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An optimization-simulation model for a simple LNG process

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ABSTRACT

A gradient free optimization-simulation method for processes modelled with the simulator Aspen HYSYS is developed. The tool is based on a Tabu Search (TS) and the Nelder-Mead Downhill Simplex (NMDS) method. The local optima that result from the TS are fine-tuned with NMDS to reduce the required number of simulations. The tool has been applied to find the total refrigerant flow rate, composition and the refrigerant suction and condenser pressures that minimize the energy requirements of a Prico process. The main strength of this method is that it has a high probability of obtaining a better solution with significantly fewer simulation runs than other metaheuristic methods. Also, by changing the TS step size it is possible to influence the initial search pattern, thereby taking advantage of already gained process knowledge to decrease the optimization time. The method is general and can be applied to other processes modelled in Aspen HYSYS.

1. Introduction

Energy and petrochemical process plants consist of unit operations such as separators, valves, expanders, compressors and heat exchangers. Each of these unit operations contributes its own set of more or less realistic thermodynamic equations as well as mass and heat balances. Such equation systems normally have a few degrees of freedom. The units are linked to each other by the material and energy streams with another set of process variables, such as flow rate, pressure and temperature. The challenging task is to minimize the investment and operating costs of the plant with respect to these process variables. In general, adjustments in the operation of one of the units will have consequences for other units, and these relationships are often nonlinear.

Mathematical programming (MP) and deterministic optimization methods are widely used in process design as these methods have the ability to find the best possible solution for the mathematical model that describes the process (Edgar, Himmelblau, & Lasdon, 2001). A common example of using MP in process design is the synthesis of heat exchanger networks (HEN). Also, some attempts have been made to connect the HEN with the background process. However, only smaller problems have been solved this way. Two thorough reviews of heat exchanger network synthesis (HENS) were published by Gundersen and Naess (1988) and by Jezowski (1994a, 1994b). Furman and Sahinidis (2002) have contributed with a critical review and annotated bibliography of 461 papers on HENS. Due to physical laws and economic relations, the mathematical model commonly results in a non-convex nonlinear programming (NLP) problem. Furthermore, with discrete decisions, a mixed integer nonlinear programming (MINLP) problem has to be solved. These types of problems can be hard, or even practically impossible to solve using deterministic global optimization algorithms without further simplification of the model. The main advantage of using equation based programs and global solvers, is that it can guarantee that the global optimum of *the model* is found (Floudas, 1999). However, if the equation based model cannot be solved unless it is made too unrealistic, then the proven optimum may not be the best possible solution in the real world.

In order to model the process more rigorously and with less effort, general purpose process simulators are often used. Such process simulators can be divided in two main groups, sequential and equation based simulators. Common to all process simulators is a library consisting of three main parts; thermodynamic relations (equations), fluid properties and pre-defined unit operations (process equipment). The processes are then designed using the unit operations, which are connected by material and energy streams. Since the set of equations are too complicated to be solved analytically, they must be solved recursively to determine settings that are consistent for the entire plant.

In an equation based process simulator the equations for all unit operations as well as the thermodynamic relations are solved simultaneously to find the solution. It is therefore possible to use

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equation based process simulators together with deterministic optimization. Equation based models can be made more rigorous by adding more equations. However, for large non-convex NLP problems, no algorithms exist that solve such problems in polynomial time, thus they rapidly get intractable.

Sequential based simulators are very common in the industry as well as in academia and are widely used due to their simplicity and robustness. Another advantage with sequential based process simulators is that their graphical user interface (GUI) can make implementation of the petrochemical process models relatively less time consuming than in equation based models. In contradiction to equation based simulators, each unit operation is modelled and solved on its own given the input data in the form of material and energy streams. The units are then solved in sequence. To speed up the convergence, numerical methods such as Wegstein are often used. For complicated flow sheets there may be several recycles and the calculation order is normally set to give the lowest possible number of recycles or tear streams (Gundersen & Hertzberg, 1983). The disadvantage with the sequential approach is that gradient information that deterministic optimization methods require is less accurate and harder to obtain. Since the solutions will change slightly from one run to another due to the sequential behaviour and the tolerances, it may be difficult to develop procedures for obtaining these gradients. A sequential based process model can be looked upon as a black box model and is therefore not suitable for use in global deterministic optimization algorithms.

A process that benefits from rigorous modelling in process simulators is liquefaction of natural gas (LNG). It is an energy and cost intensive process and due to small temperature differences in the heat exchangers, inaccurate modelling is likely to result in real world infeasibility. The main contribution of this paper is a method that does not require gradients for the heuristic optimization of sequence based simulation models.

In contrast to deterministic methods, Stochastic Optimization (SO) incorporate probabilistic (random) elements either in the objective function, the constraints, or alternatively in the algorithm itself, e.g. through random parameter values, random choices or in both. A distinction can be made between Stochastic Programming, where the model is to be optimized with regard to uncertainties in the value of some variables, e.g. the volume and sales price of a product, and Stochastic Algorithms where random elements are used in the search, the latter also known as Meta Heuristic (MH) methods. In process design the most common MH are Genetic or evolutionary algorithms (GA), Tabu Search (TS), Simulated Annealing (SA) and multi-start Local Searches (MSLS) where a local optimization algorithm is started from several feasible points (Holland, 1975; Glover, 1986; Kirkpatrick, Gelatt, & Vecchi, 1983; Marti, 2003). The main strength with MH methods is that they can be used to optimize a black box model and are thereby well suited to be implemented together with sequential based process simulators to take advantage of the rigorous thermodynamic packages and unit operations that are already developed. The weakness is that MH methods, in contrast to deterministic methods, cannot guarantee that the best possible solution is found, however, the solution might still be better than for the globally optimized but simplified deterministic model.

Apart from the modifications required for the error handling in the aggregation of the objective value, the presented method is quite similar to those applied to analytical test functions presented by Chelouah and Siarry (2005) and Hedar and Fukushima (2006). Their models consist of combinations of a global Tabu Search (TS) and a local Nelder-Mead Downhill Simplex (NMDS).

Exler, Antelo, Egea, Alonso, and Banga (2008) have applied a TS based algorithm to an integrated process and control design model. They argue that mathematical programming using global optimization methods (GO) only handle problems that are small, differentiable and continuous. A system of differential and algebraic equations forms their model's restrictions. Their case is similar to the one described in this paper and assumes nothing about the topology of the objective and the model is treated as a black box.

Cavin, Fischer, Glover, and Hungerbühler (2004) apply a TS optimization algorithm to a batch plant. Batch process simulation software is used as a black box model for the process evaluations. They discuss Genetic Algorithm (GA) versus TS and conclude that there are several factors that make GA unsuitable for such applications. The crossover operations do not always generate valid solutions, and penalty and ad hoc repair operations have a risk of spending most of the computational effort in the handling of errors.

Section 2 contains a detailed description of the optimization-simulation framework, including the aggregated objective value, the global TS, the local NMDS, the combined search and the integration between Aspen Hysys and the search procedure. The industrial process that the method is applied to, Prico, a simple LNG process, is presented in Section 3. The results are presented in Section 4. A discussion of the model and the results are found in Section 5, and conclusions and plans for further work are found in Section 6.

2. Optimization-simulation framework

From the point of view of the search algorithm, the objective function of the problem addressed in this paper is a black box. It contains a sequence based simulation model and an error handling algorithm. Since the model is known to have multiple minima and cannot easily and accurately provide any gradient information, it requires global search methods such as Simulated Annealing (SA), Tabu Search (TS) or Genetic Algorithms (GA). Among these, TS is expected to be the best suited for this problem because it gives the best control over how much the solution can change from one step of the search to the next so that less effort is spent on error handling. The reason for combining the global TS with the NMDS local search or descent method, is that the local search usually converges faster to the best solution in the area the TS has detected than the TS would on its own.

The optimization engine consists of a combined TS and NMDS which is connected to a Process Simulator Aspen HYSYS (version 2004.2) through Microsoft Excel using Visual Basic for Applications (VBA). The initial expectation, which turned out to be true, is that a large part of the computation time is spent running simulations relative to running the search algorithm; therefore Visual Basic (VBA) is an adequate surrounding layer. It provides the necessary means to get access to the COM functionality of HYSYS, which was crucial for the development. Microsoft Excel is also used as a Graphical User Interface and includes the input data, the TS and NMS settings and numerical as well as graphical results.

The objective value aggregation procedure in the VBA routine consists of the HYSYS simulation and the error handling. At the beginning of each cycle, all relevant values are given to HYSYS, which is then started and runs until it either converges or warns that it is unable to. Then some of the calculated process values are retrieved, the feasibility status is checked, and the objective value aggregation procedure condenses this information into a single objective value. Seeing it in an abstract way, this procedure replaces the traditional objective function.

2.1. The aggregated objective value

The objective value aggregation consists of two parts; the simulation model and an algorithm that condenses the simulation output or the warning message into a single number. This number is a measure of the quality of the evaluated solution. If it is able