A GENERALIZED MODEL FOR DISTILLATION COLUMNS—I
MODEL DESCRIPTION AND APPLICATIONS
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Abstract—A generalized model for the dynamic simulation of distillation columns is presented. The model allows the solution of a wide variety of problems, from open- and closed-loop responses of single (and multiple) columns to operability studies (of feed changeover and start-up operations) and column instability studies (effect of plate hydraulics during transient operations). Results are given for single columns (including industrial) as well as multiple columns for different types of operations. The problems include thermodynamically close to ideal systems to highly nonideal systems. Efficient and robust numerical integrators are used to obtain reliable solutions even for difficult discontinuous operations.

Scope—Distillation is an essential operation and a high energy consumer in most chemical processes. Realistic performance of an actual column can seldom be predicted satisfactorily by excluding the simultaneous effects of heat transfer and fluid flow on the plates. Plate hydraulics is an important factor in predicting the dynamic performance. Because of its effect on heat and mass transfer calculations accurate prediction of physical properties is also important. Also, frequently, there is more than one distillation column in the process and the interactions between columns can be significant from the design as well as the operability point of view. A generalized dynamic model taking into consideration all the factors described above, and which is numerically robust, efficient in terms of computing time and storage (even for very large industrial problems) and flexible enough to allow the study of a wide variety of processes, can have a wide or significant application both in terms of research and development as well as solving practical problems. Also, it will allow the study of the relative importance of the various features of the model and hence can verify the veracity of simplifying assumptions that are made for developing simpler models.

Conclusions and Significance—The successful application of the model to solve the different types of test problems demonstrates its wide applicability and flexibility. The differences in the responses from simplified and more complex versions of the model have been shown, and the importance of choosing the proper model (with the required degree of complexity) for a particular problem has been illustrated. The good matching of the industrial data show that the model is reliable and can be used for the study of industrial processes. Even where the industrial data were not available, the results obtained when analyzed qualitatively, seemed to be very reasonable. All this points to the potential use of the model in areas of design (related to operability and control), in understanding causes of column instability (plate hydraulics) and for detailed study of the dynamics of multiple columns and a possible extension to separation processes.

INTRODUCTION
There has been a continuous development of dynamic models of distillation columns with emphasis on process control and fast, approximate models in strategies for maintaining product specifications. Very few of these models, however, consider the solution of the material and energy balances on each plate using models to represent plate hydraulics and approaches to equilibrium. Tyreus et al. [1], and more recently Ballard and Brosilow [2] and Gallun and Holland [3], have modeled distillation columns accounting for variations in liquid holdup using a semi-implicit Runge–Kutta method and Gear’s method, respectively. Prokopakis and Seider [4] have developed a model for simulating azeotropic distillation problems. Murphy [5] developed a dynamic model for the study of heat integration of multiple distillation columns.

A need, however, exists for a dynamic model (or package) that is flexible enough to handle different
column (or columns) configurations and is versatile enough to allow the study of different processes and operations (e.g. start-up). It should be able to solve large industrial problems and should be numerically robust, efficient and reliable.

With these objectives in mind, the proposed generalized model has been developed. It is based on the model of Gani [6]. The model uses the equation-oriented approach to flow-sheeting to solve the set of ordinary differential equations (ODEs) representing the processes and the sequential modular approach to solve each of the decomposed subsets of procedures which allow the evaluation of the functions [i.e. the right-hand sides (r.h.s.) of the ODEs].

For the particular problem being solved, the model defines a set of ODEs and a set of procedures to represent the process. The ODEs represent the mass and energy balances of the process, while the procedures account for the thermodynamics, plate hydraulics, controllers, reboilers, condensers, special configurations etc. Decomposing the set of procedures into subsets, the procedures are solved to determine the r.h.s. of the ODEs needed by the numerical integrator. The numerical integrator selects the type of method to be used (Adams-Moulton, BDF or DIRK), calculates the Jacobian matrices (if necessary) by finite differencing, taking into account their sparsity, and employs a sparse matrix solver for solution of the ODEs. The purpose of this is to save as much computing time as possible so that difficult problems (i.e. discontinuous problems) or very large problems can be solved.

The paper is divided into two parts. Part I describes the development of the model and presents the dynamic results obtained from solving the different test problems. Part II [7, this issue, pp. 1%211] describes the numerical integration techniques that have been used, the analysis of the integrator performance and the integration statistics of the test problems solved. The test problems selected cover different systems (ideal to nonideal), single- or multiple-column dynamics, the effects of column hydraulics and examples of application for operability studies (start-up problem), design (multiple-column problem) and the study of control structures (closed-loop responses).

In the case of closed-loop responses, the model allows the inclusion of user-supplied routines (for controllers) or the selection of built-in procedures to provide the forcing functions.

DEVELOPMENT OF THE MODEL

The model will consist of a set of ODEs to be obtained from mass and energy balances around each plate of the distillation column and a set of algebraic equations/correlations (to be known as procedures) which will be used to predict the physical properties, the plate hydraulics, the mass and heat transfer and a set of optional procedures (for the dynamics of the reflux drum and reboiler and types of controllers). The variables that appear on the l.h.s. of the ODEs will be termed the “differential” variables, all other variables except time will be termed as “algebraic” or “procedure” variables. Time will be the independent variable.

Three assumptions are made in the development of the proposed model:

(i) the molar vapor holdup is negligible compared to the molar liquid holdup;
(ii) the liquid and vapor leaving each plate are in thermal equilibrium;
(iii) the definition of Murphree plate efficiency will apply for each plate and the liquid and vapor are perfectly mixed on each plate.

Assumption (i) is quite reasonable since in most systems, the vapor density is considerably smaller than the liquid density. The assumption of perfect mixing and Murphree plate efficiency is necessary to reduce the complexity of the problem. Models of mixing on plates are very complex and involve partial differential equations. Similarly more accurate efficiency models are very complex and add to the complexity of the problem. The accuracy that can be achieved with these complex models at the expense of the dimension of the problem and computing time was considered and it was decided to use the simplifying assumptions.

Balance equations

For a typical plate in a distillation column (Fig. 1a), mass- and energy-balance equations are defined thus:

**Component mass balance around plate p of column c for component i**

\[
\frac{dC_{p,i}^c}{dt} = F_{V,p}y_{i,p}^e + F_{L,p}x_{i,p}^e + V_{p-1,i}y_{p-1,i} + E_{p,i} + L_{p+1,i} + X_{p+1,i} + E_{p+i} - (P_{V,p} + V_{p} + E_{p,i})y_{p,i}
\]

**Total energy balance around plate p of column c**

\[
\frac{dE_{p}}{dt} = F_{V,p}H_{p}^e + F_{L,p}H_{p}^e + E_{p} - V_{p-1}H_{p-1} - E_{p-1}H_{p-1} - L_{p+1}H_{p+1} - E_{p+1}H_{p+1} - (P_{V,p} + V_{p} + E_{p,i})H_{p}
\]

**Total mass balance around plate p of column c**

\[
\frac{dL_{p}}{dt} = F_{V,p} + F_{L,p} + V_{p-1} - E_{p-1} - L_{p+1} - E_{p+1} - P_{V,p} - P_{L,p}
\]
Algebraic equations/correlations

The set of algebraic equations is divided into three parts: the first contains the equations defined to describe a particular variable; the second consists of the equations/correlations used to predict the physical properties; and the third part consists of the correlations that describe the plate hydraulics.

Equations by definition. The total mass holdup \( C_{i,p} \) on plate \( p \) and the total energy holdup \( C_{\ell,p} \) on plate \( p \) are defined by

\[
C_{i,p} = \sum_{i=1}^{\infty} C_{i,p}^i \tag{4}
\]

and

\[
C_{\ell,p} = h_p^\ell C_{T,p}^\ell \tag{5}
\]

By definition, the summation of the mole fractions should be unity, hence

\[
\sum_{i=1}^{\infty} x_{i,p}^i = \sum y_{i,p}^i = 1; \tag{6}
\]

thus,

\[
x_{i,p}^f = \frac{C_{i,p}^f}{C_{T,p}^f} \quad \text{and} \quad h_p^f = \frac{C_{\ell,p}^f}{C_{T,p}^f}. \tag{7}
\]

Use of equation (7) therefore means redundancy of equation (3). The Murphree plate efficiency is defined thus:

\[
y_{i,p}^{y\ell} = \frac{y_{i,p}^{y\ell} - y_{i,p-1}^{y\ell} + y_{i,p-1}^{y\ell}}{ME_p^\ell}. \tag{8}
\]

Physical properties correlations. The equilibrium relation between a vapor phase and a liquid phase is represented by

\[
y_{i,p}^V = K_{i,p} x_{i,p}^L \tag{9}
\]

with the equilibrium ratio, \( K_{i,p} \), being determined from

\[
K_{i,p} = f(x_{i,p}^L, y_{i,p}^V, \Theta, \Pi). \tag{10}
\]

The enthalpies of the liquid and vapor phases are also...
defined as functions of temperature, pressure and composition as

\[ H_p = f(y_p, \Theta_p, \Pi_p) \]  

(11)

and

\[ h_p = f(x_p, \Theta_p, \Pi_p) \]  

(12)

The densities are determined from

\[ \rho_L = \sum \rho_{L,i} x_i \]  

(13)

and

\[ \rho_V = \sum \rho_{V,i} y_i \]  

(14)

where the individual component densities are determined from

\[ \rho_{L,i} = f(\Pi_p, R, \Theta_p, Z_{L,i}) \]  

(15)

and

\[ \rho_{V,i} = f(\Pi_p, R, \Theta_p, Z_{V,i}). \]  

(16)

The molecular weight of each phase is determined from

\[ M_L = \sum M_{L,i} x_i \]  

(17)

and

\[ M_V = \sum M_{V,i} y_i. \]  

(18)

Equations (10), (11), (12), (15) and (16) will depend on the type of thermodynamic package being used.

**Hydraulic correlations.** The plate pressure drop is determined from the adjacent plate pressures:

\[ \Delta P_p = P_{p-1} - P_p \]  

(20)

The liquid flow rate, vapor flow rate, entrainment rates, weeping rate and flooding of the plates are all functions of the plate geometry, the liquid holdup on the plates and the plate pressure drops:

\[ V_p = f(\Delta P_p, \text{plate geometry}), \]

\[ L_p = f(C_p, \text{plate geometry}), \]

\[ L_{\text{vap}} = f(C_p, V_p, \text{plate geometry}), \]

\[ V_{\text{vap}} = f(V_p, L_p, \text{plate geometry}), \]

\[ E_{L_p} = f(C_p, \Delta P_p, \text{plate geometry}) \]

(19)

and

\[ E_{V_p} = f(C_p, \Delta P_p, \text{plate geometry}) \]

The total liquid rates of equations (1)–(3) correspond to \( L_p + L_{\text{vap}} \) of equation (19).

The detailed correlations for the above equations for the different types of plates are given in the Appendix.

**Optional equations**

**Reflux drum and reboiler.** The accumulation of liquid in the reflux drum and reboiler is taken into account through component mass-balance equations around them. For the reflux drum we have

\[ \frac{dM_{\text{RD}}}{dt} = V_{\text{RD}} y_{\text{RD}} - (L_\text{RD} + D) x D. \]  

(20)

and, for the reboiler,

\[ \frac{dM_{\text{RB}}}{dt} = L_\text{RB} x_{\text{RB}} - B x_{\text{RB}} - V_{\text{RB}} y_{\text{RB}}. \]  

(21)

**Controller equations.** Equations for the proportional (P), proportional–integral (PI) and proportional–integral–derivative (PID) controllers are included as follows:

P controller,

\[ u = k_1 e + u_\text{*}; \]  

(22)

PI controller,

\[ u = k_1 e + k_2 \int e dt + u_\text{*}; \]  

(23)

PID controller,

\[ u = k_1 e + k_2 \int e dt + k_3 \frac{de}{dt} + u_\text{*}; \]  

(24)

where \( e = m - m_\text{*}, k_1, k_2 \) and \( k_3 \) are the parameters of the controller, \( u \) is the manipulated variable, \( m \) is the measured variable and an * signifies the steady-state value.

In the case of the PI and PID controllers, the integral part, i.e.

\[ \int e dt, \]

is redefined as

\[ \frac{dA}{dt} = e, \]

where

\[ A = \int e dr. \]

Thus for PI and PID controllers, additional ODES are required. It should be noted that although these ODES are added to the set of ODES representing the distillation column, they do not affect the model ODES except through the controller-forcing functions represented by equations (22)–(24). In the case of no control, the us of equations (22)–(24) are specified variables.

**External heat input/output.** It is possible to specify the external heat input to a plate or extraction from a plate. Alternatively, it is also possible to predict the heat exchanged with the surroundings and include its effect in the balance equations. It is assumed that the temperature is uniform in the space between two plates. The heat transfer between the column wall and the surroundings is then determined from

\[ Q_p = U_p A_p \Delta \Theta_p, \]
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where:

- $U_p$, the heat transfer coefficient, is given by
  
  \[ U_p = \frac{h_0}{h} + k \alpha_p A_p, A_p, A_p, \theta_p, \theta_p \]

- $\Delta \theta_p$, the temperature difference, is given by
  
  \[ \Delta \theta_p = \theta_{\text{surf}} - \theta_p \]

and

- $h_0$, the heat transfer coefficient between the surroundings and the column external surface, is given by
  
  \[ h_0 = \frac{k \alpha_{\text{surf}} N_{\text{surf}}}{P_d + 2 t_{\text{surf}}} \]

For the simplest case, $1/(A_p h)$, the term related to the heat transfer coefficient between the inside surface of the column wall and the liquid and vapor phases inside the column can be neglected. Neglecting also the resistance to heat transfer of the column wall material compared to the insulation material requires the prediction of heat transfer due to forced convection between the surroundings and the external column wall and due to conduction through the insulation material. For this case, the external area of heat exchange, $A_p$, is given by

\[ A_p = (P_d + 2 t_{\text{surf}}) \times 3.14 P_d, \]

the logarithmic mean area, $A_p$, is given by

\[ A_p = \frac{P_d \times 2 t_{\text{surf}} \times 3.14}{\ln \left( \frac{P_d + 2 t_{\text{surf}}}{P_d} \right)} \]

and $h_0$ is given by

\[ h_0 = \frac{k \alpha_{\text{surf}} N_{\text{surf}}}{P_d + 2 t_{\text{surf}}} \]

where

- $t_{\text{surf}}$ — the thickness of the insulation,
- $k \alpha$ — the thermal conductivity,
- $N_{\text{surf}}$ — the Nusselt number,
- $P_d$ — the column diameter

and

- $\theta_{\text{surf}}$ — the temperature of the external surface.

**SOLUTION OF THE MODEL EQUATIONS**

The number of equations (ODEs, procedures and optimal procedures) will depend on the type of problem being solved and the type of model being used. The generalized model will be the most detailed and consequently will involve almost all the equations described previously. Simplified forms of the generalized model can be obtained by assuming constant rate of change of the energy holdup on each plate or constant total molar holdup. Unlike the generalized model, the plate pressures in these cases will be constant with respect to time. The different options to be employed will also affect the number of equations to be solved. The solution procedure, however, will be the same irrespective of the problem type or model type.

For each problem and corresponding model, the number of ODEs required to be solved will be defined. Simultaneously, the procedures required to determine all the algebraic variables of the ODEs will be defined. The optional equations (which will be defined by the problem definition) will be included in the list of ODEs and procedures. Starting from the initial state, when it is assumed that the differential variables will be known, the solution of the ODEs and the procedures representing the model for a particular problem will involve the following:

(a) determining the algebraic variables by using the defined procedures and determining the r.h.s.s (or the function values) of all the ODEs.

(b) determining values of the differential variables at time $t_j = t_{j-1} + \Delta t$ and repeating from (a) for $j = 1, 2, \ldots, \text{end}$. Thus at each time $t_j$, a set of ODEs and procedures are solved simultaneously in a manner similar to an equation-oriented package.

**SOLUTION OF THE PROCEDURES**

The procedures will include the algebraic equations/correlations required to determine all the algebraic variables of the ODEs. This means prediction of physical properties, plate hydraulics, optional equations (if they are procedures) and column interactions (if there are multiple columns). The set of procedures representing the model is decomposed into subsets to ease numerical solution and reduce computations and storage requirements. The decomposition, however, is based purely on heuristics and physical insights. Before the method employed for the decomposition of the procedures can be described, the variables that must be specified need to be defined.

**Variables to be specified**

Three types of variables must be specified: the differential variables at the initial state; the physical (design) variables, like the details of the plate geometry, column configuration, control structure, etc.; and the input/output algebraic variables, like the fresh feed flow rate, composition and state, the side-product flow rates and external heat input (or output) to a plate. All other input/output "algebraic" variables will be considered as manipulated variables whose steady-state values will have to be specified. In the case of an open-loop response, this steady-state value will be taken as the specified variable. In the case of the output variables, however, one product rate (distillate or bottoms) and one heat duty (reboiler or condenser) must be left unspecified. In the case of multiple columns, all the “linking” informa-
tion must be provided. In the case of linked columns, the product of one column will be the feed of another. In this case, the feed to another column may be considered as a manipulated variable. This will allow the control of feed flow rate to the column or change of state of the stream before entering the column.

Decomposition of the procedures

The starting point of all calculations is the values of the "differential" variables at time $t_j$. The first set of procedures should therefore be those that relate these variables. Using the definition equations (4)-(7), the total molar liquid holdup, the liquid-phase compositions and the liquid-phase enthalpies on each plate can be determined. In the case where equation (2) is transformed into an algebraic equation, the liquid-phase enthalpies will be determined by another subset. In these cases, the plate pressures will be specified. Each procedure in this subset contains only one variable which is unknown and hence no iteration is involved.

Knowing the liquid-phase compositions and enthalpies (or pressures in the case of simplified models) of each plate and each column, the next logical step will be to perform an "equilibrium" calculation on each plate to determine the equilibrium vapor-phase composition, plate temperatures and pressures (generalized model only). This set of procedures will involve the thermodynamic packages for the prediction of equilibrium. Also, as will be shown later (Solution of the "equilibrium" subset subsection), iteration loops will be involved here.

The next subset of procedures will include the calculation of the actual vapor-phase compositions through the definition of Murphree plate efficiencies and the physical properties. Here again a thermodynamic package can be used for the prediction of the physical properties. As all the procedures in this subset contain only one unknown variable, no iteration is involved here.

Once the compositions of each phase and their corresponding physical properties have been determined for all the plates of all the columns, the subset of procedures to determine the plate hydraulics can be employed. This subset will calculate the liquid and vapor flow rates, check for flooding, weeping or entrainment conditions and determine the weeping and entrainment rates. The solution of this subset of hydraulic procedures, will depend on the degree of complexity and details of desired plate hydraulics. Consequently, only for the most detailed calculations will iteration loops be involved.

The last subset of procedures will include those defined in the Optional equations subsection, the "linking" procedures (in the case of multiple columns). This subset of procedures therefore includes all the manipulated variables and "linked" inputs (in the case of multiple columns). As all the procedures involved in this subset will contain only one unknown variable, no iteration is involved here.

It should be noted that all the balance equations are defined by the ODEs and the procedures only involve the determination of the instantaneous values of the algebraic variables, given the instantaneous values of the differential variables. The decomposition of the procedures are done in such a way that it is possible to simulate processes with recycle streams (in the case of multiple columns) without any difficulty. This is because the recycle streams will be contained in the last subset of procedures and by that time the flow rates, compositions and physical properties of all plates for all columns will be known. It should also be noted that each subset of procedures will include all the plates of all the columns, i.e. the solution of each subset of procedures will provide values of these variables for all the columns.

Solution of the "equilibrium" subset

Two types of problems will need to be solved, depending on the type of model being used. For the generalized model, the problem to be solved is defined thus:

Given The liquid-phase composition and the liquid-phase enthalpy

Determine The equilibrium vapor-phase composition, temperature and pressure.

For all other cases, the problem to be solved is the following:

Given The liquid-phase composition and pressure

Determine The equilibrium vapor-phase composition and temperature.

The step-by-step solution technique applicable for both problems is the following:

Step I Assume initial estimates of temperature and pressure (if the generalized model).

Step II In the case of the generalized model, determine the liquid-phase enthalpy, given $\Theta, \Pi,$ and $x_{p,i}, i = 1,2,\ldots,N_c,$ and continue. Otherwise, go to Step V.

Step III If $|h_{m,i} - h_i| < \text{ERROR}_1,$ go to Step V. Otherwise, continue.

Step IV Update $\Theta$ and repeat from Step II.

Step V Given, $\Theta, \Pi,$ and $x_{p,i}, i = 1,2,\ldots,N_c,$ calculate $K_{x_i}$ and hence $y_{p,i}$ from $y_{p,i} = K_{x_i}x_{p,i}.$

Step VI If $|\Sigma y_{p,i} - 1.0| \geq \text{ERROR}_2,$ go to Step VII. Otherwise, stop.

Step VII In the case of the generalized model, update $\Pi,$ and repeat from Step II. Otherwise, update $\Theta,$ and repeat from Step V.

Newton-Raphson or Secant methods can be used to update $\Pi$ and $\Theta$. Usually about four iterations are required to satisfy a value of $\text{ERROR}_1$ and $\text{ERROR}_2$ of $10^{-4}$ [6]. A high accuracy is required.
especially for the pressure loop because a small variation in pressure causes a considerably higher variation in the pressure drops and, consequently, in the calculation of the plate hydraulics [6].

Unlike other models [3], the variables and equations corresponding to the equilibrium subset are not included in the set of equations to be solved simultaneously. This means that the equilibrium subset involves only bubble-point calculations (since the liquid-phase compositions and enthalpies or plate pressures are known from the "differential" variables). Thus the solution procedure only requires the initial conditions of the "differential" variables and the initial estimates of plate temperatures and pressures (in the case of the most complex version), or only plate temperatures in the case of the simplest version. The initial estimates for the first function evaluation can be the feed temperature and pressure. In the subsequent function evaluations, the last calculated values are used. This manner of decomposing the equilibrium subset from the set of equations to be solved simultaneously does not require good initial estimates for the state variables (which could be compositions or component flows), and at the same time reduces the size of the problem (as far as the numerical method is concerned) quite considerably. Also, it is possible to start the simulation from any initial condition and not from an initial steady state. In all the problems solved, no difficulty in attaining convergence was encountered by the equilibrium subset.

Solution of the "hydraulic" subset

The correlations used for determining the hydraulic variables are mainly empirical. The particular set given in the Appendix should not be regarded as the best available, but instead, as being fairly typical of those in use. Four different types of plates are considered: sieve plates, two types of valve plates and bubble-cap plates. Figure 1b shows the hydraulic variables of a typical plate. The solution technique employed provides several options. The simplest case is when only the liquid and vapor flow rates are calculated by considering plate hydraulics. Flooding, weeping and entrainment conditions will be checked if required but will not enter the balance equations. Also, the dynamics of the downcomer hydraulics are neglected. If the plate pressures are constant with respect to time, the vapor flow rates are determined from the transformed algebraic energy-balance equations [equation (2)]. A more complex form of the model is when the dynamics of the downcomer hydraulics are considered. In this case, as the description of the step-by-step solution will show, an iterative method will be required. The most complex case is when, in addition to the liquid and vapor flow rates and dynamics of the downcomer hydraulics, the flooding, weeping and entrainment rates are determined and included in the balance equations. Generally, two types of problems will need to be solved depending on the type of model to be considered. For the most complex case, the problem to be solved is defined as below:

**Given** The total molar holdup and total pressure drop

**Determine** The liquid and vapor flow rates across the plate, weeping, flooding and entrainment rates (if any).

For the simpler cases, the problem to be solved is as follows:

**Given** The total molar holdup

**Determine** The liquid flow rate across the plate and check (optional) the hydraulic behavior of the plate.

The step-by-step solution is as follows:

**Step 1** Select the downcomer hydraulic optional calculation procedure and calculate the liquid flow rate [equations (A.1)–(A.3)]. Three options are provided:
(a) neglect downcomer hydraulics (may be used in simpler cases);
(b) assume constant downcomer holdup;
(c) downcomer hydraulics considered—this case, an iterative solution technique is necessary for the liquid rates.

**Step 2** Check for downcomer hydraulic seal. If it is not sealed, calculate "blown" vapor flow rate [equation (A.4)] and possible gas-liquid counter-current flooding [equation (A.5)].

**Step 3** Calculate the vapor flow rate taking into account the type of plate:
(a) bubble-cap plates with the choice of two different calculation procedures [equations (A.6)–(A.10)];
(b) valve plates including flat check orifice and venturi orifice types [equations (A.11) and (A.12)];
(c) sieve plates, including the choice of two different procedures [equations (A.13)–(A.15)].

**Step 4** Check for weeping and calculate weeping flow rate (if any). Includes three optional correlations [equations (A.16)–(A.24)]. If there is any weeping, then the weeping rate is added to the liquid flow rate through the downcomer.

**Step 5** Check for wave formation on plates [equation (A.25)]. Warning given if there is wave formation.

**Step 6** Check for an excessive hydraulic gradient [equations (A.26)–(A.31)]. Warning given if there is an excessive hydraulic gradient.

**Step 7** Check for downcomer backup flooding [equation (A.32)]. Warning given if
equation (A.32) is true. See the Appendix for stopping criterion.

Step 8 Calculate entrainment rates [equations (A.33) and (A.34)].

Note: Steps 4–8 are optional in the simulation—any or all of them may be considered.

The start-up procedure

The start-up procedure employed is a more realistic version of that given by Gani [6]. The objective here was first to consider a realistic but simple start-up procedure with which to develop (and/or modify) an efficient numerical integration technique that can handle the discontinuities and to check the calculation of plate hydraulics during this type of operation. The next step (in future) would be to improve on the start-up procedure and develop an optimal control policy during these operations. The procedure in brief is given below:

\[
\begin{align*}
\text{Time} & \\
\quad t = 0 & \text{The column is empty.} \\
\quad t = t_1 & \text{Feed is introduced into the feed plate. If it is a vapor–liquid mixture, cooling is introduced.} \\
\quad t = t_2 & \text{Liquid reaches the bottom plate and the reboiler starts to increase its holdup.} \\
\quad t = t_3 & \text{The reboiler has a certain specified volume of liquid (normally dependent on the flow rate of the feed). Heat into the reboiler is introduced at this time.} \\
\quad t = t_4 & \text{If the feed was only liquid, cooling is introduced at this time. Run the column at total reflux until the vapor flow rate from the top plate is equal to the specified reflux rate.} \\
\quad t = t_5 & \text{The vapor flow is equal to the reflux rate, allow for holdup of liquid in the reflux drum and then draw out the distillate product.} \\
\quad t = t_6 & \text{Continuous operation starts.}
\end{align*}
\]

In addition to the description above, the start-up procedure will involve special control structures and plate hydraulic calculations (see Solution of "hydraulic" subset subsection). In the control structures, the plate pressure, temperature and height of liquid in the reflux drum will be controlled by manipulating the cooling water rate, the reflux rate and the distillate rate.

APPLICATIONS

The proposed model has been used for the simulation of the open-loop dynamic response of industrial columns, the study of the influence of plate hydraulics during operation, verification of plate hydraulics design, application to control, the study of the dynamics of different start-up operational procedures and the study of the dynamics of multiple columns. A selection of the dynamic results along with the test problem specifications are given in this section. The purpose here is to show the applicability and capability of the model rather than a detailed study of any of the problems mentioned above.

Details of the five test problems are given in Tables 1a and 1b. The first three columns are industrial, details of the fourth were taken from Ruiz [8] and the fifth was designed to test the model for multiple columns. Of the three industrial columns, the first is a depropanizer, the second is a debutanizer and the third is a stripping column separating a mixture of aromatics, paraffins, water and a solvent. The multiple-column problem configuration is shown in Fig. 2.

The manner in which the model is loaded into the computer for a particular run allows it to define the storage requirement for the particular problem. For the simplest problems (e.g., ideal mixtures, polynomial functions for thermodynamic properties prediction, plate hydraulics not considered), the storage requirement can be small enough to facilitate use even on a minicomputer. The results presented in this work were obtained using a VAX 11/780 and a PDP 11/70 computer.

### Table 1a. Specifications of the different distillation columns simulated

<table>
<thead>
<tr>
<th>Variable</th>
<th>Problem I Industrial depropanizer</th>
<th>Problem II Industrial debutanizer</th>
<th>Problem III Industrial extractive stripper</th>
<th>Problem IV Ruiz [8]</th>
<th>Problem V. Multiple-column problem</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of actual plates</td>
<td>8</td>
<td>40</td>
<td>30</td>
<td>8</td>
<td>Column 1: 20</td>
</tr>
<tr>
<td>Number of components</td>
<td>6</td>
<td>6</td>
<td>10</td>
<td>2</td>
<td>Column 2: 20</td>
</tr>
<tr>
<td>Plate efficiency</td>
<td>60%</td>
<td>70%</td>
<td>50%</td>
<td>100%</td>
<td>100%</td>
</tr>
<tr>
<td>Number of effective plates</td>
<td>22</td>
<td>28</td>
<td>15</td>
<td>8</td>
<td>Column 1: 20</td>
</tr>
<tr>
<td>simulated</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Column 2: 20</td>
</tr>
<tr>
<td>Actual feed plate position</td>
<td>21</td>
<td>33</td>
<td>30</td>
<td>5</td>
<td>Column 1: 11</td>
</tr>
<tr>
<td>Plating spacing (cm)</td>
<td>60</td>
<td>50</td>
<td>60</td>
<td>45.7</td>
<td>Column 2: 6 or 18</td>
</tr>
<tr>
<td>Plate dia (cm)</td>
<td>250</td>
<td>167.6</td>
<td>274</td>
<td>76.2</td>
<td>183</td>
</tr>
<tr>
<td>Type of condenser</td>
<td>Total</td>
<td>Total</td>
<td>Total</td>
<td>Total</td>
<td>Total</td>
</tr>
<tr>
<td>Type of reboiler</td>
<td>Total</td>
<td>Total</td>
<td>Total</td>
<td>Total</td>
<td>Total</td>
</tr>
<tr>
<td>Feed condition</td>
<td>Two phase</td>
<td>Two phase</td>
<td>Below</td>
<td>Bubble</td>
<td>Bubble point</td>
</tr>
<tr>
<td>Feed temperature (K)</td>
<td>300</td>
<td>338</td>
<td>361</td>
<td>291.8</td>
<td>point</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>point</td>
</tr>
</tbody>
</table>

The manner in which the model is loaded into the computer for a particular run allows it to define the storage requirement for the particular problem. For the simplest problems (e.g., ideal mixtures, polynomial functions for thermodynamic properties prediction, plate hydraulics not considered), the storage requirement can be small enough to facilitate use even on a minicomputer. The results presented in this work were obtained using a VAX 11/780 and a PDP 11/70 computer.
In this paper, most of the results reported will belong to the debutanizer column (except for the start-up and multiple-column problems). The results of the stripping column were given by Gani et al. [9] and the results of the depropranizer by Gani et al. [10]. The open-loop dynamic response of the debutanizer column is given in Fig. 3. From an initial condition, a reference steady state was reached. This is the period defined in Fig. 3 as the "steady-state search." At the steady state obtained (i.e. the reference steady state), perturbations were made and the dynamic response studied. It should be noted that if a different initial condition is used but the "design" specifications are kept unchanged, the reference steady state should again be reached. This can also be seen from Fig. 3. In addition, Fig. 3 also compares the open-loop transient responses obtained by the model using different degrees of complexity. In this case, it can be seen that although, approximately the same steady state is reached by all the versions, the transient paths are different. The matching of the transient responses depends on the size of the perturbations and the sensitivity of the variable being perturbed. Simplified (or reduced-order) models should therefore be used with caution (for control design), since the corresponding transient responses can lead to erroneous transfer functions. Details of one of the initial conditions, the reference steady state and the second steady state are given in Table 2a. Table 2b compares the reference steady state obtained from dynamic simulation with plant data for the depropanizer column. In this case, the initial condition was the feed condition (i.e. same composition and temperature on all plates).

Application of the generalized model to different aspects of tray hydraulics are discussed next. Figure 4a shows the differences in the response times (for the debutanizer column) between the variables which depend on plate hydraulics and the variables which

![Fig. 2. Multiple-column configuration.](image-url)
Table 2a. The initial condition and steady states for Problem II and the reference steady state for Problem III

<table>
<thead>
<tr>
<th>Composition</th>
<th>Initial condition</th>
<th>Distillate</th>
<th>Bottoms</th>
<th>Reference steady state</th>
<th>Distillate</th>
<th>Bottoms</th>
<th>Second steady state</th>
<th>Distillate</th>
<th>Bottoms</th>
<th>Reference steady state</th>
<th>Distillate</th>
<th>Bottoms</th>
</tr>
</thead>
<tbody>
<tr>
<td>Comp. 1</td>
<td>0.37692</td>
<td>0.09000</td>
<td>0.41061</td>
<td>0.08856</td>
<td>0.40587</td>
<td>0.11125</td>
<td>0.00811</td>
<td>0.00000</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Comp. 2</td>
<td>0.50664</td>
<td>0.11000</td>
<td>0.58937</td>
<td>0.06511</td>
<td>0.59413</td>
<td>0.08803</td>
<td>0.26836</td>
<td>0.00000</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Comp. 3</td>
<td>0.07312</td>
<td>0.20000</td>
<td>0.00000</td>
<td>0.18754</td>
<td>0.00000</td>
<td>0.17601</td>
<td>0.11928</td>
<td>0.00000</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Comp. 4</td>
<td>0.00861</td>
<td>0.25000</td>
<td>0.00001</td>
<td>0.25586</td>
<td>0.00000</td>
<td>0.24304</td>
<td>0.02072</td>
<td>0.00005</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Comp. 5</td>
<td>0.00700</td>
<td>0.15000</td>
<td>0.00000</td>
<td>0.16546</td>
<td>0.00000</td>
<td>0.15612</td>
<td>0.15362</td>
<td>0.02628</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Comp. 6</td>
<td>0.03171</td>
<td>0.20000</td>
<td>0.00000</td>
<td>0.23927</td>
<td>0.00000</td>
<td>0.23555</td>
<td>0.11728</td>
<td>0.06444</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Comp. 7</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>0.03534</td>
<td>0.03625</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Comp. 8</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>0.00029</td>
<td>0.00056</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Comp. 9</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>0.00178</td>
<td>0.86323</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Comp. 10</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>0.26413</td>
<td>0.017194</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Flow rate (kmol/h) 220.00 237.50 236.86 266.18 219.81 238.21 172.62 2411.81
Temperature (K) 363.00 385.00 320.10 365.40 315.04 356.65 391.76 455.22
Pressure (kPa) 560.00 587.80 527.50 555.30 506.34 534.16 195.56 217.83

Table 2b. Comparison of the final steady state predicted by the dynamic model with the plant data (Problem I)

<table>
<thead>
<tr>
<th>Plant data</th>
<th>Steady state*</th>
<th>Plant data</th>
<th>Steady state*</th>
</tr>
</thead>
<tbody>
<tr>
<td>Distillate</td>
<td></td>
<td>Bottoms</td>
<td></td>
</tr>
<tr>
<td>Mole fraction</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Propane</td>
<td>0.0433</td>
<td>0.0357</td>
<td>0.0018</td>
</tr>
<tr>
<td>Propylene</td>
<td>0.7975</td>
<td>0.8107</td>
<td>0.0005</td>
</tr>
<tr>
<td>Propane</td>
<td>0.1547</td>
<td>0.1526</td>
<td>0.0004</td>
</tr>
<tr>
<td>1-Butene</td>
<td>0.0032</td>
<td>0.0007</td>
<td>0.0070</td>
</tr>
<tr>
<td>n-Pentene</td>
<td>0.0010</td>
<td>0.0007</td>
<td>0.1677</td>
</tr>
<tr>
<td>n-Butane</td>
<td>0.0003</td>
<td>0.0001</td>
<td>0.0960</td>
</tr>
<tr>
<td>n-Pentane</td>
<td>1.8 × 10⁻⁵</td>
<td>1.8 × 10⁻⁵</td>
<td>0.1385</td>
</tr>
<tr>
<td>Benzene</td>
<td>7.5 × 10⁻⁹</td>
<td>2.7 × 10⁻⁹</td>
<td>0.0880</td>
</tr>
<tr>
<td>Total flow rate (kmol/h)</td>
<td>16.9</td>
<td>16.42</td>
<td>24.54</td>
</tr>
<tr>
<td>Temperature (K)</td>
<td>310.13</td>
<td>313.27</td>
<td>380.53</td>
</tr>
</tbody>
</table>

*Final steady state reached by the dynamic model.
Fig. 4a. Comparative response of the hydraulic and thermodynamic variables (Problem II).

Fig. 4b. Effect on plate hydraulics due to +50% change in reboiler heat duty (Problem III); top temperature means top-plate temperature.
depend on thermodynamics. It can be seen that the plate pressures which depend on thermodynamics have a larger time constant than the plate pressure drops, liquid and vapor rates, which depend on plate hydraulics. Also, for small perturbations around the steady state, the hydraulic variables are not very sensitive. However, for large changes (which can be brought about by feed changeover or sudden failure of some equipment), the column can become unstable due to the hydraulic variables. Results of two tests are given here. In the first test, the reboiler heat duty is increased by ±50% from the steady-state value of Problem III (industrial extractive stripper). The simulated results (Fig. 4b) shows that even though there is an immediate sharp rise in the vapor flow rate, no hydraulic instability was encountered and the column gradually reaches a new steady state. If, however, along with a +50% increase in the reboiler heat duty, 25% of the valves stop functioning (second test), hydraulic instability was encountered and the column flooding near the bottom is encountered. For this operational procedure, "flooding" or "entrainment" can take place. Figures 5a and 5b show the dynamic response of Column IV for the start-up operational procedure described previously. Figure 5a shows the liquid flow rates of each plate as a function of time, and Fig. 5b shows the vapor flow rate through the downcomers (i.e. before sealing) as a function of time. The bottom- and top-plate temperatures are also shown in Fig. 5b. For this operational procedure, "flooding" or "entrainment" did not occur. "Weeping" and downcomer "sealing" phenomena were observed as can be seen from Figs 5a and 5b. It can be seen that as liquid sealing is achieved on each plate, the vapor flow rate through the downcomers (i.e. before sealing) becomes zero (Fig. 5b) and this happens before the maximum value of the liquid rates are reached. In these two figures, the discontinuous nature of the responses are clearly evident. Also, in Fig. 5b, it can be seen that the hydraulic variables reach a steady state much earlier than the thermodynamic variables.

Simplified versions of the model have been used for control studies [10–12]. In this work only a closed-loop response for the depropanizer is given in Fig. 6. The purpose here was to test the model for its ability to predict the dynamic behavior with different types of controllers. From the open-loop responses, the model first evaluates the process gains and time constants to determine the controller parameters before predicting the closed-loop responses.

For the multiple-column problem, the dynamic results are given in terms of the steady state obtained, the effects of changes in the first column on the dynamic response and the effects of changes in the second column on the dynamic response. Figures 7a and 7b show these results. The degree of interaction between the two columns are related to design, operability and control of these columns. This point is illustrated with a simple example. It can be seen that the degree of interaction is very sensitive to the location of the feed in the second column. From Fig. 7b, it can be seen that location of the feed in the top half of the column (second) is much better than in the bottom half.

Current work is looking at the development of generalized control strategies for start-up, shutdown
Fig. 5a. Liquid flow rates during start-up operation (Problem IV).

Fig. 5b. Vapor blown through downcomers, bottom and top temperatures during start-up operation (Problem IV).
Fig. 6. Prediction and comparison of closed-loop responses (Problem I).

Fig. 7a. Multiple-column dynamics. Column 2 bottoms for different feed-plate locations (Problem V).
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and feed changeover operations, the development of reduced-order models and adaptation of the proposed model into an equation-oriented package for dynamic simulation of separation processes involving distillation columns, intermediate flash tanks and heat exchangers.

**NOMENCLATURE**

- $a_i$: Inside cross-sectional area of bubble cap (in²)
- $a_o$: Annular area between cap and riser (in²)
- $d_r$: Riser area per cap (in²)
- $A_d$: Downcomer cross-sectional area (ft²)
- $A_{min}$: Minimum area under downcomer apron (ft²)
- $A_t$: Total holer area per tray (ft²)
- $A_r$: Total riser area per tray (ft²)
- $A_a$: Active area per tray (ft²)
- $A_e$: Area available for weeping per tray (ft²)
- $B$: Bottoms flow rate (mol/h)
- $B_d$: Hydraulic stability parameter (dimensionless)
- $C$: Component molar holdup on plate (mol)
- $C_g$: Liquid gradient factor (dimensionless)
- $C_e$: Energy holdup on plate (H)
- $C_L$: Liquid holdup on plate (M)
- $C_v$: Vapor load correction factor (dimensionless)
- $C_L$: Liquid correction factor for liquid gradient (dimensionless)
- $D$: Distillate flow rate (M/s)
- $d_r$: Riser inside diameter (in.)
- $e_{dw}$: Downcomer equivalent diameter (ft)
- $e_{LV}$: Liquid entrainment ratio (lb liquid/lb vapor)
- $E_i$: Liquid entrainment flow rate (M/s)
- $E_o$: Vapor entrainment flow rate (M/s)
- $f_s$: Friction factor for froth cross-flow (dimensionless)
- $f_v$: Friction factor for vapor flow
- $F$: Flow parameter ([ft/s]·[lb/ft²])²
- $F_i$: Liquid feed to plate (M/s)
- $F_F$: Flow parameter at the weep-point ([ft/s]·[lb/ft²])²
- $F_L$: Liquid load per foot mean tray width ratio (gal/min per ft)
- $F_v$: Vapor feed to plate (M/s)
- $g$: Acceleration of gravity (32.2 ft/s²)
- $g^L$: Liquid flow rate through downcomer (gal/min)
- $h$: Liquid enthalpy (H/M)
- $h_b$: Head loss due to bubble formation in liquid
- $h_b$: Liquid enthalpy calculated (H/M)
- $h_d$: Downcomer clearance height (in.)
- $h_o$: Height of froth on tray (in.)
- $h_e$: Liquid enthalpy given by the generalized model (H/M)
- $h_{v_o}$: Height of liquid crest over weir (in.)
- $h_{w_o}$: Head loss due to aerated liquid (in. liquid)
- $h_{v_b}$: Dry-cap head loss, excluding slots (in. liquid)
- $h_{v_d}$: Head loss due to liquid flow under downflow apron (in. liquid)
- $h_{f_e}$: Liquid feed enthalpy on plate (H/M)
- $h_{f_v}$: Height of clear liquid on plate (in.)
- $h_{max}$: Maximum liquid height permissible for weeping (in. liquid)
- $h_{w}$: Weir height (ft)
- $h_F$: Liquid feed enthalpy (H/M)
- $h_T$: Head loss due to vapor flow through dry plate (in. liquid)
- $h_D$: Height of liquid in the downcomer (including froth)
- $h_{L}$: Height of liquid in the downcomer (including froth)
- $k$: Liquid–vapor equilibrium constant (dimensionless)
- $K_w$: Dry-cap head loss coefficient (dimensionless)
- $K_w$: Dry-value head loss coefficient (dimensionless)
- $l$: Total free width between caps normal to flow (in.)
- $l_d$: Downcomer height (ft)
- $l_L$: Liquid flow rate (M/s)
- $l_L$: Liquid flow rate through downcomer (M/s)
- $l_F$: Liquid flow rate from plate (M/s)
- $M_{r_b}$: Reboiler mass holdup (M)
- $M_{v_o}$: Reflux drum mass holdup (M)
- $M_L$: Liquid molecular weight
- $M_v$: Vapor molecular weight
- $N_c$: Total number of components
- $N_p$: Total number of plates
- $N_h$: Number of rows of caps normal to flow
- $N_t$: Total number of trays
- $P_i$: Plate spacing (ft)
- $Q$: External heat input/output (H/s)
- $Q^*$: Vapor flow rate (ft²/s)
- $R$: Ideal gas constant
- $R_e$: Ratio of distance between caps on parallel liquid pass to that on oblique liquid pass
- $R_h$: Reynolds number (dimensionless)
- $R_h$: Hydraulic radius for froth cross-flow (ft)
- $R_i$: Ratio of distance between risers to distance between caps
- $S$: Effective plate spacing (ft)
- $u^*$: Weeping liquid velocity (ft/s)
- $U_v$: Vapor velocity based on active area (ft/s)
- $U_i$: Vapor velocity based on hole area (ft/s)
- $U_f$: Maximum vapor velocity for downcomer flooding (ft/s)
- $V$: Vapor flow rate from plate (M/s)
- $V^*$: Vapor flow rate through hole (ft/s)
- $V^o$: Vapor flow rate through hole (M/s)
- $W$: Weir length (in.)
- $x$: Liquid mole fraction on plate
- $x_L$: Liquid mole fraction on plate
- $X_F$: Liquid feed mole fraction
- $y$: Vapor mole fraction on plate
Greek letters

\( \beta \) = Aeration factor on the plate
\( \beta^D \) = Aeration factor in the downcomer
\( \Delta_a \) = Liquid gradient for the tray (in.)
\( \Delta' \) = Uncorrected liquid gradient for the tray (in.)
\( \varepsilon \) = Eddy diffusivity (m²/s)
\( \sigma_L \) = Liquid surface tension (dyne/cm)
\( \theta \) = Temperature
\( \mu \) = Viscosity (lb/ft·s)
\( \rho_L \) = Liquid density (lb/ft³)
\( \rho_v \) = Vapor density (lb/ft³)
\( \rho_w \) = Fraction of liquid weepage (dimensionless)

Subscripts/superscripts

B = Bottoms
c = Column number
C = Condenser
D = Downcomer
f = Flooding
i = Component number
L = Liquid
p = Plate number
RB = Reboiler
RD = Reflux drum
T = Total
V = Vapor
w = Weeping
W = Weir

REFERENCES


APPENDIX

Hydraulic Subset Correlations

Liquid flow rate and downcomer hydraulics [6]

(A.1)

(A.2)

and

and

(A.3)

Downcomer sealing [13]

If \( h_{L, j}^D < h_{L, j} \), then the downcomer is not sealed and

is calculated from

(A.4)

and

(A.5)

where \( F_1 \) and \( F_2 \) are constants.

Vapor flow-rate calculation

Bubble-cap plates [14].

(A.6)

(A.7)

and

(A.8)

where \( R_i = \frac{1}{d_i} \).
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\[ A_s = \text{total slot area per tray (ft²)}, \]
\[ h_a = \text{slot height (in.)}, \]
\[ d_n = \text{top slot width (in.)}. \]
\[ d_s = \text{bottom slot width (in.)}. \]
\[ Q^n_s, \text{ then} \]
\[ h^n_s = h_a \left( \frac{Q^n_s}{Q^n_a} \right)^2, \]
where \( Q^n_s \) is the vapor flow rate for 100% slot opening.

**Wave formation**

\[ B_s = \frac{U_s \cdot h_s \cdot \rho_v \cdot g}{P_d \cdot \rho_s \cdot \rho_v} \]  
(A.25)

If:

- \( B_s < 0.5 \cdot 10^{-3} \), stable condition;
- \( 0.5 \cdot 10^{-3} < B_s < 2.5 \cdot 10^{-3} \), full waves;
- \( B_s > 2.5 \cdot 10^{-3} \), half waves;

where \( P_d \) is the plate diameter (ft).

**Hydraulic gradient**

The hydraulic gradient is considered excessive if [14]:

\[ \frac{AP}{h_s} > 0.5 \]  
(seive or valve trays)

\[ \frac{AP}{h_s} > 0.5 \]  
(bubble-cap tray).

**Sieve and valve trays** [18]

\[ f_h = \frac{g \cdot R_o \cdot \Delta_p}{120 \cdot U_s^2} \]  
(A.26)

\[ R_o = \frac{R_s \cdot U_s \cdot \rho_{L,P}}{\mu_{L,P}} \]  
(A.27)

and

\[ f_h = f(R_o). \]  
(A.28)

**Bubble-cap trays** [14]

\[ \sqrt{\Delta_p} \left\{ \frac{3}{2} \left( \frac{N_i}{N_j} - 1 \right) + \frac{2}{1 + \frac{1 + N_i}{R_o}} \right\} \]

+ \( 3 \cdot N_i \cdot \left( h_s^2 + h_w \left( R_o - 1 \right) \right) \)

\[ = \frac{N_i \cdot q'}{4} \frac{C_i}{C_f} \]  
(A.29)

where

\[ \Delta_p = C_v \cdot \Delta_p \]  
(A.30)

and

\[ C_v = f(F_{lt}), \]  
(A.31)

**Weeping condition**

Fair’s procedure [14]:

\[ h_{\text{max}}^s = C_i \cdot (h_{dp}^s + h_w)^i. \]  
(A.16)

Hughmark and O’Connell’s procedure [18]:

\[ F_s = A_s \cdot h_{\text{max}}^s + h_{dp}^s + h_w \]  
(A.17)

where the constants \( A \) and \( B \) are obtained by the fitting data of Hughmark and O’Connell.

Wada et al. procedure [19]:

\[ \log \omega = f(F_s - (F_s)_{0.98}) \]  
(A.18)

\[ (F_s)_{0.98} = 22.4 \cdot \rho_v \cdot \frac{0.03048 \cdot h_w}{\sigma_{L,P}} \]  
(A.19)

and

\[ L_w = \frac{\omega}{1 - \omega} \]  
(A.20)

**Weepage-rate calculation** [20]

\[ A_w = \left( 1 - \delta \right) A_s, \]  
(A.21)

\[ \delta = \frac{1}{1 + \left( \frac{u^n_s}{U_s} \left( \frac{\rho_v}{\rho_{L,P}} \left( \frac{C_i}{C_G} \right) \right) \right)^{1/3}}, \]  
(A.22)

\[ u^n_s = 0.6 \left( \frac{2.9 \cdot h_{\text{min}}}{12.0} \right)^{1/2} \]  
(A.23)
Liquid entrainment [22-24]

\[ e_{LV,P} = \frac{a}{\sigma_{LV}} \left( \frac{U_L}{S_L} \right)^b, \]

where \( a \) and \( b \) are function of plate type and \( S_L = P - h_1 \).

\[ E_{LP} = e_{LV,P} \frac{V_L}{M_{LV}}, \]  
(A.34)

Vapor entrainment

Because we have not yet found a satisfactory correlation, the model asks for user-supplied correlations (if any).