Convergence Characteristics of Augmented Hessian Models for Separations

R. W. Frantz[a]; V. Van Brunt[a]

[a] Department of Chemical Engineering, Swearingen Engineering Center The University of South Carolina, Columbia, SC

PLEASE SCROLL DOWN FOR ARTICLE

CONVERGENCE CHARACTERISTICS OF AUGMENTED HESSIAN MODELS FOR SEPARATIONS

R. W. Frantz and V. Van Brunt
Department of Chemical Engineering
Swearingen Engineering Center
The University of South Carolina
Columbia, SC 29208

ABSTRACT

Previous research has shown that the form and
number of MESH equations used to describe
distillation/extraction systems can change both
the linearity and convergence characteristics.
In this paper, the structures of the equation
sets for distillation and extraction models
are analyzed in terms of the form of the three
dimensional Hessian associated with them. It is
known that for highly nonlinear equilibrium
stage problems the $N(2C+1), N(2C+3)$ variable
forms used in the Naphthali-Sandholm model are
more difficult to converge than newer models of
Ricker-Nakashio-King and Krishnamurthy-Taylor
that have $N(4C)$ and $N(5C+1)$ variables
respectively. The convergence behavior of
specific equation sets that augment the size of
the Hessian are compared with the standard
forms.

Alternative models specifically designed to
augment the Hessian are analyzed in terms of
their convergence behavior. The convergence
behavior is compared to MESH equation models. By
creating models that specifically increase the
equation set at points known to be poorly scaled
and at the nonlinearity locations, improved
convergence rate and solution stability can be
achieved.

INTRODUCTION

        Traditional modeling of distillation and
extraction systems has progressed from the Lewis-
Matheson and Thiele-Geddes methods to matrix methods
that are simultaneously converged(1,2). These matrix
methods initially reduced the full equation set that
described the system to isolate and converge subsets of
the equations. This "tearing" procedure characterizes
the early steady-state modeling(2,3). However, beginning
with Newman(4) and Naphtali(5) and Naphtali and
Sandholm(6) modeling represented refined description of
the M(material balances), E(equilibrium relations),
S(summation of phase mole fractions) and H(energy)
equations. These MESH equations have traditionally been
written in two forms based on physical reasoning(7).
Recently, expanded equation sets have been used(8).
These expanded models include those of Ricker-Nakashio-
King(8) and Krishnamurthy-Taylor(9). Reported
convergence of these expanded models is faster than the
traditional MESH equation models. This paper examines
these models mathematically, i.e. in terms of their
linearity and convergence character, and suggests
alternative equation sets with different convergence
properties.

        The MESH equation set models assume that there are
C components and N stages. The Naphtali-Sandholm model
consists of C component material balances, C component
equilibrium relations, and an energy balance for each of
the N stages, thus having a total of N(2C+1) equations.
The balances are written in terms of the component
flowrates in each phase(6). Alternatively, the material
balances can be written in terms of component mole
fractions and total molar flows. In such terms, two
additional equations per stage are needed (for the
total flow variables). Usually, the summation of mole
fractions is used. The model consists of C component
material balances, C equilibrium relations, one energy
balance and two summation mole fraction equations per
stage. The total number of equations to be converged to
a solution is N(2C+3)(7,10).

        Newer models increase the number of variables and
equations. They are based on representation of staged
equipment in terms of mass transfer rather than an
approach to equilibrium. The models consider the
interface between the phases in addition to the bulk
phases.

        For the isothermal Ricker-Nakashio-King model,
there are two additional concentrations per stage

representing the interfacial compositions. The
additional equations represent the component flux across
the interface and an additional material balance. The
equations per stage represent C component material
balances for phase I, C component material balances for
phase II, C component equilibrium relations between the
interfacial phase compositions, and C steady-state flux
equations across the interface. The resulting equation
set has N(4C) equations. Convergence of extraction
systems with complex equilibria is rapid, without
special scaling required(8).

The Krishnamurthy-Taylor model for distillation is
a nonisothermal distillation model. Iteration is on
temperatures as well as concentrations. In addition,
the fluxes of each component are computed. Since both
component material balances and fluxes are computed for
each phase, one flux can be obtained by subtraction and
is not independent. For each stage, the model has C
component material balances for the vapor, C component
material balances for the liquid, C-1 steady-state flux
equations to the interface, C-1 component flux equations
from the interface, C component equilibrium relations
between interfacial compositions, two energy
balances(one for each phase), and one energy flux
equation across the interface. The total number of
equations in this model is N(5C+1). Convergence of this
model is usually with fewer iterations than convergence
with the Naphtali-Sandholm N(2C+1) model(11,12).

The formulation of these models relies on
traditional notions of the physics and chemistry
occurring in process equipment. Difficulties with
convergence of these nonlinear models have forced
consideration of techniques other than multivariate
Newton and Quasi-Newton procedures. Indeed, multiple
steady-state solutions have been obtained
(11,13,14,15,16,17,18,19). The state of the art is
summarized elsewhere(13,16). Many of the difficult
separations have only been solved using differential-
homotopy continuation(11,18). However, the convergence
criteria for multivariate Newton's method may be used
to suggest a modeling procedure based on mathematics
combined with physical description.

A MATHEMATICAL BASIS FOR MODELING STAGED SEPARATIONS

In our previous work(20) we developed a strong criterion
for the quadratic convergence of multivariate Newton's
method. This criterion expresses the required magnitudes
of the norms of three quantities. The criterion is the
multivariate version of the single variable requirement:

Newton's method will converge to a root quadratically
provided that

$$| f(x) f''(x) | < | f'(x) | \qquad\qquad [1]$$

With scaler variables and functions, the first and
second derivatives are scalers too. Thus, this criterion
only states requirements in terms of absolute values.
However, for vector variables and functions, of length
N, the criterion becomes:

$$||(f'(x)) || \; ||f''(x)|| \; || \Delta x || < 1 \qquad\qquad [2]$$

where $(f'(x))$ is the inverse of the Jacobian, an N x N
matrix (second order tensor) and $f''(x)$ is the Hessian, a
third order tensor, and Δx is a vector. The criterion
holds for appropriately defined norms (all scaler
quantities).

In particular, the norms may be considered the
magnitudes of the largest elements in each of the terms
on the left hand side. Specifically, consider what is
the effect of starting an iteration too far away from
the root. Clearly the norm of Δx is large and probably
dominates the expression. Convergence is difficult. The
norm of the inverse of the Jacobian is difficult to,
apriori, predict. How can one improve the chances of
success for Newton's method, even from a poor initial
estimate? The norm of the Hessian is considered,
because if it can be made sufficiently small,
convergence will be quadratic, even from poor starting
points, because the inequality criterion will be met. A
modeling procedure based on this reasoning is to
formulate models for separations in such a way as to
minimize the nonlinearities in the Jacobian and thereby
reduce the number and magnitude of the elements in the
Hessian. Scaling is just another way of stating that the
elements in the Hessian should be on the order of one.

The Hessians for distillation models are described
below. The MESH equations form the well known block
tridiagonal Jacobian. The Hessian for a set of
equations representing a staged system is shown in
figure 1. The second derivatives of each function are
needed. The block tridiagonal Jacobian translates to a
sparse three dimensional stack of tensor elements
extending from those on the first stage to those on the
last one. The nonzero elements for the Jacobian of the
Naphtali-Sandholm MESH equations for each stage are
given in the original paper(6).

The N(2C+3) model and equation set are presented
in figure 2 and by equations 3 - 7.
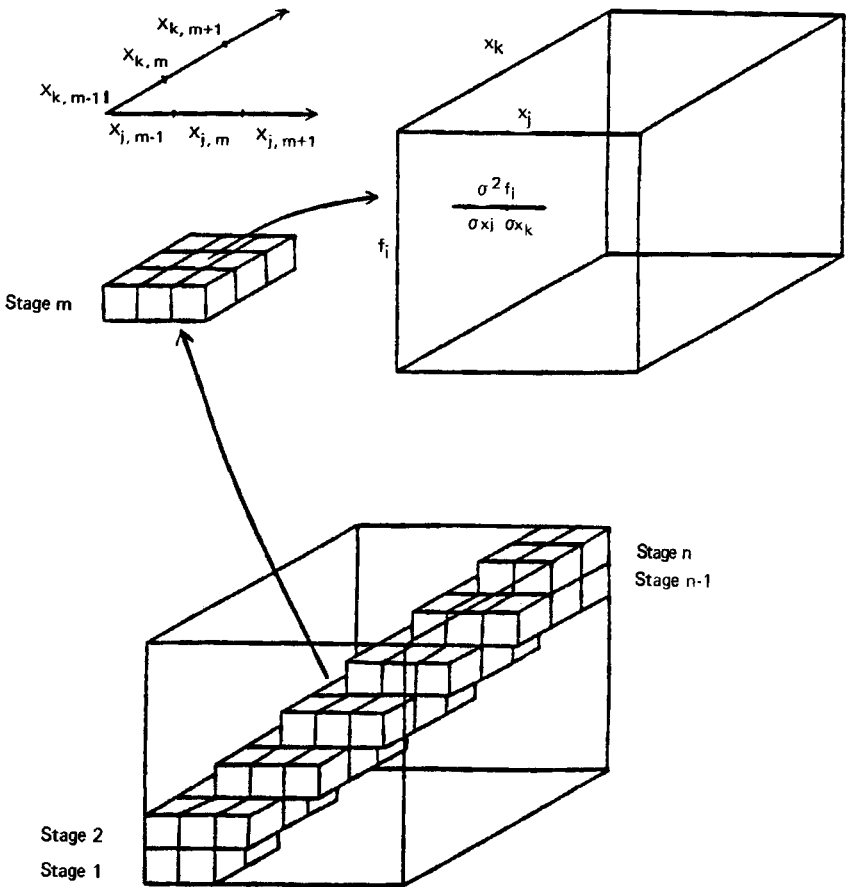
Figure 1 Structure of the Hessian of the MESH Equations

$$M_i = Y_{i,n-1}V_{n-1} + x_{i,n+1}L_{n+1} + q_{n+1}Y_{i,n+1}V_{n+1} +$$
$$r_{n-1}x_{i,n-1}L_{n-1} - (1 + S_n + q_n)Y_{i,n}V_n \qquad [3]$$
$$- (1 + T_n + r_n)x_{i,n} L_n + f_{i,n}F_n$$

$$E_i = Y_{i,n} - (\eta_n - 1)Y_{i,n-1} - \eta_n k_i x_{i,n} \qquad [4]$$

$$S_1 = \sum_i y_{i,n} - 1 \qquad\qquad [5]$$

$$S_2 = \sum_i x_{i,n} - 1 \qquad\qquad [6]$$

$$H = Hv_{n-1}V_{n-1} + Hl_{n+1}L_{n+1} + q_{n+1}Hv_{n+1}V_{n+1} +$$
$$r_{n-1}Hl_{n-1}L_{n-1} - (1 + S_n + q_n)Hv_nV_n - \qquad\qquad [7]$$
$$(1 + T_n + r_n)Hl_nL_n + Hf_nF_n - Q_{Ln}$$

The corresponding elements of the Hessian, to the best of our knowledge, have never been examined. They are listed in table 1.
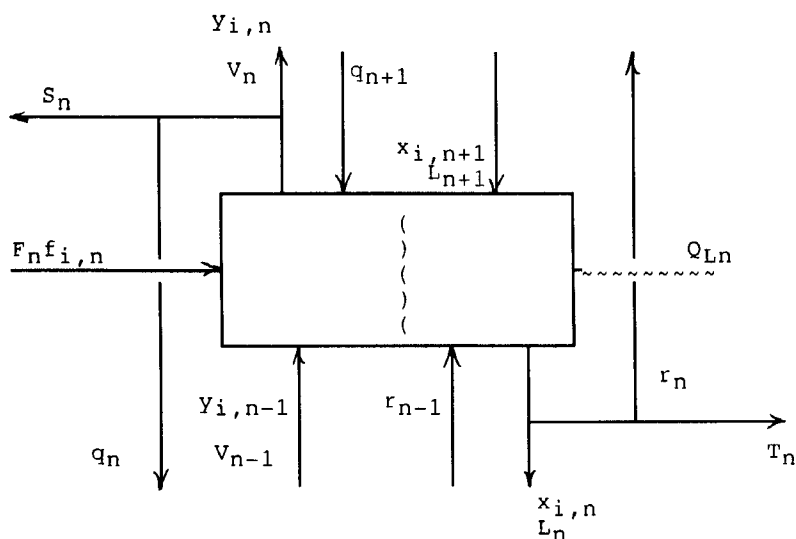
Figure 2. Equilibrium Stage Representation
Stage = n, Component = i

Table 1.
Elements of the Hessian of the MESH Equations

Hessian elements assuming: $r_n = q_n = \dfrac{\partial k_i}{\partial y_i} = 0$ [8]

and

$$\eta_n = 1 \qquad\qquad [9]$$

From the mass balances

$$\frac{\partial^2 M_i}{\partial L_n \partial x_i} = \frac{\partial^2 M_i}{\partial x_i \partial L_n} = -(1 + T_n) \qquad [10]$$

$$\frac{\partial^2 M_i}{\partial V_n \partial y_i} = \frac{\partial^2 M_i}{\partial y_i \partial V_n} = -(1 + S_n) \qquad [11]$$

$$\frac{\partial^2 M_i}{\partial L_{n+1} \partial x_{i,n+1}} = \frac{\partial^2 M_i}{\partial x_{i,n+1} \partial L_{n+1}} =$$

$$\frac{\partial^2 M_i}{\partial V_{n-1} \partial y_{i,n-1}} = \frac{\partial^2 M_i}{\partial y_{i,n-1} \partial V_{n-1}} = 1 \qquad [12]$$

From the equilibrium relations

$$\frac{\partial^2 E_i}{\partial x_i^2} = -2 \frac{\partial k_i}{\partial x_i} - x_{i,n} \frac{\partial^2 k_i}{\partial x_{i,n}^2} \qquad [13]$$

$$\frac{\partial^2 E_i}{\partial T \partial x_i} = - \frac{\partial k_i}{\partial T} - x_{i,n} \frac{\partial^2 k_i}{\partial T \partial x_{i,n}} \qquad [14]$$

$$\frac{\partial^2 E_i}{\partial T^2} = - x_{i,n} \frac{\partial^2 k_i}{\partial T^2} \qquad [15]$$

$$\frac{\partial^2 E_i}{\partial x_i \partial T} = - \frac{\partial k_i}{\partial T} - x_{i,n} \frac{\partial^2 k_i}{\partial x_i \partial T} \qquad [16]$$

No Hessian elements from S_1 and S_2

From the energy balance

$$\frac{\partial^2 H}{\partial L_n \partial x_{i,n}} = \frac{\partial^2 H}{\partial x_{i,n} \partial L_n} = -(1 + T_n)\overline{Hl}_{i,n} \qquad [17]$$

$$\frac{\partial^2 H}{\partial T \partial x_{i,n}} = -(1+T_n)L_n\overline{Cpl}_{i,n} \qquad [18]$$

$$\frac{\partial^2 H}{\partial T \partial y_{i,n}} = -(1 + S_n)V_n\overline{Cpv}_{i,n} \qquad [19]$$

$$\frac{\partial^2 H}{\partial T \partial L_n} = -(1 + T_n)\frac{\partial Hl_n}{\partial T} \qquad [20]$$

$$\frac{\partial^2 H}{\partial V_n \partial y_{i,n}} = \frac{\partial^2 H}{\partial y_{i,n} \partial V_n} = -(1 + S_n)\overline{Hv}_{i,n} \qquad [21]$$

$$\frac{\partial^2 H}{\partial T \partial V_n} = -(1 + S_n)\frac{\partial Hv_n}{\partial T} \qquad [22]$$

$$\frac{\partial^2 H}{\partial L_{n+1} \partial x_{i,n+1}} = \frac{\partial^2 H}{\partial x_{i,n+1} \partial L_{n+1}} = \overline{Hl}_{i,n+1} \qquad [23]$$

$$\frac{\partial^2 H}{\partial T \partial x_{i,n+1}} = L_{n+1}\overline{Cpl}_{i,n+1} \qquad [24]$$

$$\frac{\partial^2 H}{\partial T \partial L_{n+1}} = \frac{\partial Hl_{n+1}}{\partial T} \qquad [25]$$

$$\frac{\partial^2 H}{\partial V_{n-1} \partial y_{i,n-1}} = \frac{\partial^2 H}{\partial y_{i,n-1} \partial V_{n-1}} = \overline{Hv}_{i,n-1} \qquad [26]$$

$$\frac{\partial^2 H}{\partial T \partial y_{i,n-1}} = V_{n-1} \overline{Cpv}_{i,n-1} \qquad [27]$$

$$\frac{\partial^2 H}{\partial T \partial V_{n-1}} = \frac{\partial Hv_{n-1}}{\partial T} \qquad [28]$$

$$\frac{\partial^2 H}{\partial V_n \partial T} = -(1 + S_n)\frac{\partial Hv_n}{\partial T} \qquad [29]$$

$$\frac{\partial^2 H}{\partial L_n \partial T} = -(1 + T_n)\frac{\partial Hl_n}{\partial T} \qquad [30]$$

$$\frac{\partial^2 H}{\partial y_{i,n} \partial T} = -(1 + S_n)V_n \overline{Cpv}_{i,n} \qquad [31]$$

$$\frac{\partial^2 H}{\partial x_{i,n} \partial T} = -(1 + T_n)L_n \overline{Cpl}_{i,n} \qquad [32]$$

$$\frac{\partial^2 H}{\partial T^2} = -(1 + S_n)V_n \frac{\partial H^2 v_n}{\partial T^2} - (1 + T_n)L_n \frac{\partial^2 Hl_n}{\partial T^2} \qquad [33]$$

$$\frac{\partial^2 H}{\partial V_{n-1} \partial T_{(n-1)}} = \frac{\partial Hv_{n-1}}{\partial T_{(n-1)}} \qquad [34]$$

$$\frac{\partial^2 H}{\partial y_{i,n-1} \partial T_{(n-1)}} = V_{n-1} \overline{Cpv}_{i,n-1} \qquad [35]$$

$$\frac{\partial^2 H}{\partial L_{n+1} \partial T_{(n+1)}} = \frac{\partial H l_{n+1}}{\partial T_{(n+1)}} \qquad [36]$$

$$\frac{\partial^2 H}{\partial x_{i,n+1} \partial T_{(n+1)}} = L_{n+1}\overline{Cpl}_{i,n+1} \qquad [37]$$

As can be seen, the nonzero elements in the Hessian are due to the nonlinear terms in the Jacobian. The magnitude of the energy balance terms dominate over almost all others. Also, only $N(3C)$ terms derived from equilibrium relations include first order derivatives of K, the rest are second order effects. The terms resulting from material balances are constants. The terms resulting from the energy balance include zeroth, first and second order terms. No less than $N(8C)$ elements include partial molar enthalpies, and $N(8C+6)$ elements include heat capacities. Even for correct values for all variables, the Hessian for this system has large magnitude terms.

Scaling of the energy balance will only reduce the magnitude of these terms, not make them disappear. An alternative is to increase the number of variables with the goal of eliminating the large magnitude terms in the Hessian.

Augmenting the Variables from (y,V,T,L,x) and the Equations from (M,E,S_1,S_2,H)

This work investigates the convergence characteristics of two unique augmented systems. The first augmented equation set is formed by considering the partial molar enthalpies to be independent variables. This formulation increases the number of equations per stage from $2C+3$ (i.e. x,y,T,L,V) to $4C+3$. The new variable set is,

Variable	Number
x_i	C
y_i	C
$\overline{Hv}_i$	C
$\overline{Hl}_i$	C
T	1
L	1
V	$\underline{1}$
	$4C+3$

[38]

       To completely define the system, 2C additional
equations must be added per stage. The logical choice
for these equations is the difference between the new
variables and their model description. Thus the new
equation set would be,

Equation	Number

Component Mass Balance	C
Component distribution balance	C
Energy balance	1
Summation of $x_i - 1 = S_1$	1
Summation of $y_i - 1 = S_2$	1
$\overline{Hv}_i - fHv_i(y_i,T) = P1_i$	C
$\overline{Hl}_i - fHl_i(x_i,T) = P2_i$	C
	$\overline{4C+3}$

[39]

       The second augmented system is formed by
considering the stream enthalpies as independent
variables. This formulation increases the number of
equations per stage from 2C+3 (i.e. x,y,T,L,V) to 2C+5.
The new variable set is,

Variable	Number
x_i	C
y_i	C
Hv	1
Hl	1
T	1
L	1
V	1
	$\overline{2C+5}$

[40]

       To completely define the system, 2 additional
equations must be added per stage. The logical choice
for these equations is the difference between the new
variables and their model description. Thus the new
equation set would be,

Equation	Number

Component Mass Balance	C
Component distribution balance	C
Energy balance	1
Summation of $x_i - 1 = S_1$	1
Summation of $y_i - 1 = S_2$	1
$Hv - fHv(y_i,T) = Ev$	1
$Hl - fHl(x_i,T) = El$	1
	$\overline{2C+5}$

[41]

        Let us for a moment consider the Hessian of the
first augmented equation set. The partial derivatives of
the material,distribution, and summation equations will
all be equal to zero. The terms of $P1_i$ and $P2_i$ will be
weak functions of x,y,and T. The most significant terms
of the Hessian are from the cross partials in the energy
balance. Explicitly, the energy balance for the first
augmented system is given by:

$$H = V_{n-1} \sum y_{i,n-1}\overline{Hv}_{i,n-1} + L_{n+1} \sum x_{i,n+1}\overline{Hl}_{i,n+1} +$$

$$q_{n+1}V_{n+1} \sum y_{i,n+1}\overline{Hv}_{i,n+1} - (1+S_n+q_n)V_n \sum y_{i,n}\overline{Hv}_{i,n} -$$

$$\text{[42]}$$

$$(1+T_n+r_n)L_n \sum x_{i,n}\overline{Hl}_{i,n} + r_{n-1}L_{n-1} \sum x_{i,n-1}\overline{Hl}_{i,n-1} +$$

$$Hf_nF_n - Q_{Ln}$$

Where $\overline{Hl}_i$ and $\overline{Hv}_i$ denote the partial molar liquid and
vapor enthalpies respectively. It can be seen from this
equation that the energy balance is a function of all of
the system variables except temperature. The temperature
dependence of the energy balance has been eliminated and
incorporated into the partial molar enthalpy equations
$P1_i$, and $P2_i$. It can also be seen that the terms of the
Hessian will contain system variables as some of the
terms of the matrix. Specifically, some elements of the
Hessian will contain partial molar enthalpies. These
are typically three to five orders of magnitude and will
tend to make the norm of the Hessian very large.

        In contrast to the 4C+3 formulation, the 2C+5
formulation has an energy balance of the form given in
equation [7] with the assumptions of equation [8]. The
Hessian of this system has nonzero values of the
following form.

$$\frac{\partial^2 H}{\partial V_{n-1}\partial Hv_{n-1}} = \frac{\partial^2 H}{\partial Hv_{n-1}\partial V_{n-1}} = 1 \qquad \text{[43]}$$

$$\frac{\partial^2 H}{\partial L_{n+1}\partial Hl_{n+1}} = \frac{\partial^2 H}{\partial Hl_{n+1}\partial L_{n+1}} = 1 \qquad \text{[44]}$$

$$\frac{\partial^2 H}{\partial V_n \partial Hv_n} = \frac{\partial^2 H}{\partial Hv_n \partial V_n} = -(1 + S_n) \qquad [45]$$

$$\frac{\partial^2 H}{\partial L_n \partial Hl_n} = \frac{\partial^2 H}{\partial Hl_n \partial L_n} = -(1 + T_n) \qquad [46]$$

These equations are identical to the mass balance Hessian equations. In the 2C+5 formulation, both the component mole fractions as well as the temperatures have been eliminated from the energy balance derivatives. Furthermore, the values of the derivatives are orders of magnitude less than those found in the 4C+3 formulation. The additional terms of the Hessian due to these equations are:

$$\frac{\partial^2 Ev}{\partial T \partial y_i} = \frac{\partial^2 Ev}{\partial y_i \partial T} = \frac{\partial^2 fHv}{\partial y_i \partial T} = \overline{Cp}v_i \qquad [47]$$

$$\frac{\partial^2 El}{\partial T \partial x_i} = \frac{\partial^2 El}{\partial x_i \partial T} = \frac{\partial^2 fHl}{\partial x_i \partial T} = \overline{Cp}l_i \qquad [48]$$

$$\frac{\partial^2 Ev}{\partial T^2} = \sum y_i \frac{\partial \overline{Cp}v_i}{\partial T} \qquad [49]$$

$$\frac{\partial^2 El}{\partial T^2} = \sum x_i \frac{\partial \overline{Cp}l_i}{\partial T} \qquad [50]$$

Where,

$$\overline{Hl}_i = Hl_i + H_{il}^{EX} \qquad [51]$$

$$\overline{Hv}_i = Hv_i + H_{iv}^{EX} \qquad [52]$$

and,

$$\frac{\partial \overline{Hl}_i}{\partial T} = \overline{Cp}l_i \qquad \frac{\partial \overline{Hv}_i}{\partial T} = \overline{Cp}v_i \qquad [53]$$

RR=8.1 $\begin{cases} D=12.24 \\ x_1=0.103 \\ x_2=0.897 \\ x_3=0.000 \end{cases}$

$\left.\begin{array}{l} F_{12}=76.74 \\ x_1=0.0 \\ x_2=0.0 \\ x_3=1.0 \\ T=181.4°C \end{array}\right\}$

$\left.\begin{array}{l} F_7=23.23 \\ x_1=0.5 \\ x_2=0.5 \\ x_3=0.0 \\ T=103.0°C \end{array}\right\}$

stg 21

stg 12

stg 7

stg 1

Qcond=34999J/hr
Tcond=101.02°C

P=1 atm

Qreb=45746 J/h
Treb=150.68°C

$\begin{cases} B=87.76 \\ x_1=0.118 \\ x_2=0.007 \\ x_3=0.874 \end{cases}$
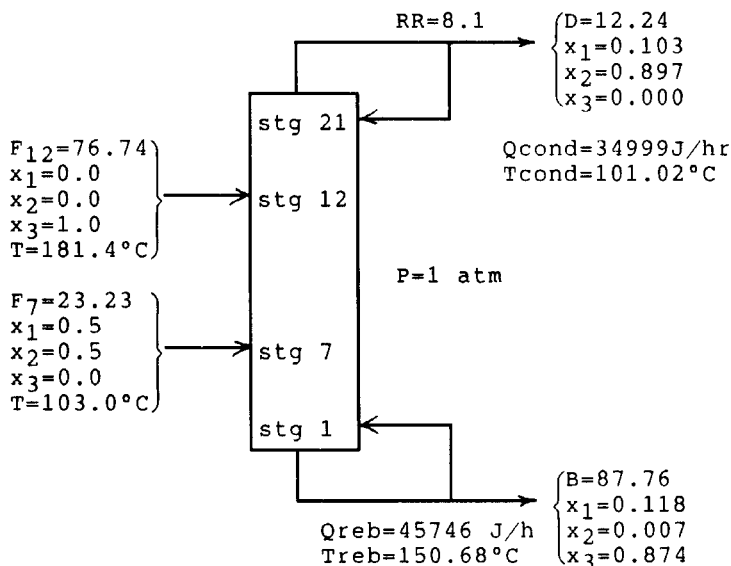
**Figure 3. Toluene(1),Methylcyclohexane(2),Phenol(3)
System**

EXAMPLES AND RESULTS

The examples chosen were representative azeotropic
distillation, extractive distillation and an
alcohol/water ternary distillation with difficult
convergence properties(11). The azeotropic distillation
is the methylcyclohexane/toluene/phenol column analyzed
by Smith(21) and Fredenslund et al.(22). The extractive
distillation system is the toluene/2-butanone/n-heptane
system also previously examined (21,22). The
methanol/ethanol/water column has been previously solved
to meaningful results only with a customized homotopy
procedure(11). The configuration of these systems along
with the converged solutions are presented in figures 3,
4, and 5 respectively .

The equilibria were modeled using the DECHEMA
Wilson parameters(23). Parameters from ternary data were
used to model the alcohol/water system(23). Vapor
pressures were predicted using the Antoine equation.
Both liquid and vapor component enthalpies were
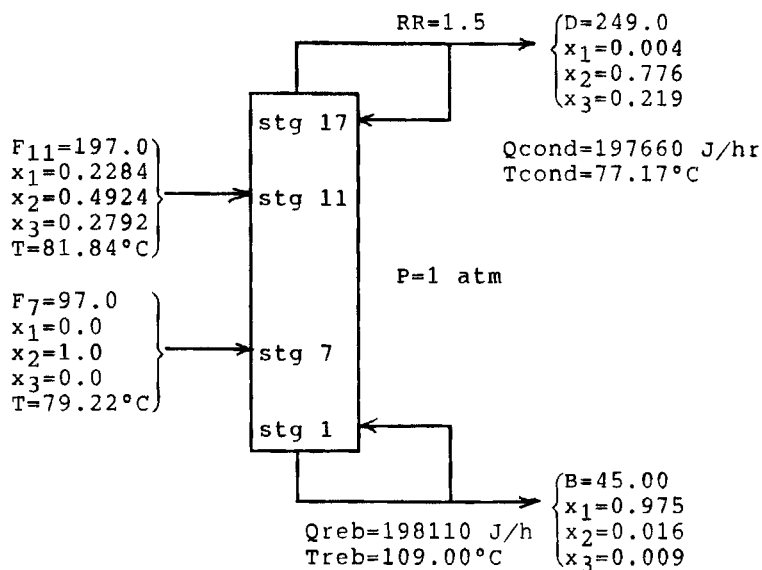calculated using a standard state of zero degrees

RR=1.5 $\begin{cases} D=249.0 \\ x_1=0.004 \\ x_2=0.776 \\ x_3=0.219 \end{cases}$

stg 17

$\left.\begin{array}{l} F_{11}=197.0 \\ x_1=0.2284 \\ x_2=0.4924 \\ x_3=0.2792 \\ T=81.84°C \end{array}\right\}$ stg 11

Qcond=197660 J/hr
Tcond=77.17°C

$\left.\begin{array}{l} F_7=97.0 \\ x_1=0.0 \\ x_2=1.0 \\ x_3=0.0 \\ T=79.22°C \end{array}\right\}$ stg 7

P=1 atm

stg 1

$\begin{cases} B=45.00 \\ x_1=0.975 \\ x_2=0.016 \\ x_3=0.009 \end{cases}$

Qreb=198110 J/h
Treb=109.00°C

**Figure 4. Toluene(1),2-Butanone(2),n-Heptane(3)
        System.**

Celsius and one atmosphere pressure. Heat of mixing
effects were taken into account for the liquid phase.
The vapor phase was assumed to be ideal at the column
pressure (one atmosphere).

Results of Numerical Experimentation

The results of numerical experimentation of the
two outlined augmented equation sets with the three
simulations presented above are:

.1.   It is possible to obtain a meaningful solution to
the alcohol/water problem using Newton's method with
line search provided ones initializes close to the
operation condition.
2.   The first augmented Hessian model (4C+3) did not
perform as effectively as the 2C+3 model.
3.   The second augmented Hessian model performed as
effectively as the 2C+3 model but not quicker or with a
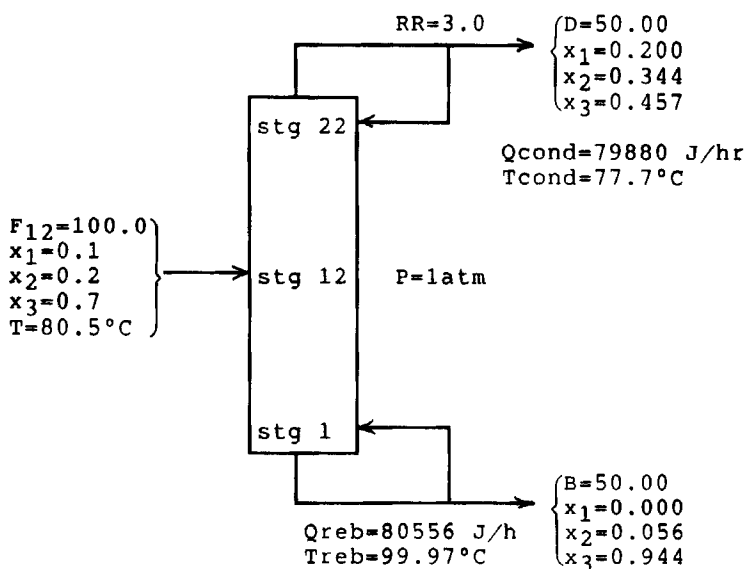noticeably greater linearity.

RR=3.0   D=50.00
                x_1=0.200
                x_2=0.344
                x_3=0.457

stg 22

Qcond=79880 J/hr
Tcond=77.7°C

F_{12}=100.0
x_1=0.1
x_2=0.2   stg 12   P=1atm
x_3=0.7
T=80.5°C

stg 1

Qreb=80556 J/h   B=50.00
Treb=99.97°C x_1=0.000
                   x_2=0.056
                   x_3=0.944

Figure 5. Methanol(1),Ethanol(2),Water(3) System

CONCLUSIONS

As a result of numerical experimentation:

1. Systems of equations designed to augment the
Hessian do not appear to converge faster than
nonaugmented systems when the initial estimates are
within the domain of attraction of both equation sets.

2. Although some experimental investigation has
been done, the exact range of the domain of attraction
of the augmented systems compared to the MESH systems is
still unknown. Work is continuing in this area.

3. Augmenting the MESH variables with the stream
enthalpies yields a Hessian that is far better scaled
than the MESH variables augmented with the partial molar
enthalpies. Numerical experimentation with both equation
sets has shown that the stream enthalpy model converges
more readily than the partial molar enthalpy model.

NOMENCLATURE

B	molar bottoms flow rate(moles/hr)
C	number of components
$\overline{Cpl}_{i,j}$	partial derivative of the liquid partial molar enthalpy of component i on stage j w.r.t. temperature
$\overline{Cpv}_{i,j}$	partial derivative of the vapor partial molar enthalpy of component i on stage j w.r.t. temperature
D	molar distillate flow rate(moles/hr)
E_i	equilibrium relationship for component i
El	Liquid enthalpy equation
Ev	Vapor enthalpy equation
EX	excess thermodynamic function
F_i	molar feed rate to stage i(moles/hr)
$f_{i,n}$	feed mole fraction of component i to stage j
$fHl(x_i,T)$	Liquid stream enthalpy model(function of liquid phase composition and temperature)
$fHv(y_i,T)$	Vapor stream enthalpy model(function of vapor phase composition and temperature)
H	energy balance equation
Hl_i	stream liquid enthalpy for stage i
$\overline{Hl}_{i,j}$	partial molar enthalpy for liquid component i on stage j
Hv_i	stream vapor enthalpy for stage i
$\overline{Hv}_{i,j}$	partial molar enthalpy for vapor component i on stage j
k_i	distribution value for component i(y_i/x_i)
L_n	molar liquid rate from stage n
M_i	molar mass balance for component i
N	number of stages
n_i	tray efficiency for tray i
P	column pressure(atmospheres)
Pl_i	first partial molar enthalpy balance for component i
$P2_i$	second partial molar enthalpy balance for component i
Q_{Ln}	heat input to stage n
q_n	fraction of vapor entrained from stage n
Qcond	condenser heat duty(Joules/hour)
Qreb	reboiler heat duty(Joules/hour)
RR	reflux ratio(L/D)
r_n	fraction of liquid backmixed from stage n
S_n	fractional vapor sidestream from stage n
S_1	first summation relationship
S_2	second summation relationship
stg	stage
T	temperature(deg. C)
T_n	fraction of liquid sidestream from stage n
Treb	reboiler temperature
Tcond	condenser temperature

V_n molar vapor rate from stage n
$x_{i,j}$ liquid mole fraction of component i on stage j
$y_{i,j}$ vapor mole fraction of component i on stage j

REFERENCES

1. King,C.J., Separation Processes, 2nd.ed.,
    McGraw Hill, NY, pp 351-354(1980)

2. Henley,E.J. and J.D.Seader,Equilibrium-Stage
    Separation Operations in Chemical Engineering,
    Wiley,NY(1981)

3. Wang,J.C. and G.E. Henke,Tridiagonal Matrix for
    Distillation, Hydrocarbon Processing, 45, No.8,
    155,No.9169(1966)

4. Newman, J., UCRL-17739 (1967)

5. Naphtali,L.M.,The Distillation Column as a Large
    System,AIChE Mtg.,SanFrancisco,CA(1965)

6. Naphtali,L.M. and D.P.Sandholm,Multicomponent
    Separation Calculations by Linearization,
    AIChE Journ., 17, 148-153(1971)

7. Holland,C.D.,Fundamentals of Multicomponent
    Distillation, McGraw Hill, NY, (1984)

8. Ricker,N.L.,F. Nakashio, and C.J.King, An
    Efficient,General Method for Computation of
    Countercurrent Separation Processes with Axial
    Dispersion, AIChE Journ.,27,277-284(1981)

9. Krishnamurthy,R. and R. Taylor,A Nonequilibrium
    Stage Model of Multicomponent Separation
    Processes, AIChE Journ., 31, I&II, 449-460,
    III,1973-1983(1985)

10. Kovach,III,J.W. and W.D.Seider, Heterogeneous
    Azeotropic Distillation-Homotopy-Continuation
    Methods,AIChE Mtg., Miami Beach, FL(1986)

11. Vickery,D.J. and R. Taylor, Path-Following
    Approaches to the Solution of Multicomponent,
    Multistage Separation Process Problems, AIChE
    Journ., 32, 547-556(1986)

12. Taylor, R., personal communication(1986)

13. Seader, J.D.,Computer Modeling of Chemical
    Processes, AIChE Monog.,81, No.15,(1985)

14.   Lin,W.-J.,J.D. Seader and T.L. Wayburn, Computing
       Multiple Solutions to Systems of Interlinked
       Separation Columns, AIChE Journ., 33,
       886-897(1987)

15.   Wayburn,T.L. and J.D. Seader, Solutions of Systems
       of Interlinked Distillation Columns by
       Differential Homotopy-Continuation Methods,
       proceed. 2nd. Intern. Conf. on Found. of
       Computer-Aided Process Design, A.W.Westerberg &
       H.H.Chien eds., CACHE, Ann Arbor, MI,
       pp 765-862(1984)

16.   Hlavacek,V. and P. Van Rompay, Simulation of
       Countercurrent Separation Processes via Global
       Approach, Comput.Chem.Engr., 9, 343-350(1985)

17.   Vickery,D.J.,T.L. Wayburn and R. Taylor, The
       Development of Homotopy Methods for the Solution
       of Difficult Separation Process Problems,
       I.Chem.E. Brighton Conference, England(1987)

18.   Frantz, R.W. and V. Van Brunt, A Differential
       Homotopy Continuation Method for Interlinked
       Solvent Extraction Cascades, Sep.Sci.&Tech., 22,
       243-267(1987)

19.   Frantz, R.W., Development and Application of
       Continuation Methods for the Solution of
       Engineering Systems, Master of Science Thesis,
       University of South Carolina, (1986)

20.   O'Quinn, L.N., R.W. Frantz, and V. Van Brunt,
       Stability of a Steady-State Hydrometallurgical
       Solvent Extraction Model, AIChE Mtg., Miami Beach,
       FL(1986)

21.   Smith,B.D.,Design of Equilibrium Stage Processes,
       McGraw Hill, NY, pp 358-438(1963)

22.   Fredenslund,A., J.Gmehling and P.Rasmussen,
       Vapor-Liquid Equilibria using UNIFAC, Elsevier,
       NY, pp 165-196(1977)

23.   Gmehling, J.and R. Eckermann, Vapor-Liquid
       Equilibrium Data Collection, DECHEMA Deutsche
       Gesellschaft für Chemisches Apparatewesen,
       Frankfurt, W. Germany(1977)