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A PARAMETRIC TRANSFER FUNCTION MATRIX FOR PACKED BINARY
DISTILLATION COLUMNS HAVING UNEQUAL VAPOUR AND LIQUID CAPACITANCE

by

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SUMMARY

A general transfer function matrix (T.F.M) has been derived for symmetrically built packed distillation columns, separating ideal binary mixtures. This T.F.M is used to assess the adequacy of assuming zero vapour hold-up in the model and also, as previously proposed by the authors^{1,2,3}, of setting the ratio of vapour to liquid hold-ups to unity for predicting the dynamics of a general system.

The analytical results are substantiated in frequency domain . It is noted that variations in the ratio of vapour to liquid hold-ups do not greatly influence the general dynamics of packed columns and that when this ratio is set to unity, the resulting simple model proposed by us, may adequately be used for the purpose of dynamic analysis and controller design.

1. Introduction

Previous analysis^{1,2,3} has produced precise, parametric transfer function matrices for symmetrically - built packed distillation columns separating ideal mixtures in extreme cases when the ratio of vapour hold-up to that of liquid in a subsection of the column is taken as unity and zero. Clearly either of the two situations represent limiting conditions of a typical case. While for tray columns, due to large liquid hold-ups retained on the trays, the ratio of vapour to liquid hold-ups may reasonably be taken as zero, in the case of an equivalent packed tower effecting the same amount of separation, such assumption may be considerably removed from reality. Practical reports⁴ indicate a reduction of around 75% of liquid hold-up in the packed columns in a common situation.

In this report a transfer function matrix (T.F.M.) of the model is derived in the general case when no assumption is made on the numerical value of the vapour to liquid hold-up ratio. The T.F.M., besides providing a more accurate description of the process dynamics for the purpose of analysis, model approximation, controller design, etc., provides a basis for comparisons between the potentials of the two above mentioned special cases in representing the dynamics of a general case.

The results show that either of the special cases result in substantially similar frequency response to that obtained for a given general case. But the case in which the ratio of vapour to liquid capacitance is assumed to be unity is more on the safe side and easier to use for controller design.

2. Derivation of the General T.F.M.

The linearized model of the system, when the equilibrium curve is approximated by straight lines of slopes α and $1/\alpha$, where α is the mixture relative volatility, is

$$\begin{cases} c \partial y / \partial \tau - \partial y / \partial h + Gv/V = y_e - y \\ - \partial y_e / \partial \tau - \partial y_e / \partial h + \alpha G \ell / V = y_e - y \\ - \partial x' / \partial \tau + \partial x' / \partial h + G \ell / V = x' - x'_e \\ c \partial x'_e / \partial \tau + \partial x'_e / \partial h + \alpha Gv/V = x' - x'_e \end{cases} \quad (1)$$

where y and x' denote small disturbances in vapour and liquid compositions in the rectifier and stripper respectively, y_e and x'_e their associated equilibrium values, v and ℓ are the perturbations in the internal vapour and liquid rates and c is the ratio of rectifier-vapour to stripper liquid hold-up (= stripper-vapour/rectifier liquid hold-up). As discussed in 1, 2 and 3, symmetry in structure demands equal packing length in both sections of the tower and the overall mass-transfer coefficient in terms of vapour composition driving force in the rectifier to be equal to that in terms of liquid composition in the stripper. The variables h and τ define normalised length and time

$$\tau = t k / H'_\ell \quad \text{and} \quad h = h' k / V$$

where H'_ℓ is the stripper liquid hold-up per unit length, k is the overall mass-transfer coefficient, V is the vapour rate in rectifier, h' represents the distance as measured from an origin at the ends of the tower, bent into a conceptual u-tube. The parameter G denotes the normalised composition gradient in steady state and t is the actual time.

None of the assumptions made in the development of the model is unusual and have already been used by a number of authors, for example 5,6,7 and 8.

The boundary conditions at feed point and top and bottom of the column are

$$\begin{cases} y(L) = x'_e(L) - \epsilon Gv/2V \\ x'(L) = y_e(L) + \epsilon G\ell/2V \end{cases} \quad \text{at feed} \quad (2)$$

$$\begin{cases} \alpha T \frac{dy_e(o)}{d\tau} = y(o) - \alpha y_e(o) \\ \alpha T \frac{dx'_e(o)}{d\tau} = x'(o) - \alpha x'_e(o) \end{cases} \quad \text{at top and bottom} \quad (3)$$

In (2) and (3), $\epsilon = \alpha - 1$, L is the 'length' of a subsection and T is the hold-up at condenser and reboiler.

Taking a Laplace transform in time, the equations of the model can be written as follows

$$\begin{pmatrix} cp + 1 - d \\ 1 \end{pmatrix} \tilde{y} + \begin{pmatrix} -1 \\ -p - 1 - d \end{pmatrix} \tilde{y}_e = -\frac{G}{V} \begin{pmatrix} \tilde{v} \\ \alpha \tilde{l} \end{pmatrix} \quad (3)$$

$$\begin{pmatrix} cp + 1 + d \\ 1 \end{pmatrix} \tilde{x} + \begin{pmatrix} -1 \\ -p - 1 + d \end{pmatrix} \tilde{x}_e = -\frac{G}{V} \begin{pmatrix} \tilde{l} \\ \alpha \tilde{v} \end{pmatrix} \quad (4)$$

where the superscript \sim is used to indicate transformed variables, p denotes the Laplace's variable and d is an operator representing differentiation w.r.t. length. The characteristic equation of the simultaneous ordinary differential equations (4) is

$$s^2 - (1-c)ps - (1 + c + cp)p = 0$$

The roots of which are:

$$s_{1,2} = \frac{(1-c)p \pm \sqrt{(1-c)^2 p^2 + 4(1+c+cp)p}}{2}$$

Defining the variables P and q as follows

$$P = \frac{1-c}{2} p \text{ and } q = \sqrt{(1+c) p (4+p+cp) / 4} \quad (5)$$

then

$$s_{1,2} = P \pm q \quad (6)$$

The roots of the characteristic equation of (3) may easily be found to be $-s_{1,2}$.

Therefore the general solution of (3) and (4) may be written as

$$\begin{cases} \tilde{y} = E_1 e^{-s_2 h} + E_2 e^{-s_1 h} + i_1 & (a) \\ \tilde{y}_e = I_1 e^{-s_2 h} + I_2 e^{-s_1 h} + i_2 & (b) \\ \tilde{x}' = J_1 e^{s_1 h} + J_2 e^{s_2 h} + i_3 & (c) \\ \tilde{x}'_e = K_1 e^{s_1 h} + K_2 e^{s_2 h} + i_4 & (d) \end{cases} \quad (7)$$

where $E_1(2), I_1(2), J_1(2)$ and $K_1(2)$ are arbitrary functions of p and i_1 to i_4 are the particular integrals of the solution for each dependant variable, easily obtainable as

$$i_1 = -\frac{(1+p)\tilde{v}-\alpha\tilde{\ell}}{(1+c+cp)p}, i_2 = -\frac{\tilde{v}-(1+cp)\alpha\tilde{\ell}}{(1+c+cp)p}, i_3 = -\frac{\alpha\tilde{v}-(1+cp)\tilde{\ell}}{(1+c+cp)p} \text{ and } i_4 = -\frac{(1+p)\alpha\tilde{v}-\tilde{\ell}}{(1+c+cp)} \quad (8)$$

Clearly (from (3) and (4)) the arbitrary functions of (7) are related to each other and four of them are defined in terms of the others. The necessary relations between arbitrary functions are obtained noting that (1) should be identically satisfied by (7). Substituting from (7-c) and (7-d) into the second equation of (4)

$$\begin{cases} K_1 = (1+p-s_1)J_1 \\ K_2 = (1+p-s_2)J_2 \end{cases} \quad (9)$$

Similarly substituting from (7-a) and (7-b) into the first equation of (3)

$$\begin{cases} I_1 = (1+cp+s_2)E_1 \\ I_2 = (1+cp+s_1)E_2 \end{cases} \quad (10)$$

Using (5) it is crucial to note that

$$\begin{cases} 1+p-s_1 = 1+cp+s_2 \\ 1+p-s_2 = 1+cp+s_1 \end{cases} \quad (11)$$

Using (6), (9), (10) and (11) the general solution (7) may be written as:

$$\begin{cases} \tilde{y} = e^{-Ph} [E_1 e^{qh} + E_2 e^{-qh}] + i_1 \\ \tilde{y}_e = e^{-Ph} \left[\left(\frac{2+p+cp}{2} - q \right) E_1 e^{qh} + \left(\frac{2+p+cp}{2} + q \right) E_2 e^{-qh} \right] + i_2 \\ \tilde{x}' = e^{Ph} [J_1 e^{qh} + J_2 e^{-qh}] + i_3 \\ \tilde{x}'_e = e^{Ph} \left[\left(\frac{2+p+cp}{2} - q \right) J_1 e^{qh} + \left(\frac{2+p+cp}{2} + q \right) J_2 e^{-qh} \right] + i_4 \end{cases} \quad (12)$$

The boundary condition equations when transformed can be written as

$$\text{Feed: } \begin{cases} \tilde{y}(L,p) = \tilde{x}'_e(L,p) - \epsilon G\tilde{v}/2V \\ \tilde{x}(L,p) = \tilde{y}_e(L,p) + \epsilon G\tilde{\ell}/2V \end{cases} \quad (13)$$

$$\text{Top and } \begin{cases} \alpha^{-1} h_e \tilde{y}(0,p) = \tilde{y}_e(0,p) \end{cases} \quad (15)$$

$$\text{bottom } \begin{cases} \alpha^{-1} h_e \tilde{x}'(0,p) = \tilde{x}'_e(0,p) \end{cases} \quad (16)$$

The considerable resemblance between the first and the second pair of equations (12) is worth noting. Unfortunately the dependance of composition variables of each subsection of the column to those of the other at the feed boundary places an awkward barrier in the way of using this similarity by fitting the equations (12) to (13) - (16) in pairs. However, if we add and subtract the equations (13) and (14) and also the equations (15) and (16), denoting vectors \underline{q} , \underline{r} and \underline{u} as:

$$\underline{q} = \begin{pmatrix} \tilde{y}-\tilde{x}' \\ \tilde{y}+\tilde{x}' \end{pmatrix}, \underline{r} = \begin{pmatrix} \tilde{y}_e-\tilde{x}'_e \\ \tilde{y}_e+\tilde{x}'_e \end{pmatrix} \quad (a)$$

and

$$\underline{u} = \frac{G}{V} \begin{pmatrix} \tilde{v} + \tilde{l} \\ \tilde{v} - \tilde{l} \end{pmatrix} \quad (b)$$

the equations of the boundary conditions can be written as

$$\text{Feed: } \begin{cases} q_1(L,p) = -r_1(L,p) - \epsilon u_1/2 \\ q_2(L,p) = r_2(L,p) - \epsilon u_2/2 \end{cases} \quad (18)$$

$$\begin{array}{l} \text{Top and} \\ \text{bottom} \end{array} \begin{cases} \alpha^{-1} h_e q_1(o,p) = r_1(o,p) \\ \alpha^{-1} h_e q_2(o,p) = r_2(o,p) \end{cases} \quad (19)$$

in which the first row of equations are independent of the second. Now the above mentioned similarities in the equations (12) allow the alternative variables given in (17) to be substituted therein without the penalty of excessive complication. The resulting equations, although no longer possessing the property of (12), are somewhat simpler to fit to (18) and (19) than it is to fit (12) to (13) - (16). They may be written as

$$\left\{ \begin{array}{l} A_2 = q_1(o,p) -i_1 + i_3 \\ B_2 = q_1(o,p) \left[\frac{2+p+cp}{2} - \alpha^{-1} h_e \right] / q + \frac{2+p+cp}{2q} (i_3 - i_1) + \frac{i_2 - i_4}{q} \\ A_1 = q_2(o,p) - i_1 - i_3 \\ B_1 = q_2(o,p) \left[\frac{2+p+cp}{2} - \alpha^{-1} h_e \right] / q - \frac{2+p+cp}{2q} (i_1 + i_3) + \frac{i_2 + i_4}{q} \end{array} \right. \quad (22)$$

Substituting from (22) into (21) and using (8) and (17b) after some lengthy algebra, not appropriate for inclusion, the vector $\underline{q}(o,p)$ can be obtained as

$$\underline{q}(o,p) = \frac{1}{1+c+cp} \underbrace{\begin{pmatrix} \cosh(PL) g'_{11} + \sinh(PL) g'_{21} & \cosh(PL) g'_{12} + \sinh(PL) g'_{22} \\ \sinh(PL) g'_{11} + \cosh(PL) g'_{21} & \sinh(PL) g'_{12} + \cosh(PL) g'_{22} \end{pmatrix}}_{G(p)} \cdot \underline{u} \quad (23)$$

where

$$g'_{11} = \left\{ (1+c) \cosh(qL) \left[\left(\epsilon + \frac{\alpha-c}{2} p \right) e^{PL} + \left(\epsilon - \frac{1-c\alpha}{2} p \right) e^{-PL} \right] - q \sinh(qL) \left[(\alpha+c) e^{PL} + (1+c\alpha) e^{-PL} \right] - \epsilon(1+c) \left[2 + (1+c + \frac{cp}{2}) p \right] \right\} / R$$

$$g'_{21} = \left\{ -(1+c) \sinh(qL) \left[\left(\epsilon + \frac{\alpha-c}{2} p \right) e^{PL} - \left(\epsilon - \frac{1-c\alpha}{2} p \right) e^{-PL} \right] + q \cosh(qL) \left[(\alpha+c) e^{PL} - (1+c\alpha) e^{-PL} \right] - \epsilon(1-c) q \right\} / S$$

$$g'_{12} = \left\{ (1+c) \cosh(qL) \left[\left(1+\alpha + \frac{\alpha+c}{2} p \right) e^{PL} - \left(1+\alpha + \frac{1+c\alpha}{2} p \right) e^{-PL} \right] - q \sinh(qL) \left[(\alpha-c) e^{PL} + (1-c\alpha) e^{-PL} \right] - \epsilon \frac{1-c}{2} p \right\} / R$$

$$g'_{22} = \left\{ -(1+c) \sinh(qL) \left[\left(1+\alpha + \frac{\alpha+c}{2} p \right) e^{PL} + \left(1+\alpha + \frac{1+c}{2} p \right) e^{-PL} \right] + q \cosh(qL) \left[(\alpha-c) e^{PL} - (1-c\alpha) e^{-PL} \right] - 2\epsilon q \left(1+c + \frac{cp}{2} \right) \right\} / S$$

$$R = (1+c) p (1+\alpha^{-1} h_e) \cosh(qL) + 2q (1-\alpha^{-1} h_e) \sinh(qL)$$

$$S = (1+c) p (1+\alpha^{-1} h_e) \sinh(qL) + 2q (1-\alpha^{-1} h_e) \cosh(qL)$$

and as given before

$$P = \frac{1-c}{2} p \quad \text{and} \quad q = \sqrt{(1+c)p(4+c+cp)/4}$$

An outstanding property of $G(p)$ is that when $c = 1$, g'_{21} and g'_{12} vanish. Consequently from (23) clearly the systems T.F.M., $G(p)$, becomes diagonal. The elements of which are simply

$$g_1(p) = \frac{\{(\alpha-1) [\cosh(qL) - 1] p^{-1} - (1+\alpha) \sinh(qL) q^{-1} - \epsilon/2\}}{\{(1+\alpha^{-1} h_e^{-1}) \cosh(qL) + \alpha p^{-1} (1-\alpha^{-1} h_e^{-1}) \sinh(qL)\}}$$

and

$$g_2(p) = \frac{\{(\alpha-1) p (\cosh qL - 1) q^{-2} - (1+\alpha) \sinh(qL) q^{-1} - \epsilon/2\}}{\{(1+h_e^{-1}) \sinh(qL) p q^{-1} + (1-h_e^{-1}) \cosh(qL)\}}$$

3. Zero - and High - Frequency Behaviour

There is of course much information about the system dynamics which can be obtained from the behaviour of the system at zero frequency and high frequencies. Because the model is a hyperbolic system of partial differential equations, any significant wave phenomena will be predicted by analysis of the system behaviour in the high frequency region.

3.1 Zero Frequency Behaviour

At zero frequency it can easily be observed that, similar to the case of unity c , g'_{12} and g'_{21} in (23) again vanish and therefore $G(p)$ becomes diagonal, the elements of which are

$$g_1(0) = \frac{\alpha\{(\alpha-1)L^2 - (1+\alpha)L - \epsilon/2\}}{2(\alpha-1)L + 1 + \alpha}$$

and

$$g_2(0) = - \frac{\alpha\{1+\alpha\}L + \epsilon/2}{(\alpha-1)}$$

3.2 The High-Frequency asymptote of the T.F.M.

The variable q can be written as

$$q = \sqrt{(1+c)p(4+p+cp)/4} = \frac{(1+c)p}{2} \left[1 + \frac{4}{(1+c)p} \right]^{\frac{1}{2}}$$

which at high frequencies approach

$$q \underset{p \rightarrow \infty}{\approx} 1 + \frac{1+c}{2} p$$

If now both numerators and denominators of $g'_{11}, g'_{12}, g'_{21}, g'_{22}$ are multiplied by $2e^{-qL}$, in the resulting $1 \pm e^{-qL}$ terms the exponential term compared to 1 can be neglected. This is because the modulus of the exponential term at high frequencies is nearly equal to e^{-2L} and when L is as small as 2 its value will be of the order 0.018 (when $L = 5$ it will be 0.00004). It is unlikely that for a subsection of column L , the N.T.U., is less than 2. Then after some algebraic operations the elements of G can be derived as

$$g_{11} \underset{p \rightarrow \infty}{(o,p)} = \frac{-2(1+c) - \epsilon(3+c+cp)e^{-L}e^{-cpL} - \epsilon(1+3c+cp)e^{-L}e^{-pL}}{4[1+c+c/(1+c)+cp]} \quad (24)$$

$$g_{21} \underset{p \rightarrow \infty}{(o,p)} = \frac{-2(1-c) - \epsilon(3+c+cp)e^{-L}e^{-cpL} + \epsilon(1+3c+cp)e^{-L}e^{-pL}}{4[1+c+c/(1+c)+cp]} \quad (25)$$

$$g_{12} \underset{p \rightarrow \infty}{(o,p)} = \frac{-2(1-c) - \epsilon[3+c+2c/(1+c)+cp]e^{-L}e^{-cpL} + \epsilon[1+3c+2c/(1+c)+cp]e^{-L}e^{-pL}}{4[1+c+c/(1+c)+cp]} \quad (26)$$

$$g_{22} \underset{p \rightarrow \infty}{(o,p)} = \frac{-2(1+c) - \epsilon[3+c+2c/(1+c)+cp]e^{-L}e^{-cpL} - \epsilon[1+3c+2c/(1+c)+cp]e^{-L}e^{-pL}}{4[1+c+c/(1+c)+cp]} \quad (27)$$

From the above equations it is clear that at high frequencies the system response contains two waves both of initial amplitude $\frac{\epsilon}{4} e^{-L}$ but one is delayed with respect to the other by $L(1-c)$ units of normalised time.

From (25) - (27) it is clear that the rational part of the two diagonal elements, i.e. (24) and (27), dominate those of the off diagonals, i.e. (25) and (26), unless c is set to zero. Also as the term $-2(1+c)$ is evidently always much greater than the amplitudes of both waves it can be concluded that at high frequencies $G(p)$ is dominant.

When c is set to zero, from (24) to (27) it is clear that the system response is approximated by a proper T.F.M., not a strictly proper one.

This is clearly an undesirable property from the control point of view.

4. Computed Results and Discussion

The computed results presented in this section are solely discussed in the context of determination of the effect of parameter c on the system dynamics and comparison of the quality of predictions when c is set to zero and unity. Not attempt is made to discuss other properties of the parametric T.F.M. derived in section 2, i.e. $G(p)$ in (23). Such analysis is presented in full detail in (9).

As discussed at the end of section 2, when c is set to unity the system T.F.M. greatly simplifies and assumes a diagonal form. Setting c to zero does to a certain extent simplify the T.F.M., however compared to the unity case, the extent of simplification is less and it does not result in a diagonal form.

In section 3 it was shown that in general, when c is not equal to unity, the T.F.M. is diagonal at zero frequency and at high frequencies except when $c=0$. The existence of dominance at intermediate frequencies can be checked by plotting the Gershgorin circles on the loci of diagonal elements of the T.F.M. in the Nyquist diagrams. Figures (1) and (2) show the Nyquist diagrams of the elements $\hat{g}_{11}(j\omega)$ and $\hat{g}_{22}(j\omega)$ of the inverse T.F.M. for both $c=1$ and $c=0$ cases with row estimate Gershgorin circles on the loci of the latter case. The system parameters are $L=5$, $\epsilon=1$, $T=5$. As pointed out before, it is not expected that the T.F.M. when $c=0$ to sustain dominance at very high frequencies. But one could argue the validity of models derived for complex systems such as distillation columns in this region. A second point worth noting is the inclusion of the -1 point in the circles of the fig. (1). In general both $c=1$ and $c=0$ cases have very similar diagonal loci, but as the fig. (1) shows the latter case exhibits more gain margin and faster response.

Figures (3) and (4) show the Nyquist diagrams of the elements $\hat{g}_{11}(j\omega)$ and $\hat{g}_{22}(j\omega)$ of the inverse T.F.M. for the same system parameters but for $c=0.15$.

Bearing in mind the arguments so far on the dominance of the T.F.M. the system is row dominant at all frequencies. Notice that the -1 point is now excluded by the Gershgorin circles.

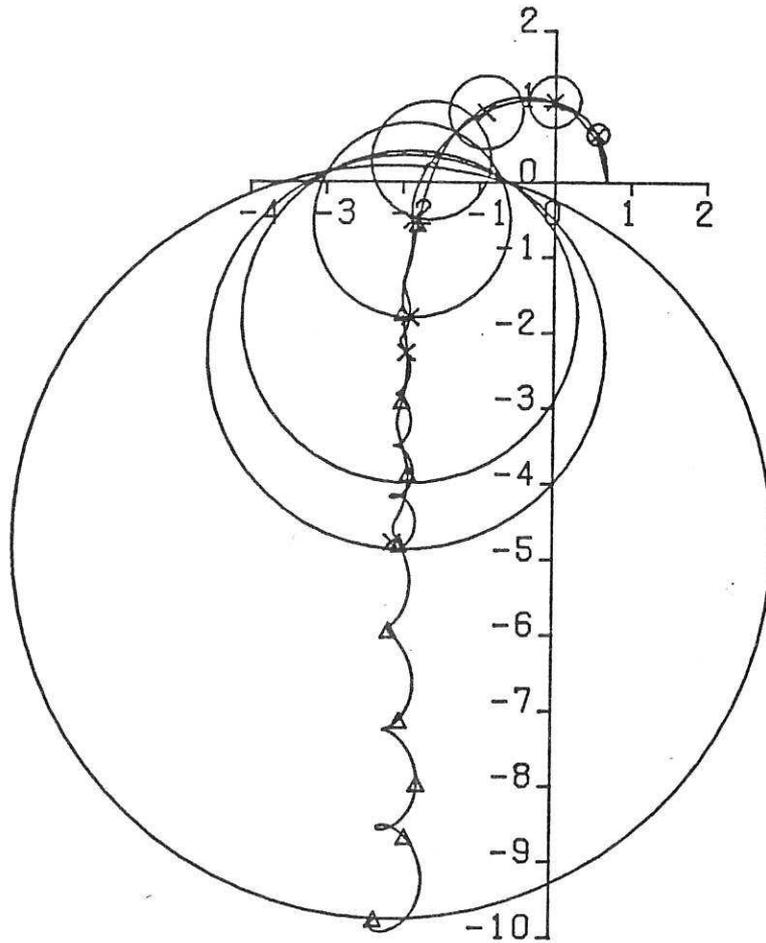
Figures (5) and (6) show the loci of $\hat{g}_{11}(j\omega)$ and $\hat{g}_{22}(j\omega)$ for the cases $c = 0.15$ and 1 . Clearly the loci of both figures are remarkably similar. The locus of $c=1$ case crosses the real axis to the right of that of $c=0.15$, hence it possesses a safe approximating property when used for controller design. Transportation delayed terms of high frequency behaviour have given rise to the lobes in loci of Nyquist diagrams shown in the Figures (1) to (6).

From what has been discussed, it is concluded that setting $c = 1$ in the model results in a simple diagonal transfer function matrix which with a high degree of robustness provides dynamic information on the general system and may more usefully be used for controller design compared to the T.F.M which results from setting $c = 0$.

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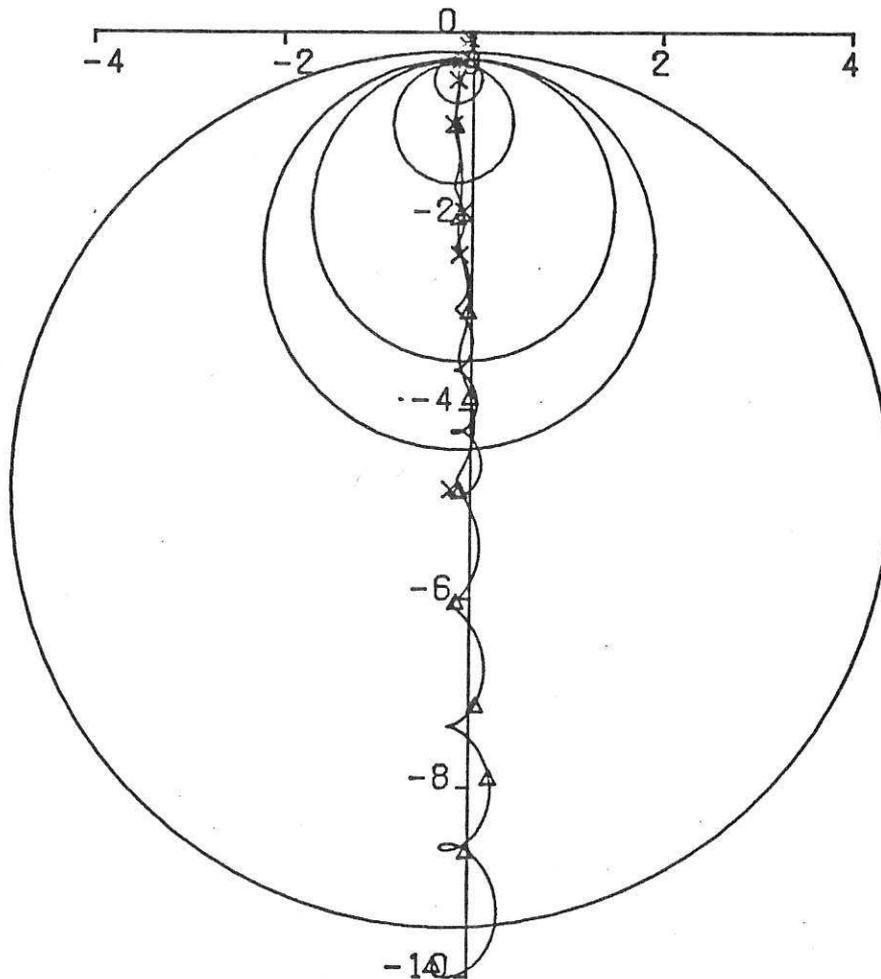
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$\Delta - \Delta$ $c = 1$, markings at frequencies of 1,2,3 10

$x - x$ $c = 0$, markings at frequencies of 0.1, 0.2,0.5,1,2,4,5,10.

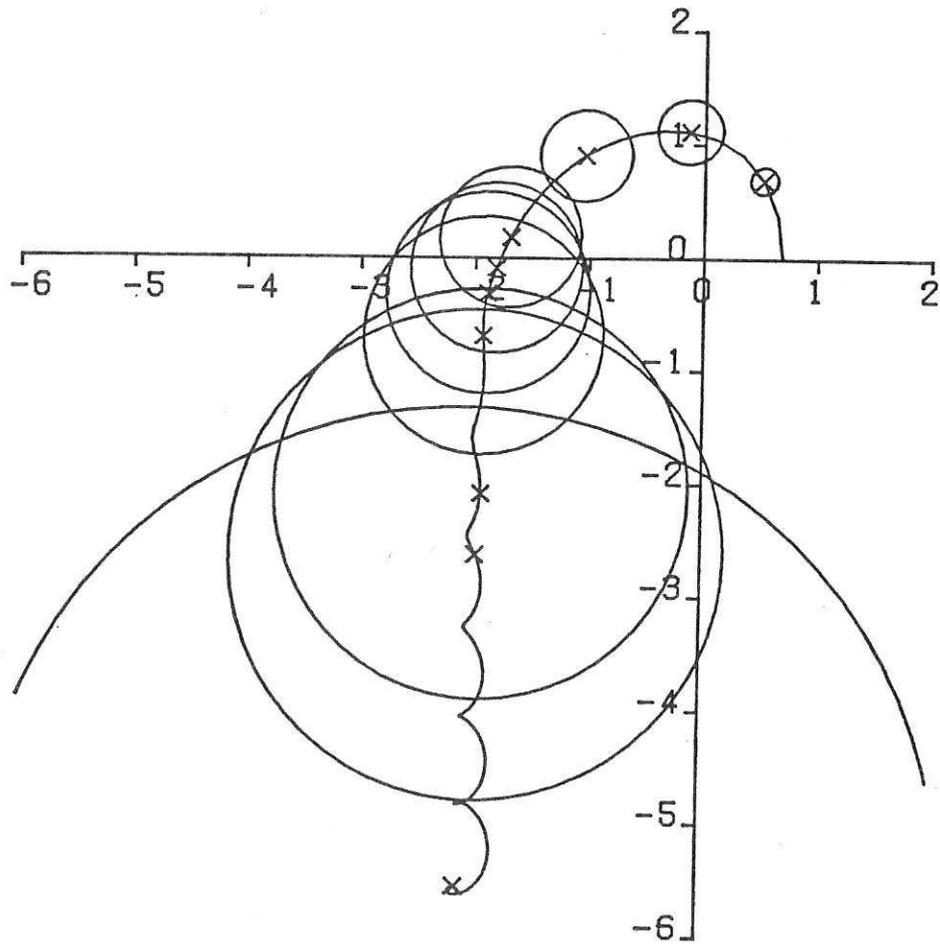
Fig. 1. Loci of $\hat{g}_{11}(j\omega)$ for $c = 1.0$ and for $c = 0.0$ with row estimate Gershgorin circles.



Δ - Δ c = 1 markings at frequencies of 1,2,3,... 10

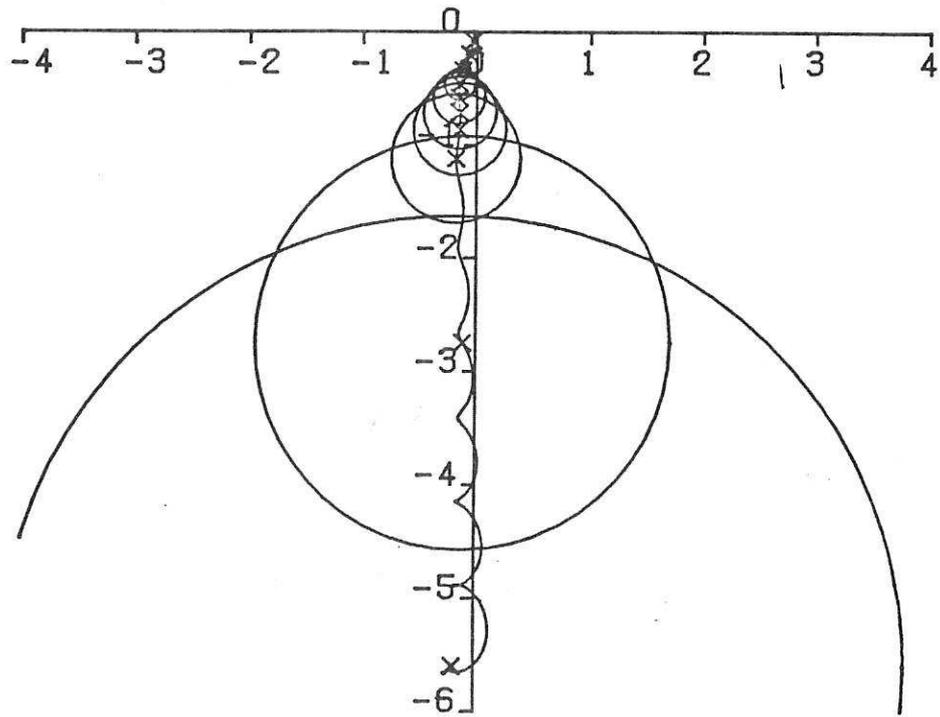
x - x c = 0 markings at frequencies of 0.1,0.2,0.5,1,2,4,5,10

Fig. 2 Loci of $\hat{g}_{22}(j\omega)$ for $c = 1.0$ and for $c = 0.0$ with row estimate Gershgorin circles.



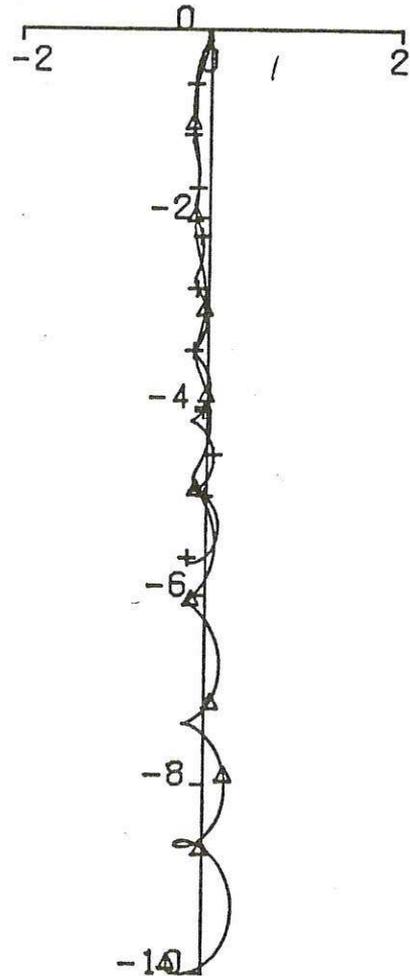
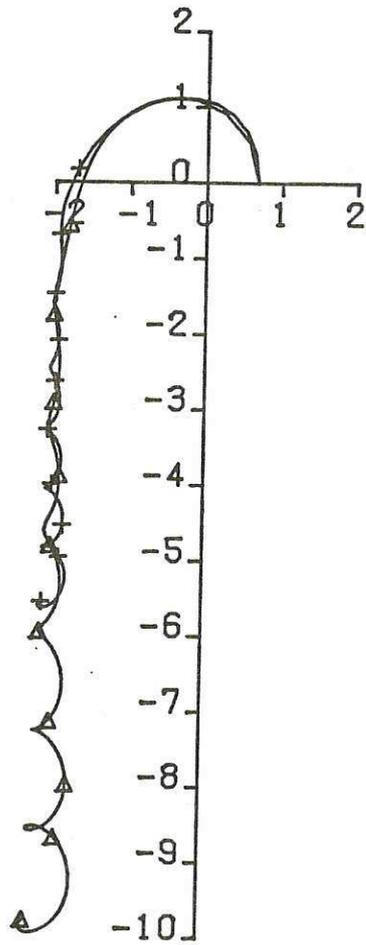
X markings at frequencies of 0.1,0.2,0.5,0.75,1,1.25,1.5,2,5,10

Fig. 3 Loci of $\hat{g}_{11}(j\omega)$ for $c = 0.15$ with row estimate Gershgorin circles



X markings at frequencies of 0.1,0.2,0.5,0.75,1,1.25,1.5,2,5,10.

Fig. 4. Loci of $\hat{g}_{22}(j\omega)$ for $c = 0.15$ with row estimate Gershgorin circles



$\Delta - \Delta - c = 1$

$\times - \times - c = 0.15$

markings at frequencies of 1,2,3,...10

Fig. 5 Loci of $\hat{g}_{11}(j\omega)$ for $c = 1$ and $c = 0.15$

Fig. 6 Loci of $\hat{g}_{22}(j\omega)$ for $c = 1$ and $c = 0.15$

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