



## Controllability analysis of alternate schemes to complex column arrangements with thermal coupling for the separation of ternary mixtures

Victoria E. Tamayo-Galván, Juan Gabriel Segovia-Hernández\*, Salvador Hernández, Julián Cabrera-Ruiz, J. Rafael Alcántara-Ávila

Universidad de Guanajuato, Facultad de Química, Noria Alta s/n, Guanajuato, Gto., Mexico 36050, Mexico

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### ABSTRACT

Thermally coupled distillation systems (TCDS) have been proposed to perform distillation separation tasks with the incentive of achieving lower energy consumption levels with respect to conventional distillation sequences. 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. That has been one of the main reasons for the lack of industrial implementation of thermally coupled distillation schemes. Recently, some alternatives 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 alternatives to the coupled systems. The results indicate that a reduction in the number of interconnections in alternate configurations does not necessarily provide an improvement of controllability properties.

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### 1. Introduction

Environmental concerns and diminishing energy resources dictate the use of highly energy-efficient process equipment in chemical industries. The separation of multicomponent mixtures into three or more products is usually performed in a sequence of simple distillation columns. Considerable energy savings can be obtained with complex distillation schemes. Complex column arrangements with or without thermal coupling are attractive options for savings in both energy and capital cost. This financial incentive has created considerable scientific interest in the last 15 years. There is a significant amount of literature analyzing the relative advantages of TCDS options for ternary separations (Tedder & Rudd, 1978; Glinos & Malone, 1988; Carlberg & Westerberg, 1989; Yeomans & Grossmann, 2000; Rév, Emtir, Sztikai, Mizsey, & Fonyó, 2001). These studies have shown that thermally coupled configurations are capable of achieving energy savings of up to 30% over conventional direct and indirect distillation sequences for the separation of feeds with low or high content of the intermediate component, and energy savings depend on the amount of the intermediate component. For zeotropic ternary, quaternary and multicomponent mixtures many functionally distinct ther-

mally coupled configurations have been published (Hernández & Jiménez, 1996, 1999a; Agrawal & Fidkowski, 1999; Rong, Kraslawski, & Nystrom, 2001; Rong, & Kraslawski, 2001; Blancarte-Palacios, Bautista-Valdés, Hernández, Rico-Ramírez, & Jiménez, 2003; Calzon-McConville, Rosales-Zamora, Segovia-Hernández, Hernández, & Rico-Ramírez, 2006). Despite the potential benefits of thermally coupled columns and some reports of successful industrial applications (Kaibel & Schoenmakers, 2002) only a limited number of such columns have been implemented in the field using the dividing wall distillation column (only one shell divided by a wall). The application of TCDS has been increasing in a variety of plants worldwide including in North America. Practical applications are especially active in Europe and Japan, where the demand for energy conservation is greater than in other places because most of the crude oil consumed there is imported from other countries (Kim, 2006). The lack of widespread use of complex columns can partly be attributed to their more difficult control properties (Agrawal & Fidkowski, 1998). In particular, the presence of recycle streams for TCDS has influenced the notion that control problems might be expected during the operation of these systems with respect to the rather well-known behavior of conventional distillation sequences. Understanding control properties of columns with thermal couplings for the separation of ternary mixtures is an issue of extreme importance since designs with economic incentives often conflict with their operational characteristics. However, recent publications report considerable progress in the identification of suitable control variables and

\* Corresponding author. Tel.: +52 473 73 20006x8142;  
fax: +52 473 73 20006x8139.

E-mail address: [gsegovia@quijote.ugto.mx](mailto:gsegovia@quijote.ugto.mx) (J.G. Segovia-Hernández).

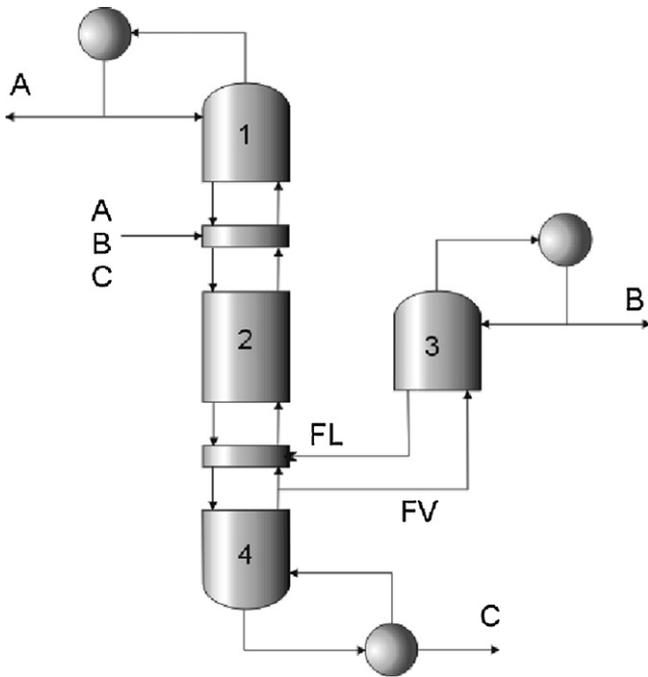


Fig. 1. Thermally coupled distillation sequence with side rectifier (TCDS-SR).

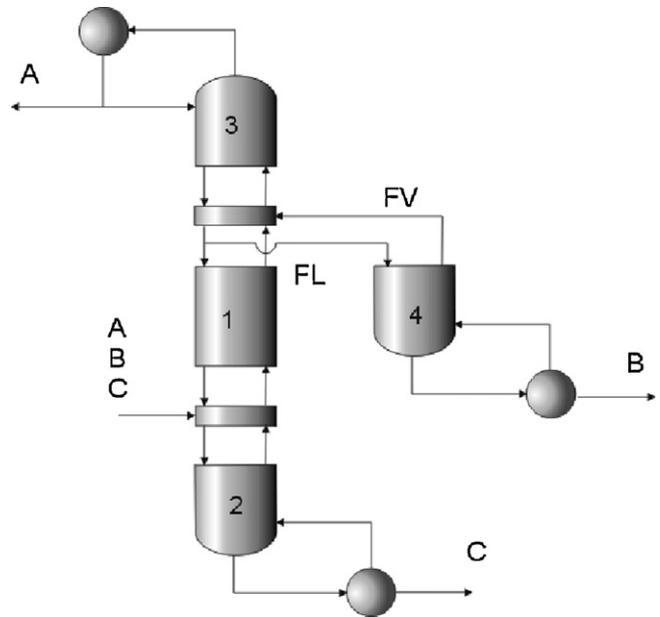


Fig. 2. Thermally coupled distillation sequence with side stripper (TCDS-SS).

control strategies for some configurations (Wolff & Skogestad, 1995; Abdul Mutalib & Smith, 1998; Halvorsen & Skogestad, 1999; Hernández & Jiménez, 1999b; Serra, Espuña, & Puigjaner, 1999, 2003; Serra, Perrier, Espuña, & Puigjaner, 2001; Jiménez, Hernández, Montoy, & Zavala-García, 2001; Segovia-Hernández, Hernández, & Jiménez, 2002a,b; Segovia-Hernández, Hernández, Rico-Ramírez, & Jiménez, 2004; Esparza-Hernández, Irianda-Araujo, Domínguez-Lira, Hernández, & Jiménez, 2005; Hernández, Gudiño-Mares, Cárdenas, Segovia-Hernández, & Rico-Ramírez, 2005; Santos-Méndez & Hernández, 2005; Segovia-Hernández, Hernández, & Jiménez, 2005a; Segovia-Hernández, Hernández, Jiménez, & Femat, 2005b; Segovia-Hernández, Hernández-Vargas, Márquez-Muñoz, Hernández, & Jiménez, 2005c). Recently, Agrawal (2000) reported several 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 thermally coupled distillation sequence with side rectifier (TCDS-SR; Fig. 1) and thermally coupled distillation sequence with side stripper (TCDS-SS; Fig. 2) designs. In this work we analyze the control properties of two alternative distillation schemes to the coupled systems and compare them to the original configuration.

## 2. Two alternatives to thermally coupled distillation sequences

Recently, Agrawal (2000) proposed two arrangements that emerge from modifications to the systems shown in Figs. 1 and 2. These new systems are shown in Figs. 3 and 4. The first modified arrangement [a direct sequence with a side stream (SDI) from the first column] eliminates the recycle stream of the TCDS-SR by reproducing the bottom section (Section 4) of the first column within the second column, which affects the structure of the original side rectifier. For the second arrangement [an indirect sequence with a side stream (SIS) from the first column], the vapor interconnection of the TCDS-SS is eliminated and the top section of the first column (Section 3) is added to the second column, affecting the

original side stripper. Therefore, the new arrangements eliminate intercolumn vapor or liquid transfers and do not contain recycle streams, and the second column of each sequence is transformed into a conventional distillation column. The resulting new structures thus seem to provide simpler systems to control and operate.

## 3. Design method

The design and optimization strategies for conventional distillation sequences involving the separation of ternary mixtures are well-known. The energy-efficient design methods for TCDS-SR and TCDS-SS schemes are described in Hernández and Jiménez (1996). Basically, preliminary designs of the TCDS options are obtained from the conventional sequences (Fig. 5). The design of the TCDS-SR sequence is obtained by using a thermal link in the vapor phase of the conventional direct sequence, which eliminates the reboiler in the second column of the conventional scheme, and the tray section (Section 4) is moved to the bottom of the first column of the conventional scheme (Figs. 1 and 5a). The vapor flow (FV) is varied

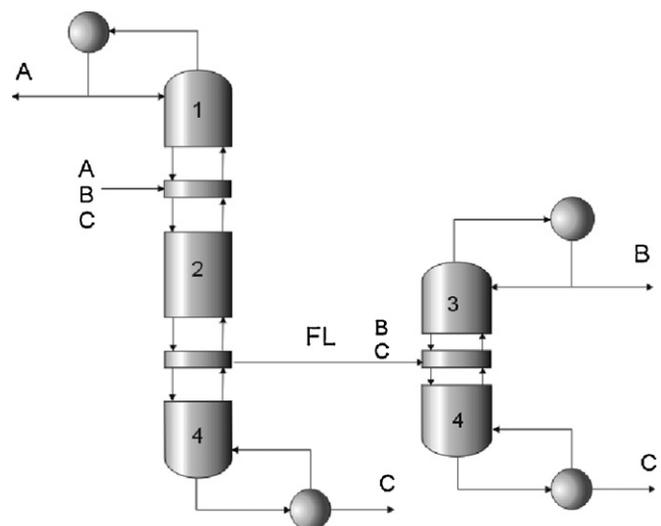


Fig. 3. Modified arrangement from the TCDS-SR (SDI).

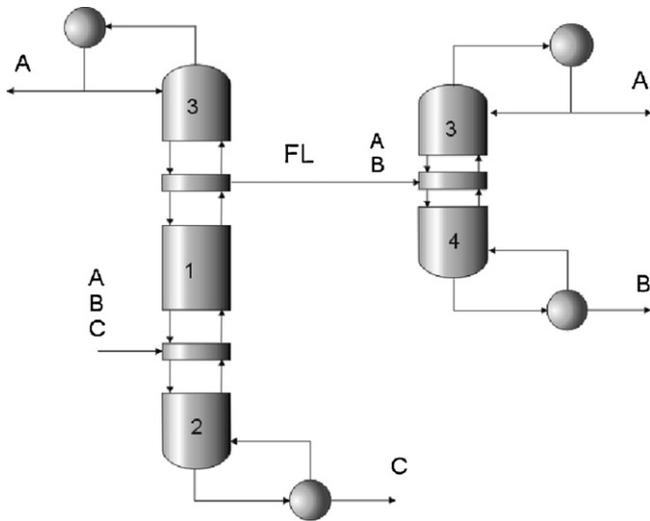


Fig. 4. Modified arrangement from the TCDS-SS (SIS).

until the minimum energy demand in the reboiler of the TCDS–SR sequence is obtained. The energy-efficient design of the TCDS–SS sequence is obtained directly from the conventional indirect distillation sequence by removing the condenser in the second column of the conventional scheme and introducing a thermal coupling in the liquid phase; the tray Section 3 is moved to the top of the first column of the conventional scheme (Figs. 2 and 5b). The liquid stream (FL) is varied until the minimum energy requirement for the TCDS–SS column is obtained.

The new schemes were then obtained directly from the TCDS arrangements following the simple tray section analogies depicted in Figs. 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 energy consumption. 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 (1985). Further details on the design and optimization procedure of alternate sequences are given by Ramírez and Jiménez (2004).

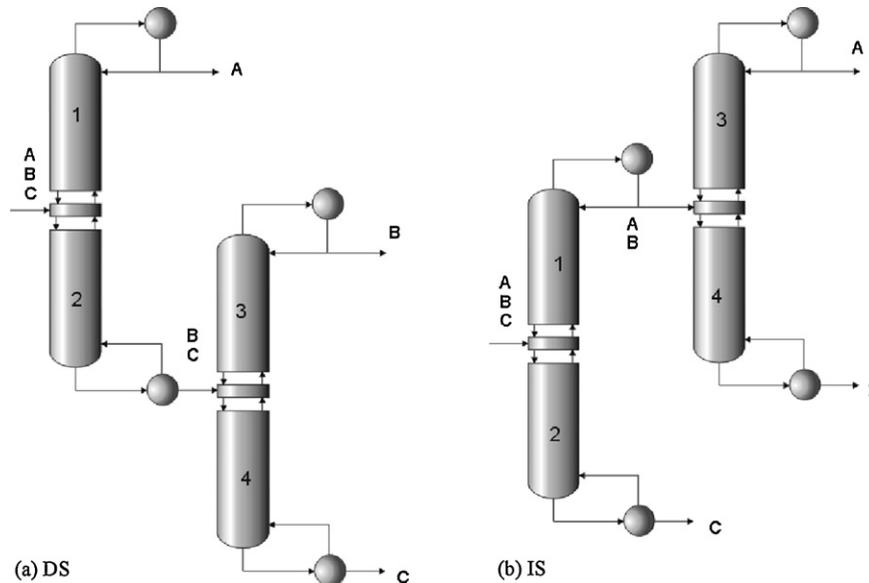


Fig. 5. Conventional distillation sequences for the separation of ternary mixtures: (a) direct sequence; (b) indirect sequence.

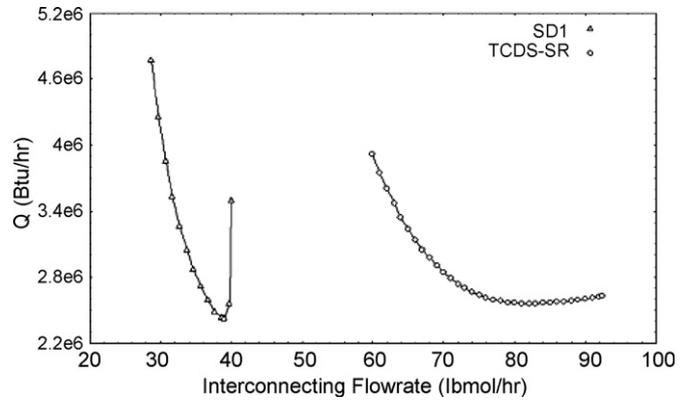


Fig. 6. Energy optimization of the TCDS–SR and SDI (case M1, F1).

#### 4. Theoretical control properties

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. Responses were obtained using Aspen Dynamics 11.1. Transfer functions were grouped into a transfer function matrix ( $G$ ) and were subjected to singular value decomposition (SVD):

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

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

$$\gamma^* = \frac{\sigma^*}{\sigma_*} \quad (2)$$

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

**Table 1**  
Transfer function matrix for TCDS–SR (M1, F1)

	R1	R2	Q1
$X_A$	$\frac{0.0072}{1 + 0.6325s}$	$\frac{0.0172}{1 + 5.3972s}$	$\frac{0.0076}{1 + 0.6325s} - \frac{0.0172}{1 + 4.09s} + \frac{3.1976}{1 + 0.6325s} + \frac{3.3316}{1 + 2.2596s}$
$X_B$	$\frac{0.0204}{1 + 3.6731s}$	$\frac{0.0208}{1 + 3.7515s}$	$\frac{0.5396}{1 + 0.0903s} - \frac{8.046}{1 + 3.0539s}$
$X_C$	$-\frac{0.0176}{1 + 3.3085s}$	$-\frac{0.0176}{1 + 3.3224s}$	$\frac{3.3336}{1 + 1.4245s}$

**Table 3**  
Transfer function matrix for TCDS–SS (M1, F1)

	R1	Q2	Q1
$X_A$	$\frac{0.0144}{1 + 0.758s}$	$-\frac{1.0408}{1 + 0.849s}$	$-\frac{4.0988}{(1 + 0.3881s)^2}$
$X_B$	$-\frac{0.0028}{1 + 0.483s} + \frac{0.0084}{1 + 6.24s}$	$\frac{1.3644}{1 + 1.6786s}$	$\frac{0.102}{1 + 0.2s} - \frac{0.7592}{0.36s^2 + 0.72s + 1}$
$X_C$	$-\frac{0.0128}{1 + 2.0659s}$	$-\frac{0.9688}{(1 + 1.1485s)^2}$	$\frac{1.0988}{0.2025s^2 + 0.54s + 1}$

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. (2001) have demonstrated the application of the SVD technique to compare the controllability properties of the thermally coupled structures of Figs. 1 and 2 to those of sequences based on conventional distillation columns (Fig. 5). It is important to highlight that the dynamic model used in each equilibrium stage includes transient total mass balance, transient component mass balances, equilibrium relationship, summation constraints and transient energy balance. Also, for the hydraulics of liquid a residence time of 5 min was assumed as a typical value (Luyben, 1992). Finally, a pressure drop of 10 psi for each distillation column was assumed in accordance with the recommendation given in Seader and Henley (2006).

## 5. Case of study

To compare the behavior of the sequences, three ternary mixtures with different values for the ease of separability index ( $ESI = \alpha_{AB}/\alpha_{BC}$ ), as defined by Tedder and Rudd (1978) were considered. The mixtures are: *n*-pentane/*n*-hexane/*n*-heptane (M1;  $ESI = 1.04$ ); *n*-butane/*i*-pentane/*n*-pentane (M2;  $ESI = 1.86$ ); *i*-pentane/*n*-pentane/*n*-hexane (M3;  $ESI = 0.47$ ). The feed flowrate was 45.36 kmol/h. The columns of the conventional sequence that provide the tray structure for the thermally coupled systems were designed assuming reflux ratios of 1.33 times the minimum values. The design pressure for each separation was chosen to ensure the use of cooling water in the condensers. 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, composition % mole, were assumed for each mixture (40/20/40; F1 and 15/70/15; F2) with a low or high content of the intermediate component.

## 6. Dynamic analysis

The design of the TCDS schemes was first developed following the approach proposed by Hernández and Jiménez (1996). The design method involves a search procedure on the interconnec-

tion streams LF or VF (Figs. 1 and 2) until a minimum energy consumption is detected. A similar optimization procedure, in the connection stream, is carried out in the alternate sequences (Figs. 3 and 4) as explained by Ramírez and Jiménez (2004). The resulting structures provided the designs that were then subjected to dynamic analysis using Aspen Dynamics 11.1.

As far as energy consumption is concerned, the optimized steady-state design for the TCDS–SR and TCDS–SS options provides energy savings in the range of 20–30% over conventional distillation sequences (see Hernández & Jiménez, 1996). The alternate schemes, SDI and SIS, are thermodynamically equivalent to TCDS–SR and TCDS–SS, respectively (i.e., similar energy consumption and thermodynamic efficiencies). In this work we used the steady-state design variables, for all cases of study, shown in Ramírez and Jiménez (2004).

The SVD technique requires transfer function matrices, which are generated by implementing step changes in the manipulated variables of the optimum design of the distillation sequences (base designs) and registering the dynamic responses of the three products. For the distillation sequences presented in this work, three controlled variables were considered, product composition A–C (in the case of the alternate structure, four controlled variables were considered, since one component is obtained in two streams). Similarly, three manipulated variables were defined: the first two variables are the reflux ratios and the heat duties supplied to the reboilers for the system; the third variable is selected based on structure (in the case of the alternate structure, four manipulated variables were considered, since one component is obtained in two streams). Fig. 6 shows the minimization of energy consumption for the case of the TCDS–SR and SDI sequences shown in Figs. 1 and 3 in order to obtain the steady-state design. It is important to emphasize that energy requirements in the reboiler depend strongly on the LF or VF streams. During the search for optimum energy consumption, three design specifications for product purities A–C were set in order to avoid deviations in the required purities.

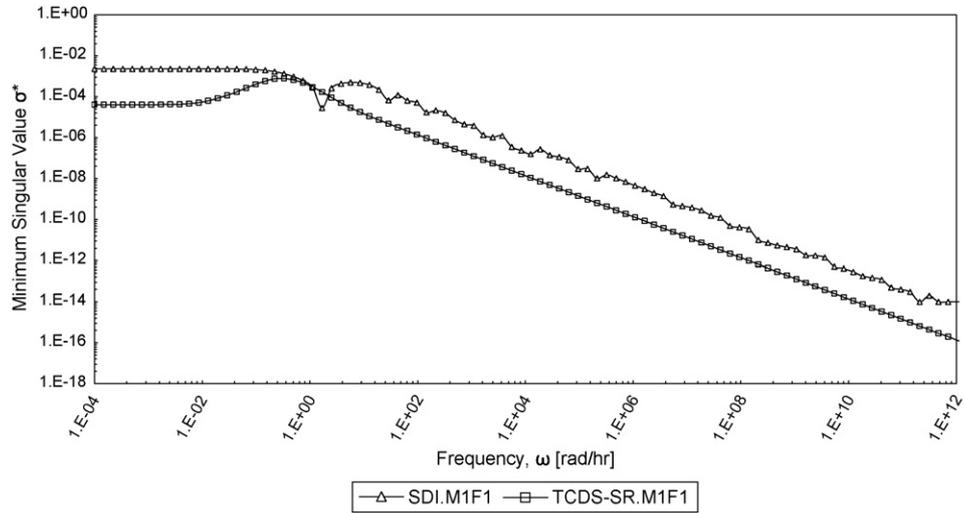
After optimum designs were obtained, open-loop dynamic simulations were carried out in Aspen Dynamics 11.1 in order to obtain the transfer function matrix. For the case of study considered here, Table 1 shows the transfer function matrix generated by using step

**Table 2**  
Transfer function matrix for SDI (M1, F1)

	R1	R2	Q1	Q2
$X_A$	$\frac{0.01e^{-0.05s}}{1 + 1.7776s}$	$\frac{0.0104e^{-0.05s}}{1 + 2.1516s}$	$\frac{2.9992}{1 + 0.6461s}$	$\frac{0.0104e^{-0.05s}}{1 + 2.2366s}$
$X_B$	$\frac{0.004}{1 + 0.7s} - \frac{0.0028}{1 + 1.6s}$	$\frac{0.004e^{-0.07s}}{1 + 0.75s} - \frac{0.0028}{1 + 2.1s}$	$\frac{1.572}{1 + 0.16s} - \frac{3.792}{1 + 1.8s}$	$-\frac{2.5708}{1.0946s^2 + 2.467s + 1}$
$X_{C1}$	$-\frac{0.0008e^{-0.27s}}{1 + 0.316s} + \frac{0.002}{1 + 4.545s}$	$-\frac{0.0008e^{-0.27s}}{1 + 0.5s} + \frac{0.002}{1 + 4.585s}$	$\frac{0.768}{1 + 0.136s} - \frac{0.4252}{1 + 0.237s}$	$-\frac{0.0008e^{-0.27s}}{1 + 0.38s} + \frac{0.002}{1 + 5.1s}$
$X_{C2}$	$\frac{0.006}{1 + 0.45s}$	$\frac{0.006}{1 + 0.18s}$	$\frac{2.9024}{1 + 1.1379s}$	$\frac{2.5908}{1 + 1.2157s}$

**Table 4**  
Transfer function matrix for SIS (M1, F1)

	R1	Q1	Q2	R2
<b>XA1</b>	$\frac{0.0068}{1 + 0.58 s}$	$\frac{1.8208}{1 + 0.4325 s}$	$\frac{0.0068}{1 + 0.4325 s}$	$\frac{0.0064}{1 + 0.4582 s}$
<b>XB</b>	$\frac{0.0152 e^{-0.09 s}}{1 + 1.1 s} + \frac{0.01}{1 + 2.8 s}$	$\frac{0.6224}{1 + 0.1162 s} - \frac{4.6532}{1 + 1.974 s}$	$\frac{1.1616}{1 + 0.623 s}$	$\frac{0.0152 e^{-0.09 s}}{1 + 1.1 s} + \frac{0.01}{1 + 2.8 s}$
<b>XC</b>	$\frac{0.0216}{1 + 1.9932 s}$	$\frac{1.8784}{1 + 0.8506 s}$	$\frac{0.0204}{1 + 1.7208 s}$	$\frac{0.0228}{1 + 3.0401 s}$
<b>XA2</b>	$\frac{0.0428}{1 + 1.6074 s}$	$\frac{10.4832}{0.4904 s^2 + 1.4807 s + 1}$	$\frac{3.5908}{0.2799 s^2 + 1.0999 s + 1}$	$\frac{0.0436}{1 + 1.9172 s}$

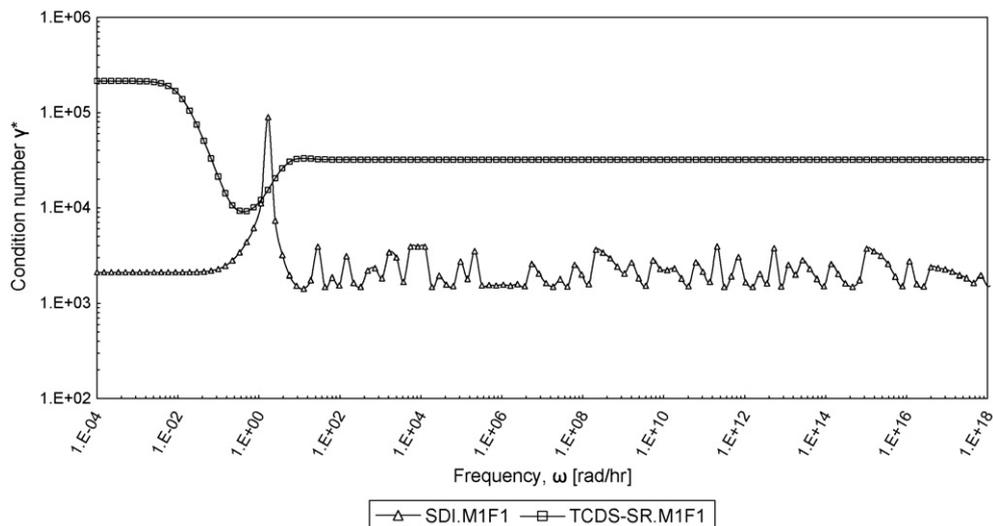


**Fig. 7.** Minimum singular value TCDS–SR and SDI (M1, F1).

changes in the manipulated variable and recording the dynamic behavior of the three product compositions (A–C). The transfer function matrix shown in Table 1 corresponds to TCDS–SR (M1 F1). It can be observed that dynamic responses can be adjusted to first order or parallel processes. Table 2 shows the transfer function matrix for the SDI (M1 F1). Similar transfer function matrices can

be obtained for TCDS–SS and SIS (Tables 3 and 4; M1 F1) and for all cases of study.

For the case of study of TCDS–SR and SDI, we obtained the following results: for the case M1 F1 (Figs. 7 and 8), the SDI arrangement presents higher values of the minimum singular value and lower condition number for the entire frequency range; therefore,



**Fig. 8.** Condition number TCDS–SR and SDI, M1, F1.

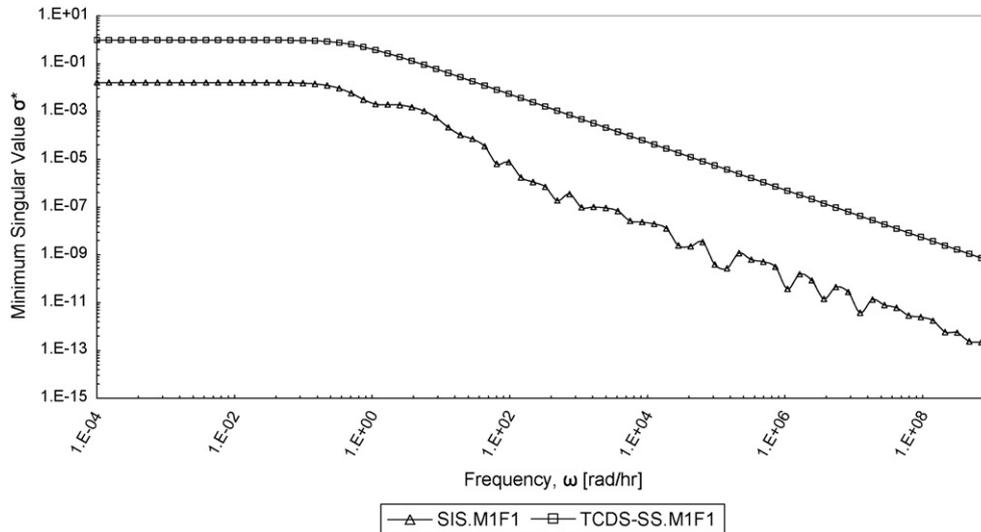


Fig. 9. Minimum singular value TCDS-S and SIS (M1, F1).

it can be expected that the SDI system will exhibit better control properties than the other sequence under feedback control, and is better conditioned to the effect of disturbances than the other distillation scheme. Figs. 9 and 10 show the minimum singular value and condition number for the case of study M1 F1. The TCDS-SS presents higher values of  $\sigma^*$  and lower values of condition number for the entire frequency range. Therefore, the TCDS-SS is expected to require less effort control under feedback operation and is better conditioned to the effect of disturbances than the SIS scheme. For the case of M2 F1, Figs. 11 and 12 show that at low frequencies TCDS-SR exhibits higher values of  $\sigma^*$  than the other scheme, but as the frequency increases, the minimum singular value decreases drastically, and SDI offers the best values for this parameter. In the case of the number condition, TCDS-SR shows the lowest values at low frequencies. In general, we can say that TCDS-SR offers better conditioning properties for model uncertainties and process disturbances than the other arrangement at low frequencies. According to SVD (Figs. 13 and 14) for the case of M2 F1, TCDS-SS shows better control properties than SIS, because that scheme presents lower values for condition number and similar minimum singular values in comparison with the SIS arrangement.

Figs. 15 and 16 show  $\sigma^*$  and condition number for the case of M3F1. SDI has the highest values of  $\sigma^*$  and the lowest condition number for the entire frequency range when compared to TCDS-SR. SDI is, therefore, better conditioned to the effect of disturbances. Similar results can be obtained for other cases of study. In general, it can be concluded that SDI presents better control properties than TCDS-SR. The results indicate that a reduction in the number of interconnections of the alternate configuration provides an improvement in controllability properties.

In the case of M3 F1 (Figs. 17 and 18), TCDS-SS seems to be the best choice because it has the highest values of  $\sigma^*$  and the lowest condition number at low frequencies when compared to the SIS arrangement. Similar results can be obtained for other cases of study. In general, it can be concluded that TCDS-SS presents better control properties than SIS. The results indicate that a reduction in the number of interconnections of the alternate configuration does not necessarily provide an improvement in controllability properties.

Based on the trends observed, a distinction is seen between the best control option for TCDS-SR and TCDS-SS with their alternate schemes, respectively. In the case of TCDS-SR and SDI, the

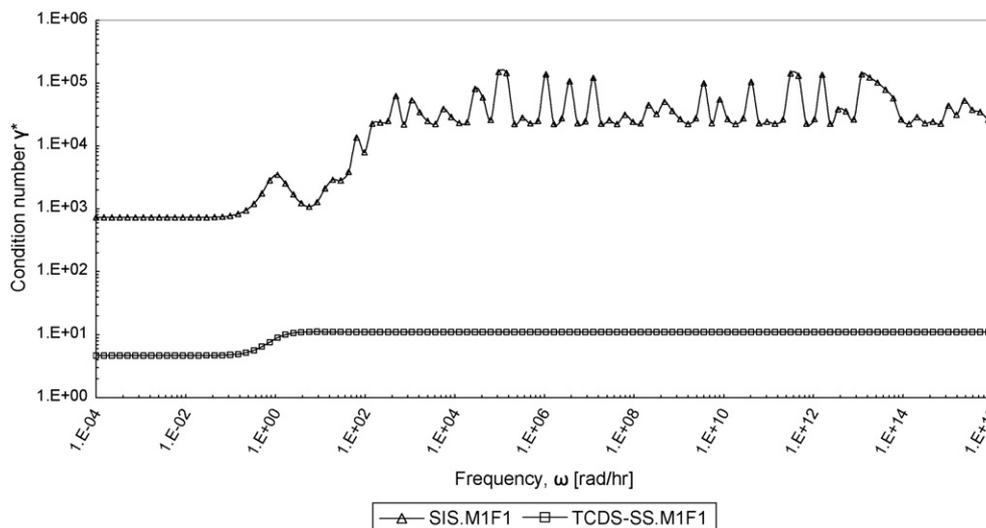


Fig. 10. Condition number TCDS-SS and SIS (M1, F1).

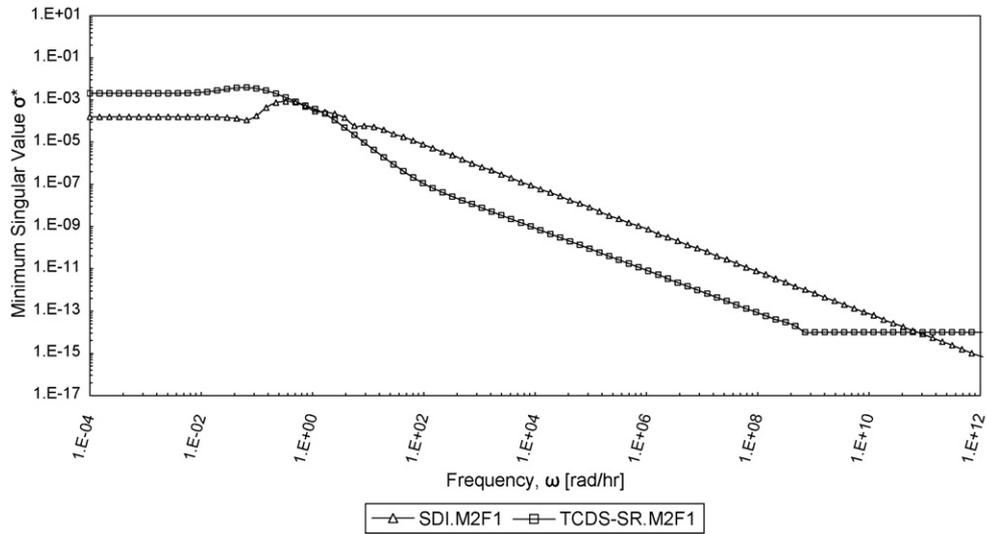


Fig. 11. Minimum singular value TCDS–SR and SDI (M2, F1).

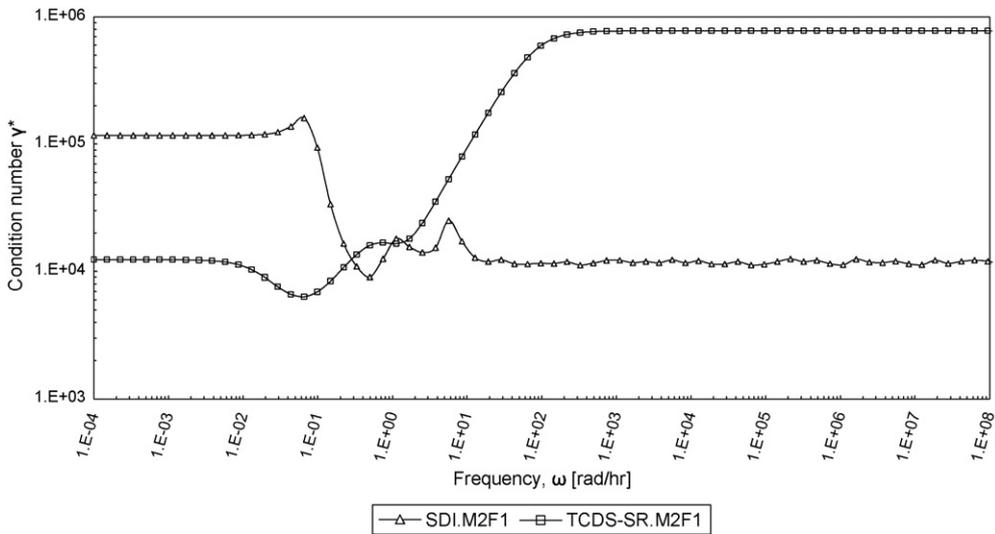


Fig. 12. Condition number TCDS–SR and SDI (M2, F1).

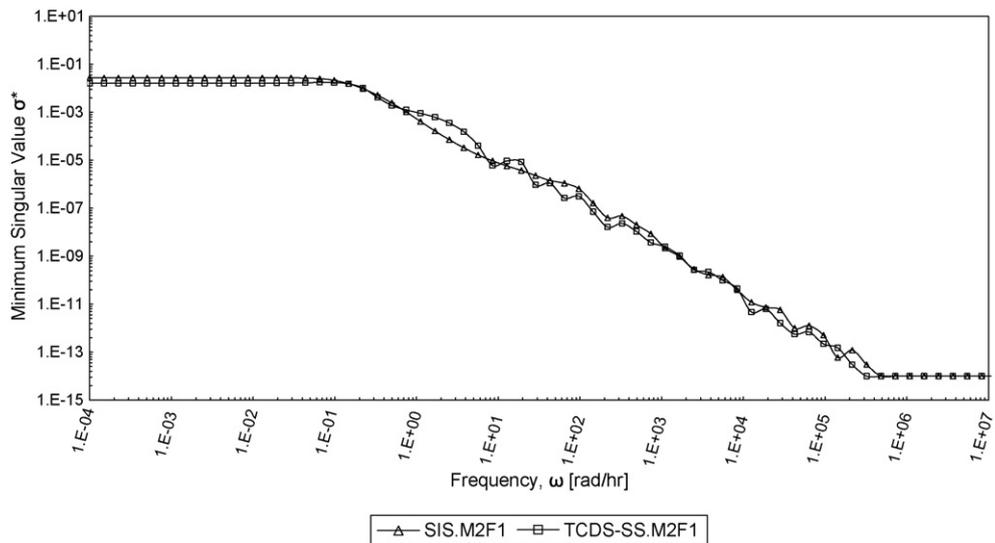


Fig. 13. Minimum singular value TCDS–SS and SIS (M2, F1).

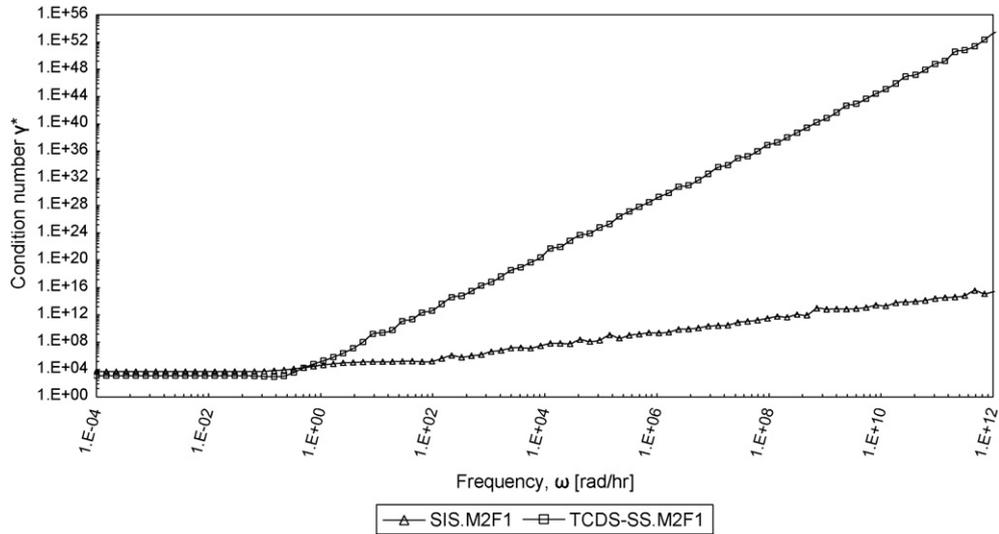


Fig. 14. Condition number TCDS-SS and SIS (M2, F1).

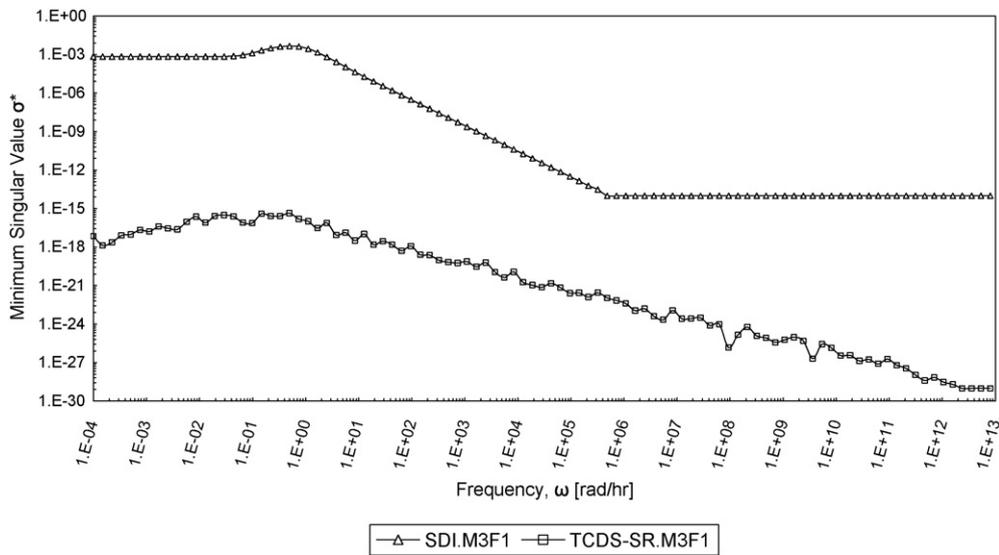


Fig. 15. Minimum singular value TCDS-SR and SDI (M3, F1).

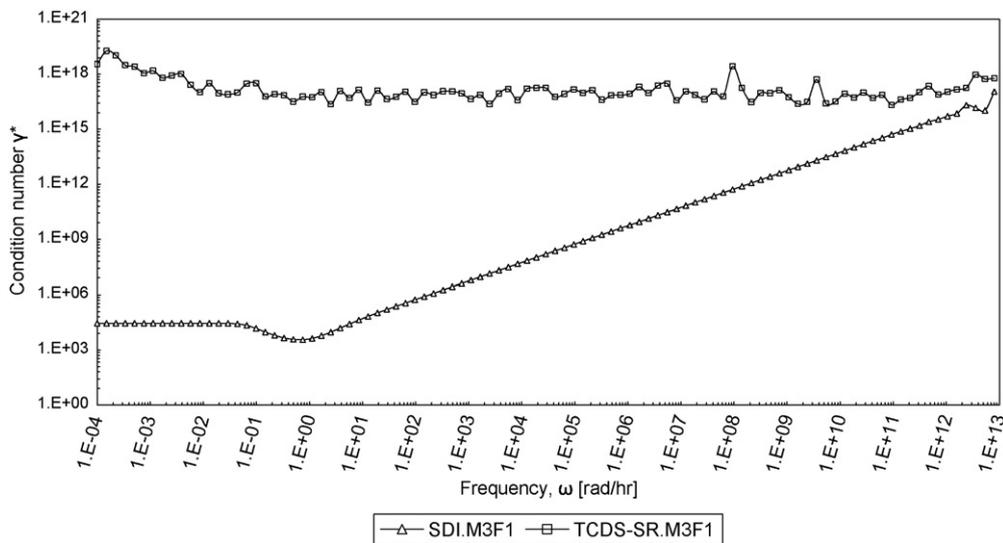


Fig. 16. Condition number TCDS-SR and SDI (M3, F1).

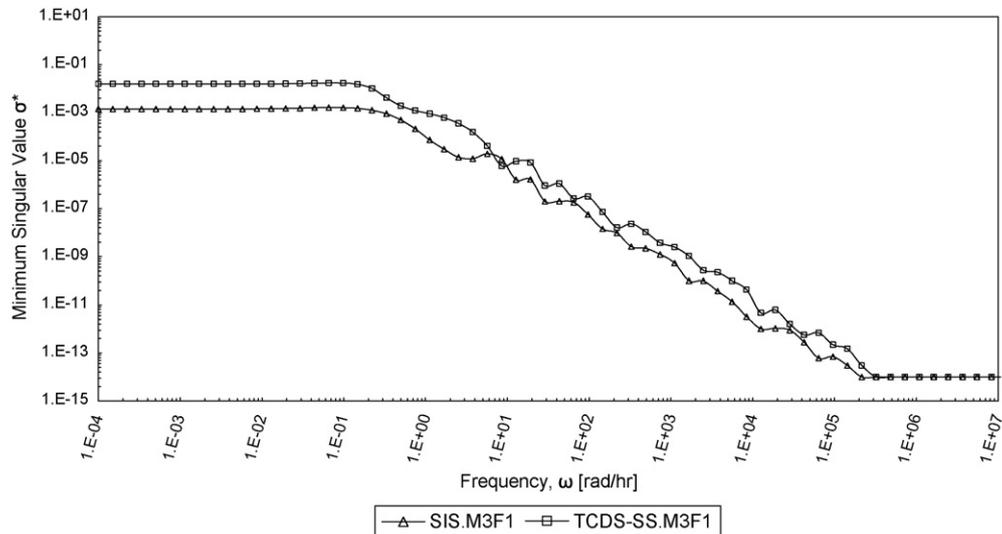


Fig. 17. Minimum singular value TCDS–SS and SIS (M3, F1).

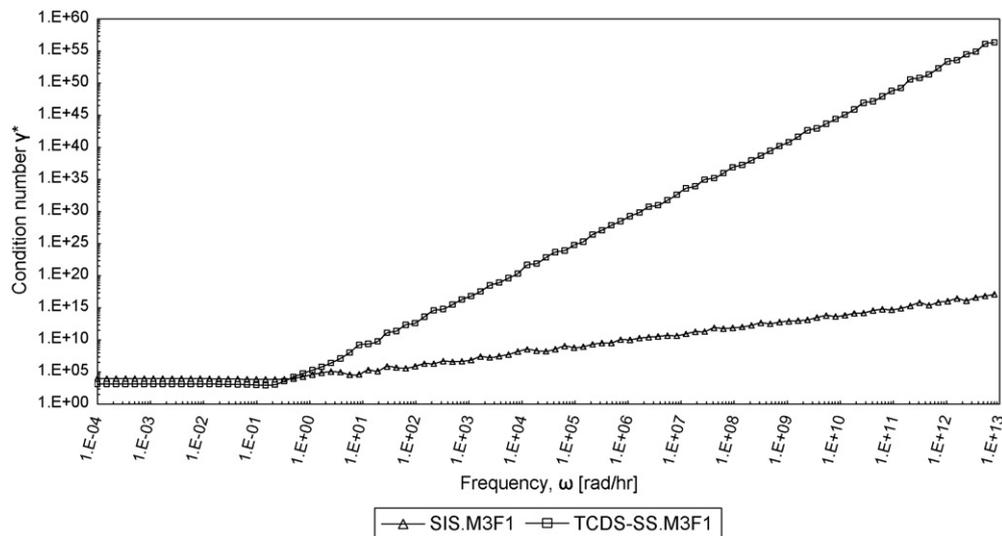


Fig. 18. Condition number TCDS–SS and SIS (M3, F1).

alternate structure has better control properties; for TCDS–SS and SIS options, the arrangement with thermal coupling is expected to require less control efforts under feedback operation. A remark on structures can be established. When B component is obtained as distillate product (TCDS–SR or SDI) the better structure is with reduction in the number of interconnections. When B component is obtained as bottoms product (TCDS–SS or SIS) the better structure is without reduction in the number of interconnections. Finally, to complement the study of theoretical control properties, closed-loop dynamic responses under the action of some specific controller are required in order to determine potential control problems such as saturation of control valves, because it is expected that the presence of recycle streams might contribute to the attenuation of the effect of disturbances in some cases (Alatiqi & Luyben, 1986).

## 7. Conclusions

An analysis of control properties of two distillation sequences that arise from modifications to thermally coupled systems with side columns has been presented. Results from singular value decomposition indicate, in general, that the SDI system is bet-

ter than the TCDS–SR, and the TCDS–SS is better than the SIS scheme. The results from theoretical control properties indicate that a reduction in the number of interconnections does not necessarily provide the operational advantages originally expected given the resulting, simpler, structural design. The results also suggest that control properties are governed by the position where B component is obtained in the scheme (top or bottom): when B component is obtained as distillate product (TCDS–SR or SDI) the better structure is with reduction in the number of interconnections. When B component is obtained as bottoms product (TCDS–SS or SIS) the better structure is without reduction in the number of interconnections. In general, it is apparent that the presence of recycle streams, instead of deteriorating the dynamic behavior of separation sequences, may contribute positively to their dynamic properties. This situation depends on structure and the position where B component is obtained in the arrangement.

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