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Generalised Optimisation Framework for the Synthesis of Thermally Coupled Distillation Columns in the Equation-Oriented Environment

Chao Liu[a], Yingjie Ma[b], Dongda Zhang[a], Jie Li[a,*], Li Sun[c]

[a]Centre for Process Integration, Department of Chemical Engineering, The University of Manchester, Manchester, M13 9PL, UK
[b]Department of Chemical Engineering, Massachusetts Institute of Technology, 02139, Cambridge, MA, USA
[c]The University of the West of Scotland, Technology Ave, Blantyre, Glasgow G72 0LH, UK
jie.li-2@manchester.ac.uk

In this paper, a novel superstructure optimisation method – The Generalised Optimisation Framework, is presented for the synthesis of a thermally coupled distillation system in the equation-oriented environment. The superstructure derived from a previous work considers all the sequencing alternatives from conventional sequences to fully thermally coupled distillation sequences. In our optimisation framework, a novel mathematical model is formulated to address the common failure of simulations when zero flowrate of streams enters units by using the "IF structure" syntax in Aspen Custom Modeller (ACM). The side rectifier configuration with the lowest total annualised cost (TAC) of 478,667 \$ y^{-1} from a ternary complex distillation column superstructure is determined in conjunction with our previously proposed feasible path-based branch and bound method as the solution algorithm.

1. Introduction

Distillation is the most widely used separation technology. The optimal synthesis of the distillation network remains a major problem in process design, and it has the potential to save significant capital and substantial energy for overall operations. Superstructure-based optimisation methods have been extensively used as they can systematically synthesise optimal distillation networks from a superstructure that incorporates all the alternative configurations. These problems are typically formulated as Mixed Integer Nonlinear Programming (MINLP) problems and simulated and optimised in the equation-oriented (EO) environment, which has distinct advantages over the sequential modular environments, such as efficient large-scale solvers and low-cost sensitivity analysis. However, many commercial process simulators that use EO approaches suffer various drawbacks. Except for gPROMS, other commercial process simulators, such as Aspen Custom Modeler (ACM), have limited model formulation flexibility for MINLP problems. Even when the models are reformulated as relaxed NLP problems, simulations may fail due to no flows entering some units, which is prevalent in complex column sequencing problems. if the equipment is not selected, the material flow through this equipment naturally becomes zero. For some simple units like splitters and valves, zero flows do not affect the units. But in other, more complex units such as distillation columns, "disappearing" flows dispatch errors, causing the failure of simulation. Setting the lower bound of the flowrate to a small value (e.g., 1×10^{-20}) is not always working. The best approach to circumvent the zero flow effect is to deactivate the associated constraints for calculating the mass and energy balance and the physical and chemical equilibrium. Generalized Disjunctive Programming (GDP) proposed by Yeomans and Grossmann (2000) succeeds in this regard by using Boolean variables to enforce the selection of a certain set of constraints representing the units, which provides an alternative to MINLP modelling and avoids numerical singularities in the nonlinear equations that are due to the disappearance of columns, sections of columns, and streams. Only GAMS algebraic modelling language supports GDP model implementation (Chen and Grossmann, 2019). However, GAMS is a generic optimisation platform and does not have any unit operation models, physical property database and flowsheeting capabilities.

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Ideal liquid or gas behaviour is often assumed, and the accuracy of thermodynamics calculations may be compromised. Reliable convergence to optimum requires elusive good initial points due to the highly nonconvexities of rigorous distillation models.

To address the aforementioned zero flows and good initial guesses issues, we propose a novel modelling framework that can be implemented in equation-oriented-based process simulators such as Aspen Custom Modeler. When the inlet flow of a unit model becomes zero, a different set of equations is activated by using the "structural IF" conditions. A pseudo flow is triggered for the VLE calculations. The outlet ports of the unit are directly linked to inlet ports to avert the flowsheeting impact on other unit blocks that are connected to them. A binary variable is assigned to each unit block that allows the explicit specifications of logical propositions for the unit interconnection principles. Our previously proposed feasible path-based branch and bound algorithm (Liu et al., 2022) are employed for the outer layer optimisation, which demonstrates good convergence performance from easy-choosing initial points. A case study for BTX (benzene, toluene and o-xylene) separation based on a ternary complex distillation column superstructure is presented to validate the proposed framework.

2. Superstructure for complex distillation systems

The problem addressed in this work can be defined as follows: given a ternary zeotropic mixture. The objective is to find an optimal configuration that separates the mixtures into their constituent components using the superstructure-based optimisation method. The superstructure is derived from the work of Proios and Pistikopoulos (2005), incorporating all the possibilities from simple conventional columns and partially or fully thermally coupled complex sequences, as illustrated in Figure 1. ABC is ordered by decreasing relative volatilities. This superstructure consists of column segments, condensers, reboilers, mixers and splitters.

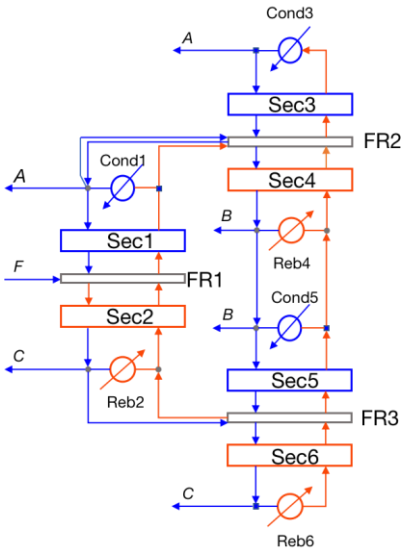

Figure 1: Ternary complex distillation column superstructure

Generic explanations are provided as follows:

(1) Column sections (Sec) are divided to rectify sections and stripping sections. If a column section is placed above a feed tray, it is considered a rectifying section. If it is located below a feed tray, it is defined as a stripping section.
(2) A rectifying section, a feed tray and a stripping section constitute a pseudo column. For example, Sec1, FR1 and Sec2 form a distillation column.
(3) Feed trays (FR) may receive single feed, multiple feeds or no feed at all.
(4) Feed trays may have vapour sidedraw, liquid sidedraw or no sidedraw at all.
(5) If no flow is fed into a feed tray, it should not have any sidedraws. Its associated rectifying section and stripping section should not have any thermally link to other columns. This is stipulated by logic constraints. For example, if there is no flow from Sec2 to FR3, Sec5 will not thermally link with Sec4.
(6) The vapour or liquid sidedraw fractions in the feed trays are defined as decision variables to determine the optimal structure.
(7) Mixers and splitters are used for stream mixing and splitting. Splitting fractions of streams are defined as decision variables to determine the optimal structure.

(8) Total 10 alternative configurations can be generated using the presented superstructure, including direct sequence, indirect sequence, 3 columns prefractionator, Petlyuk, side Petlyuk, side stripper, side rectifier, RV column and SL column.

3. Mathematical model for complex distillation systems

The fundamental concept for formulating the models of units that may suffer from zero flow effect is to construct the models by using the "Run-Time IF" syntax to change the model equations by evaluating the condition while running the simulation. If the inlet flowrate into a unit becomes zero, a different set of equations are evoked to assign a pseudo flowrate to the inlet stream to avoid simulation difficulty caused by zero flow. The general IF structure syntax used in our modelling framework in Aspen Custom Modeler is demonstrated in the following:

IF condition **THEN**

Statements1; (A set of equations to be executed if the condition is **True**);

ELSE

Statements2; (The other set of equations to be executed if the condition is **False**)

ENDIF

The mathematical models for columns, sections and feed trays are presented in below without explicitly including all the well-known equations.

3.1 Rectifying and stripping sections

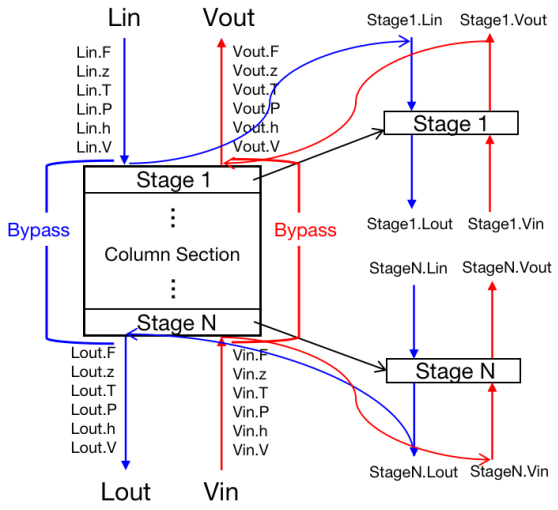

Figure 2: Port connections for a single column section

Both rectifying section and stripping section are connected with 4 ports - Lin (Liquid inlet stream), $Lout$ (Liquid outlet stream), Vin (Vapour inlet stream), and $Vout$ (Vapour outlet stream) as shown in Figure 2. Each port carries properties including flowrate, pressure, temperature, enthalpy, molar fraction and molar volume, which can be represented as *Port.property*, for instance, $Lin.F$ (the flowrate of the inlet liquid stream). In the simulation, the inlet liquid and vapour flowrates into a column section are evaluated as the "IF" condition to determine which set of equations to activate. If both of them are larger than ε (a small number, in our case, 1×10^{-4}), Eq(1) to Eq(4) are activated. The liquid inlet flow port (Lin) is connected to the inlet liquid flow port of the 1st stage (top) of column section ($Stage(1).Lin$), which means they will have the same value for each property. Likewise, the vapour inlet flow port (Vin) is connected to the inlet vapour flow port of the bottom stage of column section ($Stage(N).Vin$). For the outlet ports, the liquid outlet port of the bottom stage of column section ($Stage(N).Lout$) is linked to the liquid outlet flow port ($Lout$) while the vapour outlet port of the 1st stage of column section ($Stage(1).Vout$) is linked to the vapour outlet flow port ($Vout$). Conversely, if either of the inlet flows of a column section is less than ϵ, Eq(5) to Eq(10) are activated. Pseudo flowrates are triggered by assigning a "false" value μ (eg., 10) to the inlet streams $Stage(1).Lin.F$ and $Stage(N).Vin.F$. In this way, the difficulties of converging VLE and MESH equations in trays are overcome when either the liquid or the vapour phase disappears in a column section. As for the outlet streams, $Vout$ is directly connected to Vin and $Lout$ is directly connected to Lin. This column section is "bypassed". When a column section is bypassed, its bypass efficiency for each tray tends to be zero. The capital cost of a column section is associated with the sum of its bypass efficiencies and will also be zero. The PTC distillation model proposed in our previous work (Ma et al., 2018), as indicated in

Eq(11), is adopted for each tray. The bypass efficiency method (Dowling and Biegler, 2014) is used to determine the number of stages in a column section. We present the column section model in Figure 3, for comparison, two sets of equations are put in parallel.

IF $Vin.F > \varepsilon$ and $Lin.F > \varepsilon$ **THEN**		**ELSE**	
Link Lin and $Stage(1).Lin$	(1)	$Stage(1).Lin.F = \mu$	(5)
		$Stage(1).Lin.z/T/P/h/V = Lin.z/T/P/h/V$	(6)
Link Vin and $Stage(N).Vin$	(2)	$Stage(N).Vin.F = \mu$	(7)
		$Stage(N).Vin.z/T/P/h/V = Vin.z/T/P/h/V$	(8)
Link $Lout$ and $Stage(N).Lout$	(3)	Link $Lout$ and Lin	(9)
Link $Vout$ and $Stage(1).Vout$	(4)	Link $Vout$ and Vin	(10)
PTC model for each tray			(11)

Figure 3: Generalised tray by tray model for distillation sections

3.2 Feed tray

IF $Feed.F > \varepsilon$ **THEN**		**ELSE**	
$V = Feed.F * Vf$	(12)	$V = 1$	(23)
$L = Feed.F * (1 - Vf)$	(13)	$L = 1$	(24)
$Vout.F = (Vin.F + V) * (1 - s\_frac)$	(14)	$Vout.F = Vin.F + V$	(25)
$Vout.z * Vout.F + SideDraw.F * SideDraw.z = Vin.z * Vin.F + y * V$	(15)	$Vout.z * Vout.F = Vin.z * Vin.F + y * V$	(26)
$Vout.h * Vout.F + SideDraw.F * SideDraw.h = Vin.h * Vin.F + h_y * V$	(16)	$Vout.h * Vout.F = Vin.h * Vin.F + h\_V * V$	(27)
$SideDraw.F = (Vin.F + V) * s\_frac$	(17)	$SideDraw.F = 0$	(28)
$SideDraw.z = Vout.z$	(18)	$SideDraw.z = Vout.z$	(29)
$SideDraw.h = Vout.h$	(19)	$SideDraw.h = Vout.h$	(30)
$Lout.F = Lin.F + L$	(20)	$Lout.F = Lin.F + L$	(31)
$Lout.z * Lout.F = Lin.z * Lin.F + x * L$	(21)	$Lout.z * Lout.F = Lin.z * Lin.F + x * L$	(32)
$Lout.h * Lout.F = Lin.h * Lin.F + h\_L * L$	(22)	$Lout.h * Lout.F = Lin.h * Lin.F + h\_L * L$	(33)
$x, y, Vf, h\_L, h\_V = flash(P, Feed.z, Feed.h)$			(34)

Figure 4: Generalised feed tray model

Using Feed tray 3 (FR3) in Figure 1 as an example to present the feed tray model. The flowrate of feed is evaluated as the “IF” condition. If it is larger than ε, Eq(12) to Eq(22) are activated, and material and energy balances are calculated. Else, Eq(23) to Eq(33) are activated, and pseudo flashed vapour (V) and liquid (L) flowrates are assigned and the sidedraw flowrate becomes zero. A flash submodel, as presented in Eq(34) in

ACM is employed to implement a flash calculation to determine the vapour fraction (Vf), liquid and vapour molar fraction (x, y) and specific enthalpy (h_L, h_V) of the outlet streams.

4. Optimisation algorithm

The mathematical model constructed above is an MINLP problem and is solved by our previously proposed feasible path-based branch and bound algorithm (Liu et al., 2022).

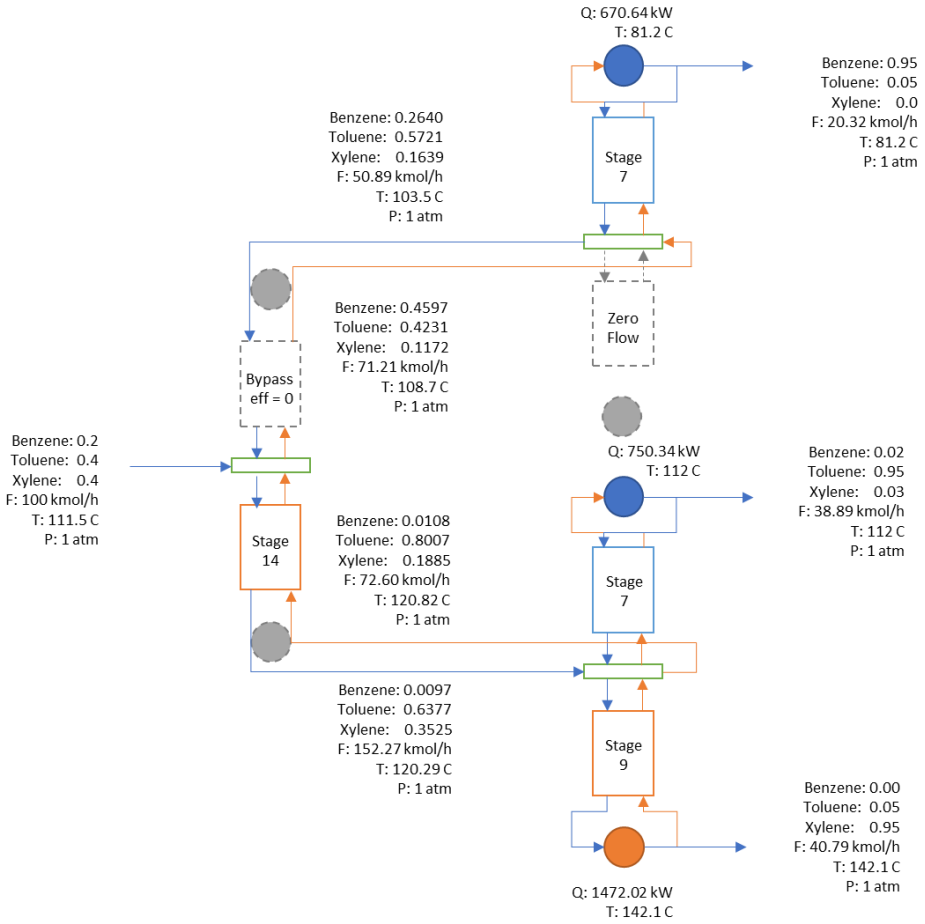

Figure 5: Optimal distillation column configuration

In our branch and bound algorithm, the NLP subproblem at each node is solved using a feasible path-based algorithm. The feasible path-based algorithm divides variables $\mathbf{x}$ into independent variables $\boldsymbol{x_I}$ and dependent variables $\boldsymbol{x_D}$ and expresses $\boldsymbol{x_D}$ as an implicit function of $\boldsymbol{x_I}$. In this way, the dimension of the problem to be optimised is reduced. The NLP subproblem at each node is decomposed into two layers, the outer layer is a small optimisation problem, while the inner layer is a process simulation problem. To foster the convergence of simulation, steady state and PTC simulation algorithm is employed. For each iteration, a steady state simulation is performed first. Only when it fails, dynamic simulation will be conducted as the PTC model is embedded.

4.1 Implementation

The mathematical model is written in ACM, and feasible path based branch and bound algorithm is executed in Python. Information such as derivatives and iterative values of variables transferred between Python and ACM is via ACM automation interface.

5. Case study

The separation of benzene, toluene and o-xylene mixture using the superstructure in Figure 1 is used to illustrate the capability of the Generalised Optimisation Framework. Table 1 presents all the information of this problem. The column operating pressure is fixed in this example. The Peng-Robinson model is selected to calculate

phase equilibrium. Medium-pressure steam is utilised as a hot utility. The example is solved on a desktop with a 2.90 GHz Intel core i7 processor, 32 GB RAM and a Windows 64-bit operating system.

Table 1: Data for hydrocarbon mixture

Mixture components A/B/C	benzene/toluene/o-xylene
Composition mole %	20 / 40 / 40
Pressure (atm)	1
Product purities	0.95 / 0.95 / 0.95
Feed flowrate (kmol h^{-1})	100
Feed condition	Saturated liquid

The optimisation problem involves 19,628 equations, 23 inequality constraints and 22,063 variables, including 189 decision variables. Among these decision variables, 180 are binary variables. The objective is to minimise Total Annualised Costs (TAC). The initial points are randomly generated. The optimal configuration is a side rectifier with TAC at 478,667 \$ y^{-1} illustrated in Figure 5. A total of 30 trays exist in the main column, and 7 stages are in the side rectifier. The bypass efficiencies of Column Section 1 (Sec1) are all zeros which mean no vapour and liquid mass and heat transfer, and Sec1 functions as a pipeline. Column Section 4 (Sec4) disappears as no flows enter it. Condenser 1 (Cond1), Reboiler 2 (Reb2) and Reboiler 4 (Reb4) are bypassed. The computational time for simulation is 79 mins.

6. Conclusions

This work presents a Generalised Optimisation Framework, including a novel mathematical model that addresses the zero flow effect and corresponding solution algorithm for the design of a complex distillation column system. The result of the case study validates the capability of handling the issue of zero flows entering distillation column sections. It also demonstrates the superiority that no tailor-made initialisation procedure is required to foster the convergence to optimum. The computational time is acceptable. In the future, we will extend this novel framework to more complex process synthesis problems using superstructure coupled with reactors and separators.

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