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Nonlinear wave modeling and dynamic analysis of high-purity heat integrated air separation column

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ABSTRACT

A new natural wave velocity of heat integrated air separation column (HIASC) is first derived to describe the concentration traveling tendency of each tray, where the disturbing wave is analyzed on the basis of the natural wave velocity distribution. In order to describe the whole concentration wave of HIASC and to consider the change of the wave profile, a wave profile trial function is further introduced to obtain another useful new wave velocity expression, i.e. instant wave velocity. Then a nonlinear wave model of HIASC is finally established based on above instant wave velocity, and the comparative researches with the mechanistic model built in our previous work are carried out to test the precision of the wave model, whose integral absolute value of error is around 2×10^{-5} and integral square value of error is around 4×10^{-9}. At last, nonlinear dynamic behaviors of HIASC are analyzed based on the wave model. The research results show the validity of the proposed nonlinear wave model of HIASC.

1. Introduction

Air separation unit is a core element of many industrial processes. Pure oxygen, nitrogen and other rare gas, like argon, are largely used in the steelmaking, food processing, integrated gasification combined cycle (IGCC), etc. Cryogenic air separation technology has been successfully employed for many years for the large-scale production of pure oxygen and nitrogen and has more advantages than the pressure swing adsorption, membrane separation and chemical absorption for the high-purity production [1–5].

However, cryogenic air separation unit consumes a large amount of energy, which impacts the widespread commercialization of many systems. For example, more than 80% of the total electricity use within IGCC is consumed by the air separation unit [6]. So a lot of researches about modeling and optimal design were carried out to reduce its energy consumption. The heat integrated distillation column (HIDiC) has long been regarded as a promising energy-saving technique since first conceptually introduced by Mah and co-workers [7]. Many researchers carried on analytical research on HIDiC and gained much success [8–16]. Then a lot of national projects have applied this technology to the air separation and proved that the heat integrated air separation column (HIASC) could save more energy than the conventional air separation column (CASC) [17–22]. Nonetheless, the previous work by our group investigated the behavior analysis of the HIASC process and revealed that the behaviors of HIASC process was quite different compared to the CASC process [22–24]. Some special characteristics of the HIASC, such as the high nonlinearity, asymmetry and inverse response, bring many difficulties to modeling, optimization and controller design, especially for the high-purity columns. Traditional linear approximating models cannot deal with the rich nonlinear behaviors of HIASC well [25–28]. Although mechanistic model can capture the rich nonlinear dynamics, the many partial differential equations lead to a complex structure and bad efficiency [29–32]. Data-driven model is so sensitive to changes in the operating conditions, and its regulatory performance drastically deteriorates [33]. So a suitable reduced dynamic model of HIASC is required.

With the development of separation processes, researchers find out that there exists a common special dynamic behavior among the systems with distributed parameters which resembles traveling waves [34,35]. This phenomenon leads to the nonlinear wave theory which is well used by Luyben for distillation columns, and he proposed profile position control of distillation columns with the propagation of temperature profiles [36]. Han et al. estimated the profile position and distillate composition from selected tray temperature measurements by observers for batch distillation based on the work of Luyben [37]. Marquardt et al. and Hwang derived expressions for the wave propagation velocity and studied dynamic behaviors of concentration waves, respectively [38–40].

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Nomenclature

Symbols

A	heat transfer area, m^2
F	feed flow rate, kmol/h
G	gas side stream rate, kmol/h
H	liquid holdup, kmol
H^*	liquid holdup per unit length, kmol/m
L	liquid flow rate, kmol/h
N	number of the whole column stages
t	time, h
U	liquid side stream rate, kmol/h
U_{ov}	heat transfer coefficient, W/(m^2 K)
V	vapor flow rate, kmol/h
x	liquid mole fraction
y	vapor mole fraction
z	feed mole fraction

Subscripts

i	a certain component of nitrogen, oxygen or argon
j	stage number

Abbreviations

CASC	conventional air separation column
HIASC	heat integrated air separation column
HIDiC	heat integrated distillation column
HPC	high pressure column
IAE	integral absolute value of error
IGCC	integrated gasification combined cycle technology
ISE	integral square value of error
LPC	low pressure column
WLN	low-purity liquid nitrogen

Kienle et al. presented a new approach to the development of low-order dynamic models for multicomponent distillation processes, which made direct use of well-known spatio-temporal pattern formation phenomena also termed as nonlinear wave propagation [41]. Henson and co-workers derived a simple mathematical model capable of describing the essential column dynamics to track the wave front propagating of a cryogenic distillation column, and an on-line model adaptation was proposed as a possible approach to overcome the constant wave shape assumption [42,43]. Gruner et al. developed a general framework for analyzing and understanding the dynamics of reactive separation processes based on equilibrium theory and nonlinear waves [44]. Kim and co-workers proposed a profile position control scheme based on wave propagation theory for the control of the column under multiple steady states, and the proposed control scheme using profile positions as controlled variables was shown to give an excellent performance for the control of the reaction conversion and product purity in the reactive distillation [45]. With the internal thermally coupled technology introduced into distillation, some researches were carried out for HIDiC based on nonlinear wave theory. Liu and co-workers established a completed nonlinear wave model of HIDiC for benzene–toluene system by combining the proposed wave velocity with thermal coupling relations and material balance relations, and the group also designed a nonlinear model predictive control based on wave model for HIDiC [46,47]. Later, Cong and co-workers proposed a generalized generic model control based on the wave model for HIDiC which could even handle a very-high-purity benzene–toluene system of HIDiC with top product composition of 0.99999 [48].

So, the nonlinear wave theory is a promising method for a suitable reduced dynamic model of HIASC. However, the air separation process is a three-component non-ideal system which is quite different from conventional HIDiC, such as the benzene–toluene system. Furthermore, the internal thermally coupled technology makes the characteristics of HIASC more complex than those of CASC. So the nonlinear wave model of HIDiC or CASC cannot be applied in HIASC directly, and there are few reports carried out on it. In this work, in order to build a nonlinear wave model for the high-purity HIASC, a new natural wave velocity of HIASC is derived, which describes the partial concentration traveling tendency of each tray, and the disturbing wave is analyzed on the basis of the natural wave velocity distribution. In order to describe the whole concentration wave of HIASC and considering the change of the wave profile, a wave profile trial function is introduced to develop a new wave velocity expression, called instant wave velocity. Then the instant wave velocity is employed to establish a nonlinear wave model of HIASC, which is compared with the mechanistic model built in our previous work [23,24]. At last, some special behaviors of HIASC are analyzed based on the established nonlinear wave model.

2. Wave velocity of HIASC

2.1. Derivation of natural wave velocity

In this work, the wave of component concentration is mainly considered because of its monotonic change along the column [46]. In order to understand the special nonlinear wave behavior of the HIASC well, a description of the wave traveling tendency on each tray called the natural wave velocity is proposed.

Considering the simplification in mathematic derivation, the following expressions are approximated as continuous problem, and the approximation formations of the material balance equations [23] are expressed as follows:

$$H^*\frac{\partial x_i}{\partial t}=\frac{\partial[(V+G)y_i]}{\partial Z}-\frac{\partial[(L+U)x_i]}{\partial Z}+\frac{\partial[Fz_i]}{\partial Z} \tag{1}$$

where x is liquid mole fraction, L is liquid flow rate, V is vapor flow rate, G is gas side stream flow rate, y is vapor mole fraction, U is liquid side stream flow rate, F is feed flow rate, and z is feed mole fraction, respectively. The subscripts i represents a certain component of nitrogen, oxygen or argon, $Z=\bar{Z}/\Delta Z$, ΔZ is the height equivalent to a theoretical plate and $\bar{Z}$ represents the space coordinate of a certain position. After this transform, Z becomes a dimensionless variable that can describe a certain position of the HIASC, $H^*=\bar{H}/\Delta Z$, which represents the liquid holdup per unit length.

Integrate Eq. (1) from $j-1$ to j, and the following equation is got:

$$\int_{j-1}^{j}H^*\frac{\partial x_i}{\partial t}dZ=\int_{j-1}^{j}\left(\frac{\partial[(V+G)y_i]}{\partial Z}-\frac{\partial[(L+U)x_i]}{\partial Z}+\frac{\partial[Fz_i]}{\partial Z}\right)dZ \tag{2}$$

Define a position between the trays $j-1$ and j as $S|_{j-1}^{j}$, which represents the position of the wave profile between the two trays. Define $\varepsilon(t)=Z-S|_{j-1}^{j}(t)$ and then transfer Eq. (2) from the ordinary coordinate system $x-Z$ to a wave traveling coordinate system $\tilde{x}-\varepsilon$, which is always centered at the wave position. After the mathematical manipulation, the expression of Eq. (2) in the new coordinate system is: