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Rapid and robust resolution of Underwood equations using convex transformations

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ABSTRACT

In this work, a new method is proposed for solving Underwood's equations. Newton methods cannot be used without interval control, and may require many iterations or experience severe convergence problems if the roots are near poles and the initial guess is poor. It is shown that removing only one adjacent asymptote leads to convex functions, while removing both asymptotes leads to quasi convex functions which are close to linearity on wide intervals. Using a change of variable, a pair of convex functions is defined; at each point within the search interval one of the two functions is guaranteed to satisfy the monotonic convergence condition for Newton methods. The search interval is restricted to narrow solution windows (simple and costless) and a simple high quality initial guess can be obtained using their bounds. Two solution algorithms are presented: in the first one, Newton (including higher-order) methods can be safely applied without any interval control using the appropriate convex function; in the second one, Newton iterations are applied to a quasi-convex function, and convex functions are used only if an iterate goes out of its bounds. The algorithms are tested on several numerical examples, some of them recognized as very difficult in the literature. The proposed solution methods are simple, robust, very rapid (quadratic or super-quadratic convergence) and easy to implement. In most cases, convergence is obtained in 2–3 Newton iterations, even for roots extremely close to a pole.

1. Introduction

The Underwood equations (Underwood, 1932, 1948, 1949) are used to estimate the minimum reflux ratio for simple distillation. The following equations hold for the rectifying section

$$\sum_{i=1}^{n} \frac{\alpha_i x_{Di}}{\alpha_i - \theta} = 1 + R \tag{1}$$

(also known as Underwood II equation) and for the stripping section

$$\sum_{i=1}^{n} \frac{\alpha_i x_{Bi}}{\alpha_i - \theta} = -S \tag{2}$$

where α_i are relative volatilities defined as $\alpha_i = K_i/K_r$, x_{Di} and x_{Bi} are distillate and bottom mole fractions, R and S are the molar reflux and reboil ratios in the distillation column, respectively.

Summing up Eqs. (1) and (2) and taking into account the mole balance equation $Dx_{Di} + Bx_{Bi} = z_i$, the equation

$$\sum_{i=1}^{n} \frac{\alpha_i z_i}{\alpha_i - \theta} = 1 - q \tag{3}$$

is obtained (also known as Underwood I equation), where q is the liquid fraction of the feed. For $q = 0$, the feed is a saturated vapor (dewpoint feed); for $q = 1$, the feed is a saturated liquid (bubble point feed). A value $q > 1$ indicates a subcooled liquid, while $q < 0$ indicates a superheated vapor.

The functions in Eqs. (1)–(3) exhibit n vertical asymptotes (at $\theta = \alpha_i$) and have n real distinct roots if the right hand side is non-zero; only the $n-1$ roots comprised between $\alpha_{\min}$ and $\alpha_{\max}$ have physical sense (they can be common roots to Underwood equations for the feed stream and for the distillate). The iterative procedure for solving the equations must be highly accurate.

The above equations are of the form

$$F(\lambda) = \sum_{i=1}^{n} \frac{a_i}{\alpha_i - \lambda} - \psi = 0 \tag{4}$$

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List of symbols

a	new variable
a_i	known positive constant
$\bar{a}_0$	first bound of solution window
$\bar{a}_L$, $\bar{a}_R$	bounds of solution window WA
$\bar{\bar{a}}_L$, $\bar{\bar{a}}_R$	bounds of solution window WAα
b	new variable, $b = 1/a$
c	variable
F	equation to be solved in λ
F	quasi-convex function
F_1	quasi-concave function
G	convex transformation
G_1	convex transformation
H	convex transformation
H_1	convex transformation
K_i	equilibrium constants
L	modified function
n	number of components
q	liquid fraction of the feed
S_k	$= \sum_{i=1}^{k} a_i$
S_{k+1}	$= \sum_{i=k+1}^{n} a_i$
$\bar{\bar{S}}_k$	sum in the expression of WAα bounds
$\bar{\bar{S}}_{k+1}$	sum in the expression of WAα bounds
z_i	feed composition

Greek letters

α_i	relative volatilities
Δ	$= \alpha_{k+1} - \alpha_k$
Δ_k	$= \lambda - \alpha_k$
Δ_{k+1}	$= \alpha_{k+1} - \lambda$
$\Delta_{\lambda L}$	$= \bar{\lambda}_{L0} - \alpha_k$
$\Delta_{\lambda R}$	$= \alpha_{k+1} - \bar{\lambda}_{R0}$
λ	variable
$\bar{\lambda}_0$	first bound of solution window
$\bar{\lambda}_L$, $\bar{\lambda}_R$	bounds of solution window WA
$\bar{\lambda}_{L0}$, $\bar{\lambda}_{R0}$	bounds of solution window WA at $\Psi = 0$
$\bar{\bar{\lambda}}_L$, $\bar{\bar{\lambda}}_R$	bounds of solution window WAα
ν	iteration level
Ψ	$=1 - q$
Ψ'	$\Psi\Delta$

Subscripts

i, k	integer indices
L	left
R	right
r	reference component
0	initial guess

Superscripts

*	at the root
(k)	on interval (α_k, α_{k+1})

Several particular cases of Eq. (4) are given in Vacahern and Monroy-Loperena (2012).

Despite their limitations and the development of sophisticated rigorous methods for distillation calculations, the so-called shortcut methods are still widely used in distillation design (Ramírez-Corona et al., 2010; Ghadrdan et al., 2011; Adiche and Vogelpohl, 2011; Kraemer et al., 2011; Nawaz and Jobson, 2011; Halvorsen et al., 2013; Monroy-Loperena and Vacahern, 2013, to mention only a few recently presented applications).

The function in Eq. (4) is non-convex on each interval between two adjacent vertical asymptotes. Thus, Newton-type methods cannot be used without interval control (for instance, a combination of Newton and bisection methods can be used, Michelsen and Mollerup, 2004). Several calculation methods have been proposed. Billingsley (2002) proposed a second-order method for solving Eq. (4) for all roots. Gritton et al. (2001) used homotopy continuation methods. Leibovici and Nichita (2010) proposed two simple algorithms, one using a logistic function and the other removing both adjacent asymptotes. Kocak (2011) used a modified Ostrowski (1966) fourth-order method, and warned that such methods should be used with caution because iterates can fall out of the search interval. Monroy-Loperena (2012), Monroy-Loperena and Vacahern (2012) and Vacahern and Monroy-Loperena (2012) presented an elegant solution by solving the problem as a generalized eigenvalue problem (finding all at once all the roots of Eq. (4) by calculating the eigenvalues of a companion matrix). In fact, certain secular equations are of this type, whether they arise in eigenvalue problems, or in the update of the singular value decomposition of matrices, or in some least square type problems, etc. (Melman, 1997a, 1998).

The Rachford and Rice (1952) (RR) equation, which is very important in phase equilibrium calculations, is similar in nature (for $\Psi = 0$, $a_i = z_i$, $\alpha_i = 1/(1 - K_i)$ in Eq. (4)) and has also received some attention in the recent years (Juanes, 2008; Li et al., 2012; Gaganis et al., 2012). Most proposed methods have a certain degree of complexity. Recently Nichita and Leibovici (2013) showed how convex transformations within a search region enable Newton-type updates to be used without the need for bound checking and interval reduction, in a simple, robust and efficient manner. In the present paper, we propose two methods for solving Eq. (4) using convex transformations and solution windows.

Even though the resolution of Underwood equations, and, more generally secular equations is well documented in the literature, here an original approach is presented; the novelty of the paper consists in (i) applying the methodology of Nichita and Leibovici (2013) (in which convex transformations of the original function ensure a monotonic convergence of Newton methods irrespective to the initial guess) to Underwood equations and analyzing some features specific to these equations; and (ii) deriving entirely new narrow solution windows containing the roots.

The paper is structured as follows: first, convex and quasi-convex transformations of the original function are presented (their derivatives are given in an appendix), then several solution windows (with their detailed derivations in two appendices) are proposed. Two solution algorithms are proposed and applied to various numerical examples before concluding.

2. Proposed methods

The components ore ordered according to equilibrium ratios, from the lightest to the heaviest component, $K_1 > \ldots > K_k > \ldots > K_n$, or, in terms of relative volatilities, $\alpha_n < \ldots < \alpha_k < \ldots < \alpha_1$. There are $n-1$ real roots between poles, $\lambda^{(k)} \in (\alpha_k, \alpha_{k+1})$, and if $\Psi \neq 0$ the nth root is either $\lambda^{(n)} < \alpha_n$ if $\Psi > 0$ (as in Eq. (1)) or $\lambda^{(1)} > \alpha_1$ if $\Psi < 0$ (as in Eq. (2)). For $\Psi = 0$, there are only $n-1$ real roots located between poles.

Through this paper, the formalism is presented using the more natural ordering from a mathematical point of view, that is, the poles are ordered according to the relative volatilities, $\alpha'_1 < \ldots < \alpha'_k < \ldots < \alpha'_n$, with $\alpha'_k = \alpha_{n-k+1}$ (implicitly the roots are rearranged as $\lambda'^{*}_k = \lambda^{*}_{n-k+1}$). After solving the equation, the roots can