

# Towards Implementing a Total Capital Cost Budgeting Constraint in MILP-Based Approximations to MIFP Problems

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Budgeting the total capital cost of a chemical engineering project is integral to its future financial success. It is often difficult to know beforehand how costly a project will be, but if the final price grows larger than an internal budget, problems can arise. The project may have to be prematurely cancelled, reflecting a large lost sunk cost. Alternatively, the project could be completed, but at the cost of shelving other pursuits. Neither result is desirable. Capping the total estimated capital cost of the project in preliminary optimisation studies could pre-emptively circumvent some of these problems. This work explores the challenge of integrating a capital cost budgeting constraint into a nonconvex, MIFP chemical process network unit production cost minimisation model, and introduces a novel solution strategy and algorithm to find the globally optimal solution. The algorithm incorporates an inexact parametric algorithm based on Newton's method with successive piecewise linear approximations and NLP subproblems to guarantee feasibility of the nonconvex objective function. The result is an MILP problem with NLP subproblems. The efficiency of the proposed algorithm is demonstrated by minimising the unit production cost of a large chemical conversion network. The problem is solved with several general purpose MINLP solvers in addition to the proposed method. Computational results show that the proposed method shows promise to outperform general-purpose MINLP solvers when solving large MIFP network optimisation problems.

## 1. Introduction

Industrial-sized processes can have enormous capacities and corresponding capital investment costs. For example, Malaysian-based PETRONAS purchased a 47 % share of a 170,000 bbl/d oil refinery in Malacca, Malaysia from Philips 66 for  $635 \times 10^6$  \$ late in 2014 (Reuters, 2014). Larger industrial projects can command price tags of over  $1 \times 10^9$  \$. With so much capital on the line, extensive planning of such industrial processes can take a number of years and resources.

In the chemical engineering community, strides are always being made to minimise the capital cost of important unit processing equipment, such as heat exchangers (Chew et al., 2014). Such work certainly lowers the capital costs of facilities. However, when novel projects or processes are developed in the chemical engineering community, such as recent advances in liquid fuel production from bioresources (Gürsel et al., 2014) or waste heat recovery systems (Bellqvist et al., 2014), uncertainty arises in how to budget capital when planning these projects. Thus, a natural step could be to implement capital cost budgeting into process design and optimisation models.

To date, a number of models have been constructed that calculate the total capital cost of the resulting process selection and processing pathway structure. However, the user has no direct influence over the final capital cost of the facility. To the best of our knowledge, no network-based processing pathway optimisation work has incorporated a capital budget constraint directly into the model. The lack of such a constraint is likely due to the nonconvex scaling effects of a project's capital cost with its capacity (Seider et al., 2009). These nonconvex scaling effects increase the difficulty of finding globally optimal solutions. Additional solution strategies should be considered when solving these problems. To that end, a general survey of initial work in mathematical programs involving capital budgeting was compiled by Bernhard

(1969). At the time, many models that considered capital budgets did so with fixed capital costs for the various projects. These models emphasized financial analysis – concepts of borrowing, lending, and the use of other financial instruments and strategies were modelled. However, parameters more of interest to the chemical engineering community such as capacities, input costs, and energy & material flows were absent from these models. The financial analysis of these early models has been expanded by allowing fractions of projects to move forward (Laínez et al., 2009). This approaches the concept of allowing the capacities of the various projects to change, but does not take into account the nonlinearly scaling aspect of capital cost with capacity. The optimal design (and re-design) of supply chains under capital budgeting has also been considered (Narahariseti et al., 2008) but the capacities of the available projects were not allowed to vary.

This work presents a novel, and by far the most efficient, computational method to solve MIFP network-based processing pathway optimisation problems using a tailored MILP piecewise linear approximation algorithm with NLP subproblems within an inexact parametric algorithm based on Newton's method. Piecewise linear approximations are used to approximate the nonconvex capital cost scaling functions, and the NLP subproblems serve to find a feasible upper bound within the context of an overall capital cost budget constraint. To the best of our knowledge, such a challenging MINLP problem with capital budget constraints were considered intractable for rigorous global optimization before. This method is then compared with directly solving the original MIFP with general purpose MINLP solvers.

## 2. Global Optimisation Strategy and Algorithm

Mixed-integer fractional programs (MIFPs) are a special class of mixed integer nonlinear programs (MINLP) that have a fractional term or terms in the objective function. Such problems can arise naturally from a number of process engineering scenarios. A particularly common problem might be the minimisation of the production cost of a processing pathway, with the denominator in this case being the amount of product produced. Other fractional objectives might arise from a desire to minimise the unit emissions (GWP, etc.) from a facility following the functional unit methodology in life cycle optimization (Yue et al., 2013). Thus, solving optimisation problems within the framework of MIFPs is integral. In this work, the aim is to minimise the unit production cost of a large-scale process network. The general representation of the problem to be solved in this work is as follows:

$$\min \left\{ \frac{\sum_j a_j \cdot X_j^{sf_j} + \sum_j b_j \cdot X_j + \sum_i c_i \cdot S_i}{\sum_i d_i \cdot S_i} \right\} \quad (\text{P0})$$

$$\text{s.t.} \quad \sum_j f_j \cdot X_j^{sf_j} \leq ccb \quad (1)$$

$$\sum_i g_{ik} \cdot S_i + \sum_j h_{jk} \cdot X_j + \sum_j l_{jk} \cdot Y_j \leq m_k, \forall k \quad (2)$$

$$X_j \in \mathfrak{R}_+^n, S_i \in \mathfrak{R}_+^m, Y_j \in \{0,1\}^n \quad (3)$$

where the indices  $i$  and  $j$  correspond to variables  $S_i$  and  $X_j$ .  $Y_j$  is a set of binary integer variables for the discrete design and synthesis decisions of the process network. The index  $k$  represents the set of model constraints. Upper case letters indicate variables, and lower case letters indicate parameters. The parameter  $ccb$  represents the capital cost budget. Note that the addition of the scaling factors  $sf_j$  introduce concave terms to the model. Eq(1) is the capital budget constraint, and Eq(2) represents a generic form of general mixed-integer linear constraints. There are key solving challenges that arise in this model. Nonconvexities arise not only within the fractional structure of the objective function but also within the capital cost scaling terms in the objective function (Gong and You, 2014). The capital cost budget constraint in Eq(1) provides an additional solving challenge due to the nonconvex nature of the capital cost function. We approach these complexities systematically in the sections below.

### 2.1 Inexact Parametric Algorithm using Newton's method

There are a number of algorithms for solving MIFP problems, such as the branch-and-bound method (Gao et al., 2015), but parametric algorithms have been shown to be the most efficient approach for nonlinear MIFP problems (Chu et al., 2013). For P0 above, a parameter  $pp$  is introduced as the following fraction:

$$pp = \frac{\sum_j a_j \cdot X_j^{sf_j} + \sum_j b_j \cdot X_j + \sum_i c_i \cdot S_i}{\sum_i d_i \cdot S_i} \quad (4)$$

Thus, problem P0 can be rewritten as:

$$F(pp) = \min \left\{ \sum_j a_j \cdot X_j^{sf_j} + \sum_j b_j \cdot X_j + \sum_i c_i \cdot S_i - pp \cdot \sum_i d_i \cdot S_i \right\} \quad (P1)$$

with all constraints the same as P0. The objective function of this problem is a function of  $pp$  and is denoted as  $F(pp)$ . While this function is a “nested optimization” problem and does not have a close-form analytical solution, it has been mathematically proved that the equation  $F(pp) = 0$  has only one solution which also serves as the globally optimal solution to problem P0 (Zhong et al., 2014). Thus, efficient, iterative root-finding algorithms can be used to find the solution of problem P0. In this work, inexact Newton’s method is used for solving this non-convex MIFP.

## 2.2 Successive piecewise linear approximations for concave capital cost functions

We next approximate the concave capital cost functions for all technologies in the processing network with piecewise linear approximations using SOS1 variables, resulting in a mixed integer, linear programming (MILP) problem (P2):

$$F'(pp) = \min \left\{ \sum_j RX_j + \sum_j b_j \cdot X_j + \sum_i c_i \cdot S_i - pp \cdot \sum_i d_i \cdot S_i \right\} \quad (P2)$$

s.t. Eq(2) and (3)

$$X_j = \sum_n W_{j,n} \cdot u_{j,n}, \forall j \quad (5)$$

$$RX_j = CC_j \geq \sum_n W_{j,n} \cdot val_{j,n}, \forall j \quad (6)$$

$$\sum_n W_{j,n} = 1, \forall j \quad (7)$$

$$\sum_n EX_{j,n} = 1, \forall j \quad (8)$$

$$W_{j,1} \leq EX_{j,1}, \forall j \quad (9)$$

$$W_{j,n} \leq EX_{j,n-1} + EX_{j,n}, \forall j, n > 1 \quad (10)$$

$$W_{j,n} \leq EX_{j,n-1}, \forall j, n = N \quad (11)$$

where the set  $n$  denotes the number of grid points in the piecewise linear approximation,  $u_{j,n}$  are the values of the grid points in the  $X_j$  space,  $W_{j,n}$  are continuous, weighted terms for each  $u_{j,n}$  in each interval,  $val_{j,n}$  are equal to the value of the original nonconvex capital cost function at each grid point,  $RX_j$  serves as a substitute for the capital cost of each technology  $CC_j$ , and  $EX_{j,n}$  are SOS1 variables that determine in which interval the MILP solution is located. Note that the constraints in P0 also apply here.

Solving the MILP branch and refine algorithm with piecewise linear approximations provides a valid lower bound for the capital cost, and an upper bound could be obtained by substituting the optimal solution of the MILP problem into the original objective function of P1 (You et al., 2011). However, the resulting upper bound could result in an infeasible objective value with under a capital cost budget constraint (Figure 1). The capital cost for the MILP solution is feasible and serves as a lower bound for the original problem (Gong et al., 2015). In contrast, the corresponding capital cost calculated at the capacity of this solution using the original capital cost equation is infeasible as it violates the budget constraint. Another method must be followed to ensure a feasible global upper bound and convergence to the global optimum.

## 2.3 Implementation of NLP subproblems to ensure feasibility

The novel contribution of this work is the development of a nonlinear programming (NLP) subproblem solution method. In formulation P1, the only binary variables are the decision variables on whether or not a technology is chosen to be in the final processing pathway. Thus, if one can determine a set of candidate technologies, these binary variables can be fixed as parameters, resulting in an NLP subproblem that can be more readily solved. Any feasible, local solution to this NLP subproblem can function as a valid upper bound for the original problem. This advantageous property is employed in the algorithm described in this work. A flowchart of this algorithm is given in Figure 2. First, the MILP problem is solved with the branch

and refine algorithm with piecewise linear approximations for each technology's capital cost. The binary variables that determine the selection of technologies are then fixed as parameters. Solving the resulting NLP subproblem, if it is feasible, will give a valid, global upper bound for the original problem.

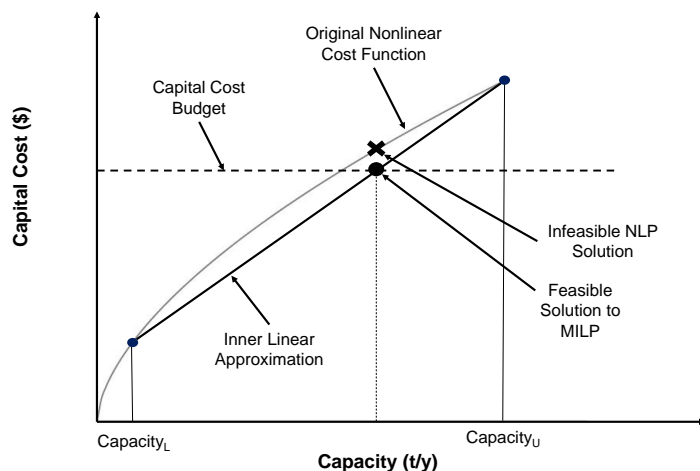


Figure 1: Original nonlinear capital cost function, inner linear approximation, and a capital cost budget constraint is shown. Also shown is the possibility for an infeasible solution to the NLP subproblem but a feasible solution to the MILP problem

If some tolerance between the objective value of the MILP solution and the objective value of the NLP solution is satisfied, the algorithm terminates with the output of the NLP as the final solution. If not, more points can be added to the piecewise linear approximation, and the algorithm repeats until convergence is satisfied. The proposed algorithm bears some resemblance to the outer-approximation algorithms for MINLP problems (Duran and Grossman, 1986). A key difference here, however, is that the underlying NLP has nonconvex terms, requiring a different approach. It should be noted that a key property of the present algorithm is its ability to find a feasible upper bound to the original MINLP model, ensuring convergence to a global optimum.

### 3. Case Study, Results, and Discussion

All experiments were performed on a DELL OPTIPLEX 790 desktop PC with an Intel(R) Core(TM) i5-2400 CPU @ 3.10 GHz and 8 GB RAM. All models and solution procedures were coded in GAMS 24.3.3 (Brooke, 2009). The original MINLP problems were solved with BARON 14.0.3 (Tawarmalani and Sahinidis, 2005), SBB, DICOPT, and SCIP 3.0. MILP problems were solved with CPLEX 12.6, and NLP subproblems were solved with CONOPT 3. The results shown were obtained with the proposed algorithm. A network of chemical conversion technologies was constructed based on previous work (Garcia and You, 2015). Data obtained for each technology in the network included bases for the capital and operating costs and corresponding capacities. Large sets of candidate reactants and products are included in the network, providing the user a wide array of options. Demand for three primary products was to be satisfied by processing any amount of a variety of feedstocks with a variety of distinct processing pathway choices. Other secondary products and byproducts could also be produced and sold. The unit production cost was the objective to be minimised in the model. A capital budget of  $145 \times 10^6$  \$ was fixed.

A production cost of  $-1.044$  \$/kg was achieved; the negative sign indicates that the final processing pathway is profitable. The optimal processing pathway results in a capital cost of  $142.9 \times 10^6$  \$ – just under the limit set before the optimisation. Table 1 compares the computational performance of solving the problem directly with general purpose MINLP solvers with that of the proposed algorithm. The proposed algorithm is shown to perform one order of magnitude faster than BARON. SCIP could not find an optimal solution after the maximum computation limit of 10,000 s, while SBB and DICOPT encountered infeasibility errors. It should be noted that the problem size in terms of numbers of equations and variables is larger in the MILP than that of the original MINLP formulation, due to the addition of the piecewise linear approximations. The NLP subproblem has the same number of equations as the original MINLP formulation, but no longer has binary variables, eliminating some complexities of the original model. This elimination of computational complexity is manifested in the time taken to solve each problem. These results could suggest that as the problem size increases with larger processing pathway networks and

more feedstock and product choices, the proposed algorithm might demonstrate significant decreases in computation times compared to solving the MIFP formulation directly.

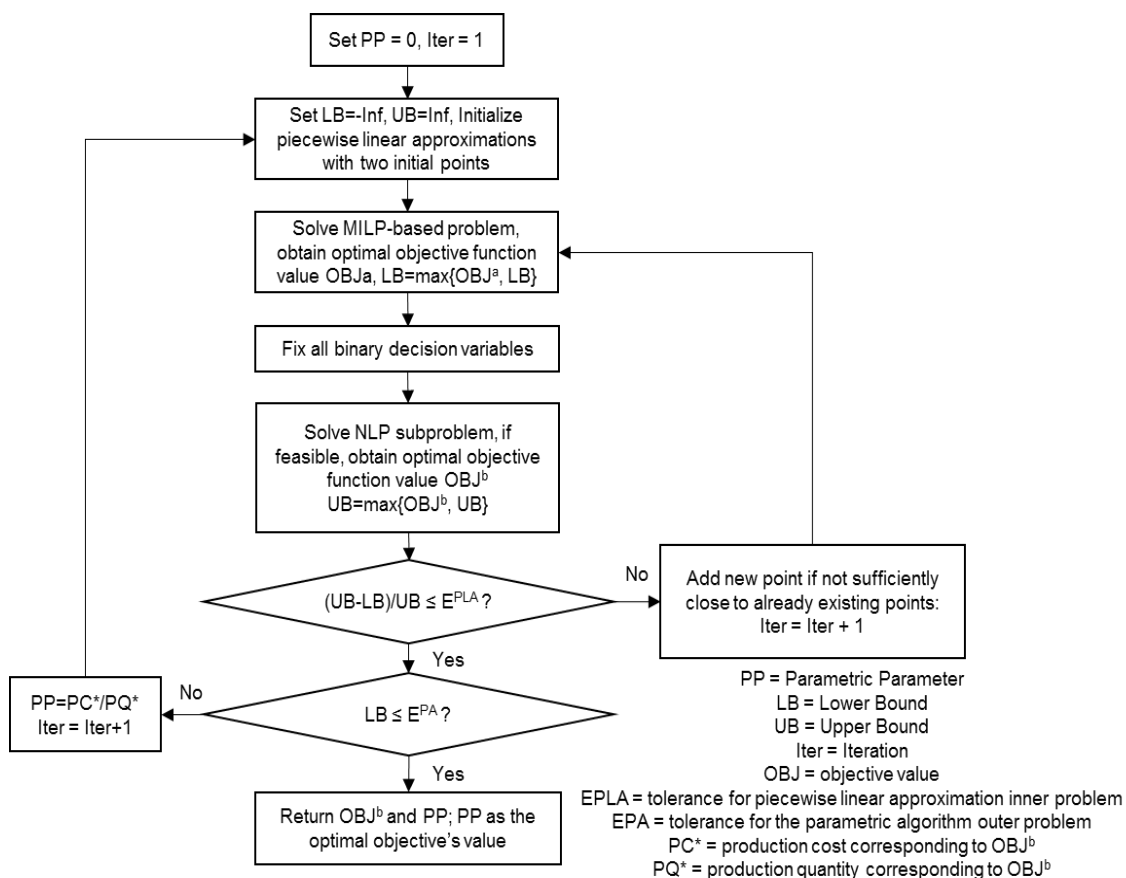


Figure 2: Flowchart for the proposed algorithm to solve MIFP problems with capital cost budget constraints using a parametric algorithm, piecewise linear approximations, and NLP subproblems to ensure feasibility and optimality (details about implementation and computer programs are given in Section 3).

Table 1: Computational results. 10,000 s was the maximum solving time allowed

	BARON 14.0.3	SCIP 3.0	SBB	DICOPT	Proposed algorithm
Obj. Value (\$/kg)	-1.044	[-38.92, -1.02]	Locally infeasible	Locally infeasible	-1.044
Continuous Variables	1,090	1,090	1,090	1,090	4,690 (in MILP); 1,090 (in NLP)
Integer/Binary Variables	200	200	200	200	400 (in MILP); 0 (in NLP)
Constraints	1,375	1,375	1,375	1,375	4,175 (in MILP); 1,375 (in NLP)
Solving Time (CPUs)	338.1	10,000	N/A	N/A	68.6

#### 4. Conclusion

A novel method for handling capital budget constraints in process selection and planning stage optimisation models was summarized. A general MIFP formulation was built to model a processing

technology network and minimise its unit production cost with a constraint on the overall capital cost of the processing pathway. A branch and refine algorithm using piecewise linear approximations to the nonlinear terms in the capital cost functions for each technology in the network was employed to enhance the computational efficiency of solving the problem, resulting in an iterative MILP problem. Solving this MILP provided a valid lower bound to the unit production cost. To ensure feasibility under the presence of a capital cost budget, the binary decision variables were fixed upon solution of the MILP, and then an NLP subproblem was solved to obtain a global upper bound. The proposed algorithm was shown to find the globally optimal solution more quickly than directly solving the original MIFP with general purpose MINLP solvers. Such a method can allow project designers and managers to quickly and effectively determine which projects should be built to minimise unit production costs under capital budget constraints. This capability will be especially useful for smaller or newer industries, such as the renewable energy sector.

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