Plant-wide Controllability and Structural Optimization of Plants with Recycles
Groenendijk, A.J.

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Chapter 3

Plantwide Controllability of Impurities in a Plant with Recycles

3.1 Introduction

Recycle loops strongly affect dynamics and control of a complex plant. The stability of control structures for component inventories may be influenced by recycle interactions and by connectivity, which leads to flowsheet alternatives possessing different control properties. The previous chapter presented a simulation-based methodology for evaluating these phenomena and finding the best flowsheet structure from controllability point of view. Steady state and dynamic simulations are combined with controllability analysis tools, both static and in the frequency domain, which enables to get more value from simulation than the usual sensitivity studies. The power of this approach will be demonstrated in this chapter by an industrial case study about the handling of impurities in a Vinyl Chloride Monomer plant.

3.2 Problem definition

The removal of impurities in a balanced Vinyl Chloride Monomer (VCM) process is known to be difficult. Significant market fluctuations require a wide operating window, while maintaining product purity under economical conditions. Higher reaction conversion or plant throughput typically yields more secondary products and impurities that may accumulate and cause unstable operation.
3.2.1 Reactions

A balanced VCM process contains three main reactions, which may be described as follows:

- **Chlorination**: \( \text{C}_2\text{H}_4 + \text{Cl}_2 \rightarrow 1,2\text{-C}_2\text{H}_4\text{Cl}_2 \text{ (DCE)} + \text{impurities} \)
- **Cracking**: \( \text{DCE} \rightarrow \text{C}_2\text{H}_3\text{Cl} \text{ (VCM)} + \text{HCl} + \text{impurities} \)
- **Oxychlorination**: \( \text{C}_2\text{H}_4 + 2 \text{HCl} + \frac{1}{2} \text{O}_2 \rightarrow \text{DCE} + \text{H}_2\text{O} + \text{impurities} \)

The intermediate product 1,2-dichloroethane (DCE) is produced by the direct chlorination of ethylene with fresh chlorine. The cracking of this intermediate gives Vinyl Chloride (VCM). The Hydrogen Chloride that is produced as a byproduct of the cracking process will be used to chlorinate more ethylene in the oxychlorination process. Oxygen is added here to remove hydrogen. As a result all fresh chlorine that is added to the process will be used finally to produce VCM. There is no net production of HCl. Therefore the process is said to be in balance.

3.2.2 Impurities

The oxychlorination process may also use HCl waste streams from other plants as chlorine source. This will reduce the net consumption of fresh chlorine but may also introduce additional impurities in the process. In general, waste and impurities in the effluent of the three reactors may originate from (1) feed impurities, (2) secondary reactions with the main reactant(s) and (3) supplementary reactions with feed impurities.

Each reaction section may have its own separation system, but some of the impurities from different reactors may be collected and eliminated in a central separation system. Recycling of impurities over more than one reactor may generate even more waste material. Generally, the impurities lead to operation problems. Their upper limit concentration must be strictly controlled to prevent polymerization or fouling. However, in special cases some impurities may be useful catalyzing or inhibiting some reactions and their concentration has to be kept at an optimum value by balancing formation and elimination rates. Thus, impurity control and main component control are strongly coupled. A special feature of impurity dynamics is the fact that some of them are always in transient state, hence a simultaneous steady state optimization of both is impossible. However, an accurate steady state plant simulation model contributes to understand and to evaluate quantitatively formation and elimination mechanisms as well as interactions between them.
3.3 Plant structure

Figure 3.1 presents the flowsheet of the balanced VCM process. The reactions take place in the reactors R1 (Chlorination), R2 (Cracking) and R3 (Oxychlorination). The washing/drying section S0 removes unconverted reactants. A first amount of (light) impurities is removed by column S1. Three main recycle loops cross in the distillation column S2 whose main function is to purify fresh and recycled DCE. Three other distillation columns are involved in this operation: S3 for finishing DCE, S4 for ‘Lights’ and S5 for ‘Heavies’ removal. The column S2 will collect also impurities associated with the production and the recycling of DCE, which may contain lights, intermediates and heavies. Among the impurities three significant components are identified for this process: chloroprene (I₁), trichloroethylene (I₂) and CCl₄ (I₃). These components are lighter than the main component DCE. Both I₁ and I₂ are polymerizable and have concentration constraints in the bottom product of column S2. They can leave the plant as Lights via column S4 but significant amounts will remain in the recycle to reactor R1. There they are transformed to Heavies (C₆Cl₄), which are easily removed by column S5. They are also drawn as a side-stream from column S2, being directly recycled to reactor R1. This creates a fourth loop, also containing S2. They may also be destroyed in a supplementary reactor, R4, between the columns S2 and S4. This will decrease the impurities loading of S4, which will improve its performance. Therefore, this alternative design may have better control properties.

Figure 3.1; Flowsheet of the balanced VCM process with optional reactor R4
A major feature of the VCM process is the fact that impurity I₃ has a beneficial role since it enhances both conversion and yield of the cracking reaction. It can leave the system only via column S4 as Lights. Therefore, regarding the removal of I₁ and I₂, a compromise has to be found with an optimal concentration of I₃ in the bottom of the column S2. These considerations show that the design and operation of S2 are essential for the process as a whole. S2 is a large distillation column, operating at a very large reflux ratio. Its operation is constrained by specifications on the quality of the bottom product: $\text{spec}_1$, the maximum concentration of I₁; $\text{spec}_2$, the maximum concentration of I₂; and $\text{spec}_3$, the optimum concentration of I₃.

### 3.3.1 The nominal operating point

Rigorous steady state simulation models are used to find the nominal operating points of the basic plant structure and the alternative structure with additional reactor R4. Details of the models are given in an appendix at the end of this thesis. The nominal operating values of variables that are interesting from controllability point of view are given in Table 3.1.

Introduction of the extra reactor R4, between column S2 and S4 for the transformation of impurities I₁ and I₂ into Heavies leads to a different steady state behavior of the system. The Heavies that are produced by reactor R4 will leave column S4 through the bottom, while the impurities I₁ and I₂ left the basic system as Lights. Therefore, in this alternative design the concentration of impurity I₃ in the top distillate of column S4 is higher. To keep $\text{spec}_3$, the optimum concentration of I₃, the distillate flowrate of column S4 has been reduced with about 40%. Furthermore, the nominal values of I₁ and I₂ become significantly lower. The impact of these changes on the controllability of the system will be studied by a steady state analysis. But first the control problem has to be defined and a selection of input and output variables has to be made.

### 3.4 Plantwide control strategy

In a complex plant as the balanced VCM process, a large number of variables have to be controlled. Most of them - pressures, temperatures, levels - may be controlled locally. However, material balances in general and especially the material balances of impurities are established by interactions between the different operating units and recycles in a plant. Therefore, the control of all material balances requires a plantwide approach.
Consequently, the handling of impurities is dealt with as a multivariable control problem. Here the controlled variables (outputs) are maximum or optimum values of concentrations (flowrates) of impurities on selected streams or locations. They can be measured in an operating plant, but also set as ‘design specifications’. These specifications may be achieved by manipulating inputs as distillate flowrate, reflux ratio, reboiler duty, feed temperature, etc. These may also be seen as ‘design variables’ in a new design or revamp. It is obvious that one manipulated variable affects more than one controlled variable, so interaction between controller loops should be taken into account.

In this study we focus our attention on the material balances of the impurities $I_1$, $I_2$ and $I_3$. Since these have a slow dynamic behavior, the fast control loops are assumed to operate instantaneously. Therefore pressures, temperatures and levels are fixed in the simulation models while duties and flowrates are free (calculated). In the distillation columns S2 and S4 the reflux flow is much larger than the distillate flow, therefore we assume that the reflux flow is used to control the drum level and the bottom flow to control the reboiler level. The reboiler duties and distillate flowrates are used then to meet the specifications.

3.4.1 Inputs, outputs and disturbances

In this work we focus our attention on the slow dynamics of the material balances, therefore the concentrations of the impurities $I_1$, $I_2$ and $I_3$ in the bottom product of column S2 are the outputs of the control problem. Normally the design variables of this column S2, the distillate flowrate (D2), side stream flowrate (SS2) and reboiler duty (Q2), will be used then as the input variables of the control problem. However, by trying to satisfy the specifications on the impurities $I_1$, $I_2$ and $I_3$ in the bottom product of column S2 during the calibration of the plant steady state model, the important role of column S4 as an exit of impurity $I_3$ became evident. Simulations did not converge with a too small distillate flowrate. Impurity $I_3$ is then built up in the plant (‘snowball effect’ on impurities concentration, see also Figure 3.4). Therefore, to resolve this problem, in addition to the column S2 distillate flowrate (D2), side stream flowrate (SS2) and reboiler duty (Q2), also the column S4 distillate flowrate (D4) and reboiler duty (Q4) are taken into account as possible manipulated variables in a plantwide control structure (inputs). The main disturbance of the plant is the throughput, being modified by the flowrate of the external DCE feed ($F_{DCE}$). A second disturbance that will be taken into account is the fraction of impurity $I_3$ in this stream ($X_{I3}$).
### Table 3.1: Nominal operating values and scaling factors

<table>
<thead>
<tr>
<th></th>
<th>basic plant</th>
<th></th>
<th>alternative with R4</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>spec</td>
<td>nominal value</td>
<td>scaling factor</td>
<td>nominal value</td>
</tr>
<tr>
<td><strong>Output</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$I_1$</td>
<td></td>
<td>$&lt;100$</td>
<td>86</td>
<td>82</td>
</tr>
<tr>
<td>$I_2$</td>
<td></td>
<td>$&lt;600$</td>
<td>564</td>
<td>547</td>
</tr>
<tr>
<td>$I_3$</td>
<td></td>
<td>2000</td>
<td>2000</td>
<td>2000</td>
</tr>
<tr>
<td><strong>Input</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>D2</td>
<td></td>
<td>14.5</td>
<td>3.6</td>
<td>14.55</td>
</tr>
<tr>
<td>SS2</td>
<td></td>
<td>35</td>
<td>8.75</td>
<td>35</td>
</tr>
<tr>
<td>Q2</td>
<td></td>
<td>34</td>
<td>8.5</td>
<td>34</td>
</tr>
<tr>
<td>D4</td>
<td></td>
<td>5.59</td>
<td>1.4</td>
<td>3.53</td>
</tr>
<tr>
<td>Q4</td>
<td></td>
<td>1.0</td>
<td>0.25</td>
<td>0.9</td>
</tr>
<tr>
<td><strong>Disturbance</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$F_{DCE}$</td>
<td></td>
<td>175</td>
<td>75</td>
<td>175</td>
</tr>
<tr>
<td>$X_{13}$</td>
<td></td>
<td>0.12</td>
<td>0.12</td>
<td>0.12</td>
</tr>
</tbody>
</table>

#### 3.4.2 Scaling

Scaling of the input and output variables makes model analysis and controller design much simpler. A useful approach is to make the variables less than one in magnitude (see 2.3.3). The scaling factors of the impurities $I_1$ and $I_2$ are therefore based on their maximum allowed value while that of $I_3$ is based on the maximum expected change of its reference value. The inputs are scaled by 25% of their nominal value. Proper operation of the distillation columns should normally be guaranteed within this range, but problems may occur when the operating variables become outside this range. For each disturbance, the largest expected change is taken as scaling factor. The nominal values and scaling factors of the inputs, outputs and disturbances are given in Table 3.1. The nominal values of $I_1$ and $I_2$ become significantly lower when the extra reactor R4 is introduced. This lead to larger scaling factors. The impact of these differences on the controllability of the system will be studied next.

#### 3.5 Steady state analysis

From extensive steady state simulations a scaled gain matrix $G$ can be generated according to the relation $c = Gm$, where $c$ are the scaled plantwide control variables and $m$ are the scaled manipulated variables (eq. 2.2). With the scaled disturbances $d$, a scaled disturbance gain matrix $G_d$ is generated, according to the relation $c = G_d d$ (eq. 2.3). The introduction of scaled variables allows reformulation of the plantwide control problem. To keep the impurities within their bounds under disturbances, control is necessary when the scaled disturbance gains are greater than one.
3.5.1 Basic flowsheet

3.5.1.1 Static gains

Table 3.2 shows the static gain matrices for the basic plant structure. Control is necessary, since the scaled disturbance gains are greater than one. When regarding the sign of the input/output gains, it is noticed that both D2 and SS2 have a negative effect on the impurities I1 and I2, while the effect on I3 is positive. Increasing these manipulated variables means recycling more material through reactor R1. Impurities I1 and I2 are transformed to Heavies here (‘negative feedback’), but I3 is build up in the recycle (‘positive feedback’).

Increasing the reboiler duty Q2 will give rise to fewer impurities in the bottom product. This holds also for the distillate flowrate and reboiler duty of column S4 (D4 resp. Q4). The first is an exit for the impurities while the second will purify the recycle stream to R1, so both have a reverse effect on the controlled variables. The high gain values are in line with their important role in removing impurities, especially for I3.

<table>
<thead>
<tr>
<th>G</th>
<th>D2</th>
<th>SS2</th>
<th>Q2</th>
<th>D4</th>
<th>Q4</th>
</tr>
</thead>
<tbody>
<tr>
<td>I1</td>
<td>-0.075</td>
<td>-0.261</td>
<td>-5.742</td>
<td>-0.376</td>
<td>-0.079</td>
</tr>
<tr>
<td>I2</td>
<td>-0.212</td>
<td>-0.527</td>
<td>-3.574</td>
<td>-0.437</td>
<td>-0.071</td>
</tr>
<tr>
<td>I3</td>
<td>0.411</td>
<td>0.030</td>
<td>-0.893</td>
<td>-2.829</td>
<td>-0.616</td>
</tr>
</tbody>
</table>

3.5.1.2 Controllability indices

Table 3.3 resumes the steady state controllability analysis with RGA and SVD. The manipulated variables are arranged such that the preferred pairings are on the main diagonal. The indices show a great difference between the possible combinations of manipulated variables. Notice first that the lower singular values, also known as the Morari Resiliency Index, are less than unity for all scaled systems. This demonstrates that the outputs cannot be set independently. This is also reflected by the large condition numbers, indicating that the plant may be drawn into some directions more easily than into others.

Notice that as long as the reboiler duty of column S2, denoted as Q2, is used as one of the manipulated variables, there is still some control power into the weakest direction. However, when Q2 is not used, the lower singular value becomes almost zero and the condition number is therefore also extremely high. So, Q2 should always be used in a control structure and furthermore it is preferably paired with I1. The high static gain is dominating here.

<table>
<thead>
<tr>
<th>G</th>
<th>F_DCE</th>
<th>X_L3</th>
</tr>
</thead>
<tbody>
<tr>
<td>I1</td>
<td>4.424</td>
<td>0.132</td>
</tr>
<tr>
<td>I2</td>
<td>3.193</td>
<td>0.192</td>
</tr>
<tr>
<td>I3</td>
<td>2.606</td>
<td>1.631</td>
</tr>
</tbody>
</table>
Table 3.3; Controllability indices of the basic VCM-plant

<table>
<thead>
<tr>
<th>I₁, I₂, I₃ paired with</th>
<th>RGA diagonal elements</th>
<th>Singular Values</th>
<th>Condition Number</th>
</tr>
</thead>
<tbody>
<tr>
<td>Q₂, SS₂, D₂</td>
<td>1.48, 1.56, 1.05</td>
<td>6.84, 0.50, 0.24</td>
<td>28.8</td>
</tr>
<tr>
<td>Q₂, SS₂, D₄</td>
<td>1.47, 1.43, 1.01</td>
<td>6.91, 2.71, 0.31</td>
<td>22.0</td>
</tr>
<tr>
<td>Q₂, SS₂, Q₄</td>
<td>1.47, 1.44, 1.01</td>
<td>6.84, 0.60, 0.31</td>
<td>22.3</td>
</tr>
<tr>
<td>Q₂, D₂, D₄</td>
<td>1.43, 1.08, 0.86</td>
<td>6.89, 2.74, 0.17</td>
<td>41.8</td>
</tr>
<tr>
<td>Q₂, D₂, Q₄</td>
<td>1.47, 1.17, 0.93</td>
<td>6.83, 0.74, 0.12</td>
<td>55.0</td>
</tr>
<tr>
<td>Q₂, D₄, Q₄</td>
<td>1.10, 4.25, 2.01</td>
<td>6.90, 2.77, 0.02</td>
<td>370</td>
</tr>
<tr>
<td>Q₄, D₄, D₂</td>
<td>9.30, 5.19, 0.48</td>
<td>2.98, 0.30, 0.008</td>
<td>397</td>
</tr>
<tr>
<td>Q₄, D₄, SS₂</td>
<td>8.67, 5.17, 0.02</td>
<td>2.96, 0.58, 0.008</td>
<td>369</td>
</tr>
<tr>
<td>SS₂, D₂, D₄</td>
<td>17.6, 13.7, 3.87</td>
<td>2.91, 0.65, 0.006</td>
<td>480</td>
</tr>
<tr>
<td>SS₂, D₂, Q₄</td>
<td>71.3, 59.1, 16.6</td>
<td>0.75, 0.63, 0.001</td>
<td>605</td>
</tr>
</tbody>
</table>

The static gain matrix showed already that the effect of the distillate flowrate and reboiler duty of column S₄ (D₄ resp. Q₄) on the control variables is comparable. When they are used both as manipulated variables, the lower singular value becomes very small and the condition number correspondingly high. So it is not useful to combine them in a control structure.

This will leave five possible combinations of manipulated variables that have acceptable properties. They all have RGA diagonal elements near unity, which suggest that diagonal control would be possible without too many interactions. The combinations where the distillate flowrate of column S₂ (D₂) is used to control I₂ have a smaller Morari Resiliency Index and a higher condition number than the combinations where the side draw of this column (SS₂) is used. Furthermore, the low static gains of D₂ and Q₄ result in two singular values below unity when they are used to control I₃, while the use of D₄ will give only one singular value below unity. Therefore the combination of controllers I₁-Q₂, I₂-SS₂ and I₃-D₄ seems to be preferable from a steady state point of view. However, the four other structures should not be discarded yet, because they might have better dynamic properties.

3.5.1.3 Disturbances

A singular value decomposition of the static disturbance gain matrix gives the singular values 6.11 and 1.36, which are comparable with the magnitudes of the disturbance vectors themselves (6.05 and 1.65). The matrix with input directions is therefore almost equal to the identity matrix. This indicates that the two disturbances are almost independent of each other and their combined effect is not relevant. Therefore the rejection of the two disturbances may be treated separate.
Plantwide Controllability of Impurities in a Plant with Recycles

3.5.2 Flowsheet with impurity destroying reactor R4

3.5.2.1 Static gains

The nominal values of the impurities \( I_1 \) and \( I_2 \) become significantly lower when introducing the extra reactor. Their scaling factors are therefore larger than in the basic flowsheet. This reduced the static gains of the inputs on \( I_1 \) and \( I_2 \) slightly, as can be seen in Table 3.4.

The impact of the distillate flowrate on impurity \( I_3 \) is almost doubled. Also the sensitivity of \( I_3 \) to the side stream flowrate is increased by a factor 5. This is the result of recycle interactions. \( I_3 \) is built up in all four recycle streams originating in column S2 and the only exit is the distillate flow of column S4. By reducing this exit, the sensitivity of \( I_3 \) to the recycle interactions is increased. This increasing sensitivity to recycle interactions is a remarkable result, especially relevant in the context of waste minimization and zero discharge plants, where the impurities removal is even further reduced. It demonstrates that such design modifications meant to reduce waste have a strong impact on the performance of the system and may become detrimental in operation.

Table 3.4; Static gain matrices of VCM-plant with reactor R4

<table>
<thead>
<tr>
<th></th>
<th>D2</th>
<th>SS2</th>
<th>Q2</th>
<th>D4</th>
<th>Q4</th>
</tr>
</thead>
<tbody>
<tr>
<td>I1</td>
<td>-0.076</td>
<td>-0.184</td>
<td>-4.325</td>
<td>-0.154</td>
<td>-0.041</td>
</tr>
<tr>
<td>I2</td>
<td>-0.140</td>
<td>-0.302</td>
<td>-2.298</td>
<td>-0.215</td>
<td>-0.061</td>
</tr>
<tr>
<td>I3</td>
<td>0.737</td>
<td>0.156</td>
<td>-0.908</td>
<td>-2.136</td>
<td>-0.727</td>
</tr>
</tbody>
</table>

3.5.2.2 Controllability indices

Table 3.5 shows the steady state controllability indices for the alternative flowsheet. Only the five possible combinations of manipulated variables that have acceptable properties are shown here. The higher RGA diagonal elements indicate slightly more interaction and the lower singular values indicate a smaller operating window than in the basic plant, but the differences are very small. An SVD analysis of the static disturbance gain matrix confirms the conclusion that the two disturbances are almost independent of each other and their rejection may be treated separate. We may conclude that on the basis of the steady state analysis of both alternatives no clear preference can be assigned to the different design and control alternatives.
Table 3.5; Controllability indices of VCM-plant with reactor R4

<table>
<thead>
<tr>
<th>I₁, I₂, I₃ paired with</th>
<th>RGA diagonal elements</th>
<th>Singular Values</th>
<th>Condition Number</th>
</tr>
</thead>
<tbody>
<tr>
<td>Q₂, SS₂, D₂</td>
<td>1.49, 1.69, 1.12</td>
<td>4.99, 0.79, 0.15</td>
<td>33.67</td>
</tr>
<tr>
<td>Q₂, SS₂, D₄</td>
<td>1.49, 1.39, 0.96</td>
<td>5.03, 2.05, 0.19</td>
<td>26.36</td>
</tr>
<tr>
<td>Q₂, SS₂, Q₄</td>
<td>1.48, 1.40, 0.96</td>
<td>4.99, 0.73, 0.18</td>
<td>27.32</td>
</tr>
<tr>
<td>Q₂, D₂, D₄</td>
<td>1.48, 0.95, 0.68</td>
<td>5.03, 2.17, 0.12</td>
<td>41.08</td>
</tr>
<tr>
<td>Q₂, D₂, Q₄</td>
<td>1.45, 0.99, 0.71</td>
<td>4.99, 1.03, 0.09</td>
<td>58.43</td>
</tr>
</tbody>
</table>

3.5.3 Column S2

The control problem concentrates on the impurities level in the bottom product of the large distillation column S2. Four recycle loops cross in this column, so its operation is strongly coupled to the rest of the plant by the effect of recycle interactions. Nevertheless it is interesting to study the column as a stand-alone object, without the interaction of recycles. Table 3.6 shows that the scaled static process gains of the stand-alone column are much smaller than in the studied flowsheet structures. There is only little control power available in the column itself. A singular value decomposition of this static gain matrix gives the singular values 2.0, 0.01 and 1.5e-5. This indicates that the system can in fact be drawn into one direction only. The lower two singular values are close to zero, so there is almost no control power into these directions. This means that the impurity levels cannot be varied independently. The interactions between the controllers are such that only one impurity can be controlled properly at a time. The high and negative RGA elements also are an indication of this. It is clear that the stand-alone column cannot be controlled properly. In general, the behavior of a stand-alone unit may differ considerably from its behavior when the unit is integrated in a flowsheet. This is mainly due to the effect of recycle interactions. A control structure for the whole plant can therefore not be developed unit by unit. Only a plantwide approach can solve the problem.

Table 3.6; Scaled static process gains

<table>
<thead>
<tr>
<th>G</th>
<th>D₂</th>
<th>SS₂</th>
<th>Q₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>I₁</td>
<td>-0.0766</td>
<td>-0.1613</td>
<td>-2.0370</td>
</tr>
<tr>
<td>I₂</td>
<td>-0.0045</td>
<td>-0.0142</td>
<td>-0.0616</td>
</tr>
<tr>
<td>I₃</td>
<td>-0.0005</td>
<td>-0.0010</td>
<td>-0.0139</td>
</tr>
</tbody>
</table>

Table 3.7; RGA matrix

<table>
<thead>
<tr>
<th>Λ</th>
<th>D₂</th>
<th>SS₂</th>
<th>Q₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>I₁</td>
<td>-35.3</td>
<td>17.0</td>
<td>19.3</td>
</tr>
<tr>
<td>I₂</td>
<td>3.25</td>
<td>-0.89</td>
<td>-1.36</td>
</tr>
<tr>
<td>I₃</td>
<td>33.0</td>
<td>-15.1</td>
<td>-16.9</td>
</tr>
</tbody>
</table>
3.6 Dynamic simulation

3.6.1 Identification of main dynamics

Prior to construction of the dynamic flowsheet, model decisions have to be made regarding the flowsheet elements of which the dynamics have to be taken into account. The steady state analysis showed the important role of the impurities destruction in reactor R1 and R4. Therefore the impact of these two liquid phase reactors on the plant dynamics is considered in this part, first for the basic flowsheet then for the flowsheet with impurity destroying reactor R4.

Reactors R2 and R3 are assumed to have no contribution to the plant dynamics, because as gas phase reactors they possess a negligible holdup and residence times with orders of magnitude of seconds or minutes only and hence they are supposed to act instantaneously.

The separation system is simulated dynamically with a reduced set of components. The reactants having zero flow in the reactor outlet streams are omitted. Since phenomena concerning the impurity material balances are taking place at long time scales, level and pressure controllers are assumed to operate instantaneously. Therefore condenser pressures are fixed and total material balances in drums and reboilers are modeled assuming steady state. So, condenser duties and reflux and bottom flowrates are free while reboiler duties and distillate flowrates are specified. Details of the dynamic model are given in Appendix 1.

3.6.2 Basic flowsheet

Dynamic simulations with step perturbations on the disturbances and manipulated variables show interesting responses (for the concentration of I_3 in the bottom of S2, see Figure 3.2). All impurities will finally reach steady state values, but in different times. For steps on distillate and side stream flowrates of column S2, the manipulated variables D2 and SS2 respectively, new steady states are reached in about 24 hours. The responses are influenced by the recycle interactions. In both cases a recycle through reactor R1 is increased. More impurities I_1 and I_2 are destroyed, while I_3 is being built up, on the contrary. After two hours the concentration of I_3 will reach a maximum and then decreases to the final value. This is so because this impurity I_3 finally leaves the plant via column S4. Increasing the reboiler duty Q2 will boil out the impurities immediately. Recycles are responsible for a small increase after half an hour, but the steady state is reached within two hours, which is much faster than the responses on D2 and SS2.
Simulations of an increase in distillate flowrate (D4) or reboiler duty (Q4) of column S4 show a decrease in impurities with a dualistic character, since the response is initially fast but it continues more slowly later on. The slowest part of the response is the most significant one, but it takes about 30 hours to reach steady state. This is the time needed for all recycles to become in equilibrium. A similar dualistic response is observed from steps on disturbance variables (Figure 3.3): a long settling time of impurity I₃ after an increase of the same impurity in the external DCE feed (X₁₃) or in DCE feed flowrate (Fᵢ₄). An increased flowrate of DCE will result in a higher production rate of both product and impurities. The impurities are build up in the DCE recycle and go to the top of column S2 from where one part is recycled to R1 (destruction of I₁ and I₂) and another will flow to column S4, were the three impurities can leave the plant.

As shown in Figure 3.4, the operating window of the distillate flowrate of column S4 has a lower limit of 80% relative to its nominal value. When the flowrate is lower, feed and produced impurity I₃ cannot be purged from the plant anymore, hence I₃ will build up in the recycles and its concentration increases to unacceptable high levels. This is a kind of ‘snowball effect’ occurring to the concentration of impurities rather than to the whole system.

![Figure 3.2](image)

**Figure 3.2; Dynamic response of impurity I₃ in the bottom of S2 after a scaled step perturbation of I on resp. D2, Q2 or D4 in the basic VCM plant**

*When D2 is increased, I₃ increases fast in the beginning and later decreases slowly to its final value. Increasing Q2 gives an almost instantaneous drop of I₃, followed by a fast increase. The final value is reached must faster than after a step on D2. A step on D4 gives the slowest response. This is due to the time needed for the recycles to become in equilibrium with each other.*
Plantwide Controllability of Impurities in a Plant with Recycles

Figure 3.3: Dualistic response of impurity $I_3$ in the bottom of S2 after a scaled step perturbation of 1 on the external DCE feed $\gamma_{DCE}$ or impurity concentration $I_3$ in this feed $X_{I3}$ in the basic VCM plant

When the DCE flow is increased, more VCM will be produced and also more HCl, which is recycled and leads to a higher DCE production rate. The higher DCE production and cracking rates give rise to more production of impurities on the short term and more build up of these impurities in the recycles on the longer term. An increase of the impurity content $I_3$ in the external DCE flow also yields more build up in the recycles. The long settling time is due to the time needed for the recycles to become in equilibrium with each other.

Figure 3.4: Snowball effect of D4 on the concentration of $I_3$ in the bottom of S2

The only exit for $I_3$ is the top distillate of column S4 (D4). When this flowrate is decreased to 90% of its nominal value, $I_3$ will rise and reaches a new steady state value after about 50 hours. When D4 is decreased to 70%, $I_3$ will rise continuously and a new steady state is never reached. The amount of $I_3$ that is feed to and produced in the plant is higher than the amount that can leave the plant and therefore $I_3$ is build up in the recycles (kind of 'snowball effect'). The limiting value for D4 is about 80% of its nominal value.
3.6.3 Flowsheet with impurity destroying reactor R4

Introduction of the reactor R4 has a strong influence on the dynamic behavior of the plant. Because the impurities $I_1$ and $I_2$ in the top distillate D2 of column S2 are transformed into heavies in R4, increasing flowrate D2 results in a fast drop of $I_1$ and $I_2$ in the bottom of S2. In the same time, the feed of column S4 contains less $I_1$ and $I_2$ and therefore more $I_3$ can leave the plant via the Lights directly, compensating the build-up in the recycle. It will not reach a maximum first (in contrast to the same response in the basic flowsheet, Figure 3.2) but goes in a dual fast-slow response to its steady state value (Figure 3.5). Now $I_1$ and $I_2$ show a minimum because their transformation in R4 results in lower concentrations and therefore in less transformation in R1 through which the side steam is recycled. The dynamic characteristics of the responses on steps in the other inputs are the same as in the basic flowsheet, but their final values are changed, as was already shown in the steady state analysis.

![Figure 3.5; Dynamic response of impurities $I_1$, $I_2$ and $I_3$ (bottom S2) after a scaled step perturbation of 1 on the distillate flow D2 of column S2 in the VCM plant with extra reactor R4]

The impurities $I_1$ and $I_2$ are transformed into heavies in reactor R4, located between column S2 and column S4, so their concentrations decrease fast when the distillate flow of S2 is increased. On the longer term they increase slightly because their lower concentrations lead to less transformation in reactor R1. Impurity $I_3$ is built up in the recycle and therefore increases.
3.7 Dynamic controllability analysis

From the dynamic Speedup™ plant model a scaled linear state space description has been generated as a basis for frequency responses to be calculated in Matlab®. In this case study full order state space descriptions are used. However, state space descriptions may become very large and difficult to handle. Chapter 5 will deal with this subject.

From Figure 3.6 it can be seen that the static gains appear to hold well for frequencies up to 0.02 h⁻¹. At frequencies above 10 h⁻¹ the system is not responding anymore to disturbances and feedback control is no longer needed. Besides, the system is neither responding anymore to the manipulated variables. For oscillations with a frequency in between, the system responses feature a delay and the magnitudes are lower. This clearly demonstrates why a steady state analysis of the plant behavior falls short. During operation of the plant there will always be oscillatory disturbances with frequencies in this range, hence impurity concentrations will always be in a transient.

![Figure 3.6; Frequency responses of impurity I₃ to D₂, Q₂ and D₄](image)

The response of I₃ to an oscillation on D₄ starts to deviate from steady state at a low frequency already. Column S₄ cannot follow these fluctuations. The response of I₃ to an oscillation on D₂ starts to increase at the same frequency. The removal of I₃ by column S₄ seems to compensate the build up effect of D₂ at low frequencies. The response of I₃ to an oscillation on Q₂ remains the same for the whole frequency range where feedback control is needed. At frequencies where the system is not responding anymore to D₂ and D₄ because the recycles cannot follow these fast fluctuations, the effect of Q₂ is not yet affected. Only at frequencies that are corresponding with the time constant of the column itself, the magnitude of Q₂ on I₃ first increases before it also goes to zero. The effect of Q₂ on I₃ is only reduced by the reflux over the top of the column and is hardly affected by recycle interactions.
Taking a closer look at the frequency responses, a clear difference between D2, Q2, and D4 can be seen. The Lights removal by D4 affects the impurity concentrations in the bottom of column S2 through the recycles. At frequencies above 0.02 h\(^{-1}\) the large holdups in the main recycle paths are damping the effects and the response of I\(_3\) to D4 starts to deviate from steady state. This also affects the response of I\(_3\) to D2 (and SS2, not shown). The build up of I\(_3\) in the short recycle loop through reactor R1 can follow the intermediate frequencies, but the removal of I\(_3\) via D4 does not compensate this effect anymore. This leads to a higher magnitude for the response on D2 (and SS2) between 0.1 - 1 h\(^{-1}\). Its maximum around a frequency of 0.3 h\(^{-1}\) corresponds to the maximum in the step response (Figure 3.2). This recycle also becomes to have a delaying effect leading to damping of oscillations at frequencies around 2 h\(^{-1}\). For these values the residence time in reactor R1 corresponds to half a period and the recycle interactions are such that the responses to D2 (and also D4) are zero. At higher frequencies the direction of these inputs is opposite to steady state, which will complicate feedback control.

The response to the reboiler duty Q2 shows another behavior. It is mainly a result of the interaction between the reboiler and the column S2 itself and is hardly affected by recycle interactions. Therefore the system follows the input changes up to much higher frequencies. At frequencies between 2 – 20 h\(^{-1}\), where the period of the fluctuations is of the same order as the response time of the column, the magnitude of Q2 is increased because the opposite effect of the reflux over the top of the column is damped. The maximum gain around 12 h\(^{-1}\) corresponds to the minimum in the step response (6 min., Figure 3.2). At higher frequencies, also the reboiler does not affect the impurities anymore.

### 3.7.1 Relative Gain Array

In order to analyze the interaction behavior of the system an RGA analysis has been applied. The RGA number, defined by equation 2.27 as \(\|\text{RGA} - I\|_{\text{sum}}\), is used as indicator. Note that RGA numbers close to zero are preferred over the whole frequency range when diagonal feedback control is concerned, since such values would predict a minimum of interactions. The recycle interactions indicated above have a significant influence on the RGA elements. The direction of responses on inputs D2 and D4 at frequencies between 1 and 10 h\(^{-1}\) become opposite to that at steady state (Figure 3.6). Hence, more interactions between control loops at higher frequencies are expected. This is confirmed by high RGA numbers for the diagonal structures with I\(_1\)-Q2, I\(_2\)-SS2, I\(_3\)-D2 or I\(_1\)-Q2, I\(_2\)-SS2, I\(_3\)-D4 as control loops at these frequencies (Figure 3.7).
Figure 3.7: RGA number of two alternative control structures of the basic VCM plant

This figure shows that at low frequencies the control structure with D4 has fewer interactions than the one with D2. At higher frequencies, interaction between the different control loops increases fast for both structures.

3.7.2 Diagonal controller performance

The effects of loop closing by a diagonal pattern (input 1 - output 1, input 2 - output 2, etc.) is investigated now, realizing that any loop closing alters the interactions in a plant. The closed loop analysis follows ideas of Skogestad and Postlethwaite (1996), who utilized the Performance Relative Gain Array (PRGA) and the Closed Loop Disturbance Gain (CLDG) to tune MIMO systems with diagonal control. The closed loop analysis is based on an approximation of the closed loop error $e$ in response on disturbances $d$ and references $r$, containing PRGA ($\Gamma$) and CLDG ($\tilde{G}_d = \Gamma G_d$):

$$e = SG_d d - Sr \approx \tilde{S}G_d d - \tilde{S}\Gamma r$$ (2.51)

The crucial assumption here is that the sensitivity matrix $S$, which in principle is a complex function of all the controller gains and the whole plant behavior, is decoupled and approximated by a product of two terms, $S \approx \tilde{S}\Gamma$. The diagonal sensitivity matrix $\tilde{S} = \text{diag}\{1/(1 + k_i g_i)\}$, $g_{ij}$ being the open loop gain and $k_i$ the controller gain, has only diagonal elements. Therefore, the two terms of the error expression also are diagonal matrices of which the elements may be evaluated loop-by-loop. Due to the approximation these responses have become split into the diagonal sensitivity and the plant transfer matrices, corrected for interaction, $\tilde{G}_d$ and $\Gamma$. The diagonal form of $\tilde{S}$ allows the evaluation of the individual controllers independent from the others, which is convenient for tuning. In
Chap. 3

addition, the PRGA and CLDG allow analyzing the impact of the diagonal control structure through interaction prior to tuning. In other words PRGA and CLDG measure the changed input-output behavior under diagonal closing, which helps to predict the impact of each diagonal controller, before it is actually implemented. Thus, PRGA and CLDG have some resemblance to RGA, which also describes the impact of loop closing on the input-output behavior, but in a different manner, as will be explained in the next section. As regards the physical interpretation of the PRGA and CLDG matrices, it will be explained how they represent real responses on setpoint changes and disturbances. Here, we will first explain the significance of PRGA in comparison with RGA in the context of setpoint tracking and illustrate this on the VCM example. Then along similar lines CLDG will be explained as serving disturbance rejection. After that, PRGA and CLDG will be applied to the tuning of the diagonal controller.

3.7.2.1 Performance Relative Gain Array

The performance relative gain array (PRGA) may be explained with the ordinary RGA as a reference. The RGA measures the interaction characteristics of a plant by comparing the open loop performance to the closed loop performance assuming ideal setpoint tracking of the outputs. It is used to identify the optimal input-output pairing in diagonal control, but not all elements are usable to analyze the performance of the controller. Only the elements corresponding to the selected input-output pairs - preferably being closest to 1 and positioned on the diagonal of the RGA - are relevant. The PRGA also measures plant interaction, but in a different way, allowing to analyze the controller performance. From the derivation of the PRGA (Γ) in chapter 2 (eq. 2.49) it may be realized that the diagonal elements of G follow as

\[ \tilde{G} = \Gamma G, \]

in other words, Γ represents the inverse of the off-diagonal plant elements. Since these off-diagonal elements are responsible for the interaction, causing other outputs to change rather then changing the desired output, Γ is a certain measure for this interaction. More precisely stated, the closed loop response of any output i on a unit step change of the setpoint of one output r_j follows from Γ as element γ_{ij}, be it under the following assumptions. Firstly, every loop is assumed to be closed according to a diagonal control structure, and secondly, the controller gain k_i is assumed to be zero. Hence, in equation 2.51 \( \tilde{S} = I \) and the response becomes equal to Γ for a setpoint change of 1. Hence, these values have a clear, physical meaning in the performance analysis of the diagonal controller with unit setpoint changes. Exact setpoint tracking would imply values equal 1 for the diagonal elements of Γ,
meaning absence of interaction. Since RGA and PRGA diagonal elements are equal, PRGA does not give more information as regards the diagonal. However, the off-diagonal PRGA elements are a measure of the interactions in the diagonally controlled plant. Zero values mean no interactions. Non-zero values show quantitatively to which extent the setpoint tracking of one particular output has impact on the other outputs. If control on boundaries rather than setpoint tracking is acceptable for those other outputs, then the criterion is that PRGA elements should not exceed one. This means that the setpoint tracking of one output does not lead to violation of boundaries for the other outputs that evidently are automatically kept under control. However, values larger than 1 indicate violations of boundaries indeed, which means that the setpoint tracking of one output simultaneously requires additional control action to keep other outputs within boundaries. The tuning of such a controller is discussed in section 3.8.

As another interesting difference between RGA and PRGA it should be realized that PRGA is also the more sensitive instrument, since it not only allows for 2-way interactions like RGA, but also takes 1-way interactions into account. If an open loop input-output pair has a zero gain, meaning no direct influence of the input on that output, the corresponding PRGA may have a finite value $>0$, indicating that this particular output is affected by the input indirectly via the diagonal control structure, hence by pure interaction. Note that the PRGA is analyzed in the frequency domain, which should represent physically realistic fluctuations in setpoint tracking, supposed to take place for operational reasons.

We will perform now a PRGA analysis on the VCM plant. Figure 3.8 shows the effect of a setpoint change of impurity $I_3$ between the bounds [-1,1] as a function of frequency, assuming that the diagonal control structure $I_1$-Q2, $I_2$-SS2, $I_3$-D2 is implemented in the basic flowsheet. The setpoint tracking of $I_3$ in itself is effective at low frequencies, while the unwanted impact on $I_1$ and $I_2$ is acceptable. The PRGA elements for these two impurities are close to zero, that for $I_2$ being somewhat higher. At higher frequencies, where the interactions between the control loops become significant, all impurities will exceed their bounds, so feedback control is no longer effective. Figure 3.9 shows the performance of the alternative diagonal structure $I_1$-Q2, $I_2$-SS2, $I_3$-D4 for the same setpoint tracking problem. Again, at low frequencies $I_3$ is controlled effectively, while the impurities $I_1$ and $I_2$ are only slightly affected. However, $I_1$ will exceed bounds at somewhat lower frequency than before. Note that although both structures show violations at high frequencies, this is not expected to be a problem in operation since the setpoint of the initiator for the cracking process is not normally changed
at such high frequencies. In conclusion, the PRGA analysis shows both diagonal structures to be nearly equivalent: if only \( I_3 \) is controlled on setpoint, the other impurities are automatically kept between boundaries, so no additional control action is required.

Now, it is interesting to see the impact of a flowsheet change - the addition of an extra impurity-destroying reactor R4 - on the setpoint tracking performance, when the same two control structures are implemented. Figure 3.10 shows the performance of the control structure \( I_1\text{-}Q2, I_2\text{-}SS2, I_3\text{-}D2 \) to be similar to that of the same structure in the base case flowsheet (Figure 3.8), although the unwanted impact on \( I_1 \) and \( I_2 \) is somewhat smaller. The same holds for the second diagonal control structure, \( I_1\text{-}Q2, I_2\text{-}SS2, I_3\text{-}D4 \) (Figure 3.11), which shows a similar performance as that structure in the base case. In conclusion, the introduction of the extra reactor R4 in the alternative flowsheet has only a minor improving effect on the performance of the diagonal controller when setpoint tracking is concerned.

![Figure 3.8; Performance Relative Gain Array elements for the effect of a reference change of \( I_3 \) on the outputs \( I_1, I_2 \) and \( I_3 \) with the diagonal control structure \( I_1\text{-}Q2, I_2\text{-}SS2, I_3\text{-}D2 \) in the basic VCM plant](image)

The figure shows that \( I_3 \) is controlled close to its new reference value of 1 while \( I_1 \) will remain close to zero. \( I_2 \) is greatly affected as a result of the interaction between the control loops at low frequencies. At higher frequencies this effect is reduced. All PRGA elements show a fast increase at frequencies where the response of the system goes to zero. At these frequencies feedback control is no longer effective.
The control of $I_3$ with $D_4$ follows the fluctuation of the reference value of $I_3$ between $-1$ and $1$, while $I_1$ and $I_2$ are hardly affected. The decreased magnitude of $D_4$ at intermediate frequencies is reflected by an increased effect of the reference change of $I_3$ on the control of $I_1$. However, reference values are seldom changed at these frequencies.

The magnitude of $D_2$ on $I_3$ is larger in the plant with reactor $R_4$, relative to the base case (Figure 3.8), while the magnitude of $D_2$ on $I_2$ is lower. This is reflected by this figure of PRGA elements. The impurities $I_1$ and $I_2$ are less affected by a reference change of $I_3$ than in the base case.
Figure 3.11: Performance Relative Gain Array elements for the effect of a reference change of $I_3$ on the outputs $I_1$, $I_2$ and $I_3$ with the diagonal control structure $I_1$-Q2, $I_2$-SS2, $I_3$-D4 in the alternative flowsheet with additional reactor R4

If this figure is compared to Figure 3.9, we see that the effect of a reference change of $I_3$ on $I_1$ and $I_2$ remains low for a larger frequency range. This is a result of the lower magnitude of $D_4$ on $I_1$ and $I_2$, relative to the base case.

3.7.2.2 Closed Loop Disturbance Gain

The performance of diagonal feedback control with respect to disturbance rejection is studied by calculating the closed loop disturbance gains (CLDG), denoting the effect of a disturbance on the outputs when a diagonal control structure is implemented. This is another tool, also introduced by Skogestad and Postlethwaite (1996) to analyze the output sensitivity of the plant as changed by the diagonal control structure, before actually tuning it. In this respect the CLDG may be compared to the open loop disturbance gain of the outputs. When scaled open loop disturbance gains remain below 1 then, according to the acceptable control criterion, one would guess that control is not necessary at all for such outputs, since they would stay within bounds even without control. Applying the same reasoning to a diagonally closed plant, finding closed loop gains below 1 would imply that no control for the associated outputs is needed, since these stay within boundaries for any disturbance. This is reflected in the elements of CLDG that physically represent the closed loop responses on disturbances for a diagonal control structure and zero controller gains. According to equation 2.51 this means $\bar{S} = I$, so the response equals $\bar{G}_d$. When CLDG elements are below 1, the corresponding outputs are automatically under control due to the diagonal control structure and the
interactions invoked by this. Note that this is the result of the concerted action of all the manipulated variables acting on this output under the diagonal control structure. It might well be that not all of these manipulated variables do have an open loop effect on this output. In such a case disturbance rejection is realized only because of interaction. Now, if a CLDG element exceeds 1, then indeed extra control action is necessary to realize disturbance rejection and keep this output within boundaries. The tuning of such a controller is discussed in the next section.

The CLDG analysis has been applied on the VCM example for two disturbances, the feed stream $F_{DCE}$ and the concentration of impurity $I_3$ in this feed stream, $X_{13}$, under the 2 diagonal control structures mentioned above, for both flowsheet alternatives. The results are shown in Figure 3.12 to Figure 3.19. Figure 3.12, showing all CLDG elements to be above one, indicates the necessity of extra control action to reject disturbances of the feed flow $F_{DCE}$ on any of the impurity levels for the structure $I_1$-$Q_2$, $I_2$-$SS_2$, $I_3$-$D_2$ in the base case. Figure 3.13 indicates for the other disturbance ($X_{13}$), that impurity $I_1$ in this case automatically stays within acceptable bounds when only $I_2$ and $I_3$ are controlled, hence the system is almost indifferent to the presence or absence of the controller $I_1$-$Q_2$.

Figure 3.14 shows the behavior of the alternative control structure $I_1$-$Q_2$, $I_2$-$SS_2$, $I_3$-$D_4$ to be improved with respect to disturbance $F_{DCE}$, since here impurity $I_2$ does not require control, while $I_1$ and $I_3$ still do. Figure 3.15 also shows improvement for the other disturbance, since under the alternative structure only $I_3$ needs control and $I_2$ and $I_1$ do not. Hence, in the base case flowsheet the structure $I_1$-$Q_2$, $I_2$-$SS_2$, $I_3$-$D_4$ performs best, since impurity $I_2$ never requires control. Figure 3.16 shows a result for the alternative flowsheet containing the reactor $R_4$. Disturbance $F_{DCE}$ in structure $I_1$-$Q_2$, $I_2$-$SS_2$, $I_3$-$D_2$ requires impurities $I_1$ and $I_3$ to be controlled only, so the controllability of this flowsheet is slightly better than that of the base case. Figure 3.17 shows this situation even to be improved for the $X_{13}$ disturbance, only requiring control for $I_3$. Figure 3.18 and Figure 3.19 indicate that the alternative control structure $I_1$-$Q_2$, $I_2$-$SS_2$, $I_3$-$D_4$ does not lead to further improvement in this flowsheet, like it did in the base case. For disturbance $F_{DCE}$ $I_1$ and $I_3$ and for $X_{13}$ again only $I_3$ have to be controlled.

In conclusion, both the alternative control structure and the alternative flowsheet structure perform better than the base case. Choosing the best alternative, still always $I_3$ has to be controlled with $D_4$, while for disturbance $F_{DCE}$ also $I_1$ has to be controlled with $Q_2$. 
Figure 3.12; Closed Loop Disturbance Gains for the feed disturbance $F_{DCE}$ on the outputs $I_1$, $I_2$ and $I_3$ with the diagonal control structure $I_1$-Q2, $I_2$-SS2, $I_3$-D2 in the basic VCM plant

The figure shows that all three impurities are affected by the feed disturbance in this closed loop system and therefore need to be controlled.

Figure 3.13; Closed Loop Disturbance Gains for the impurity disturbance $X_{13}$ on the outputs $I_1$, $I_2$ and $I_3$ with the diagonal control structure $I_1$-Q2, $I_2$-SS2, $I_3$-D2 in the basic VCM plant

This figure shows that $I_1$ is hardly affected by the impurity disturbance with this control structure, while $I_2$ and $I_3$ need only to be controlled at low frequencies.
Figure 3.14; Closed Loop Disturbance Gains for the feed disturbance $F_{DCE}$ on the outputs $I_1$, $I_2$ and $I_3$ with the diagonal control structure $I_1$-Q2, $I_2$-SS2, $I_3$-D4 in the basic VCM plant.

This figure shows that $I_2$ is hardly affected by the feed disturbance in this control structure with $D4$. This is in contrast with the base case, where $I_3$ is controlled with $D2$.

Figure 3.15; Closed Loop Disturbance Gains for the impurity disturbance $X_{I3}$ on the outputs $I_1$, $I_2$ and $I_3$ with the diagonal control structure $I_1$-Q2, $I_2$-SS2, $I_3$-D4 in the basic VCM plant.

The impurities $I_1$ and $I_2$ are hardly affected by the impurity disturbance, while $I_3$ is only affected at low frequencies.
Figure 3.16; Closed Loop Disturbance Gains for the feed disturbance $F_{DCE}$ on the outputs $I_1$, $I_2$ and $I_3$ with the diagonal control structure $I_1$-$Q2$, $I_2$-$SS2$, $I_3$-$D2$ in the alternative flowsheet with additional reactor R4.

The introduction of reactor R4 lowers the closed loop disturbance gains. As a result of the controller interactions, $I_2$ will be kept between its bounds and does not need to be controlled itself for this disturbance.

Figure 3.17; Closed Loop Disturbance Gains for the impurity disturbance $X_{13}$ on the outputs $I_1$, $I_2$ and $I_3$ with the diagonal control structure $I_1$-$Q2$, $I_2$-$SS2$, $I_3$-$D2$ in the alternative flowsheet with additional reactor R4.

The Closed Loop Disturbance Gain of $I_3$ becomes larger with R4, but that of $I_2$ is lower.
Figure 3.18; Closed Loop Disturbance Gains for the feed disturbance $F_{DCE}$ on the outputs $I_1$, $I_2$ and $I_3$ with the diagonal control structure $I_1$-$Q_2$, $I_2$-$SS_2$, $I_3$-$D_4$ in the alternative flowsheet with additional reactor $R_4$

The Closed Loop Disturbance Gains with reactor $R_4$ are all lower than without this reactor.

Figure 3.19; Closed Loop Disturbance Gains for the impurity disturbance $X_{I3}$ on the outputs $I_1$, $I_2$ and $I_3$ with the diagonal control structure $I_1$-$Q_2$, $I_2$-$SS_2$, $I_3$-$D_4$ in the alternative flowsheet with additional reactor $R_4$

With reactor $R_4$ included, both $I_1$ and $I_2$ are not affected by the impurity disturbance.
3.7.2.3 Relative Disturbance Gain

The ratio between the closed loop disturbance gain and the open loop disturbance gain, giving the change in input-output behavior due to diagonal feedback control, is called the relative disturbance gain (RDG). The elements of this matrix are preferably smaller than one, which would mean that the interactions between the controllers are such that they reduce the apparent effect of the disturbance. In such cases relatively small gains are sufficient for the individual loops. However, they may also be larger than 1, indicating that the apparent effect is enhanced instead, implying high gains for the loops concerned.

Assuming the structure I₁-Q₂, I₂-SS₂, I₃-D₄ in the base case flowsheet and the concentration of impurity I₃ in the DCE feed (X₁₃) as the disturbance this time, RDG values have been plotted in Figure 3.20 for all three impurities. At low frequencies they are below one, so the system can be controlled with small controller gains. At frequencies between 1 and 10 h⁻¹ the RDG elements rise to high values, indicating an opposite direction of the controller interactions, which complicates control of the impurities. At these frequencies control would not even be possible, but this is not a problem since according to the CLDG elements, the impurities are automatically kept between their bounds, hence control is also not required.

![Graph showing RDG values](image)

**Figure 3.20; Relative Disturbance Gains of impurity I₃ in the external DCE feed X₁₃ for the outputs I₁, I₂, and I₃ with diagonal control structure I₁-Q₂, I₂-SS₂, I₃-D₄ in the basic VCM plant**

This figure shows that the apparent effect of the disturbance on I₂ with this control structure implemented is reduced enormously at low frequencies, so a low controller gain would be enough. At higher frequencies, the closed loop disturbance gains are higher than the open loop disturbance gains due to negative controller interactions. However, the absolute values are low in this frequency range and therefore no control is needed.
Figure 3.21: Relative Disturbance Gains of the external DCE feed flowrate $F_{\text{DCE}}$ for the outputs $I_1$, $I_2$, and $I_3$ with diagonal control structure $I_1$-Q2, $I_2$-SS2, $I_3$-D4 in the basic VCM plant

This figure shows that the apparent effect of the flow disturbance on $I_2$ with this control structure implemented is also reduced enormously at low frequencies, so a low controller gain would be enough. At higher frequencies, the closed loop disturbance gains are again higher than the open loop disturbance gains due to negative controller interactions.

Another disturbance, the step on the DCE feed ($F_{\text{DCE}}$), gives also rise to RDG elements less than one at low frequencies (Figure 3.21), but they are not so high at intermediate frequencies. So, for this disturbance the apparent effect of the controller interactions is such that the open loop behavior is less affected.

Especially the RDG values of $I_2$ at low frequencies are very small for both disturbances. The controller interactions are such that the apparent effect of the disturbances on $I_2$ is reduced enormously and only small controller gains are needed. This is in agreement with the conclusion from the CLDG analysis that $I_2$ does not need to be controlled because it is automatically kept between its bounds due to controller interactions.

3.8 Tuning the diagonal controller

The tuning of MIMO control systems with classical (SISO) tuning methods like Cohen-Coon and Ziegler-Nichols is frustrated by interaction, since tuning of one loop is influenced by tuning of the other ones. This problem is overcome using the controllability tools PRGA and CLDG that provide means to perform tuning of a diagonal control system loop-by-loop, by
capturing the interaction impact in one matrix, the PRGA matrix \( \Gamma \). This may clearly be seen from equation 2.51, showing the error to be approximated by terms that each are products of the diagonal sensitivity matrix \( \tilde{S} \) with \( \tilde{G}_d \) and \( \Gamma \) for disturbance rejection and reference tracking, respectively. Evidently, small errors are realized by small \( \tilde{S} \) or small \( \tilde{G}_d \) and \( \Gamma \) values. The impact of the latter has been discussed in the previous section. Here, we are interested in tuning criteria, also derived from the mentioned error expression.

In chapter 2 it has been shown that for disturbance rejection in order to keep the outputs between their bounds \([-1,1]\), the value of \((\tilde{S})^{-1} = \text{diag}\{(1 + k|g_{ij}|)\}\) should be larger than the closed loop disturbance gain \( \tilde{G}_d \) over the whole frequency range where control is needed (eq. 2.53). Since \( \tilde{S} \) has diagonal elements only and so has the product of \( \tilde{S} \) with \( \tilde{G}_d \), this inequality may be tested for each loop individually by comparing the diagonal elements \((1 + k|g_{ii}|)\) with \( \tilde{g}_{ai} \). The proportional gains then are determined by plotting \((1 + k|g_{ii}|)\) and \( \tilde{g}_{ai} \) for all disturbances in one frequency graph and choosing \( k_i \) in such a way that the former curve always lies above the latter ones in the required part of the frequency domain.

This has been carried out for the VCM case, resulting in Figure 3.22 to Figure 3.25. From the previous section it was concluded that for the base case flowsheet and control structure \( I_1\)-Q2, \( I_2\)-SS2, \( I_3\)-D2 impurities \( I_2 \) and \( I_3 \) always would have to be controlled. Now, we will investigate whether this is possible indeed, first for \( I_2 \) then for \( I_3 \). Figure 3.22 shows the impact on impurity \( I_2 \) for changes in the two disturbances analyzed before: \( F_{DCE} \) (dashed curve) and \( X_{13} \) (dotted curve), the former having a more serious impact. The figure shows the open loop gain of the manipulated variable to control \( I_2 \), in this structure being \( g_{22} = SS2 \). Since this gain is lower than the CLDG curves, there is not enough input magnitude to control \( I_2 \) on setpoint. On the other hand, the curve of \((1 + k_2g_{22})\) for a maximum (scaled) controller gain of 1 lies entirely above the CLDG of the \( I_3 \) disturbance of the DCE feed \( \tilde{g}_{d2} \) (\( d = X_{13} \)), so this disturbance can be rejected and control of \( I_2 \) within bounds for this disturbance is possible. However, at low frequencies \((1 + k_2g_{22})\) is smaller than \( \tilde{g}_{d2} \) (\( d = F_{DCE} \)), so there is lack of control power for the feed disturbance and \( I_2 \) will become outside its bounds.
Figure 3.22; Input magnitude of SS2 and loop transfer function of I2−SS2 with the Closed Loop Disturbance Gains for the diagonal control structure I1−Q2, I2−SS2, I3−D2 in the basic VCM plant

This figure shows that the effect of the disturbances in a closed loop system is higher than the available control power (input magnitude). Therefore I2 cannot be controlled on setpoint with SS2 in this control structure. It also shows that SS2 has not enough magnitude to keep I2 between its bounds. The closed loop transfer function with the maximum controller gain of I has still a lower value than the closed loop disturbance gain of the feed step.

Figure 3.23; Input magnitude of D2 and loop transfer function of I3−D2 with the Closed Loop Disturbance Gains for the diagonal control structure I1−Q2, I2−SS2, I3−D2 in the basic VCM plant

This figure shows that D2 has not enough input magnitude and I3 can not be controlled between its bounds in this control structure at low frequencies.
Chapter 3

Figure 3.24: Input magnitude of SS2 and loop transfer function of $I_2-SS2$ with the Closed Loop Disturbance Gains for the diagonal control structure $I_1-Q2$, $I_2-SS2$, $I_3-D4$ in the basic VCM plant.

This figure shows that the apparent effect of the disturbances in this control structure is such that the impurity $I_2$ remains between its bounds and therefore does not have to be controlled (controller gain zero). However, there is enough input magnitude to control $I_2$ on setpoint.

Figure 3.25: Input magnitude of D4 and loop transfer function of $I_3-D4$ with the Closed Loop Disturbance Gains for the diagonal control structure $I_1-Q2$, $I_2-SS2$, $I_3-D4$ in the basic VCM plant.

From this figure it is seen that D4 has enough input magnitude to control $I_3$ on setpoint. To keep $I_3$ only between its bounds, the control capacity available is not even fully required. A scaled controller gain of 0.36 is sufficient.
Figure 3.23 shows a similar plot for impurity I₃, in this control structure to be controlled with D₂. It shows that D₂ lacks control power to control either of the two disturbances on setpoint or within bounds. In conclusion, where the previous analysis indicated the necessity to control I₂ and I₃ indeed, finally it turns out from the tuning procedure, that control within bounds is not possible in this case.

Regarding the alternative control structure I₁-Q₂, I₂-SS₂, I₃-D₄, in the previous section it has been concluded that never control was required for I₂, while control is needed always for I₃ and sometimes for I₁. Figure 3.24 confirms this conclusion for I₂, showing \((1 + k₂g₂₂)\) always to be larger than \(g_{d₂}\), even with zero gain. In contrast, impurity I₁ needs control and from Figure 3.25 it indeed appears to be possible for a controller gain even below the maximum.

In conclusion, the closed loop controllability tools indeed are able to discriminate between various control and flowsheet alternatives, proving that the two flowsheets are controllable with the alternative control structure, while they are not with the basic control structure. The closed loop tuning technique proved to confirm this conclusion and was successfully used to tune the alternative controller with respect to the control of I₃ with D₄.

### 3.9 Closed loop simulations

Closed loop simulations with the full nonlinear dynamic model have been carried out to compare with the results of the controllability analysis. Figure 3.26 and Figure 3.27 show the response of impurities I₂ and I₃, respectively, on a feed disturbance \(F_{DCE}\) for the base case flowsheet and several control structures. Implementing only one controller, I₁ with Q₂, automatically yields effective control of I₂, but that is not so for I₃, although the response is suppressed to some extent. Again assuming a 1-controller system but this time controlling I₂ with SS₂ gives surprisingly bad results for I₂ itself and the result for I₃ is even worse. Another 1-controller system that is evaluated, I₃ with D₂, produces bad performance for both impurities. However, controlling I₃ with D₄ works out very well for I₃, but only poorly for I₂. Hence, none of the 1-controller systems works satisfactorily for both impurities, which is in agreement with the controllability analysis.

Two 2-controller systems have been implemented. The system I₁-Q₂, I₂-SS₂ performs very well for I₂ but does not keep I₃ within bounds, even when a 3rd controller is added, I₃-D₂, which is in agreement with the controllability results, predicting bad performance for all
impurities in case of control structure $I_1$-$Q_2$, $I_2$-$SS_2$, $I_3$-$D_2$. The 2-controller system $I_1$-$Q_2$, $I_3$-$D_4$ works well for all impurities, which also fits with the controllability analysis, indicating a better performance for the alternative control structure $I_1$-$Q_2$, $I_2$-$SS_2$, $I_3$-$D_4$. Hence, it is also confirmed that a 3rd controller, to control $I_2$, is not necessary.

Closed loop simulations with the controller structure $I_1$-$Q_2$ and $I_3$-$D_4$ implemented in the flowsheet with reactor R4 showed that the disturbances are reduced with about the same amount. Since the nominal values of impurities $I_1$ and $I_2$ are lower in this flowsheet structure, their values stay lower in the closed loop simulations with disturbances. Impurity $I_3$ follows the same pattern. However, all impurities show a small oscillation on their main pattern with a period of about 10 minutes. A closer examination shows that this is caused by $Q_2$. The step response has an overshoot on all disturbances in the first 10 minutes. In the closed loop simulations, the controllers are continuously correcting this overshoot on a short time period, while on the longer term they also control the disturbance. Although this oscillatory behavior is a disadvantage, the lower values of $I_1$ and $I_2$ make this alternative flowsheet preferable above the base case, which again confirms the controllability conclusions.

![Figure 3.26; Closed Loop Dynamic responses of $I_2$ to a step disturbance on $F_{DCE}$](image)

*Figure 3.26; Closed Loop Dynamic responses of $I_2$ to a step disturbance on $F_{DCE}$*

*When only the controller $I_1$-$Q_2$ is implemented, $I_2$ is kept between its bounds, while only implementing the controller $I_2$-$SS_2$ this is not the case. $SS_2$ will reach its bound in that situation. When both controllers are combined ($I_1$-$Q_2$ and $I_2$-$SS_2$) $I_2$ is kept between its bounds. When the controller $I_3$-$D_2$ is the only active one, $I_2$ is increased relative to the open loop response, while the controller $I_3$-$D_4$ has a reducing effect on $I_2$.***
Control of $I_1$ with $Q2$ reduces the effect of the disturbance on $I_3$ more than when $I_3$ itself is controlled with $D2$. In this case $D2$ reaches its bound and $I_3$ cannot be controlled further. This is still the case when all three controllers $I_1-Q2$, $I_2-S2$ and $I_3-D2$ are implemented. However, $I_3$ can be controlled with $D4$. Because this also reduced the disturbance effect on impurity $I_1$, the closed loop response of $I_3$ with both controllers $I_1-Q2$ and $I_3-D4$ is slightly higher, but the impurity is kept well between its bounds $[-1,1]$.

### 3.10 Conclusions

In chapter 2 we have presented a simulation based methodology for evaluating flowsheet design and control alternatives on their controllability and closed loop behavior. In this chapter the systems approach is illustrated with an industrial case study concerning the removal of impurities in a balanced VCM process. It is shown that the combination of steady state and dynamic simulations, together with a linear controllability analysis in the frequency domain improves understanding of the behavior of a large plant with complex recycle structure to a greater extent than extensive steady state simulations only.

It is furthermore shown that the material balance of impurities in the VCM plant is a plantwide problem. It is demonstrated how the interaction between recycles may be exploited to create flowsheet and control alternatives with feasible plantwide control properties that cannot be reached with the stand-alone column. Using the positive feedback effects of the recycle streams and the negative feedback effects of chemical reactors and exit streams gives a flowsheet design and control structure alternative with acceptable control properties. In this
structure the manipulated variables belong to different units, as already could be expected from the steady state analysis. The interaction between the controllers is such that all three impurities can be kept between their bounds with only two controllers implemented. This was predicted by the controllability analysis and confirmed by the closed loop simulations, but a steady state analysis alone turned out to be insufficient to obtain this result. This proves that a linear controllability analysis in the frequency domain with tools like PRGA and CLDG is useful and is capable to discriminate between flowsheet and control alternatives in an effective way. Especially, using the controllability analysis it appeared that the problems mainly originate from the interaction between the different units in the flowsheet. This also illustrates the difference in nature between the controllability characteristics of a plant as compared to those of a single column. Column dynamics may be complex as well, but they do not offer such a wide variety of problem causes distributed in unknown ways over the system and consequently do not possess so many unexpected ways to solve those problems. These solutions also are less well detectable by intuitive means, and stress the importance of controllability tools even more.

The case study was devoted to a large complex plant, the Vinyl Chloride Monomer plant. It showed that the material balance of impurities is always in a transient with time constants in the order of days, making a dynamic analysis unavoidable. The steady state analysis suggested to use the side stream SS2 as a manipulated variable to control one of the impurities (I2). However, dynamic simulations showed that this gives a serious inverse response. Controllability analysis tools indicated the shortcoming of input magnitude and closed loop simulations showed that a new steady state could not even be achieved. Changing the control loop for another impurity, using D4 instead of D2 to control I3, reduces the apparent effect of the disturbance such that control of I2 is no longer needed. The improved performance of this control alternative could never have been predicted by intuition.

The introduction of an additional reactor to destroy impurities that are difficult to remove was expected to give an improved performance. We have seen that the behavior of the alternative flowsheet structure, both steady state and dynamic, is different, especially with respect to D2. It was shown that control of I2 is not needed even with the basic control structure. However, also this design alternative does not have enough control power to keep I1 and I3 between its bounds under disturbances with this control structure. Again the alternative control structure should be used. So, the control structure turned out to be more important than the design.
However, the design alternative has lower levels of impurities, resulting in larger scaling factors. In fact this implies more operational freedom and therefore this design alternative, in combination with the alternative control structure, is preferable.

The introduction of the extra reactor gives access to alternative flowsheets with different recycle structures. The effect of these design modifications on the performance of the system will be studied in the next chapter.