

## Controllability Applications of Multicomponent Chemical Systems in Distillation Columns at High Purity Products

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### ABSTRACT

Controllability analysis of multicomponent chemical systems at high purity product distillation columns in steady-state modes are evaluated for the separation of five multicomponent chemical systems with multicomponent composition at 97 and 93 mol % product purity in order to obtain the best configuration between the controlled and manipulated variables based on steady-state control indices measurements. The following controllability indices are used to screen the best controllability features:- The Niederlinski index (NI), the Morari resiliency (MRI), the relative gain array (RGA) and the condition number (CN). This study proved that for many different chemical systems with different composition of distillation process and at a certain product purity there must be one common control structure which is found to be (D1-L2-B2) for 97% purity and (L1-L2-Q2) for 93 % purity showing the minimum interaction between control variables.

**Keywords:** controllability; steady-state; (NI); (MRI); (CN).

### 1. Introduction

A control mechanism is introduced that makes changes to the process in order to cancel out the negative impact of disturbances. To achieve this, instruments must be installed to measure the operational performance of the plant. These measurements could include temperature, pressure, flow rate, composition, level, pH, density and particle size. The low concentrations required of many environmentally significant compounds prior to discharge from a chemical plant have created a need for a new class of separation methods and have focused attention on many techniques that often have been ignored. In terms of operation it is important to identify the optimal way a system can be operated so that the product purity which is expecting is actually achieved. Most of the columns studied have had product purities that were low to moderate (0.1 to 5 mol % impurity). Very few papers consider the dynamics and control of high purity columns, despite of their industrial importance. Boyd (1975) used a double differential control scheme to maintain overhead purities of about 10 ppm in a benzene/ toluene/m-xylene separation. A highly nonlinear behavior was reported. The control problems with high-purity columns have been so severe that many process designers try to avoid making high-purity products out of both ends of a column simultaneously. It is a very common practice in the chemical industry to build two columns instead of one and to provide large intermediate tanks to handle recycle flows between these columns. Pure products are produced out of one end of each column. This practice increases both capital investment and energy costs. The steady state behavior was investigated by linear analysis and by digital simulation of a nonlinear mathematical mode. (Imter and ...) process disturbances such as feed rate, feed composition, product flow rates, or product compositions required for sizing of the relevant equipment as well as for the selection of control structure. Assali and McAvoy (2010) proposed an approach based on optimal control to define dominant measurements and manipulated variables. Jørgensen and Jørgensen (2000) suggested a special mixed integer linear programming (MILP) tied to Parseval's theorem combined with relative gain array (RGA) and internal model control (IMC) concepts. Chen et al. (2011) proposed a method based on IMC theory and optimization for designing Smith predictor in a multivariable process. The methodology of self-optimizing control (SOC) belongs to the third category mentioned above. This technique is thought to maintain the process working at its optimal state using linear combinations of measurements as CVs to reject disturbances effects. It is important to note that most of the aforementioned works reported the use of the classic relative gain array (RGA) (Bristol, 1966) for input-output pairing purposes which drives to a

decentralized control structure. In fact, several authors have analyzed the RGA properties, its implications on control performance, and its drawbacks when the process is ill-conditioned or close to the singularity (Grosdidier et al., 1985; Garcia and Morari, 1985; Skogestad and Morari, 1987; Skogestad and Postlethwaite, 2005). Other authors have proposed modifications to handle non-square processes (Chang and Yu, 1990; Khaki-Sedigh and Moaveni, 2009; Skogestad and Postlethwaite, 2005), disturbances (Chang and Yu, 1992, 1994; Lin et al., 2009) and dynamic information (McAvoy et al., 2003; He et al., 2009). A complete review and trends were given in Khaki-Sedigh and Moaveni (2009). In Yuan et al. (2011) was presented a technique for manipulated variables (MVs) selection, based on controllability for the multivariable chemical process. A criteria for measurements selection accounting only steady-state information and SOC was proposed in Hori et al. (2005) and Hori and Skogestad (2008). A systematic approach for MIMO controller design with different interaction levels was proposed in Shen et al. (2010) using the relative normalized gain array (RNGA) (He et al., 2009). All of these works demonstrate that multivariable control for chemical processes is still an open research field. The continuous emergence of new strategies is a clear demonstration of this issue. The recently appeared minimum square deviation (MSD) methodology suggested by Molina et al. (2011) can be considered in the third category. The MSD approach can be divided in two sequential combinatorial problems addressing the CVs selection and controller design. The former is based on minimizing the sum of square deviations (SSD) of the uncontrolled variables (UVs) from their operating points assuming the perfect control for the CVs (Chang and Yu, 1990; Hori et al., 2005; Skogestad and Postlethwaite, 2005). From this step a diagonal control structure can be obtained. The MSD is extended with the net load evaluation (NLE) index to define a new multivariable control structure taking into account change of references and disturbances effects on CVs. This last stage can provide proper sparse control structures. It is important to note that the SSD index is directly related to the non-square relative gain (NRG) array, suggested by Chang and Yu (1990) and perfect SS indirect control opportunely proposed by Hori et al. (2005). Hence, the SSD approach is used here as a tool for defining a proper CVs selection. Therefore, the main contribution of the MSD procedure is done by the use of the NLE index, which extends and generalizes the approach presented by Chang and Yu (1994). Hence, the new NLE scalar index allows to evaluate and sort different controller structures designed in the context of internal model control (IMC) theory. In addition, a stability test at steady-state (Garcia and Morari, 1985) to focus the search towards a feasible set of solutions is included.

## 2. Material and Methods

It is very important in this work to explore the controllability of high purity distillation columns by comparing five multicomponent feed composition. The steady state control indices of the selected distillation configuration are done. The steady state control of the open-loop system for changes in various manipulated and disturbance variables will first studied in order to gain some insight into the control difficulties associated with the operation of these columns. Then several types of closed-loop control systems will investigated (Skogestad, 2000). Steady state gains are calculated for 3x3 multivariable systems. A computer program has been done by Mat lab to calculate the steady state control indices. The following controllability indices and methods are used:

- Niederlinski index (NI) is a fairly useful stability analysis method. It can be used to eliminate unworkable pairings of variables at an early stage in the design. The settings of the controllers do not have to be known, but it applies only when integral action is used in all loops.
- Morari resiliency index (MRI) the larger it is value, the better is the control.
- The relative gain array (RGA), the diagonal elements ( $\lambda_{ii}$ ) close to unity indicates weak interaction
- The condition number (CN), the smaller the better is the control.
- Short cut method (FUG) is used for design of distillation column.
- Minimum number of trays (Nm) is calculated from short cut method which is used for the rigorous simulation.
- Minimum reflux ratio (Rm) is calculated and optimum reflux ratio is found to be 1.3 times the Rm.
- The Hyprotech's (HYSYS) professional simulation package and excel calculations are used for the modeling of steady-state simulation of the distillation schemes.

- Steady-state control indices are determined for the optimum schemes fit for different control structures and feed composition.

### 3. Results screening and Discussion

The general control objectives considered in this work is to maintain composition of the products at set points, and to select the optimum process configuration that can be used for many different feed compositions and maintain the operation close to minimum energy consumption. Composition control objective includes the control of all the five-product purities. The controlled and manipulated variables are defined for each separation system and the possible pairings of these variables.

#### Mixtures of 93 % product purity.

Best three configurations chosen from the steady state simulation for five multicomponent mixtures at 93% product purity are shown In the following tables the steady state indices are collected briefly to indicate the best candidate configuration, best NI, MRI, CN,  $\lambda_{11}$ ,  $\lambda_{22}$  And  $\lambda_{33}$  are screened as follow; NI is around one CN more than 0.1,  $1 < CN > 10$  then  $\lambda_{11}$ ,  $\lambda_{22}$  And  $\lambda_{33}$  are close to one. And then the candidate steady state indices are tabulated as below, The analysis of the investigation of all possible control structure for the conventional direct sequence show that all the structure have positive (NI), and the structure which have negative RGA or indicated some interaction between the loops are excluded from the further dynamic investigations. The remaining structures (table 3.4) which show less interaction, high MRI and low CN are: (L1-L2-Q2), (R1-D2-BR), (D<sub>1</sub>,L<sub>2</sub>,B<sub>2</sub>). The best structure which show the best control indices values is (L1-L2-Q2).

Table1. The relation between configuration and SSI (BTX93%)

composition	configuration	NI	MRI	CN	$\lambda_{11}$	$\lambda_{22}$	$\lambda_{33}$
Benzene	L1-L2-Q2	0.97	0.41	48.0	0.97	1.0	1.0
Toluene m- xylene	R1-L2-Q2	0.911	0.399	10	0.93	1.0	1.0
	D1-L2-Q2	0.92	0.55	4.7	1.01	1.2	1.2

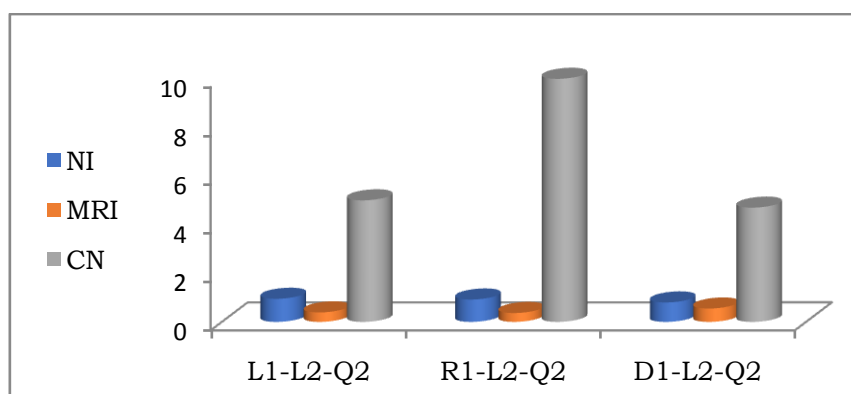


Fig 1. The relation between configuration and SSI (BTX93%)

Table 2. The relation between configuration and SSI (EPB93%)

composition	configuration	NI	MRI	CN	$\lambda_{11}$	$\lambda_{22}$	$\lambda_{33}$
Ethanol	L1-L2-Q2	0.94	0.32	4.8	0.99	1.06	1.07
Propanol	R1-D2-BR2	1.14	0.51	4.1	0.99	0.87	0.87
Butanol	R1-L2-Q2	0.92	0.42	10	0.99	1.07	1.07

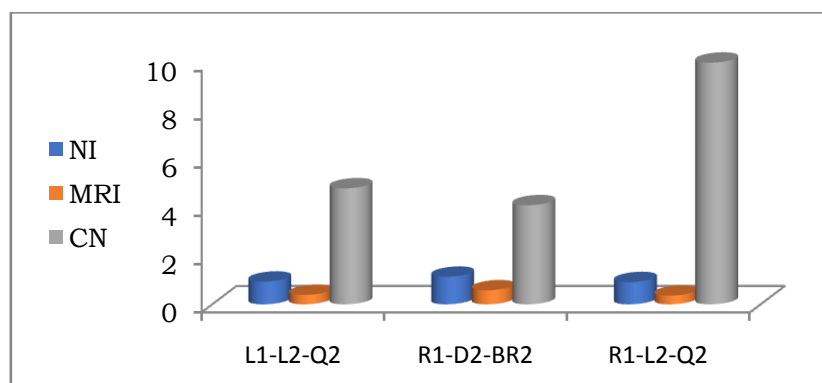


Fig 2. The relation between configuration and SSI (EPB93%)

Table3. The relation between configuration and SSI (PHH93%)

composition	configuration	NI	MRI	CN	$\lambda_{11}$	$\lambda_{22}$	$\lambda_{33}$
Pentane	L1-L2-Q2	0.98	0.23	4.98	1	1.1	1.1
Hexane	R1-R2-Q2	0.99	0.43	2.45	1.0	1.0	1.0
Heptane	R1-D2-BR2	1.17	2.0	1.08	1.08	0.99	0.99

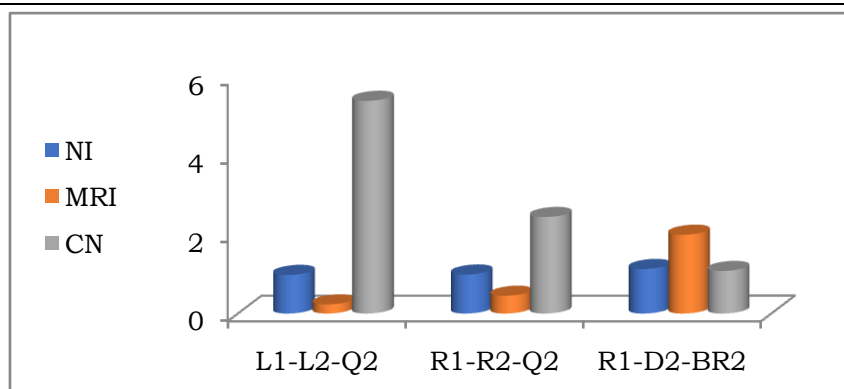


Fig 3. The relation between configuration and SSI (PHH93)

The tables show the relation between the type of configuration and the steady state indices at product purity 93%. It is obviously that the configuration ( L1 – L2 – Q2 ) which relates the reflux quantity in the first column to the reflux quantity in the second column and the energy required in the reboiler in the second column, is presented to be satisfactory and applicable and general for all the five feed composition and it gives good results in steady state indices and show less interaction and good controllability features among the loops. This achievement is very important because it indicates that there one certain configuration is successful and we can apply to many different feed composition at a certain product purity.

#### Mixture of 97% product purity.

Table1. The relation between configuration and SSI (BTX97%)

Composition	Configuration	NI	MRI	CN	$\lambda_{11}$	$\lambda_{22}$	$\lambda_{33}$
Benzene	R1-R2-B2	0.94	0.44	1.8	1.0	1.0	1.0
Toluene	D1-L2-B2	1.09	0.69	2	1.0	0.91	0.96
m-xylene	R1-L2-B2	1.18	0.66	2.1	0.77	0.98	1.0

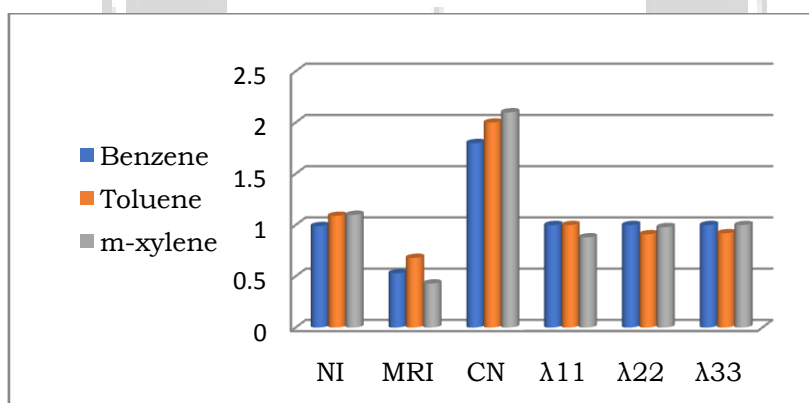


Fig 4.The relation between configuration and SSI (BTX97%)

Table2. The relation between configuration and SSI (EPB97%)

composition	configuration	NI	MRI	CN	$\lambda_{11}$	$\lambda_{22}$	$\lambda_{33}$
Ethanol	L1-R2-B2	0.99	0.010	9.32	1.25	1.26	1.01
Propanol	L1-R2-Q2	0.98	0.010	18.3	1.60	1.60	1.26
Butanol	D1-L2-B2	1.02	0.03	9.13	1.00	0.97	0.97

Table3. The relation between configuration and SSI (PHH97%)

composition	configuration	NI	MRI	CN	$\lambda_{11}$	$\lambda_{22}$	$\lambda_{33}$
Pentane	R1-R2-B2	1.10	0.17	5.1	1.0	0.93	0.91
Hexane	L1-R2-B2	1.12	0.17	5.55	1.0	0.91	0.91
Heptane	D1-L2-B2	1.03	0.23	4.7	1	0.89	0.89

In the other hand, at the product purity 97% the results obtained from the calculation of the steady state indices are shown to be very clear and obviously the configuration ( D1-L2-B2) was the most common, applicable and the RGA close to unity indicates a weak interaction among the loops and indicate possible stability.

#### 4. Conclusion

High-purity columns respond much more quickly than predicted by linear analysis as we found in the conventional direct schemes distillation columns. This fact must be recognized in specifying analyzer cycle times and in designing control systems. It is clearly illustrated that the relative volatility  $\alpha_{AB}$  and  $\alpha_{BC}$  for the five chemical systems are related inversely to the reflux ratio. The steady state controllability study shows that the conventional direct schemes distillation columns of different feed compositions and producing high-purity (93% and 97%) products can be controlled with decentralized controller structures and be effectively controlled with one specified configuration, this configuration has the ability to avoid serious interaction among loops, in the case of this study the best acceptable feature was (D1-L2-B2) for the product purity 97% and (L1-L2-Q2) for the product purity 93% at different composition . The structure (L1-L2-Q2) and the structure (D1-L2-B2) give good result in the further simulations, It give satisfied result in the steady state analysis from this we can conclude that steady state analysis, when used alone, can provide complete and sometimes leading information about the controlled distillation process.

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