

A HYBRID INTERVAL CONSTRAINT PROPAGATION AND MATHEMATICAL PROGRAMMING METHOD FOR ENERGY SYSTEMS SYNTHESIS

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Abstract:

In the last three decades the simultaneous synthesis of process and utilities systems and process optimization and HEN synthesis has become very important research field in chemical engineering. These large systems are difficult to solve and a lot of simplifying assumptions are still needed to keep these problems mathematically tractable especially in industrial applications. In this paper a hybrid method in which we are integrating constraint propagation with mathematical programming on the stand-alone modeling level for solving large energy systems synthesis is introduced. Such integration is illustrated using new formulation for solving HEN synthesis targeting problem under all possible combinations of process modifications and a CP application numerical example in which CP is used as a preparatory step to NLP solution for the total annualized cost minimization of HEN synthesis problem.

Keywords: Interval Constraints Propagation; Constraint Programming, Mathematical Programming, Process Synthesis, Constraint Satisfaction

Introduction:

Worldwide industrial community is ravenous to producing more-with-less through cost effective but benign new products and processes. Chemical process industry is known as one of the most energy-intensive manufacturing sectors in the industrial community. Waste heat recovery applications, as old as the industry itself, are nowadays a must. Many techniques emanated in the early seventies for systematic heat integration has been in use since in the industrial community and are now gaining more momentum. Finding any small room for improvement in the newly designed processes that can bring some value towards energy saving and GHG emissions reduction will be more than welcomed. For non-constrained and non-thermodynamic constrained processes process design and operation alternatives are cumbersome

and the number of alternatives that include different process structures, design parameters and operating conditions result in a combinatorial optimization problem.

Constraint Programming field, known to be a little younger than mathematical programming, is getting every day ground in reducing the computational effort needed to solve combinatorial optimization problems. A crucial component in Constraint Programming approach is the Constraint Propagation.

Constraint Propagation (CP) is a very efficient method for reducing the search space of combinatorial search and optimization problems and has become more important in the last two decades. The basic idea of constraint propagation methods is to detect and remove inconsistent variable(s) assignment(s) that can not participate in any feasible solution through the repeated analysis and evaluation of the variables, domains and constraints describing a specific problem instance.

Constraint logic Programming or sometimes called Propagation (CLP), as a technique used in Constraints Satisfaction (CS) applications, is a unique problem-solving paradigm that establishes a clear distinction between two pivotal aspects of any problem; a precise definition of the constraints that define the problem to be solved, and the algorithms and heuristics enabling to solve it. CLP is increasingly being used as a problem-solving tool for many engineering problems. It was originally developed for solving CS feasibility problems but has recently been used in optimization problems too.

Grossmann and co-workers have combined the power of both Constraint Programming and MILP on the algorithmic level to solve continuous time scheduling of multipurpose batch plants [1]. They used MILP to optimize the high level decisions and Constraint Programming to obtain feasible detailed schedule. Hooker and co-workers in 2002, referenced by Grossmann et al., specified two ways to integrate Constraint Programming and mathematical programming. One by combining them on the modeling level and try to find the algorithm that can solve such hybrid model. The second by decomposing the original problem into two sub-problems; one is MILP and the other is Constraint Programming. Each model is solved separately and information obtained from one help solving the other.

Essentially, combinatorial optimization problems can be posed as multi-level optimization one. Sub-problems can be solved using constraints propagation for feasibility checks. The decision maker inputs and the solutions of the sub-problems insights can be fed to another MP formulation to find the details of the final solution.

The HEN synthesis problem under all possible combinations of process parameters modifications is a quite large problem. Upon decomposition, to targeting and synthesis sub-problems, it can be

easily tackled using CS to find under all possible combinations of process changes the heating and cooling utilities minima and maxima targets.

In this paper a hybrid method in which we are integrating constraint propagation with mathematical programming for solving large energy systems synthesis is introduced. Such integration is illustrated using new formulation for solving HEN synthesis targeting problem under all possible combinations of process modifications sub-problem. A second example for integrating CP and MP; is using CP and NLP for total annualized cost minimization of HEN. It is a numerical example for solving minimum area HEN sub-problem to show the use of CP as a preparatory step to MP problem solution.

Interval constraint propagation at a Glance:

Interval mathematics

Because floating-point computational errors need to be estimated and controlled, interval analysis has grown considerably in the past 30 years. Interval arithmetic deals with processing intervals that bound real numbers. Consider a real variable, x , bounded by two other numbers, $x_l \leq x \leq x_u$. One can define an interval X such that $x \in X$ where $X = [x_l, x_u]$. Similarly, an interval Y can be defined to include a real variable y such that $y \in Y$. An interval arithmetic operation, $*$, (for example, addition, subtraction, multiplication, and division) is defined by:

$$X * Y = \{x * y: x \in X, y \in Y\} \quad (1)$$

A particularly useful property of interval arithmetic operations is:

$$x * y \in X * Y \quad (2)$$

which means that the sum, difference, product, and quotient of two real numbers belong to the same properties of the including intervals. Rules for interval operations include:

$$X + Y = [x_l, x_u] + [y_l, y_u] = [x_l + y_l, x_u + y_u] \quad (3)$$

$$X - Y = [x_l, x_u] - [y_l, y_u] = [x_l - y_u, x_u - y_l] \quad (4)$$

$$X * Y = [x_l, x_u] * [y_l, y_u] = [\min(x_l y_l, x_u y_u, x_l y_u, x_u y_l), \max(x_l y_l, x_u y_u, x_l y_u, x_u y_l)] \quad (5)$$

$$X / Y = [x_l, x_u] / [y_l, y_u] = [x_l, x_u] * [1/y_u, 1/y_l] \quad \text{if } 0 \notin [y_l, y_u] \quad (6)$$

Isotonicity is another useful property of interval operations. It states that for intervals $X, Y, W,$ and Z

$$\text{if } X \subset W \text{ and } Y \subset Z \text{ then } X * Y \subset W * Z \quad (7)$$

For each continuous function, $f(x)$, where x is an n -dimensional vector and $x \in X$, one can use interval arithmetic to identify bounds on the range of the function. Consider a function $f(x)$ whose range over interval X is defined as $\square f(X)$, i.e. $\square f(X) = \{f(x): x \in X\}$.

An interval function F is called an inclusion function for f over interval X if

$$\square f(X) \subseteq F(X) \quad (8)$$

Inclusion functions are extremely important in interval analysis as they provide bounds on ranges without exhaustive enumeration. There are two common methods for constructing inclusion functions: natural interval extensions and centered forms. A natural interval extension is an expression where each x in the various terms of $f(x)$ is replaced with it including interval, X , and the mathematical operators are replaced with interval operations. Centered forms are inclusion functions that represent generalization of the algebraic centered forms for real variables. A particularly useful centered form is based on the natural interval extension of Taylor's expansion of the function. More details on interval analysis are given in [2-4].

Constraint logic propagation

Constraint logic propagation known as CLP is a problem-solving paradigm that establishes a clear distinction between two pivotal aspects of a problem: a precise definition of the constraints that define the problem to be solved, and the algorithms and heuristics enabling selection of the decisions to solve the problem. Because of these capabilities, constraint programming is increasingly being used as a problem-solving tool for many engineering problems [5,6]. Constraint programming was originally developed for solving feasibility problems but has recently been used in optimization problems [7]. Although constraint programming methods are efficient in solving feasibility/targeting problems, optimization depends entirely on building the correct constrained model. To show how constraint logic propagation with interval labels works, this paper gives numerical examples one is the "Waltz" algorithm, first introduced in the mid seventies [8].

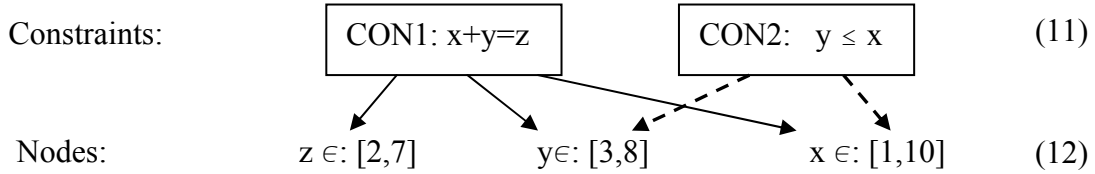
Suppose the following relations model/define our problem:

$$x+y=z, \quad y \leq x \quad (9)$$

and we can start with the following bounds:

$$x \in [1,10], \quad y \in [3,8], \quad z \in [2,7], \quad (10)$$

This would be implemented in a data structure given by the following constraint network:



The very famous old “Waltz” algorithm proceeds as follows:

The constraint queue begins with both constraints (CON1, CON2).

CON1 ($x + y = z$) is popped from the queue.

Since $x \geq 1$ and $y \geq 3$, CON1 gives $z \geq 4$; therefore reset the bounds of z to $[4,7]$.

Since $z \leq 7$ and $y \geq 3$, CON1 gives $x \leq 4$; therefore reset the bounds of x to $[1,4]$.

Since x and z have been changed, add CON2 to the queue.

CON2 ($y \leq x$) is popped from the queue.

Since $x \leq y$, CON2 gives $y \leq 4$; therefore reset the bounds of y to $[3,4]$.

Since $y \geq 3$, CON2 gives $x \geq 3$; therefore reset the bounds of x to $[3,4]$.

Since x and y have changed, add CON1 to the queue.

CON1 ($x + y = z$) is popped from the queue.

Since $x \geq 3$, $y \geq 3$, CON1 gives $z \geq 6$; therefore reset the bounds of z to $[6,7]$.

Since only z has changed and z has no other constraints beside CON1, nothing is added to the queue.

Since the queue is empty, the algorithm quits.

This simple numerical example demonstrates how to use constraint logic propagation techniques in solving engineering problems that can be modeled using constraints and interval labels consisting of deterministic bounds [9].

Combined CP and MP method for energy systems synthesis:

A system that includes equality constraints such as mass, heat balances and performance equations, inequalities constraints such as the ones including operating windows and design parameters and logical expressions constraints of superstructures and/or operating philosophies can easily be modeled in CS environment as below:

$$X^2 + 6.0x = y - 2^k;$$

$$kx + 7.7y = 2.4;$$

$$(k-1)^2 < 4;$$

$$(\ln(y+2x+12) < (k+5)) \text{ or } (y > k^2) \rightarrow (x < 0.0) \text{ and } (y < 1);$$

Where k is integer; x, y are real and \rightarrow stands for implication

The solution of the problem above exhibits several solutions that all lay in these intervals of the three variables.

$$k = [0, 2];$$

$$x = [-6, -1e-10];$$

$$y = [0.311688, 1];$$

The exact solutions are as follows:

$$k = 0; x = -5.88301; y = 0.311688;$$

$$k = 0; x = -0.11701; y = 0.311688;$$

$$k = 1; x = -0.289055; y = 0.349227;$$

$$k = 2; x = -0.658479; y = 0.482721;$$

In real life industrial problems we can find many ways to limit the number of solutions or even push the problem further to having a unique solution via adding to the problem new constraints. Such constraints can be based upon the physico-chemical nature of the problem, using entropy balance for instance and through the insertion of decision maker's constraints and preferences such as defined ranges for objective function, operating window of some equipment, desired features in process structure and units design and so on.

In the above mentioned problem we can add one more constraint and the problem will be fully defined and has a unique solution [10].

$$X^2 + 6.0x = y - 2^k;$$

$$kx + 7.7y = 2.4;$$

$$(k-1)^2 < 4;$$

$$(\ln(y+2x+12) < (k+5)) \text{ or } (y > k^2) \rightarrow (x < 0.0) \text{ and } (y < 1);$$

$$(x < 2.5y) \rightarrow (ky < 3) \text{ and } (k > y+1);$$

This unique solution then is; $k = 2, x = -0.658$ and $y = 0.4827$

The essence of our method of integrating CS and MP in solving large optimization problems is to convert the large industrial combinatorial problem into multi-level optimization problem. We then solve using CP first at the lowest level of "followers" to define certain range of this level objective function and variables. We move from the lowest follower level up to a higher level and repeat this step of solving using CP till we reach to the upper/leader level. Again we use CP for the leader problem to tighten the range of both the variables and leader's objective function.

MP is then used to find the details of the whole problem solution after inserting bounded variables, objectives ranges of the followers.

The simultaneous HEN synthesis and process operations optimization problem can be represented as three levels optimization problems; minimize area cost subject to minimum number of units subject to minimum utility cost, or in two levels (BLPP) minimize capital cost subject to minimum energy cost.

Illustrating Examples:

In this section we introduce two examples, CP formulation for HEN synthesis energy targeting application and a numerical example in which we use CP solution of a HEN minimum capital cost synthesis as a preparatory step for the NLP application for finding the solutions details of the HEN synthesis.

The first example that shows how to formulate the CP model for solving energy targeting sub-problem under all possible combinations of process modifications, is detailed below.

Model Description and CP Formulation: (Example 1)

Hot streams temperatures shifted down one-by-one by the first set of desired minimum temperature differences, ΔT_{\min}^i , between the hot and cold resource streams to form a set of possible discrete temperature values for a continuum of possible values for ΔT_{\min}^i . ΔT_{\min}^i represents the ΔT_{\min} of hot stream (i) which refers to the minimum temperature approach between a specific hot stream and all other cold streams, can be taken here in this paper as equal to 1 F. The shifted supply and target (output) temperatures of resource hot streams, and the actual supply and the target cold streams temperatures obtained through this are then sorted in a descending order, with duplicates removed, with each successive temperature pair representing the boundaries of a temperature step and defining a new temperature step “S”. Each supply temperature and target temperature input is in the form of intervals (e.g., a pair of range boundaries) and not single discrete numbers. Each supply temperature and target temperature input interval is then divided on an equal basis according to the desired temperature precision. The completion of this step results in “N” number of process temperature steps. While not discussed in details here creating the new heat carrier streams in the hot side or in the cold side can be done with the same concept used above of temperature range division. The heat carrier stream or pump around streams exist and no exist decisions can also be modeled with supply

temperature defined by the user on a range and its target temperature and FCp too as variables defined in ranges. The target temperature range will be divided to equal temperature intervals again degree-by-degree or according to the required accuracy in temperature.

The total number of temperature steps is “N+1,” where S varies from 0,1,2,...,N and the temperature step number ”0” represents the external energy utility temperature step. In this step, known as the external energy step, energy output, initial values: $Q_{s=0}^{low_output} = 0.0$ in “energy units” and $Q_{s=0}^{high_output} = 0.0$ in “energy units.”

Each temperature step, ”S” greater than 0, where $S = 1, 2, \dots, N$, has energy surplus $Q_s^{surplus}$. Such energy surplus has two calculated values: $Q_s^{low_surplus}$ and $Q_s^{high_surplus}$. It also has energy output Q_s^{output} from one temperature step to another. Such energy output Q_s^{output} has also two calculated values: $Q_s^{low_output}$ and $Q_s^{high_output}$. These values for energy surplus $Q_s^{surplus}$ and energy output Q_s^{output} are calculated for $S=1, 2, \dots, N$:

$$Q_s^{low_surplus} = \left(\sum_{k=1}^{n_s} FCp_k^{low} - \sum_{j=1}^{m_s} FCp_j^{high} \right) (Th_s - Tc_s)$$

$$Q_s^{high_surplus} = \left(\sum_{k=1}^{n_s} FCp_k^{high} - \sum_{j=1}^{m_s} FCp_j^{low} \right) (Th_s - Tc_s)$$

$$Q_s^{low_output} = Q_{s-1}^{low_output} + Q_s^{low_Surplus}$$

$$Q_s^{high_output} = Q_{s-1}^{high_output} + Q_s^{high_Surplus}$$

Where n_s and m_s are the number of the resource hot and cold streams respectively represented in the s^{th} temperature step and Th_s and Tc_s are the higher and lower shifted temperatures for the hot streams, respectively, and actual temperature of the cold streams representing the temperature boundaries. Logic propositions such as “or, and, \rightarrow ” are used to enable modeling logics.

$[FCp_k]$ and $[FCp_j]$ are heat capacity flowrate intervals; defined as follows:

FCp_k^{low} : is the low value of the Heat Capacity Flowrate term resulted from the multiplication of the value of the flow F lower bound by the specific heat value Cp of the hot stream number k in flow-specific heat units.

FCp_k^{high} : is the high value of the Heat Capacity Flowrate term resulted from the multiplication of the value of the flow F upper bound by the specific heat value Cp of the hot stream number k in flow-specific heat units.

FCp_j^{low} : is the low value of the Heat Capacity Flowrate term resulted from the multiplication of the value of the flow F lower bound by the specific heat value Cp of the cold stream number j in flow-specific heat units.

FCp_j^{high} : is the high value of the Heat Capacity Flowrate term resulted from the multiplication of the value of the flow F upper bound by the specific heat value Cp of the cold stream number j in flow-specific heat units

$$\sum_{k \in Hs} [FCp_k] - \sum_{j \in Cs} [FCp_j] + [Qh_s] - [Qc_s] + [Q_s^{surplus}] + [Q_s^{output}] = 0.0; \quad S=1,2,\dots,N;$$

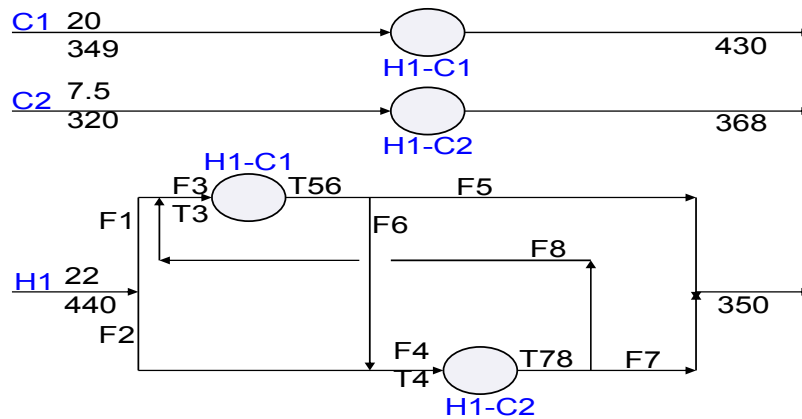
$$[Qh_s] \geq 0.0; [Qc_s] \geq 0.0; [Q_s^{output}] \geq 0.0; [Q_0^{surplus}] = 0.0; [Q_0^{output}] = 0.0;$$

Upon the calculation of utilities minima using the above formulation the selection of the heating and cooling utilities exact consumption can be decided by the decision maker from the resulted ranges. An interval collapsing algorithm using MP or other methods can now be used to select the operating conditions that render the desired level of energy consumption [11, 12].

The second example of integrating CLP and MP methods is a heat exchanger synthesis problem, to find the minimum area/cost network for desired energy consumption and defined stream matches. Table 1.0 Data for the CP Illustration Model

stream	Tin(K)	Tout(K)	FCp(kW/K)
H1	440	350	22
C1	349	430	20
C2	320	368	7.5

Exchanger minimum approach temperature is 10 K, the problem needs no heating and cooling utilities, the cost of heat exchanger is function in its area (cost = 1300*A^{0.6} \$/yr) and the network streams superstructure is shown below.(Fludas et al., 1996)



NLP can be used alone to solve this problem (Fludas et al., 1996). However combining the power of both CP and MP methods can make the solution even easier since the application of the CP first can confirm feasibility of desired objective function, reduce noticeably the search space since it rigorously define lower and upper bounds of each variable and/or parameters and enable the deletion of parts of the superstructure that are not feasible and/or undesired by the decision maker.

Note: Chen approximation for the log mean temperature difference is used.

CP Model Formulation:

$$\begin{aligned}
 &1300*A1^{0.6}+ 1300*A2^{0.6}-OF=0.0; \\
 &A1-(1620/DTA) = 0.0; \\
 &A2-(360/(0.5*DTB))=0.0; \\
 &ta-(T3- 430)=0.0; \\
 &tb-(T56-349)=0.0; \\
 &tab-(ta+tb)=0.0; \\
 &tc-(T4-368)=0.0; \\
 &td-(T78-320)=0.0; \\
 &tcd-(tc+td)=0.0; \\
 &((0.5*ta*tb*tab)^{0.3334})-DTA=0.0; \\
 &((0.5*tc*td*tcd)^{0.3334})-DTB=0.0; \\
 &F1+F2-22=0.0; \\
 &F3-F5-F6=0.0; \\
 &F4-F7-F8=0.0; \\
 &F3-F1-F8=0.0; \\
 &F4-F2-F6=0.0; \\
 &F1*440-F8*T78-F3*T3=0.0; \\
 &F2*440-F6*T56-F4*T4=0.0; \\
 &(F3*(T3-T56))-1620=0.0; \\
 &(F4*(T4-T78))-360=0.0; \\
 &T3-430 \geq 0.1; \\
 &T56-349 \geq 0.1;
 \end{aligned}$$

$T4-368 \geq 0.1$;
 $T78-320 \geq 0.1$;
 $T3 \leq 440$;
 $T56 \leq 440$;
 $T4 \leq 440$;
 $T78 \leq 440$;
 $F1; F2; F3; F4; F5; F6; F7; F8 \geq 0.0$;

CP Interval Model Solution:

$A1 = [171.678, 3764.16]$; $A2 = [11.9785, 244.221]$; $F1 = [17.4659, 19.3347]$;
 $F2 = [2.66527, 4.53409]$; $F3 = [17.8218, 19.7287]$; $F4 = [3.0025, 5.10778]$;
 $F5 = [15.4664, 19.7287]$; $F6 = [0, 2.35543]$; $F7 = [0.739738, 5.10778]$; $F8 = [0, 2.26277]$;
 $T3 = [431.214, 440]$; $T4 = [390.581, 440]$; $T56 = [349.1, 357.886]$; $T78 = [320.1, 369.519]$;
 $OF = [34262.7, 216901]$;

The objective function $OF = [34262.7:216901]$ \$/yr lower and upper bounds can be tightened more and more using repeated bisectional method followed by feasibility checks. OF can then be inserted as a new constraint in the model. The decision maker for instance; can define desired range for his/her budget (OF), if he/she gets feasible solution it means his/her desired objective is achievable and he/she can continue then using NLP to find the details of the solution.

Now let us assume that the decision maker has a budget of $OF = [40000:45000]$ \$/yr.

Inserting new budget interval value in the CP model constraints list renders the following tightened bounds for system variables.

$A1 = [180.476, 287.627]$; $A2 = [13.3803, 63.1493]$; $F1 = [17.9487, 19.2544]$;
 $F2 = [2.7456, 4.05127]$; $F3 = [18.1984, 19.5222]$; $F4 = [3.00929, 4.44035]$;
 $F5 = [16.5616, 19.5222]$; $F6 = [0, 1.63681]$; $F7 = [1.43581, 4.44035]$; $F8 = [0, 1.57349]$;
 $T3 = [433.964, 440]$; $T4 = [401.445, 440]$; $T56 = [350.981, 357.018]$; $T78 = [320.371, 358.925]$;

It is clear from the new bounds that the decision maker objective is achievable, HEN superstructure is reducible, F8 superstructure branch is close to zero and can be removed from the H1 stream superstructure, and the flow & temperature ranges have been reduced drastically, compared with normal monotonicity checks. Such insights make the NLP formulation and solution easier especially for large industrial problems.

Conclusion:

Combining CP and mathematical programming in a stand-alone fashion on the modeling level creates more powerful environment for solving optimization problems. Logical constraints that are very common in process synthesis and operation problems are easily formulated in CP environment. Formulating and solving energy systems synthesis problems in CP environment results in insights and tight bounds on the problem variables and objective function before applying MP. CP as a preparation step to large optimization problem solution makes the step of obtaining the detailed solution of the problem using mathematical programming easier.

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