

RATE-BASED MODELING OF TWO COMMERCIAL SCALE H₂S STRIPPING COLUMNS

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Abstract

This paper describes rate-based models^{1,2} of two commercial scale H₂S stripping columns in order to obtain improved prediction of column performance compared to equilibrium stage models that use component efficiencies. For one stripping column for which H₂S bottom concentrations were available the rate-based column model results are in reasonable agreement with the plant data, whereas the equilibrium stage model predicts H₂S bottoms concentrations orders of magnitude lower when a constant tray efficiency of 50% is used for all compounds. No plant data was available for the second column but the rate-based model gave results that were well in-line with operating experience.

The rate based models simulated both of the columns more or less exactly as they were constructed. The columns were modelled with 20 trays, not with 10 equilibrium stages. The feeds were directed to the appropriate locations in the column; for the equilibrium stage model the H₂S alone had to be diverted to a lower stage in order to match the plant data. Equilibrium stage models are unable to adequately model the columns under consideration because the efficiencies of different components vary in different ways depending on the component. For example, in one column the heavier components had efficiencies that varied from approximately 40% in the top to 60% in the bottom. For the light components the efficiencies varied from about 20% in the top to around 60% in the bottom. We submit that for columns such as the two H₂S stripping columns described in this exercise the proper course of action is to use a rate-based model. There were no significant disadvantages concerning calculation speed, convergence, or availability of properties for these processes that contain 60+ components, especially as the predicted efficiencies matched the observed performance.

Keywords: Hydrogen Sulfide, Stripping, Rate-based, Nonequilibrium, Efficiency

1. The Actual Columns

H₂S Stripper A had 20 valve trays with dimensions as summarised in Table 1. The main feed to the column comprised water, hydrogen, hydrogen sulphide and several light paraffins (up to n-hexane) plus 78 pseudocomponents. The stripping medium was steam injected into the base of the column. The second column was a refluxed / reboiled H₂S stripper from a PYGAS process – PYGAS (pyrolysis gasoline) is produced in an ethylene plant that processes naphtha, butane, or gasoil. The feed to this column contained 66 compounds, all of them identifiable (that is, no pseudo components). The diameter of the PYGAS column was 1.586m and the tray spacing 500 mm and equipped with Shell Calming Section trays.

Table 1: H₂S steam stripper design details

Column diameter	2.1 m	Active area	1.54 m ²
Tray spacing	600 mm	Total hole area	0.09 m ²
Number of passes	2	Downcomer area	1.92 m ²
Liquid flow path length	407 mm	Weir height	25 mm

2. The Model Columns

Both H₂S strippers had been modelled using equilibrium stage models^{3,4} with the following significant features.

1. The model columns had 10 equilibrium stages (not counting the condenser).
2. The Soave-Redlich-Kwong (SRK) model was used for the thermodynamic properties.
3. A stage efficiency of 50% was used for all components on all stages.

The existing models led to predictions of the H₂S composition in the column bottoms that was very far from that observed in practice. One of two methods had been used to improve predictions.

1. The component efficiency of H₂S (and only H₂S) was set to a much lower value than that of the other components.
2. All of the H₂S in the feed (and only the H₂S) was fed to an intermediate stage.

However, even with these “tricks” it was not always possible to obtain acceptable agreement between the model predictions and plant data.

We used the column simulation program ChemSepTM to model the H₂S strippers. The SRK model was used for the equilibrium properties and enthalpy departures with the same set of interaction parameters that was used in the earlier equilibrium stage simulations. There was little difference between the results obtained with the equilibrium stage model in ChemSep⁵ and the equilibrium stage simulations done earlier with a flowsheet simulator. The stripper that was equipped with Shell Calming section trays was modelled in two ways: as a column with valve trays and as a column with sieve trays. The PYGAS column proved to be very easy to converge. The time taken to converge a single simulation depends most notably on the flow model selected. If we select the mixed flow model for both phases (the fastest model and usually the more conservative – meaning lowest efficiencies) the time for a single simulation usually was around 50 seconds on a Dell Precision portable workstation (2.6 GHz CoreTM Duo CPU). The plug flow model typically takes 3-5 times more computer time.

The plant data for Column A that served as the basis for this simulation study showed that the concentration of H₂S in the bottoms stream was 15 ppm (mass basis). Table 2 summarises the results of a comparison between the equilibrium stage model and the rate-based model simulations for the operating conditions on that date. We see that the equilibrium stage model predicts a concentration of H₂S in the bottoms that is very far from what was observed. Note that in order to provide a fair comparison with the rate-based simulations the H₂S stream was not split from the feed to the top of the column. The best agreement with the plant data was obtained by modelling the trays as sieve trays rather than valve trays and with the Chan & Fair model for the mass transfer coefficients (for which the Chan and Fair model was developed). It is our experience that valve trays often are more effectively modelled as sieve trays (from the point of view of mass transfer only, of course).

Table 2: Comparison between simulation models

Tray type	Mass Transfer Coefficient see refs 1, 2 for details	ppm H ₂ S in bottoms (mass basis)
NA	Equilibrium stage	0.08
Valve Tray	AIChE	5
Sieve Tray	Chan-Fair	12

The liquid composition profiles for selected compounds in both columns are shown in Figure 1. Note that the composition of H₂S (in the liquid phase) falls in nearly a straight line (when plotted on a logarithmic scale). Simply adding trays will, therefore, mean that any desired composition can be attained. The liquid composition in the PYGAS column does not change much over the height of the column. The mole fraction of H₂S, however, changes a great deal (this is, of course, the point).

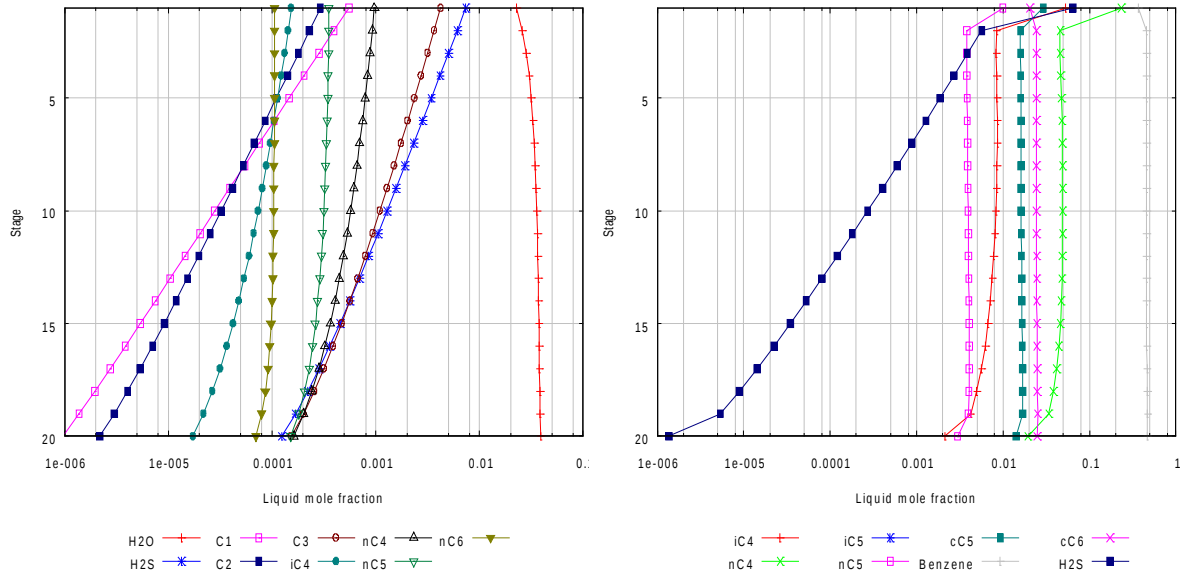


Figure 1: Predicted liquid phase composition profiles for H₂S stripping columns (PYGAS on right).

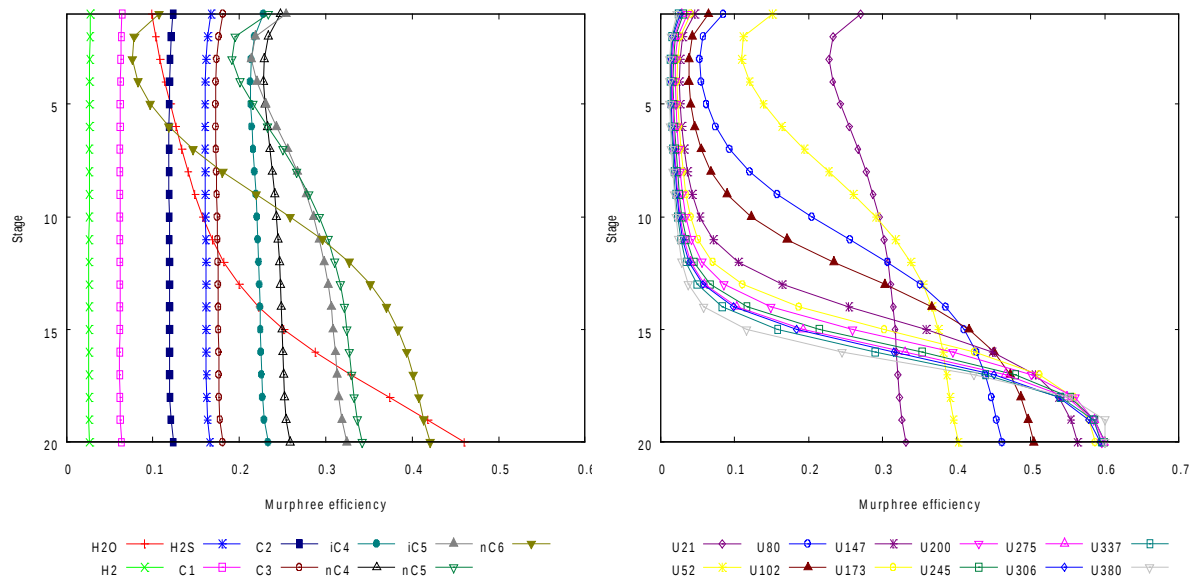


Figure 2: Predicted Murphree efficiency profiles for H₂S Stripper A.

Figure 2 shows the Murphree efficiencies¹⁻⁴ for the light boiling compounds and for selected pseudo components in Column A. The efficiencies for pseudo components not shown in Figure 2 are in between those shown here. The efficiencies of selected components in the PYGAS column are shown in Figure 3. Some observations of the predicted Murphree component efficiencies follow:

1. They vary very widely from component to component as well as along the height of the column.
2. The efficiency of water changes from around 12% near the top of the steam stripper to nearly 60% near the bottom.
3. The efficiencies of the heavier pseudo components in Column A closely approach zero in the top of the steam stripper.
4. The efficiency of most of the light gases is nearly constant over the height of the column (but still varies from component to component).
5. The Murphree efficiency of several compounds lies outside the range of zero to one on some stages in the PYGAS column.

6. The efficiency of H₂S is relatively constant in both columns; slightly less than 20% in Column A and 33% in the PYGAS column.

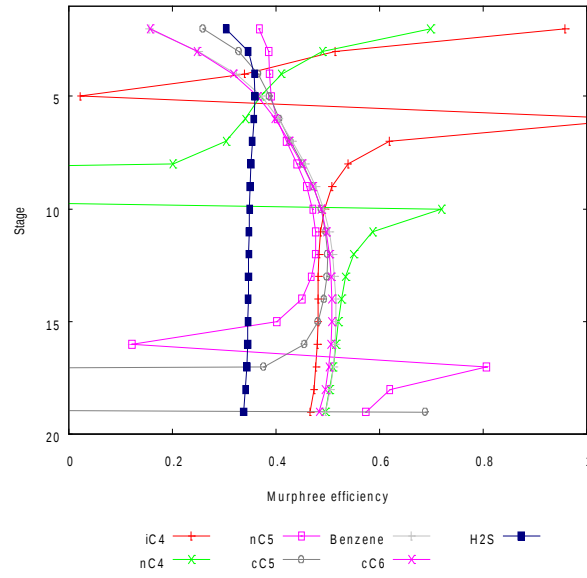


Figure 3: Predicted Murphree efficiency profiles for PYGAS column.

Arithmetic average values of component Murphree efficiencies should not be used as a simple measure of column and tray performance because the average on any tray can be significantly influenced by just one component efficient that lies far outside the expected range of values. Figure 4 shows what we term the Baur efficiency for the two H₂S strippers. Note that the Baur efficiency is not constant along the length of the column. It must be emphasised that both Murphree and Baur efficiencies were calculated from the results of a rate-based simulation; they were not used with an equilibrium stage model to predict the performance of the column.

The Baur efficiency is defined as follows⁶

$$\varepsilon = \sqrt{\sum_{i=1}^c (\Delta y_{i,L})^2} / \sqrt{\sum_{i=1}^c (\Delta y_i^*)^2} \quad (1)$$

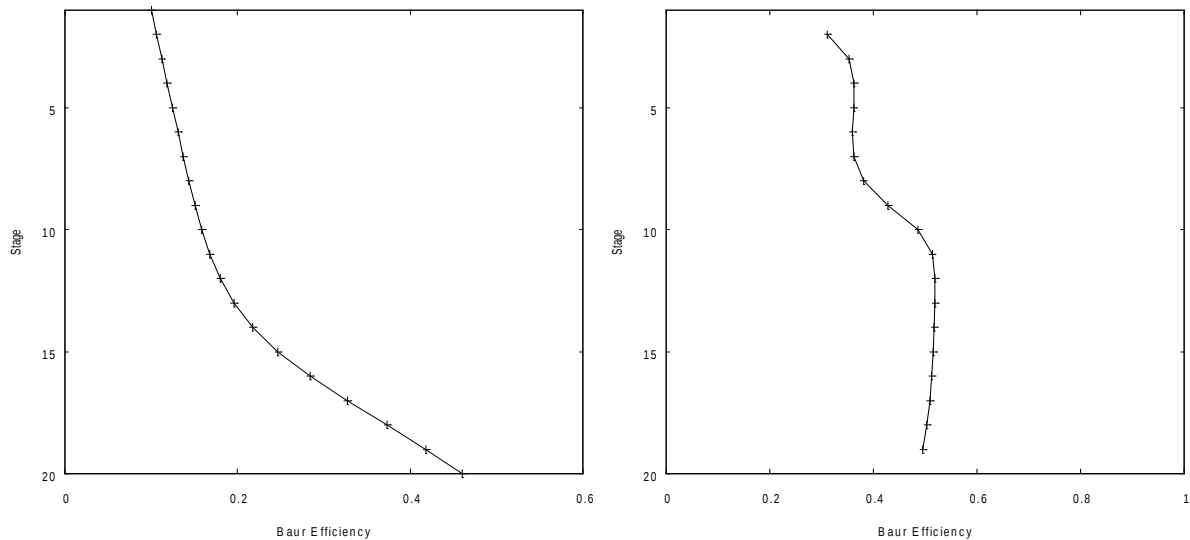


Figure 4: Baur efficiency profiles for two H₂S Stripping Columns (PYGAS on right)

The Baur efficiency as defined above has a simple and appealing physical significance: it is the ratio of the length of the actual composition profile (in mole fraction space) to the length of the composition profile from an equal number of equilibrium stages. Unlike the component Murphree efficiencies and HETPs, there is just one Baur efficiency per tray or section of packed column regardless of the number of compounds; the Baur efficiency is “well-behaved” in that it cannot be negative, or tend to infinity (although it can be greater than one). For all of these reasons we suggest that for assessing the overall performance of a column the Baur efficiency is, arguably, the most useful of the many definitions of efficiency.

3. Comparison with Design Data

A majority of the simulations of the PYGAS column were done in “design mode” wherein ChemSep determines the dimensions of the trays at the same time as the simulation is carried out. We can, therefore, compare the tray design from ChemSep with the tray design data (as noted earlier, these were available to us only after we had done our first simulation).

It must be remembered that no rate-based column model includes correlations for sizing of calming section trays. Characteristics of calming section trays include shorter flow path lengths than would be expected for a single pass sieve tray, and long weir lengths (because of the multiple downcomers arranged in the direction of the liquid flow across the tray). It is therefore, interesting to note that ChemSep “designed” a two pass sieve tray in which the flow path length is indeed shorter than the usual flow path length for a single pass tray. Again, this is something that we would expect to be the case for the calming section tray design. ChemSep estimated the diameter to be 1.66m. The actual internal diameter is 1.586m.

4. Influence of Mass Transfer, Flow Models and Thermodynamics

It is worthwhile to determine the extent to which our choice of mass transfer coefficient model and the gas/vapour and liquid flow models influences the results. Table 3 summarises some results for the PYGAS stripping column to illustrate this point.

Table 3: Comparison between models

Vapor Flow Model	Liquid Flow Model	Mass Transfer Coefficient	H ₂ S in bottoms (mass ppm)	H ₂ S Efficiency	Baur Efficiency
Mixed	Mixed	Chan & Fair	0.53	35.00%	30-50%
Mixed	Mixed	AIChE	0.52	35.00%	30-60%
Plug	Mixed	Chan & Fair	0.53	35.00%	31-51%

It is interesting to note that for this particular process there is very little difference between the models when it comes to predicting the concentration of hydrogen sulphide in the column bottoms. Normally, one would expect that a plug flow model would lead to an increase in the efficiency of a few percentage points (perhaps as much as 5 or 6 points). It is, therefore, somewhat surprising to find that the vapour flow model has so little influence in this case. Further, the Chan & Fair correlation normally provides more optimistic estimates of the efficiencies than does the AIChE method. (Put another way, the AIChE method is more conservative.) We see that in this case there is essentially no difference between the correlations. The good news here is that with these model variations all producing about the same overall result we can be reasonably confident in our predictions.

Additional simulations showed the importance of the thermodynamic model. In addition to the standard SRK model we carried out simulations with several other widely used models including the SRK model with different mixing rules, and with the Chao-Seader method. Simply changing the thermodynamic model lead to predictions of the H₂S concentration that differed by several orders of magnitude.

5. Concluding Remarks

While the importance of the proper selection of thermodynamic models cannot be underestimated it is the selection of an appropriate mass transfer model that is key to being able to model separation processes that should be considered rate-based as opposed to equilibrium based. It is in the widely varying component efficiencies that we find the explanation for the inability of the equilibrium stage model to predict the performance of these columns. It is not unusual in modeling distillation operations to see efficiencies that are far larger than one on one stage and far less than zero on another. However, such behavior usually is indicative of a maximum in the concentration profile of those components and the mass transfer rates of those compounds are typically very low indeed under those circumstances. What we see here is very large differences between the largest and smallest component efficiencies. In the stream stripper, for example, the efficiencies of the light boiling compounds vary from less than 5% to more than 50%. The efficiencies of the pseudo components also vary widely from near zero at the top of the column to more than 60% at the bottom. A model that assumes constant average component efficiencies over the height of the column or even on a per stage basis cannot mimic this behavior. The underlying reasons are rooted in the very different resistances to mass transfer for the various compounds. The numbers of vapor phase mass transfer units are very high (> 4) but very low (< 1) in the liquid phase for the light boiling compounds, for the heavier compounds the numbers of transfer units are low in both phases. Assuming that all species have the same facility for mass transfer is simply wrong. Rate-based models may take longer to solve a given computer simulation but they eliminate having to guess the number of equilibrium stages and/or the component efficiencies needed to model a particular process.

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