Control Properties and Thermodynamic Analysis of Two Alternatives to Thermally Coupled Distillation Systems with Side Columns

J. G. Segovia-Hernández[+], E. A. Hernández-Vargas,
J. A. Márquez-Muñoz, S. Hernández, and A. Jiménez*
Universidad de Guanajuato, Facultad de Química, Noria Alta s/n,
Guanajuato, Gto., 36050, México.
*Instituto Tecnológico de Celaya, Departamento de Ingeniería Química,
García Cubas y Av. Tecnológico s/n, Celaya, Gto. 38010. Mexico.

The thermally coupled distillation configurations have received considerable attention because of their efficiency to reduce the energy required for the separation of ternary mixtures. The structure of the complex systems offers some control challenges arising from the transfer of vapor (or liquid) streams between the columns. Recently, some alternate schemes to thermally coupled distillation arrangements, that might provide better operational properties than the complex columns, have been proposed. In this work, we analyze the control properties of two alternative distillation schemes to the coupled systems. The theoretical control properties are analyzed with the application of the singular value decomposition technique. The results indicate that a reduction in the number of interconnections of the alternate configurations does not necessarily provide an improvement of its controllability properties. Also, second law calculations and energy consumptions were performed for the two alternate distillations schemes.

Keywords:
Thermally coupled distillation schemes, control properties, energy consumption

Introduction

In chemical and petrochemical industry distillation units are the most widely used separation techniques for fluid mixtures. The main disadvantage of the distillation is its high – energy requirements. Several techniques are used to overcome this problem like integration of the distillation column with the overall process which can give significant energy savings (*Smith* and *Linnhoff*[1], *Mizsey* and *Fonyo*[2]) but this kind of improvement can be limited. Significant energy savings can be reached by the use of complex distillation arrangements such as thermally coupled distillation sequences (TCDS), heat integrated distillation systems, and the heat pumping techniques.

In the case of the TCDS, through the implementation of a vapor-liquid interconnection between two columns, a condenser or a reboiler of one of the columns is eliminated, and if a proper search on the operating conditions is performed, such an interconnection can provide energy savings (*Hernández* and *Jiménez*,[3] *Hernández* and *Jiménez*[4]). TCDS for ternary mixtures have particularly been analyzed with special interest due to the remixing in the intermediate component (presented

naturally in the conventional distillations sequences and associated with higher demands of energy) which is reduced and the use of the energy improved (*Triantafyllou* and *Smith*,[5] *Hernández et al.*[6]). Two of the schemes that have received special attention are the systems with side columns: the thermally coupled system with a side rectifier (TCDS-SR, Figure 1) and the thermally coupled system with a side stripper (TCDS-SS, Figure 2). Theoretical studies (*Tedder* and *Rudd*,[7] *Annakou* and *Mizsey*,[8] *Dünnebier* and *Pantelides*,[9] among others) have shown that those thermally coupled
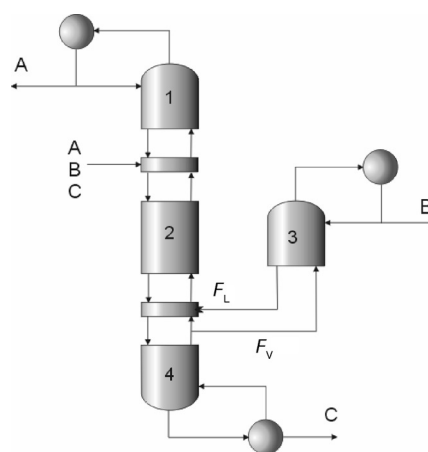

F i g . 1 – *Thermally coupled distillation sequences with a side rectifier (TCDS – SR)*

[+]Author to whom all correspondence should be addressed,
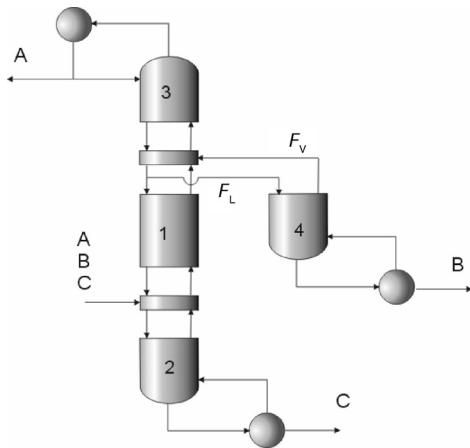e-mail: gsegovia@quijote.ugto.mx, tel: (52) 473 73 20006 ext 8142.

F i g . 2 – *Thermally coupled distillation sequences with a side stripper (TCDS – SS)*

distillation schemes with side columns are capable of achieving typically 30 % of energy savings compared with the conventional schemes.

The understanding of the control properties of columns with thermal couplings for the separation of ternary mixtures is an issue of extreme importance, since many times designs with economic incentives conflict with their operational characteristics. *Fidkowski* and *Krolikowski*,[10] among others, pointed out that despite their energy savings, TCDS options may show controllability problems because of their integrated nature. In particular, the presence of recycle streams for TCDS schemes has influenced the notion that control problems might be expected during the operation of those systems with respect to the rather well-known behavior of conventional distillation sequences. For that reason, TCDS options have not been implemented extensively in the process industries until recent times (*Kaibel* and *Shoenmakers*[11]). In many works, some authors (*Wolff* and *Skogestad*,[12] *Abdul-Mutalib* and *Smith*,[13] *Jiménez* et al.,[14] *Segovia – Hernández* et al.,[15] *Segovia – Hernández* et al.,[16] *Segovia – Hernández* et al.,[17] *Cardenas* et al.,[18] *Hernández* et al.[19]) have found the rather unexpected result that the control properties of the integrated sequences were better than those of the conventional schemes in many cases, so that the predicted savings in, both, energy and capital would probably not be obtained at the expense of operational and control problems. Recently, *Agrawal*[20] have reported some alternate configurations to TCDS schemes for the separation of ternary mixtures, eliminating the recycle streams that appear to have some operational advantages over expected dynamic properties of the designs of TCDS-SR and TCDS-SS. In this work we analyze the control properties of two alternative distillation schemes to the coupled systems and compare them to the original configuration. Also,

second law calculations and energy consumptions were performed for the two alternate distillations schemes

Alternative schemes to TCDS with side columns

Agrawal[20] has proposed two arrangements that emerge from modifications to the systems shown in Figures 1 and 2. Such new systems are shown in Figures 3 and 4. The alternate arrangement to TCDS-SR, a direct sequence with a Side stream from the first column (ATCDS-SR, Figure 3) eliminates the recycle stream of the TCDS-SR sequence by reproducing the bottom section (section 4; see Figure 3) of the first column within the second column, which affects the structure of the original side rectifier. In the other case, the alternate arrangement to TCDS-SS, an Indirect Sequence with a Side stream from the first column (ATCDS-SS, Figure 4), the vapor interconnection of the TCDS-SS scheme, is eliminated and the top section of the first column (section 3; see Figure 4) is added to the second column, affecting the original side stripper.
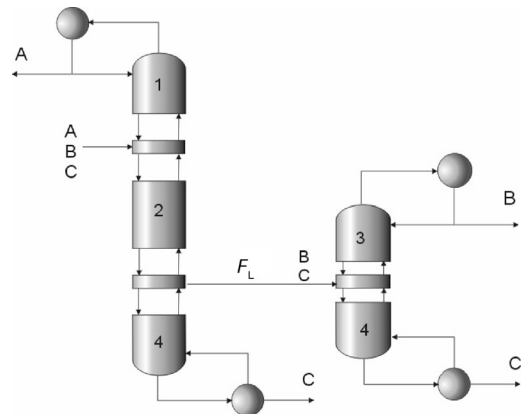

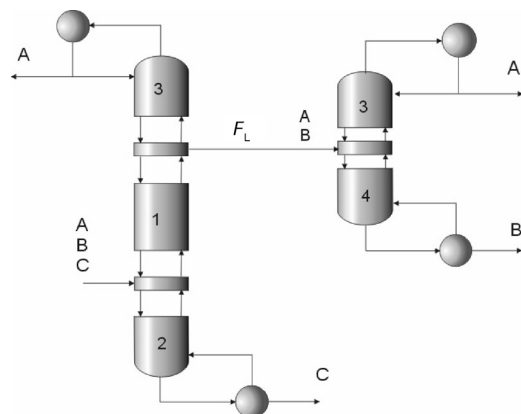F i g . 3 – *Alternate arrangement to the TCDS – SR sequence (ATCDS-SR)*

F i g . 4 – *Alternate arrangement to the TCDS – SS sequence (ATCDS-SS)*

Therefore, the new arrangements do not contain recycle streams, and the second column of each sequence is transformed into a conventional distillation column. The resulting new structures, therefore, seem to provide simpler systems to control and operate.

Energy – efficient designs

The design and optimization strategies for conventional distillation sequences, involving the separation of ternary mixtures (Figure 5), are well known. The energy – efficient design methods for TCDS – SR and TCDS – SS schemes are described in *Hernández* and *Jiménez*.[3] Basically, preliminary designs of the TCDS options are obtained from the conventional sequences (Figure 5). The design of

TCDS – SR column is obtained by using a thermal link in the vapor phase in the conventional direct sequence, which eliminates the reboiler in the second column of the conventional scheme, and the tray section (named 4) is moved to the bottom of the first column of conventional scheme (Figure 1 and 5a). The vapor flow (FV) is changed until the minimum energy demand in the reboiler of the TCDS – SR sequence is obtained. The energy – efficient design of TCDS – SS option is obtained directly from the conventional indirect distillation sequence by removing the condenser in the second column of conventional scheme and introducing a thermal coupling in the liquid phase; the tray section named 3 is moved to the top of the first column of conventional scheme (Figure 2 and 5b). The liquid stream (FL) is varied until the minimum energy requirement for TCDS – SS column is obtained.

The new schemes were then obtained directly from the TCDS arrangements following the simple tray section analogies depicted in Figures 1 – 4. The new systems were also subjected to an optimization procedure to detect the values of the side stream flowrates from the first column that minimized their energy consumptions. It should be noted that the range for the search procedure for these structures is more restricted than for the TCDS structures because of mass balance considerations. Those bounds for columns with side streams have been explained by *Glinos* and *Malone*.[21] (For more details to optimization method of alternate sequences, see *Ramírez* and *Jiménez*.[22])

Singular value decomposition (SVD)

Open loop dynamic responses to set point changes around the assumed operating point (which corresponds to that with minimum energy consumption for each configuration) were obtained. The responses were obtained through the use of Aspen Dynamics. Transfer function matrices (G) were then collected for each case, and they were subjected to SVD:

$$G = V\Sigma W^H \qquad (1)$$

where $\Sigma = \text{diag } (\sigma_1,.....,\sigma_n)$, σ_i = singular value of $G = \lambda_i^{1/2}(GG^H)$; $V = (v_1, v_2,.....)$ matrix of left singular vectors, and $W = (w_1, w_2,....)$ matrix of right singular vectors. Two parameters of interest are the minimum singular value, σ_*, and the ratio maximum to minimum singular values, or condition number:

$$\gamma^* = \sigma^* / \sigma_* \qquad (2)$$

(a) DS

(b) IS
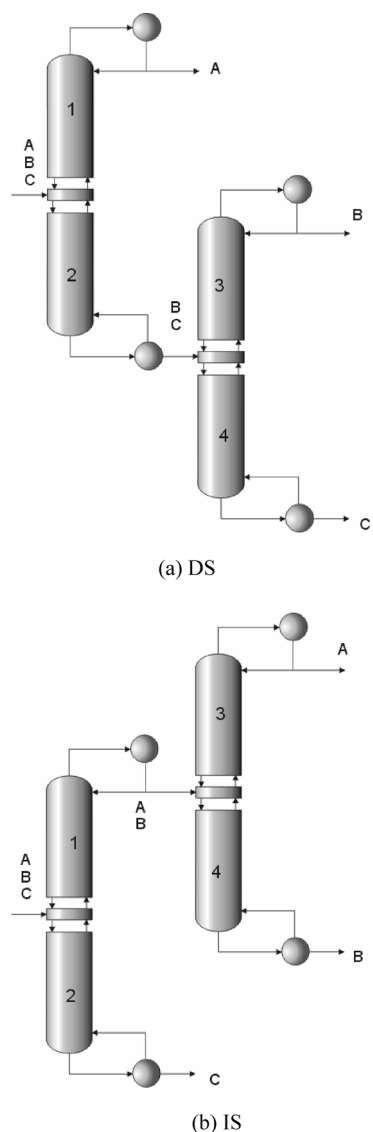
F i g . 5 – *Conventional distillation sequences for the separation of ternary mixtures: (a) direct sequence; (b) indirect sequence*

The minimum singular value is a measure of the invertibility of the system and represents a measure of the potential problems of the system under feedback control. The condition number reflects the sensitivity of the system under uncertainties in process parameters and modeling errors. These parameters provide a qualitative assessment of the theoretical control properties of the alternate designs. The systems with higher minimum singular values and lower condition numbers are expected to show the best dynamic performance under feedback control. *Jiménez* et al.[14] have shown the application of the SVD technique to compare the controllability properties of the thermally coupled structures of Figure 1 and 2 to those of sequences based on conventional distillation columns (Figure 5).

A full SVD analysis should cover a sufficiently complete range of frequencies. For this initial analysis of the alternative schemes to the coupled configurations, we simply estimated the SVD properties for each separation system at zero frequency. Such analysis should give some preliminary indication on the control properties of each system around the nominal operating point.

Cases of study

To compare the behavior of the sequences three ternary mixtures with different values of the ease of separability index (ESI = α_{AB}/α_{BC}), as defined by *Tedder* and *Rudd*,[7] were considered. The mixtures description is given in Table 1; the feed flowrate was 45.36 kmol hr^{-1}. The columns of the conventional sequence that provide the tray structure for the thermally coupled systems (*Hernández* and *Jiménez*[3]) were designed assuming reflux ratios of 1.33 times the minimum values. The design pressure for each separation, in alternate sequences, was chosen to ensure the use of cooling water in the condensers. In the case of the integrated schemes, the pressure operation was chosen to guarantee the use of cooling water to condenser of the light component (A). It is well known that the energy savings obtained in the TCDS structure for ternary separations depend strongly on the amount of intermediate component. For that reason, two feed compositions were assumed for each mixture (Table 2) with a low or high content of the intermediate component.

Table 1 – *Mixtures analyzed*

Mixture	Components (A, B, C)	ESI
M_1	n-pentane / hexane /n-heptane	1.04
M_2	n-butane / i-pentane / n-pentane	1.86
M_3	i-pentane /n-pentane / hexane	0.47

Table 2 – *Feed composition*

Feed	Composition, % mole
F_1	40 / 20 / 40
F_2	15 / 70 / 15

Results

First, energy consumption and thermodynamic efficiencies for the separation of ternary mixtures were calculated. When the results were analyzed, in general, the TCDS options and alternate arrangements presented energy savings in the range between 10 and 35 %, in contrast to conventional distillation sequences (Tables 3–5). These results are in agreement with the classical result of energy savings around 30 %. Two trends for TCDS and alternate arrangements were obtained: for both types of feed compositions, the TCDS and alternate schemes required less energy consumption to achieve the separation, in comparison to the conventional sequences; the TCDS sequences and their alternate schemes have similar energy consumptions, but energy savings were higher in the TCDS than the alternate schemes (Table 6). In general, the new systems can perform the ternary separations with similar energy consumption as the thermally coupled systems (mixture M_1, feed F_2; Table 3) or deteriorate the energy savings provided by the thermally coupled options (mixture M_3; Table 5), although, even in those cases they still provide energy savings with respect to the conventional sequences.

Table 3 – *Power consumptions (kW) and thermodynamic efficiencies for mixture M_1*

Feed	Distillation sequence	Total heat duty Q_d / kW	η / %
F_1	DS	941.5	16.8
	TCDS-SR	724.3	22.1
	ATCDS-SR	746.9	22.2
	IS	846.4	22.7
	TCDS-SS	624.1	27.2
	ATCDS-SS	636.91	27.7
F_2	DS	1314.8	7.7
	TCDS-SR	1042.7	9.8
	ATCDS-SR	987.9	10.2
	IS	1239.3	11.9
	TCDS-SS	945.6	13
	ATCDS-SS	931.3	12.9

T a b l e 4 – *Power consumptions (kW) and thermodynamic efficiencies for mixture M_2*

Feed	Distillation sequence	Total heat duty Q_d / kW	η / %
F_1	DS	2130.8	7.5
	TCDS-SR	1590.1	8.6
	ATCDS-SR	1578.4	9.16
	IS	2493.0	9.9
	TCDS-SS	1540.3	10.6
	ATCDS-SS	1568.7	11.1
F_2	DS	2834.8	5.5
	TCDS-SR	1939.5	9.0
	ATCDS-SR	1930.4	9.1
	IS	2274.1	8.0
	TCDS-SS	1959.5	9.0
	ATCDS-SS	1968.2	8.8

T a b l e 5 – *Power consumptions (kW) and thermodynamic efficiencies for mixture M_3*

Feed	Distillation sequence	Total heat duty Q_d / kW	η / %
F_1	DS	1020.3	17.4
	TCDS-SR	862.3	17.6
	ATCDS-SR	931.0	17.5
	IS	1060.3	25.0
	TCDS-SS	918.4	27.8
	ATCDS-SS	987.4	28.1
F_2	DS	1090.1	17.9
	TCDS-SR	982.7	14.6
	ATCDS-SR	1017.1	14.8
	IS	1215.4	21.9
	TCDS-SS	1027.7	25.8
	ATCDS-SS	1034.2	26.1

T a b l e 6 – *Energy savings in thermally coupled and alternate schemes*

Mixture	Feed	Distillation sequence	Part of energy savings (%) (in comparison to the respective conventional sequence)
M_1	F_1	TCDS-SR	23.0
		ATCDS-SR	20.6
		TCDS-SS	26.3
		ATCDS-SS	24.75
M_1	F_2	TCDS-SR	20.7
		ATCDS-SR	24.9
		TCDS-SS	23.7
		ATCDS-SS	24.8
M_2	F_1	TCDS-SR	25.4
		ATCDS-SR	25.9
		TCDS-SS	38.2
		ATCDS-SS	37.1
M_2	F_2	TCDS-SR	31.6
		ATCDS-SR	31.9
		TCDS-SS	13.8
		ATCDS-SS	13.4
M_3	F_1	TCDS-SR	15.5
		ATCDS-SR	8.75
		TCDS-SS	13.4
		ATCDS-SS	6.9
M_3	F_2	TCDS-SR	15.4
		ATCDS-SR	6.7
		TCDS-SS	15.4
		ATCDS-SS	14.9

The second law efficiencies calculated for all of the schemes show that, in general, the introduction of links (as in TCDS or in alternate schemes) increased the thermodynamic efficiencies, in contrast to conventional schemes. However, coupled and alternate schemes have obtained similar efficiency values (Tables 3–5). These increments were not superior to 6 % because the conventional distillation schemes and the corresponding TCDS sequences and new arrangements have the same levels of temperatures in some products streams. The difference is the introduction of the thermal link. The optimization of these links causes significant energy savings and improve the values of the thermodynamic efficiencies. At this point, it is important to say that the second law efficiency calculated in integrated and alternate schemes is similar, despite the fact that the levels of temperature are different in the streams of each sequence.

In general, the results show that the alternate schemes, which were proposed as alternatives with better operational properties than the TCDS with side columns, have similar energy consumptions and second law efficiencies. It can be interpreted, as the alternate schemes to TCDS- SR and TCDS-SS are almost thermodynamically equivalent.

Tables 7–9 give the results for the SVD test for each sequence. The thermally coupled distillation systems, TCDS – SR and TCDS – SS, have the lowest value of the condition number, which im-

T a b l e 7 – *Minimum singular value and condition number for each structure (mixture M_1)*

Feed F_1

scheme	σ_*	γ^*
TCDS – SR	29.3	80.9
ATCDS – SR	0.0603	16356.24
TCDS – SS	80.4	12.2
ATCDS – SS	0.1	29392

Feed F_2

scheme	σ_*	γ^*
TCDS – SR	1.8	1984
ATCDS – SR	0.6	3231.5
TCDS – SS	1.7	2483
ATCDS – SS	0.0006	181674

T a b l e 8 – *Minimum singular value and condition number for each structure (mixture M_2)*

Feed F_1

Scheme	σ_*	γ^*
TCDS – SR	41.4	125.8
ATCDS – SR	0.1	8166.1
TCDS – SS	120.8	8.9
ATCDS – SS	0.1	98594

Feed F_2

Scheme	σ_*	γ^*
TCDS – SR	4.4	851.9
ATCDS – SR	2	1603.2
TCDS – SS	7.5	1328.8
ATCDS – SS	0.0018	273873.7

T a b l e 9 – *Minimum singular value and condition number for each structure (mixture M_3)*

Feed F_1

Scheme	σ_*	γ^*
TCDS – SR	21.7	85.8
ATCDS – SR	1.7	4064.2
TCDS – SS	257.5	34.57
ATCDS – SS	0.04	10315.63

Feed F_2

Scheme	σ_*	γ^*
TCDS – SR	5.8	977.8
ATCDS – SR	0.1	69816
TCDS – SS	3	1401.3
ATCDS – SS	0.02	17057

plies that these sequence are better conditioned to the effect of disturbances than the alternate arrangements; such sequences also show the highest value of the minimum singular value, which means that the coupled columns are expected to require lower control efforts under feedback operation than the other alternate sequences. On the other side of the analysis, the modified structures show the worst values of the SVD parameters, which implies that, from the set of structures, these sequences are worst conditioned to the effect of disturbances. Since the new structures were conceived to improve the control properties of the thermally coupled distillation sequences, it should be highlighted that the complex configurations do not show the worst control properties of the four sequences. The SVD parameters indicate that the theoretical properties of the modified structures (ATCDS – SR and ATCDS – SS), obtained through the elimination of one interconnecting stream, are expected to be worse than those of the original complex arrangements. Moreover, one can also notice that the reduction of one interconnection from the coupled arrangements deteriorate the theoretical controllability properties of the complex structures. The best compromise on the theoretical controllability properties, provided by the SVD application, seems to be provided by the thermally coupled structures.

Overall, the results from this test indicate that the reduction in the number of interconnections that provides simpler designs does not necessarily drive to the expected operational advantages with respect to the original complex configurations.

Conclusions

An analysis on energy consumption, thermodynamic efficiency and control properties of two new distillation sequences that arise from modifications

to the thermally coupled systems with side columns, has been presented. It has been shown, that the new systems can perform the separations tasks with similar energy demands in the reboilers and second law efficiencies, as the thermally coupled systems with side columns for ternary mixtures. When the mixtures were analyzed, the TCDS and alternate schemes presented savings up to 20 % or more in contrast to the conventional direct and indirect distillation sequences. Regarding thermodynamic efficiency, in general, the introduction of thermal links (or interconnection) increased its value; such an increment is caused by reduction in the energy consumption through the use of thermal link. These results are very important because let conclude that the ATCDS-SR and ATCDS-SS are thermodynamically equivalent schemes to TCDS-SR and TCDS-SS, respectively. The results from the theoretical control properties, evaluated from the singular value decomposition method, indicate that a reduction in the number of interconnections does not necessarily provide the operational advantages originally expected, given the resulting, simpler, structural design. Two major conclusions can be addressed from this initial study on control properties. First, the controllability properties of the complex columns were not improved by all of the alternative sequences that were conceptually designed aiming to do that; even more, the thermally coupled distillation sequences. Second, the properties of the complex arrangements can be deteriorated by the reduction in the number of interconnections.

Appendix

When continuous – flow and steady – state – flow systems, such as those shown in Figures 1 through 5, are analyzed under the laws of thermodynamics, thermodynamic efficiencies (η) can be computed through standard expression as explained in the work of *Seader* and *Henley*[23]. These equations are:

Energy balance:

$$\sum_{\text{out}} (nH_{\text{m}} + Q + W_{\text{S}}) - \sum_{\text{in}} (nH_{\text{m}} + Q + W_{\text{S}}) = 0 \quad (1)$$

Entropy balance:

$$\sum_{\text{out}} \left(nS_{\text{m}} + \frac{Q}{T_{\text{S}}} \right) - \sum_{\text{in}} \left(nS_{\text{m}} + \frac{Q}{T_{\text{S}}} \right) = \Delta S_{\text{irr}} \quad (2)$$

Availability balance:

$$\sum_{\text{in}} \left[nB_{\text{m}} + Q \left(1 - \frac{T_0}{T_{\text{S}}} \right) + W_{\text{S}} \right] - \sum_{\text{out}} \left[nB_{\text{m}} Q \left(1 - \frac{T_0}{T_{\text{S}}} \right) + W_{\text{S}} \right] = W_{\text{L}} \quad (3)$$

Minimum work of separation:

$$W_{\text{min}} = \sum_{\text{out}} nB_{\text{m}} - \sum_{\text{in}} nB_{\text{m}} \quad (4)$$

Second law efficiency:

$$\eta = \frac{W_{\text{min}}}{W_{\text{L}} + W_{\text{min}}} \quad (5)$$

where $B_{\text{m}} = H_{\text{m}} - T_0 \, \Delta S_{\text{m}}$ is the availability function, $W_{\text{L}} = T_0 \, \Delta S_{\text{irr}}$ represents the lost work in the system, and η is the thermodynamic efficiency. Second law efficiencies for all of the schemes considered can be computed from enthalpies, entropies and optimal heat consumptions in the reboilers.

Nomenclature

B_{m} – molar availability function, kJ kmol^{-1}
F_{L} – interconnecting liquid flow rate, kmol h^{-1}
F_{V} – interconnecting vapor flow rate, kmol h^{-1}
G – transfer function matrix
H_{m} – molar enthalpy, kJ kmol^{-1}
W_{L} – lost work in the system, kJ
n – amount of substance, kmol
Q – heat, kJ
S_{m} – molar entropy, kJ kmol^{-1} K^{-1}
T_0 – temperature of the surroundings, K
T_{s} – temperature of the system, K
V – matrix of left singular vectors
W – matrix of right singular vectors
W_{min} – minimum work for the separation, kJ
W_{s} – shaft work, kJ
ΔS_{irr} – production of entropy, kJ K^{-1}
η – second law efficiency
σ^* – maximum singular value
σ_* – minimum singular value
γ^* – condition number
Σ – matrix of singular values
λ_{i} – eigenvalue i

Superscripts

H – transpose and conjugated

Subscripts

in – entering system
out – leaving system

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