for AIChE J.*.

Briesen, H. (2002). *Adaptive Composition Representation for the Simulation and Optimization of Multicomponent-Mixture Processes*. VDI-Verlag, Düsseldorf.

Briggs, W., Henson, V., and S. McCormick (2000). *A Multigrid Tutorial*. SIAM, Philadelphia.

Gill, P., Murray, W., Saunders, M., and M. Wright (1986). Users Guide for NPSOL (Version 4.0). *System Optimization Laboratory, Stanford University, USA*.

Katzer, J., Ramage, M., and A. Sapre (2000). Petroleum refining: Poised for profound changes. *Chem. Eng. Process.*, July, 41-51.

Mizoguchi, A., Marlin, T.E. and A.N. Hrymak (1995). Operations optimization and control design for a petroleum distillation process. *Can. J. Chem. Eng.*, **73**, 896-907.

Pedersen, C.C. (2000). The road ahead to refinery wide optimization. *Proceedings for Aspen World 2000*, Orlando, USA.