

Calculation of the HETP at Total Reflux: Generalization of the Fenske Equation

Brian Hanley  
Koch-Glitsch, Inc.  
4111 East 37<sup>th</sup> Street North  
Wichita, KS 67220

Prepared for Presentation at the 2001 AIChE Annual Meeting/November 4-9/ Distillation Equipment and Applications II

© Koch-Glitsch, Inc.  
June, 2001

Unpublished

AIChE shall not be responsible for statements or opinions contained in papers or printed in its publications.

## Abstract

The Fenske<sup>1</sup> and Smoker<sup>2</sup> equations for calculating the number of theoretical plates necessary to achieve a desired level of separation for binary systems with constant relative volatilities have been generalized to account for any vapor/liquid equilibrium behavior. The generalization is achieved by considering the number of stages as a continuous variable and differentiating the standard equations with respect to mole fraction of the more volatile component. The resultant integral for the number of theoretical stages can be evaluated numerically without difficulty.

The great advantage of such a formulation comes from the fact that the stage calculation can now be easily linked to the average column operating pressure, the quality of the feed, the pressure at the top and bottom of the column (and hence to the vapor and liquid physical properties at these locations) as well as to models for flooding and for the HETP. The calculations allow for rapid exploration of the parameter space for the separation. An example of the operation of such a calculational procedure will be given using TKSolver, a declarative rule-based programming environment, that provides great flexibility for solving the coupled, nonlinear equations necessary for packed column design and rating.

## Introduction

The Fenske and Smoker equations represent, in essence, the graphical construction of the McCabe-Thiele method in analytical form. Both utilize the assumptions of constant relative volatility and constant molar overflow. At the time of their development, graphical methods for column design represented the “state of the art”. However, all such graphical methods become inconvenient and prone to error if a large number of stages are required to effect a given separation. This often occurs if the relative volatility is close to one or if extremely pure products are required. An example of an industrially important separation where large numbers of stages are often needed is that of ethylbenzene

---

<sup>1</sup> Fenske, M.R., *Ind. Eng. Chem.*, **24**, 1932.

<sup>2</sup> Smoker, E.H., *Trans. AIChE*, **34**, 1938.

from styrene monomer. This system conforms rather well to the assumptions behind the Fenske and Smoker equations. Calculation of the number of stages with these analytical methods is literally orders of magnitude faster than graphical constructions even when “primitive” computing tools (like a slide rule and paper and pencil) are the only ones available.

With the advent of computers the utility of the Fenske and Smoker equations increased again. Now, the stage calculations could be easily connected to the hydraulic rating equations for column sizing. The coupled nonlinear equations for the design were now subject to great computational power. Alternative designs and design optimizations subject to physical and/or monetary constraints could now be analyzed in a way previously unavailable. Table 1 presents a simple example of some “pseudo” computer code that links stage calculations from the Smoker equation with hydraulic calculations for column design or rating of a packed section.

Industrially important binary separations are not limited to having constant relative volatilities nor do they always conform to the assumption of constant molar overflow, although this condition is nearly met for a majority of systems. For these separations the Fenske and Smoker equations are not generally applicable. However, it is possible to employ them over small increments where the relative volatility is essentially constant. In fact, *this observation is the key to our generalization of these equations to systems with variable relative volatility.*

Advanced software tools for the simulation of complex separations – like *Aspen*, *ProSim*, or *SimSci* - are now readily available. These packages often include simplified methods, like the Smoker equation or Edminster’s method, alongside rigorous approaches where very few assumptions about VLE or process flows need to be made. In addition, these packages sometimes include tools for optimization. Why, then, is there a need for a generalized Fenske equation or Smoker equation? The answer lies in the tradeoff between rigor, time, extensibility, and control. The development here is not in any way meant to supersede the calculational prowess of these software packages but rather to complement them for a

limited set of separations – binary or pseudo-binary systems where the assumption of constant molar overflow is reasonable. How does a generalized Fenske or Smoker equation complement the aforementioned simulation tools?

In most preliminary process evaluations one would like to “explore” alternatives rapidly but as thoroughly as is practicable given limited time or manpower, for example. In addition, there may arise the need to “solve” the problem in ways not really amenable to the solution scheme(s) envisioned by the software manufacturers. Further, there may be a need to “extend” the code beyond the options available in the simulation package. Consider the following example: one must perform a separation where the total pressure drop across the section is limited. One might envision that the column diameter is a variable but one that is constrained between a minimum and maximum value. Further, the engineer might consider in-house pressure drop correlations superior to those found in the software. First, the time required to set up such a process simulation from “scratch” in any of the available software simulators is considerable – including the time to figure out how to use “object linking and embedding” – OLE – for doing the pressure drop calculations outside the programming environment if OLE is even offered as an option in the simulator. Second, the simulators are usually designed to handle “scratch” problems in a particular manner – for example, the pressure drop is handled as an “output” rather than as an “input”. In such a situation the engineer can either a) solve the simple simulation over and over again, keeping track of the pressure drop as she/he changes conditions manually, or b) spend additional time trying to reconfigure the simulator to handle the special case.

On the other hand, inexpensive software tools are readily available that are capable of treating all variables as either inputs or outputs and which can solve multiple coupled nonlinear equations in a relatively straightforward way. These programs also usually include extensive libraries of mathematical procedures – like integration, differentiation, or optimization – that are readily and easily implemented. Finally, these packages are easily extensible to include subroutines specific to the problem at hand – via

OLE, for example. *TKSolver* v4.0 is an example of one such software tool and it is the one upon which we shall focus attention in the remainder of this paper.

Thus, the process engineer in the preliminary stages of a design might prefer to do initial screening evaluations in a software environment where speed and flexibility are maximized and where some design rigor is sacrificed. At the end of this evaluation process, the most appealing design can be simulated in a more rigorous process simulation environment to verify and finalize the concept.

### Development

By treating the number of stages as a continuous variable, it is straightforward to show that the Fenske equation for the number of stages required to achieve a given level of separation at total reflux in a binary separation can be generalized to:

$$N = \int_{x_B}^{x_T} \frac{dx}{x \alpha(x) (1-x)} - 2$$

where we have assumed that the relative volatility is independent of pressure for the range of pressures encountered between the bottom and top of the column (this requirement can be relaxed at the expense of an additional differential equation). The relative volatility as a function of composition can be obtained in any number of ways. For example, such information can be generated in *Aspen* quite easily by choosing the components and the VLE model to be used.

Similarly, the Smoker equation can be generalized to:

$$N_{\text{rec}} = \int_{x_i}^{x_D} \frac{(\alpha(x) - mc(x)^2) dx}{x' [\alpha(x) - mc(x)^2 - x'(\alpha(x) - 1)mc(x)] \ln \left( \frac{\alpha(x)}{mc(x)^2} \right)} - 1$$

$$N_{\text{strip}} = \int_{x_B}^{x_i} \frac{(\alpha(x) - mc(x)^2) dx}{x' [\alpha(x) - mc(x)^2 - x'(\alpha(x) - 1)mc(x)] \ln \left( \frac{\alpha(x)}{mc(x)^2} \right)} - 1$$

$$N = N_{\text{rec}} + N_{\text{strip}}$$

where “k” is the root between 0 and 1 of:

$$m(\alpha(x) - 1)k^2 + [m + b(\alpha(x) - 1) - \alpha(x)]k + b = 0$$

and

$$m = \frac{R}{R+1} \text{ in the rectifying section OR } m = \frac{R x_F + q x_D - (R+q)x_B}{(R+1)x_F + (q-1)x_D - (R+q)x_B} \text{ in the stripping section}$$

$$b = \frac{x_D}{R+1} \text{ in the rectifying section OR } b = \frac{(x_F - x_D)x_B}{(R+1)x_F + (q-1)x_D - (R+q)x_B} \text{ in the stripping section}$$

$$c = 1 + (\alpha(x) - 1)k$$

$$x' = x - k(x)$$

$x_i$  is the mole fraction at the intersection of the operating line in the rectifying section and the q-line passing through  $x_F$ .

Note that the calculations envisioned in Table 1 for the packed section can now be performed by calling an integration routine that carries out the requisite numerical integrations described above. Recall that any variable that appears in the problem can be treated as an input or an output. Clearly, the utility of such a tool is obvious.

### Example

Consider as an example the rectification at total reflux, of the binary system cyclohexane/n-heptane at 24 psia. Figure 1 shows the relative volatility versus composition for this system estimated via several VLE methods as implemented in *AspenPlus* v10.0. Figure 2 is a plot for calculating the minimum number of theoretical stages from the generalized Fenske equation for the various solution models presented in Figure 1.

First, it is interesting to note the variation in predicted dependence of the relative volatility with composition for this relatively well-understood system. Second, even the relatively modest changes in the relative volatility seen with this system (irrespective of the solution model) lead to noticeable changes in the required number of stages. Certainly, the situation is worse for systems where the relative volatility changes more drastically with composition.

## **Conclusions**

Integral versions of the Fenske equation and the Smoker equation have been developed. The resulting integrals are valid even if the relative volatility changes with composition. In addition, they are easy to solve numerically if relative volatility data are available. The generalized Smoker equation can be used to quickly explore the separation/hydraulics parameter space before going to a more rigorous simulation.

**Table 1: Partially Complete “Pseudo” Computer Code for Stage Specification and Hydraulic Design/Rating for a Packed Section**

```

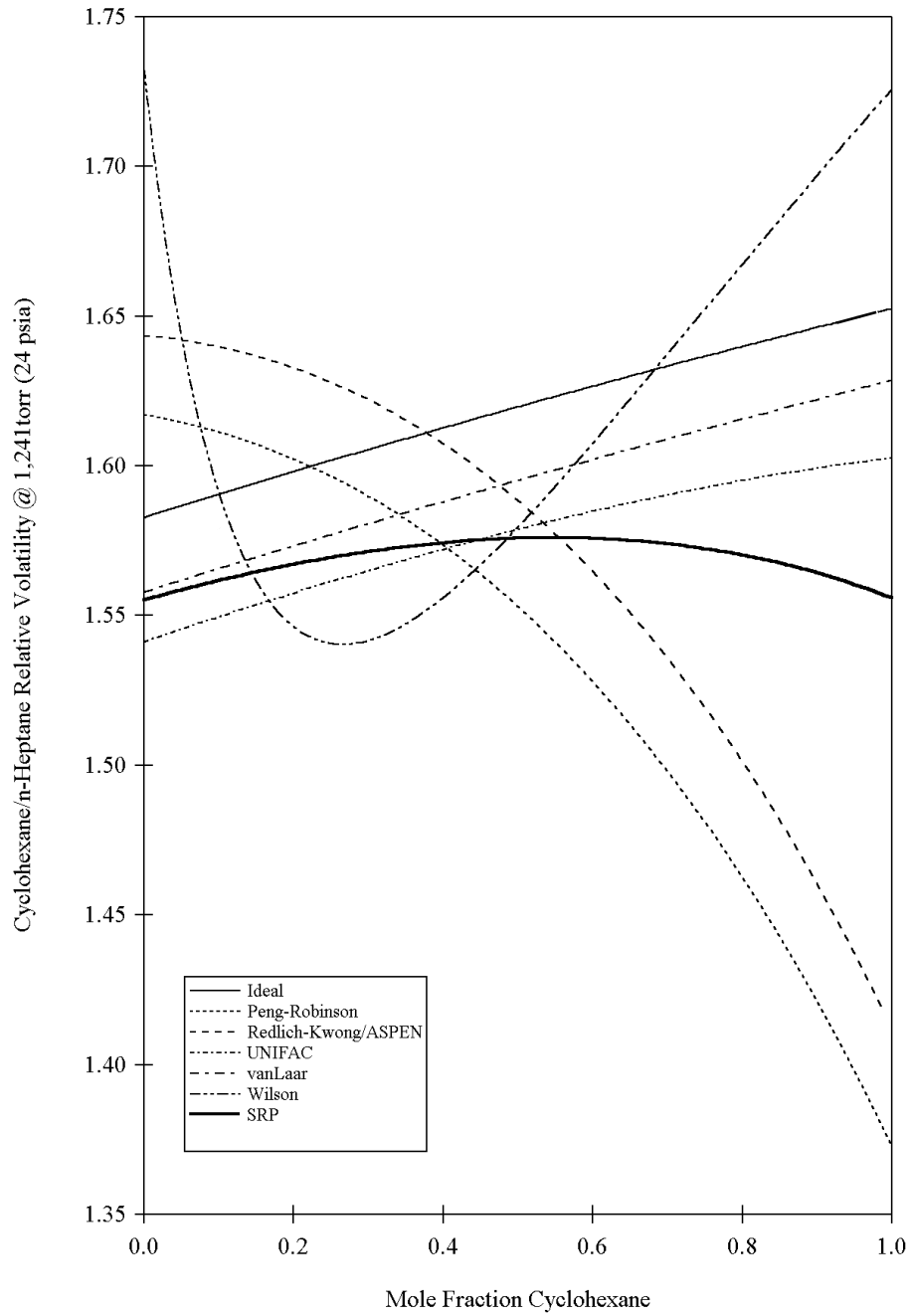
xq=(-(R+1)^(-1)*xD*(q-1)-xF)/(R/(R+1)*(q-1)-q)
N_rect=Smoker(α,xq,xD)-1
N_strip=Smoker(α,xB,xq)-1
Nideal=N_rect+N_strip
call property_estimate(top conditions)
call property_estimate(bottom conditions)
Bottoms=Distillate*(xD-xF)/(xF-xB)
Feed=Bottoms+Distillate
call pdrop(Cv_top,pltop,Cl_top,Clflood_top;Δp_rect)
call pdrop(Cv_bot,plbot,Cl_bot,Clflood_bot;Δp_strip)
Cl_top=R*Distillate*MW_top/pltop/(pi()*Dtop^2/4)
Cl_bot=(R*Distillate+q*Feed)*MW_bot/plbot/(pi()*Dbot^2/4)
Cv_top=(R+1)*Distillate*MW_top/(pvtop)/(pi()*Dtop^2/4)*abs(sqrt(pvtop/pltop))
Cv_bot=(Distillate*(R+1)+Feed*(q-1))*MW_bot/pvbot*abs(sqrt(pvbot/plbot))/(pi()*Dbot^2/4)

```

*Symbol Definitions*

xq: mole fraction of the light component for the “q-line”  
xD: mole fraction of light component in the distillate product  
xF: mole fraction of light component in the feed  
xB: mole fraction of light component in the bottom product  
R: reflux ratio  
Pbot: pressure at the bottom of the section  
Ptop: pressure at the top of the section  
Cv: flow capacity factor  
Cl: liquid loading  
D: column diameter  
Distillate: molal flow rate of the distillate product  
Feed: molal flowrate of the feed  
Bottoms: molal flow rate of the bottom product

Figure 1: Variation in Relative Volatility with Composition for the Binary Cyclohexane/n-Heptane at 24psia



**Figure 2: Minimum Number of Stages Required Calculated from the Generalized Fenske Equation**

