IMPLEMENTATION OF OPTIMAL OPERATION FOR HEAT INTEGRATED DISTILLATION COLUMNS

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ABSTRACT

A multi-effect distillation where the condenser of a high pressure column is integrated with the reboiler of a low pressure column has been studied. The method of self-optimizing control has been used to provide a systematic procedure for the selection of controlled variables, based on steady state economics. The heat integrated distillation system was optimized to find the nominal operating point and it was found that a temperature in the low pressure column has good self-optimizing properties. The study also shows how there can be multiplicities in the objective function for certain variables in the system.

INTRODUCTION

Distillation is an energy consuming process that is used for about 95% of all fluid separation in the chemical industry and accounts for an estimated 3% of the world energy consumption [1]. Heat integration of distillation columns, where the condenser of one column is coupled with the reboiler of another column, is used to reduce the energy consumption of distillation. Typically the reduction in energy consumption is 50%. It is very important that such heat integrated columns are operated correctly so that the plant is operational and the energy savings are achieved. However, the task of identifying a suitable control structure for heat integrated distillation columns is not as straightforward as for a single column.

We study a system (see Figure 1) where the higher pressure in the first column allows the condensing heat from the top to be used to boil the second column. This is a forward integration as mass and heat are both integrated in a forward direction.

Other multi-effect configurations are for example dual feed and reverse integration [2].

A number of studies are concerned about the dynamics and control of multi-effect distillation. Tyreus and Luyben [3] published one of the first papers in this area.
addressing the control of the dual feed configuration. Their main conclusion was to decouple the two columns by introducing an auxiliary reboiler and condenser. Other authors have discussed the use of an auxiliary reboiler and condenser. Lenhoff and Morari [4] questioned their conclusion since they did not find such an effect. Gross et al. [5] used an auxiliary reboiler in their simulations, but noted that even if an additional reboiler provides an additional manipulated variable it may also lead to severe interaction problems.

The work by Roffel and Fontein [6] is most similar to our work. They discuss some aspects related to constrained control. Much of their discussion is based on steady state economics and active constraints.

Frey et al. [7] recommended using ratios of material flows as manipulated variables after examining four different control schemes for the dual feed case with and without mass integration. They used the relative gain array (RGA) as a controllability measure. Much of the above work used simple models that did not include important effects, like flow dynamics and heat transfer area. Gross et al. [5] presents results for a rigorous model where they used controllability analysis and non-linear simulations for a dual feed industrial heat integrated process. They conclude that a detailed model is needed in order to capture essential details.

The objective of this work has been on the selection of controlled variables, that is, finding which variables that should be controlled. We use the concept of self-optimizing control [8], which is based on steady state economics, to provide us with a systematic framework for the selection of the controlled variables. This method involves a search for the variables that, when kept constant, indirectly lead to near-optimal operation with acceptable economic loss. In self-optimizing control, rather than solving the optimization problem on-line, the problem is transformed into a simple feedback problem [8]. In practice, this means that when the plant is subject to disturbances it will still operate within an acceptable distance from the optimum, and there is no need to re-optimize when disturbances occur. This paper uses this method to find which variables should be controlled for a multi-effect distillation case so that the system will operate near the optimum.

MODELLING

The system studied is a multi-effect separation of methanol and water with small amounts of ethanol present in the feed (see Table 1 for feed and column data). The feed enters the high pressure (HP) column where methanol at 99% is the top product (see Figure 1). The bottom stream from the HP column containing methanol, water and a small amount of ethanol goes to the low pressure (LP) column where the final separation between methanol and water takes place. In the LP column the top product is also methanol at 99% and the bottom product is water at > 99% purity. The LP column has also a small side stream, below the feed stage, to prevent ethanol building up in the bottom parts of the column. Heat is transferred from the condenser in the high pressure column to the reboiler in the low pressure column.
We use a “rigorous” model where the energy, material (overall) and component balances are included. Holdup in the vapour phase has been neglected. This considerably simplifies the model and is usually a good assumption when the pressure is below 10 bar [9]. The vapour-liquid equilibrium has been modelled by assuming ideal gas and using liquid activity coefficients for the ternary system from the Wilson equation. The parameters used are from Gmehling and Onken [10]. To model the liquid flows we have used a simplified Francis weir formula. In the dynamic model the vapour flow, \( V_i \), on a stage \( i \) has been modelled using a valve type equation for the pressure drop from one stage to the next:

\[
V_i = c \sqrt{\frac{P_{i-1}^2 - P_i^2}{P_i^2 - P_{i+1}^2}}
\]  

(1)

For the integrated reboiler/condenser we have calculated the heat duty from:

\[
Q = U A (T_{THP} - T_{BLP})
\]  

(2)

where \( T_{THP} \) is the temperature at the top of the HP column and \( T_{BLP} \) is the temperature in the bottom of the LP column.

In the optimization, the area, \( A \), is treated as a degree of freedom and there is a maximum available area for the exchanger \( (A_{\text{max}}) \). An alternative to using a maximum area would be to specify an allowable temperature difference, \( \Delta T_{\text{min}} \), for the exchanger. If area is totally unconstrained and with no minimum allowable temperature difference then it would be optimal to have an infinite area.
Table 1. Feed and column data

<table>
<thead>
<tr>
<th>Feed &amp; Column Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>Feed rate: 1200 mol/s</td>
</tr>
<tr>
<td>Feed composition:</td>
</tr>
<tr>
<td>73 mol% methanol</td>
</tr>
<tr>
<td>2 mol% ethanol</td>
</tr>
<tr>
<td>25 mol% water</td>
</tr>
<tr>
<td>Feed liquid fraction:    q_F =1</td>
</tr>
<tr>
<td>No. stages HP column: 36</td>
</tr>
<tr>
<td>No. stages LP column: 48</td>
</tr>
</tbody>
</table>

SELF-OPTIMIZING CONTROL

The self-optimizing control procedure [8] consists of six steps: 1) a degree of freedom (DOF) analysis, 2) definition of cost function and constraints, 3) identification of the most important disturbances, 4) optimization, 5) identification of candidate controlled variables and 6) evaluation of loss with constant setpoints for the alternative sets of controlled variables.

The multieffect column (see Figure 1) has 11 dynamic (control) degrees of freedom: the feed rate, heat duty in the HP column, reflux in HP and LP columns, distillate flows in HP and LP column, heat transfer rate/area in the integrated condenser/reboiler, the bottom flow in the HP and LP column, the cooling in the LP column and the sidestream in the LP column. There are 4 levels (condenser and reboiler in each column) with no steady-state effect (and thus with no effect on the cost) that have to be controlled, and with the feed rate given, this leaves 6 DOFs for optimization.

In the formulation of the objective function there are two ‘conflicting’ elements; we would like to produce as much valuable product as possible, but using as little energy as possible. For a given feed, the cost function is defined as the amount of distillate (0.99 mol% methanol) multiplied by the price of methanol, minus the cost of boilup:  
\[
J = P_d (D_{HP} + D_{LP}) - P_v V_{HP} .
\]

As we would like to maximise the profit we have to minimise (-J). To simplify we have used a relative cost of energy, so the objective function to be maximised is:

\[
J = D_{HP} + D_{LP} - w_r Q_{HP}
\]  
(3)

where \(D_{HP} + D_{LP}\) (mol/s) are the top products (methanol) and \(Q_{HP}\) (MJ) is the heat load to the HP column and \(w_r = 0.6488\) mol/MJ, is the relative cost of energy.

After defining the objective function the system constraints are specified. These are the model equations, i.e. the mass, component and energy balances, for the distillation process (equality constraints) and operational constraints (inequalities) that has to be satisfied at the solution. The following operational constraints have been defined for the multi-effect system:

- The LP column must be operating at a pressure above or equal to 1 bar.
- The HP column must be operating at a pressure below or equal to 15 bar.
The product (distillate) from both columns must contain at least 99% methanol.
The bottom stream from the LP column should contain at least 99% water (i.e. no more then 0.1 % methanol and ethanol).

The optimization problem can then be formulated as:

$$\min_u (-J_u(x,u,d)) \quad \text{objective function}$$

subject to

$$g_1(x,u,d) = 0 \quad \text{model equations}$$

$$g_2(x,u,d) \leq 0 \quad \text{operational constraints}$$

where:
- x – state variables
- u – independent variables we can affect (DOF for optimization)
- d – independent variables we can not affect (disturbances)

By solving the optimization problem we find the nominal steady state operating point, i.e. the optimal operating point for the multi-effect distillation when there are no disturbances. This gives us the optimal nominal values for all the variables in the system. We then have to define the most important disturbances in the system. For this case we have considered disturbances in the feed flow of ± 20 %. Feed composition disturbances have not been considered as it is assumed that it only has small variations. The optimization problem was then solved for the disturbances to find the optimal cost (or profit) for each case, used for calculating the loss. The optimal solution for the nominal case and the two disturbances can be seen in Table 2.

From the optimization it was found that the following five constraints are active:

- the pressure in the LP column - should be 1 bar
- purity in the distillate from the HP column should be at 99 mol% methanol
- purity in the distillate from the LP column should be at 99 mol% methanol
- purity in the bottom stream from the LP column should be at 99 mol% water
- the area should be equal to the maximum area, $A_{\text{max}}$

The pressure constraint for the HP column was not an active constraint as the optimal value of 11.39 bar is below the maximum allowable pressure of 15 bar.
Table 2. Optimum solution for nominal case and for F +20% and F-20%

<table>
<thead>
<tr>
<th>F</th>
<th>J_\text{opt} (mol/s)</th>
<th>X_D,HP</th>
<th>X_D,LP</th>
<th>X_B,HP</th>
<th>X_B,LP (water)</th>
</tr>
</thead>
<tbody>
<tr>
<td>100 %</td>
<td>815.82</td>
<td>0.99</td>
<td>0.99</td>
<td>0.567</td>
<td>0.99</td>
</tr>
<tr>
<td>120 %</td>
<td>850.37</td>
<td>0.99</td>
<td>0.99</td>
<td>0.594</td>
<td>0.99</td>
</tr>
<tr>
<td>80 %</td>
<td>664.65</td>
<td>0.99</td>
<td>0.99</td>
<td>0.5013</td>
<td>0.99</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>P_{LP} (bar)</th>
<th>P_{HP} (bar)</th>
<th>L_{HT} (kmol/h)</th>
<th>V_{B,HP} (kmol/h)</th>
<th>A (m^2)</th>
<th>L_{LT,(kmol/h)}</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0130</td>
<td>11.39</td>
<td>5468.8</td>
<td>7138</td>
<td>5360</td>
<td>3744.1</td>
</tr>
<tr>
<td>1.0130</td>
<td>11.41</td>
<td>5753.4</td>
<td>7532.9</td>
<td>5360</td>
<td>3619.8</td>
</tr>
<tr>
<td>1.0130</td>
<td>11.25</td>
<td>5535.2</td>
<td>7151.5</td>
<td>5360</td>
<td>4331.7</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>V_{D,LP} (kmol/h)</th>
<th>Q_{B,HP} (MW)</th>
<th>\Delta P_{HP} (bar)</th>
<th>T_{b,LP} (K)</th>
<th>T_{2,LP} (K)</th>
<th>T_{4,LP} (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5187.5</td>
<td>66.486</td>
<td>0.76</td>
<td>412.11</td>
<td>404.69</td>
<td>386.63</td>
</tr>
<tr>
<td>5084.8</td>
<td>70.165</td>
<td>0.84</td>
<td>411.99</td>
<td>405.82</td>
<td>384.66</td>
</tr>
<tr>
<td>5284.2</td>
<td>66.612</td>
<td>0.77</td>
<td>411.61</td>
<td>401.07</td>
<td>390.77</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>T_{6,LP} (K)</th>
<th>B_{HP} (kmol/h)</th>
<th>Q_{B,HP}/F (MW/(kmol/h))</th>
<th>Q_{B,HP}/L_{HT} (MW/(kmol/h))</th>
<th>Q_{B,HP}/L_{LT,LP} (MW/(kmol/h))</th>
<th>B_{HP}/F_{HP}</th>
</tr>
</thead>
<tbody>
<tr>
<td>381.9</td>
<td>2652.5</td>
<td>0.0154</td>
<td>0.0121</td>
<td>0.0178</td>
<td>0.614</td>
</tr>
<tr>
<td>378.96</td>
<td>3407.2</td>
<td>0.0135</td>
<td>0.0122</td>
<td>0.0194</td>
<td>0.657</td>
</tr>
<tr>
<td>389.04</td>
<td>1838.5</td>
<td>0.0193</td>
<td>0.0120</td>
<td>0.0154</td>
<td>0.532</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Q_{B,LP} (MW)</th>
<th>D_{HP}(kmol/h)</th>
<th>D_{LP}(kmol/h)</th>
<th>B_{LP}(kmol/h)</th>
<th>V_{D,HP}(kmol/h)</th>
<th>S (kmol/h)</th>
</tr>
</thead>
<tbody>
<tr>
<td>58.633</td>
<td>1667.5</td>
<td>1422.7</td>
<td>993.43</td>
<td>7137.4</td>
<td>236.43</td>
</tr>
<tr>
<td>57.472</td>
<td>1776.8</td>
<td>1445.4</td>
<td>915.62</td>
<td>7531.5</td>
<td>1046.2</td>
</tr>
<tr>
<td>59.725</td>
<td>1617.5</td>
<td>930.67</td>
<td>843.76</td>
<td>7153.8</td>
<td>64.096</td>
</tr>
</tbody>
</table>

**Evaluation of loss with constant setpoints**

It is optimal that the system is operated so that the five active constraints listed above are fulfilled and we should use a control system where these variables are controlled at their constrained value (“active constraint control”). This means that there is one steady state degree of freedom left. We now want to find the most suitable controlled variable for this remaining degree of freedom, for which the best choice is not obvious.

To do this a number of candidates for the control variables were proposed. To find out which of the candidates is most suitable we evaluate the loss $L = J(u,d) - J_{\text{opt}}(d)$ for the defined disturbances, when the variables are kept constant at their nominal optimal set point. In addition to evaluating the loss at the selected disturbances the loss is also found when there are implementation errors in the controlled variables ($c_{\text{ad}}$) of 20%. The variable selected for self-optimizing control should give an acceptable loss.

From the evaluation of we found that the best variable to keep at constant setpoint is the temperature on tray six in the LP column.
Multiplicities in the Objective Function

The results in Figure 2 give some ideas about the nonlinear behaviour of the solution surface for this problem. Using a constant area in the integrated reboiler/condenser it can be seen how some of the variables are varying with the heat load to the HP column. It can also be observed in Figure 3 that there are multiplicities in the objective function of some variables. The consequence of these multiplicities in the objective function is that if these variables are used for control then a small implementation error could move the plant into a region with a very large loss or infeasibilities in the objective.

![Temperature and Water Composition in LP Column](image1)

![Pressure (at top) in HP Column](image2)

![Bottom Flow and Water Composition in HP Column](image3)

*Figure 2. Selected variables as a function of heat load to HP column*
Based on the analysis above we propose a control structure for the multi-effect columns, as shown in Figure 4. The control structure has the following features:

A) Stabilising level loops (4)
   - The distillate flows are used for level control in the condensers of both columns.
   - The bottom flow in the low pressure column, BLP is used for level control.
   - The reboiler level in the high pressure column is controlled by the boilup in the bottom of the high pressure column.

B) Active constraint loops (3)
   - The reflux flows are used for final composition control of the distillate streams from both columns.
   - The pressure in the LP column is controlled by the condensation rate in the condenser.
   - The sidestream flowrate is used for composition control in the LP column bottom stream (controlling the water concentration)
   - The maximum area in the integrated reboiler/condenser is used (not an actual control loop)

C) “Self-optimizing” loops (2)
   - The bottom flowrate in the high pressure column, BHP is used for temperature control on tray 6 in the low pressure column (this is the 'self-optimizing control loop').
DISCUSSION

Earlier we have assumed that the feedrate is set at the inlet to the plant. However, this may require reconfiguration of loops if one of the columns becomes a bottleneck. For example if there is an increase in the feedrate to the HP column then eventually this will lead to a case where either the boilup (or the pressure) in this column will reach its constrained value.

If there is a chance that one of these constraints may be reached then boilup is effectively lost as a degree of freedom for control and it will be advantageous to use an alternative control structure. An alternative could for example be to switch to using the feedrate to control the holdup in the bottom of the HP column. This configuration would require that there is a small holdup tank upstream of the HP column so that the feedrate can be manipulated.

In the self-optimization procedure only the steady state effects of the system has been considered, that is we have found the best control variables for the system based on the steady state economics. The dynamic effects have not been considered in detail. However, there may be some interesting effects with the selected control structure in Figure 4. If looking at the open loop response in the methanol concentration in the top of the HP column when making a step in the reflux (with holdup loops closed) then the response of the concentration of methanol will first increase with increasing reflux, then decrease. This happens because the boilup is used to control the liquid level in the bottom of the column. An increase in the
reflux flowrate will first give an increase in the concentration of methanol, but as the reflux reaches the bottom part of the column the level increases and thus boilup is increased. As a result there will be more of the heavy component going up the column and the methanol concentration will decrease. Dynamic effects of the selected control structure will therefore be considered in further studies.

**CONCLUSIONS**

The method of self-optimizing control has been applied to a multi-effect distillation case. We have found that five of the system variables should be controlled at their constraints: the top composition in both columns, the pressure in the LP column, the composition in the bottom of the LP column and the area in the integrated exchanger. This left one unconstrained degree of freedom for which the choice of a suitable controlled variable was not obvious. We have found that selecting a temperature in the lower part of the LP column has good self-optimizing properties. It has also been shown that certain variables may have multiplicities in the objective function and they are thus unsuitable for self-optimizing control.

**REFERENCES**


11. Larsson, T., Skogestad, S., Control of an industrial heat integrated distillation column, Presented at the AIChE Annual Meeting, Dallas, November, 1999