A NEW STRATEGY AND ALGORITHM OF MINLP BASED ON MODULE FOR SYNTHESIS OF CHEMICAL PROCESSES

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Abstract

This article presents the formulation and the solution of a class of **M**ixed-**i**nteger **N**on**l**inear **P**rogramming (MINLP) problems, applied to optimal synthesis of process systems in a modular simulator environment. The proposed algorithm makes use of module, reduces the work of calculation on model equations, makes the size of MINLP smaller. The algorithm consists of solving alternate sequences of MILP master problem and NLP subproblem whose sizes have been reduced. The NLP subproblem provides the linearization information of the nonlinear constraints that relate the output variables to input variables specified explicitly. At the same time **D**ata-**O**riented **P**rocess **S**imulation system (DOPS) technique is used in the modular simulator environment. The HDA process is taken as a case study the capabilities of the process synthesizer. It proves that the proposed solution deals with complex MINLP problems satisfactorily.

Keywords

process synthesis; modular simulator environment; MINLP; solution algorithm.

Introduction

A wide range of chemical engineering problems can effectively be framed as **M**ix-**I**nteger **N**on**l**inear **P**rogramming problem (MINLP) as this approach allows the simultaneous optimization of the continuous variables pertaining to a certain structure, and of the structure itself which is modeled via binary variables (Floudas,1995; Grossmann,1996). Such a mathematical framework has been proposed for a variety of process synthesis problems (e.g., heat recovery networks, separation systems, reactor networks), process operations problems, molecular design problems and synthesis of metabolic pathways. A number of these applications are described in Floudas (1995) and Grossmann (1996).

With the increasing reliance on modular based approaches to process design and optimization, more attention has been focused on the simulation optimization method which is the basis of these techniques. By using the simulation method, we can inherit the excellent accomplishment of process simulation. At the same time the complex chemical process synthesis problems become relatively simple problem.

In the algorithm of modular simulation environment, the synthesis problem has been distinguished into three hierarchical levels: (1) superstructure level, (2) structure level and (3) modular level. The solving of superstructure level is proven to be relatively simple. We put our effort on seeking the algorithm and strategy for the modular level and structure level, above all the conjunction between these levels.

In the modular level, the general simulation method used is the sequential module method, which goes along iterative using sophisticated unit module. The method is limited for use in simpler process synthesis problems, but the number of variables for practical interest is usually too large, which will result in prohibitive iterative calculations.

In this paper we first describe the solution strategy and algorithm of the new modular method. In the modular level, we adopt the date-driven technology and introduce the pseudo-torn streams and pseudo-variables. The use of the date-driven technology avoids large time iterative in computing the unit modules. The introduction of pseudo-torn streams and pseudo-variable transforms complex problem to a new equivalent problem whose number of variables is much smaller.

MINLP express of process synthesis problem

First we define the superstructure, the mathematical model of process synthesis is stated as:

$$\min_{\boldsymbol{y},\boldsymbol{d},\boldsymbol{s}} \ \boldsymbol{a}^{\mathrm{T}} \cdot \boldsymbol{y} + f(\boldsymbol{d},\boldsymbol{s}) \qquad (1)$$

$s.t.$

$$\boldsymbol{B}\cdot\boldsymbol{y}+h(\boldsymbol{d},\boldsymbol{s})\le 0$$
$$\boldsymbol{C}\cdot\boldsymbol{y}+g(\boldsymbol{d},\boldsymbol{s})=0$$
$$m(\boldsymbol{d},\boldsymbol{x})=0$$
$$\boldsymbol{Q}\cdot\boldsymbol{y}+\boldsymbol{E}\cdot\begin{bmatrix}\boldsymbol{d}\\ \boldsymbol{x}\end{bmatrix}\le\boldsymbol{e}$$
$$\boldsymbol{y}\in\boldsymbol{Y}=\left\{\boldsymbol{y}/\boldsymbol{y}\in\{0,1\}^{\boldsymbol{n}}\right\}$$
$$\boldsymbol{d}\in\boldsymbol{D}=\left\{\boldsymbol{d}/\boldsymbol{d}\in R^{\mathrm{m1}},\boldsymbol{d}^{\boldsymbol{l}}\le\boldsymbol{d}\le\boldsymbol{d}^{\boldsymbol{u}}\right\}$$
$$\boldsymbol{x}\in\boldsymbol{X}=\left\{\boldsymbol{x}/\boldsymbol{x}\in R^{\mathrm{m2}},\boldsymbol{x}^{\boldsymbol{l}}\le\boldsymbol{x}\le\boldsymbol{x}^{\boldsymbol{u}}\right\}$$

where y's are the binary topological variables, D is a set of continuous decision variables, x's are the continuous independence variables in the mathematical model of unit, m's are model equations of unit and the model includes materiel, energy, equilibrium equations. The element of x appears in the objective function, equation constraint g and inequality restriction h according to s which is the subsidiary element, s is the interest variables, a is a set of vector, the matrix B, C, Q have the same dimension. The equation $Q*y+E*[d\ x]^t \le e$ expresses two kinds of constraint, one is topological constraint and the other is bound constraint.

New solution strategy of MINLP problem

Using a general modular environment solving the MINLP has two problems, one is the information communication between different software, the other is that the iterative of module unit will take too much time. In order to overcome these shortcomings, we propose a new three levels model strategy. (Figure 1)

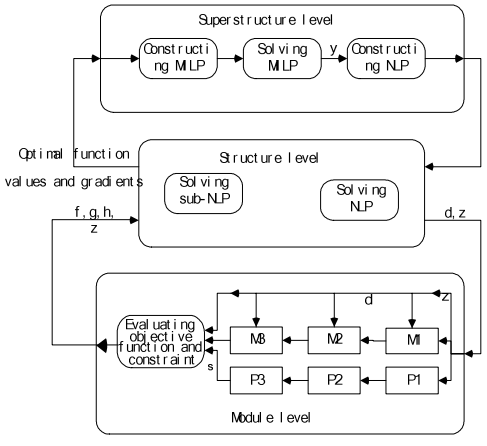

Figure.1 The modular based solution strategy of MINLP problem

Superstructure level

The superstructure level is the highest level. It includes three distinct steps: the first one is the construction of the master problem according to the OA/ER algorithm (Kocis and Grossmann, 1987). The next step will be devoted to solve MILP (**M**ix-**I**nteger **l**inear **P**rogramming) problem. The third is to construct the NLP (**N**on**l**inear **P**rogramming) problem.

Structure level

The purpose of structure level is to optimize the operation parameters. During seeking the optimization, we adopt an improved *SQP* which includes a matrix *P* (Yue Jincai, 1994). The matrix *P* is used to simplify the problem. After simulating several times, the simplified model is used to express the complicated problem. Using the simplified model in the computing process can shorten computing time and improve the convergence.

Modular level

In the modular environment, different modules correspond to different modular equations. The module is equal to process unit. After fixuping the variables y's, d's, z_{ts}'s, we adopt the technology of data-driven and introduce the matrix P to the *SQP*. The interested variables s's and the pseudo-torn streams variables z_{ts}'s are calculated simultaneously. The objective of NLP problem and the constraint function is obtained. The adopting of data-driven technology reduces difficulty in the communication of energy streams and material streams of different module by database. By doing so the modification in the modular simulation or process simulation will bring the same result in the database. By the way, data redundance is avoided and the share for the process data is realized.

New algorithm of MINLP problem

With introducing the pseudo-torn streams and the pseudo-variables, the model is expressed as follows:

$$\min\ \boldsymbol{a}^{T}\cdot\boldsymbol{y}+f\left(\boldsymbol{d},\boldsymbol{s},\underline{\boldsymbol{s}}''(\boldsymbol{d},\boldsymbol{z}_{ts},\boldsymbol{z}_{lm})\right)\qquad(2)$$

s.t

$$\boldsymbol{z}_{ts}-\underline{\boldsymbol{z}}_{ts}(\boldsymbol{d},\boldsymbol{z}_{ts},\boldsymbol{z}_{lm})=0$$
$$\boldsymbol{B}\cdot\boldsymbol{y}+\mathrm{h}\left(\boldsymbol{d},\boldsymbol{s},\underline{\boldsymbol{s}}''(\boldsymbol{d},\boldsymbol{z}_{ts},\boldsymbol{z}_{lm})\right)\le 0$$
$$\boldsymbol{C}\cdot\boldsymbol{y}+\mathrm{g}\left(\boldsymbol{d},\boldsymbol{s},\underline{\boldsymbol{s}}''(\boldsymbol{d},\boldsymbol{z}_{ts},\boldsymbol{z}_{lm})\right)=0$$
$$\boldsymbol{z}_{lm}-\underline{\boldsymbol{z}}_{lm}\left(\boldsymbol{d},\boldsymbol{z}_{ts},\boldsymbol{z}_{lm}\right)=0$$
$$\boldsymbol{s}-\underline{\boldsymbol{s}}\left(\boldsymbol{d},\boldsymbol{z}_{ts},\boldsymbol{z}_{lm}\right)=0$$
$$\boldsymbol{D}\cdot\boldsymbol{y}+\boldsymbol{E}\cdot\left[\boldsymbol{d},\boldsymbol{z}_{ts},\boldsymbol{z}_{lm},\boldsymbol{s}\right]^{\mathrm{T}}\le\boldsymbol{e}$$
$$\boldsymbol{y}\in\mathrm{Y}=\left\{\boldsymbol{y}/\boldsymbol{y}\in\{0,1\}^{\boldsymbol{n}}\right\}$$
$$\boldsymbol{d}\in\mathrm{R}^{\mathrm{m1}},\boldsymbol{d}^{\boldsymbol{l}}\le\boldsymbol{d}\le\boldsymbol{d}^{\boldsymbol{u}}$$
$$\boldsymbol{z}_{ts}\in\mathrm{R}^{\mathrm{m2}},\boldsymbol{z}_{ts}^{\boldsymbol{l}}\le\boldsymbol{z}_{ts}\le\boldsymbol{z}_{ts}^{\boldsymbol{u}}$$
$$\boldsymbol{z}_{lm}\in\mathrm{R}^{\mathrm{m3}},\boldsymbol{z}_{lm}^{\boldsymbol{l}}\le\boldsymbol{z}_{lm}\le\boldsymbol{z}_{lm}^{\boldsymbol{u}}$$
$$\boldsymbol{s}\in\mathrm{R}^{\mathrm{m4}},\boldsymbol{s}^{\boldsymbol{l}}\le\boldsymbol{s}\le\boldsymbol{s}^{\boldsymbol{u}}$$

$$\underline{\boldsymbol{s}}\in\underline{\boldsymbol{S}}=\{\underline{\boldsymbol{s}}\ \boldsymbol{computed\ at}\ \mathrm{mod}\ \boldsymbol{ule\ level}\}$$
$$\underline{\boldsymbol{z}}_{ts}\in\underline{\boldsymbol{Z}}_{ts}=\{\underline{\boldsymbol{z}}_{ts}\ \boldsymbol{computed\ at}\ \mathrm{mod}\ \boldsymbol{ule\ level}\}$$
$$\underline{\boldsymbol{z}}_{1m}\in\underline{\boldsymbol{Z}}_{1m}=\{\underline{\boldsymbol{z}}_{1m}\ \boldsymbol{computed\ at}\ \mathrm{mod}\ \boldsymbol{ule\ level}$$

These symbols are with the same meanings as shown in equation set (1).

When formulating the model to a mathematic problem,

two problems arise. One is the definition of pseudo-torn stream and pseudo-variables, while the other is the connection of constrain and the topological variables. The introduction of the nature torn streams makes the solving of NLP problem simply and the introducing of the pseudo-torn streams make the MILP problem became a large size but dimensions small and easy to solve mathematical problem.

Illustrating case: HDA problem

The HDA (hydrodesalkylation) process is used to test and demonstrate the new strategy and algorithm. The HDA process testing case consists of four kinds of possible structures (Figure 2).

The adopted softwares are DOPS (**D**ata **O**riented **P**rocess **S**imulation system) and GAMS (GAMS, **G**eneral **A**lgebraic **M**odeling **S**ystem).

In the process, a critical problem of the convergence criteria arises in the solving of the problem. We adopt the following convergence criteria. The convergence is achieved when the lower bound is greater or equal to the best upper bound. An alternative convergence criterion is used: structure repetition.

Using the arithmetic based on the data-driven modular environment to synthesis HDA process, the result is obtained and shown Table 1. Presented results are compared with the solutions from the method developed by J. M. Reneaume. By using the database technique and data sharing technique, our proposed algorithm do facilitate solving the sophisticated chemical process synthesis.

Table 1 Operating conditions for the two methods

	Reneaume	This work	Reneaume	This work
structure	[1 0 1 0]	[1 0 1 0]	[0 1 0 1]	[0 1 0 1]
c($/year)	$12.04*10^6$	$12.10*10^6$	$14.81*10^6$	$14.69*10^6$
d1(kmol/h)	673.3	671.7	661.7	666.3
d2(kmol/h)	618.1	617.7	611.6	613.9
d3(K)	298	298	298	298
d4	0.27	0.27	0.29	0.29
d5(M^3)	193	193.2		
d6(M^3)			28.9	128.7
d7(K)			290.5	288.5
d8(pa)			482307.1	473187.8

The proposed data-driven modular arithmetic for MINLP problem avoided the following shortcoming. First, the method need not set up the rigorous mathematic model as does the equation-based arithmetic. In the general arithmetic, the model is expressed by the simplified function of process unit. So the result is not rigorous. The modular method, either the method developed by Reneaume, or our method use the rigor model of the units while the size of the synthesis model does not increase. So the result from our algorithm is more accurate than the method based on equation.

By using the date-driven technology the difficulty is decreased between the communication of energy streams and material streams of different module by database. Thus the modification in the modular simulation or process simulation will bring the same result in the database. By using the method, data redundance is reduced and the sharing of the process data is easily realized.

Conclusion

A new formulation of data-driven MINLP for chemical process synthesis is proposed in a modular environment. In such an environment, rigorous mechanism models are used, even if they are described by differential equation, without increasing MINLP problem size. By using the data-driven technology, the communication of information among the different computing process is realized. In the process simulation, the information between different processes is clarity and easily communicated. The computing process is simplified and the time is saved. The HDA case study shows the proposed strategy and algorithm is promising for solving the MINLP chemical process synthesis problem.

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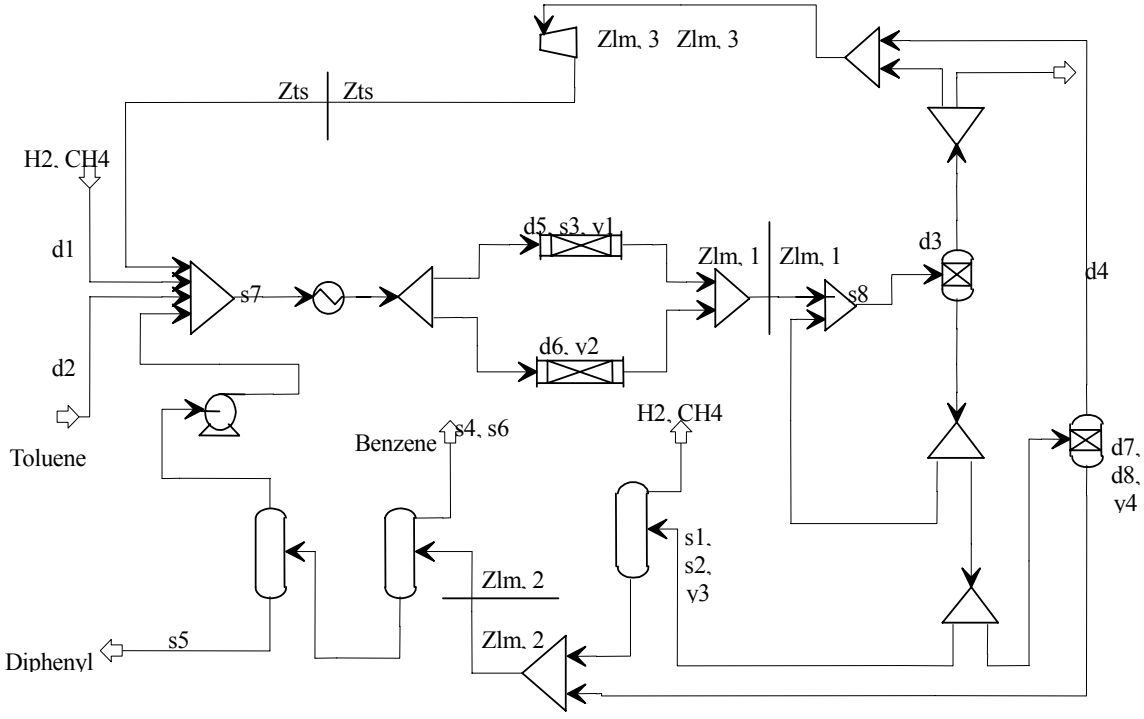

Fig. 2 The superstructure of HDA process