

**MODELING OF A DISTILLATION COLUMN
USING BOND GRAPHS**

by

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To let understanding stop at what cannot be understood is a high attainment. Those who cannot do this will be destroyed on the lathe of heaven.

Tchuan-tse

The author would like to thank the universe for not being as perversely ordered as once thought.

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ABSTRACT

Modeling and simulating distillation columns is not a new enterprise. All of the models described in the literature either contain algebraic loops or simplifying assumptions that render the model ill-equipped for dynamic simulations. The structure and the equations that represent a trayed distillation column are explored using bond graphs. Bond graphs model the power flow in a system, an inherently instructive way to view complex systems. The power of bond graphs is evident by providing a clear, graphical representation of a distillation column that systematically organizes the equations and possible approximations. The model of a distillation column is explored in general and then by using a specific model developed by Steven Gallun. Results of this study reveal several ways of eliminating the algebraic loops and producing a dynamic model. The bond graph model can be expanded by introducing other elements including chemical reactions and thermal interaction with other columns.

1.0 INTRODUCTION

The basic idea of distillation is to separate components of a mixture from each other to various degrees. A distillation column is one of the primary techniques used by industry for separating a mixture. A distillation column is a complex system that is represented by a number of models depending on what aspects of a distillation column are chosen and on what assumptions are made. The basic idea of bond graphs is to graphically model a system. As a modeling methodology, bond graphs represent a powerful approach for understanding the distillation column. This chapter presents background information for both distillation columns and bond graphs.

1.1 The basics of a distillation column

The distillation column is a widely used apparatus used to separate various chemicals, most commonly petroleum products. Historically, distillation has been around for millennia. Distillation using more than one stage has been around for a couple of centuries [1]. The theoretical basis of the separation is the different boiling points of the components being separated.

A simple example should explain this. Assume a two component mixture in a closed chamber; component A with boiling point at T_A and component B with a higher boiling point at T_B . At a temperature between T_A and T_B , an equilibrium is reached such that the percentage of component A in the vapor is higher than the percentage of component A in the liquid. With only two components, this also means that the percentage of component B in the vapor is lower than the percentage of component B in the liquid. Now, drain out the

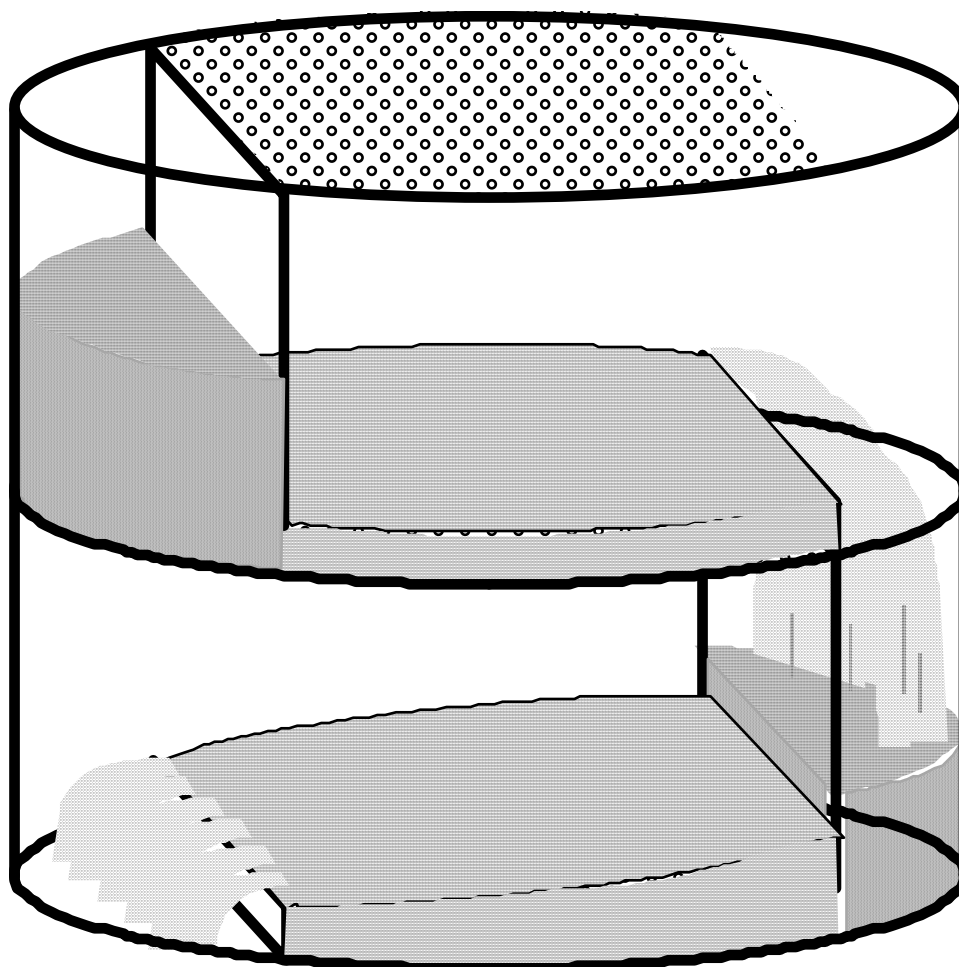


Figure 1.1. The basic stage of a distillation column.

liquid and a new equilibrium will be reached where the vapor contains an even higher percentage of component A than in the liquid that will form. If the ratio of liquid to vapor is to be about the same, the temperature will need to be lowered. As we continue the process of draining and lowering the temperature, the result will be a mixture of almost all component A at a temperature just above T_A .

This simple example describes single-stage batch distillation. A distillation column is a clever way to reproduce many chambers at the same

time. The chambers in a distillation column, called stages, are stacked on top of each other separated by a stage plate, or tray. The stage in Figure 1.1 is defined to contain the foam on the tray, the vapor above the tray and the liquid in the downcomer below the tray. Thus, Figure 1.1 shows one full stage and two half stages. Figure 1.2 illustrates a basic distillation column. The liquid is drained by gravity; the vapor migrates up due to pressure caused by heat. The liquid is forced to flow over each stage plate before it flows down a downcomer to the

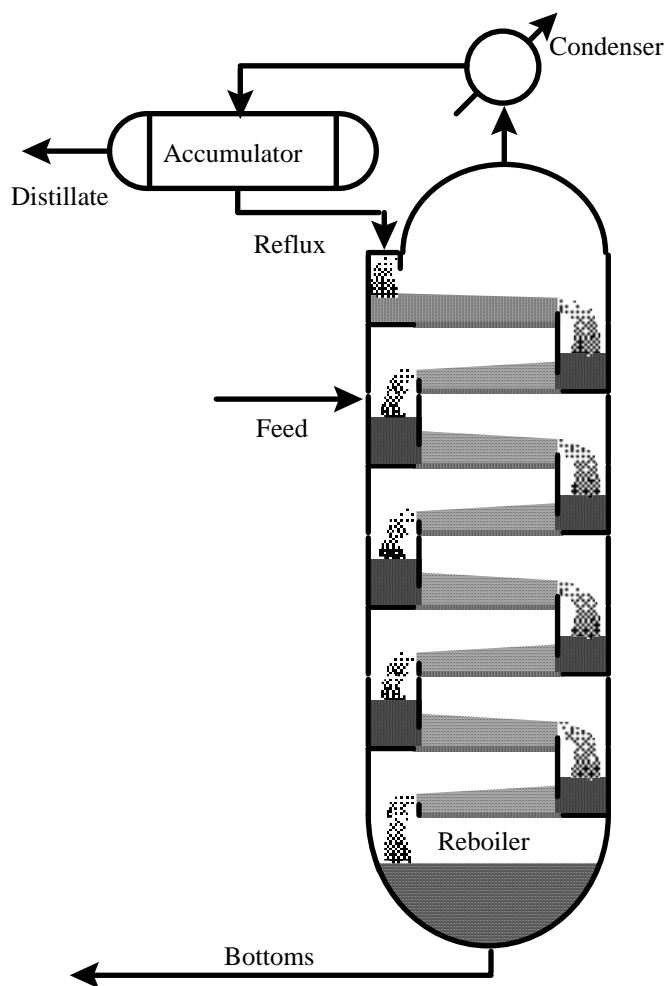


Figure 1.2. The basic distillation column.

next stage plate. The vapor is forced to flow through holes in the stage plate, and then through the liquid over the plate, thus creating good contact between liquid and vapor.

At the bottom of the distillation column is a heat source, the reboiler, and the ability to siphon off liquid, the bottoms. The top of the distillation column is a condenser that cools the vapor of the top stage into liquid and a receiver that holds the liquid and allows for some of this liquid to be

returned, the reflux, and some to be taken away as distillate. Somewhere in the middle of the column is the feed, where the original mixture to be separated is introduced into the column. Here, vapor rising from below heats the mixture such that vapor rising to the next stage has a higher percentage of the low-boiling component (component A) than the original mixture. The liquid flowing through the downcomer will have a higher percentage of the high-boiling component (component B). If all has worked well, the distillate will be a nearly pure component of the mixture, the component with the lowest boiling point. The liquid flowing down from the top stage, although initially pure, captures the high-boiling component in the vapor coming up by cooling the vapor.

In a multicomponent distillation, both the distillate and bottoms are typically composed of several of the original components. The most volatile of the components will not appear in the bottoms and the least volatile of the components will not appear in the distillate. The component appearing in both distillate and bottoms with the highest percentage in the distillate is called the high key. Similarly, the component appearing in both distillate and bottoms with highest percentage in the bottoms is called the low key. Essentially, the distillation column separates the mixture into the high key and more volatile components and the low key and less volatile components.

A real distillation process can be complicated by many factors. There might be many components. The component to be separated out has neither the highest nor lowest boiling point. The phase equilibria may not be as simple as presented above (e.g., in an azeotropic mixture, the equilibrium temperature at a specific ratio of components can be lower than the lowest boiling point of any of the pure components). The components may form multiple liquid phases. Real

distillation columns become complex in meeting the requirements. Feeds of different mixtures can come in on several stages. Distillate and bottoms may be reintroduced at various stages. Sidestreams can transport liquid or vapor off any stage to become feeds on another stage or into another column. Heat can be added or removed from any stage. Several distillation columns can be used in series (e.g. azeotropic mixtures require more than one column). Heat integrated columns allow heat flows between columns. Additional components such as solvents, may be added to facilitate separation. The condenser may not totally condense the vapor into liquid. A variety of control strategies may be used to stabilize or optimize the process. Designers of columns must consider these factors as well as deciding the number of plates, the type of plates (see [1] or [2] for the choices), whether tray plates are used at all, whether additional components should be added to facilitate separation, or whether a simple chemical reaction should occur. The ideas presented in this thesis are hoped to be basic enough and bonding graphing powerful enough to be applied to any of the possible configurations.

The purpose of a tray is to facilitate liquid and vapor interaction; this purpose is also fulfilled by a packed column, in which trays are not used at all. The column is filled, or packed, with irregularly shaped objects designed to create continuous contact between liquid falling down and vapor rising. This form of distillation column is gaining popularity in industry [3]. The non-hydraulic equations are identical with a trayed column, except a stage is no longer defined by stage plates. The form of the dynamic equations is modeled intuitively by partial derivatives; approximating this by a series of differential equations, as if it were a trayed column, makes sense. One notable difference

between a packed and trayed column is that the pressure differential is much lower in a packed column; the hydraulic equations for a trayed column could not be used. The equations for a packed column will not be discussed.

Complex distillation can lead to a variety of problems; some of these problems must be anticipated when designing or modeling a column. Weeping occurs when the liquid flows down through the holes in the plate, caused by insufficient vapor flow [2]. Flooding occurs when the liquid flows up through the plate, caused either by excessive vapor flow (entrainment flooding) or excessive liquid buildup on the stage (downcomer flooding) [1, 4]. Entrainment is either the carrying off of liquid with the vapor through the plate or the carrying off of the vapor with the liquid through the downcomer. Other problems include downcomer blocking, oscillations in the liquid holdup, and instabilities in the operations of the column. These problems can occur in any distillation column with the right provocation, although design and control systems should be able to limit the likelihood. Properly modeling and simulating a column should expose such problems.

1.2 The basics of bond graphs

A bond graph is a graphical description of a physical system that preserves the computational and topological structure of the system. Each bond represents the transport of energy as a pair of conjugate variables (effort and flow) that multiply together to represent power. Thus, bond graphs show the flow of power through a system. Table 1.1 lists several pairs of conjugate variables.

effort (e)	flow (f)
pressure	volume flow
temperature	entropy flow
force	velocity
chemical potential	molar flow
voltage	current
torque	angular velocity

Table 1.1. The basic conjugate pairs.

Bonds (half arrows) originate and terminate at various types of elements, depending on the physical system and the equations used to describe them. The basic elements describe fundamental relationships between the variables that are attached by a bond or by bonds. These basic elements are listed in Table 1.2. As suggested by their definitions, only the 0-node and 1-node accept more than one bond. These elements will not be sufficient to describe a distillation column; new elements will be developed to reflect the equational forms of the distillation

symbol	name	equation
0	0-node	$\sum f_i = 0$ $\forall i$
1	1-node	$\sum e_i = 0$ $\forall i$
R	Resistance	$e = R * f$ or $f = e/R$
C	Capacitance (Compliance)	$f = C \frac{de}{dt}$
I	Inductance (Inertia)	$e = I \frac{df}{dt}$
SF	Flow Source	$f = \text{given}$
SE	Effort Source	$e = \text{given}$

Table 1.2. The basic nodes of a bond graph.

column model and of thermodynamic systems in general.

Bond graphing a system provides more than just a graphical mapping of the system. Bond graphing inherently provides some system analysis, an easy means of expanding the system, and modularity. Each bond is assigned one causality stroke that appears at one end of the bond. The causality stroke determines which equation (represented by an element) is used to solve for each variable; the stroke is placed where the flow variable is calculated. Thus, a bond graph can determine whether a system contains algebraic loops or structural singularities. Adding an element to the system (e.g., a resistor, a chemical reaction, a heat source) can be represented by adding an element and a bond to the bond graph. The effect of such a new element on the system can be seen immediately by the placement of the causality stroke. Pieces of bond graphs can be grouped into subsystems and be represented by a new element. Hierarchical bond graphs are thus modularized to describe large systems.

It is beyond the scope of this thesis to describe bond graphs in all details. See [5], [6], or [7] for a comprehensive introduction to the subject of bond graphs and their use. For a comprehensive bibliography of bond graphs, see [8]. Bond graphs have proven to be useful in describing mechanical and electrical systems. Bond graphs also provide a framework for working with convection and with thermodynamics [9, 10, 11, 12, 13]. The use of bond graphs in chemical systems has been limited, however. Chemical systems should benefit from being bond graphed. Later sections will discuss how bond graphs can be assembled to represent a distillation column.

1.3 The assumptions of a distillation column

In forming a model for the distillation column, general assumptions about the operation of a distillation column must be made. The assumptions a model makes are the major distinctions between the models found in the distillation literature. A complete set of dynamic equations would be of a daunting size considering that a stage contains many forms of energy transformations and that a distillation column or a set of columns can contain hundreds of stages. Of course, simplifying assumptions are desirable in such a complex apparatus. Early computer models required stringent simplifying assumptions to run [14, 15, 16].

Typical assumptions deal with system constraints (i.e. the type of column and components used), heat flow, hydraulics, and dynamic equilibrium. Assumptions leading to the simplest set of equations that approximate the behavior of a distillation column are used. Assumptions can be broken down within these categories of assumptions.

System constraints: 1) The condenser may be a partial or total condenser; 2) The trays may be of several types and each requires separate models for vapor flow through them; 3) Chemical reactions must be modeled if the components react. Distillation mostly does not include components that react, though some models do allow for chemical reaction [4, 17, 18]. The most general models also allow sidestreams, feeds, and heat transfer on each stage, allowing for a specific complex column to be modeled.

Heat flow: 1) The column is adiabatic, the only heat exchanges by conduction that need be modeled are those in the condenser and reboiler; 2) The thermal capacitance of the column metal is negligible. Both of these assumptions are used by almost all distillation models.

Hydraulics: 1) Vapor holdup (of mass and energy) on each stage is negligible. The molar holdup of the vapor is usually much less than the molar holdup of the liquid, thus, the vapor holdup effects are considered small. This also allows for a great simplification in the equations as seen in the next chapter. Further, more stringent, assumptions can be made that simplify the model greatly, such as 2) constant pressure or pressures throughout the column, 3) constant liquid molar holdup, 4) constant liquid volume holdup, 5) constant reflux flow, or 6) negligible hydraulic dynamics. These simplifying assumptions are essentially the assumption of small perturbations from steady-state.

Dynamic equilibrium conditions are assumed to be reached between the vapor and the liquid before leaving the stage, which requires the intensive variables (i.e. pressure, temperature, chemical potential) of both vapor and liquid to be equal. In the simple example of single-stage batch distillation, equilibrium was reached over time before draining and lowering temperatures. In a distillation column, continuous heat and mass exchange is assumed to create a dynamic equilibrium. This is the assumption of perfect mixing of vapor and liquid on the stage. The equations detailing the vapor-liquid equilibrium (the steady-state flow between the phases resulting in equal chemical potentials) have a large variety of assumptions that determine their complexity and whether they form an algebraic loop. The assumption of vapor-liquid equilibrium is typically relaxed by using Murphree efficiency.

The assumption of negligible hydraulic dynamics is common in the literature. In making the model as simple as possible, the equations for pressure, fluid flow, and vapor flow are omitted and values are assumed. Justification of this comes from Levy, who showed that the (steady-state, algebraic) hydraulic

equations had little influence on the most influential modes, the smallest eigenvalues of a distillation system [19]. The equations dealing with the vapor-liquid equilibrium were shown to be the most influential. Thus, first or second order approximations of the distillation column could leave out the hydraulic dynamics [20]. Work by Tyreus, *et. al.* and Lagar, *et. al.* verified that the eigenvalues most influenced by the (steady-state, algebraic) hydraulic equations are independent from those due to the vapor-liquid equilibrium, but that removing the hydraulic equations does not reduce the stiffness of the system [21, 22]. The assumptions used reflect the aim of the model. If comprehensive dynamics are to be included, the hydraulic equations must be included.

Assumptions will play a large part in determining the scope and desirability of a distillation column model. The severe assumptions of steady-state, neglected hydraulics, or small perturbation models will not be considered as possibilities. Assumptions and the resultant equations will be dealt with on an element by element basis in the next chapter.

2.0 THE ELEMENTS OF A DISTILLATION COLUMN

A complete dynamic model of a distillation column must include material balance and flow, energy balance and flow, liquid to or from vapor flow within a stage, temperature, pressure, and hydraulic dynamics, system constraints, and chemical reactions. Together, these relationships can define the operations of a distillation column, as well as many other chemical and thermodynamic processes. For modeling reasons, these relationships can be seen in terms of power balances. In terms of power flow, the relationships become temperature and entropy flow, pressure and volume flow, and chemical potential and molar flow. These relationships and any bond graphs associated with them are derived as separate elements of a distillation column. This chapter will discuss the equations that form the traditional model, their origins, their possible variants, and how they might be reformed into bond graph notation.

From these equations, three models of a distillation column will be formed. Equations used in the model of Gallun will be noted with a G. The equations used in the simple modification of Gallun's model will be noted with an S. Equations that form a rigorous model that can be bond graphed will be noted with an R.

2.1 Mass balance

There is an overall balance of mass. This simple statement is carried to the stage level. The conservation of mass is described by the equation:

$$\begin{aligned} \frac{d\text{Mass}}{dt} &= (\text{rate of liquid coming in} - \text{rate of liquid leaving}) \\ &+ (\text{rate of vapor coming in} - \text{rate of vapor leaving}) \end{aligned} \quad (2-1)$$

Many forms of equation (2-1) can be and are developed, depending on the needs of the rest of the model [4]. Only a few are considered here, with the emphasis on the mass balance for each stage j . The liquid coming into each stage is mainly from the downcomer of the previous stage, the vapor coming in is mainly through the plate from the stage below. Other sources of flow can include the feed stream which is generally a liquid that comes in on only a few of the stages. Sidestreams can remove some of the vapor or liquid from a stage in the middle of the column [1]. Entrainment, both liquid-in-vapor and vapor-in-liquid, can also be included in the model [1, 2, 23]. This thesis will not consider sidestreams or entrainment, but results presented here should allow their inclusion.

Consider the mass balance in terms of molar holdup, M_j , and molar flow for stage j :

$$\frac{dM_j}{dt} = (F_j + L_{j-1} - L_j) + (V_{j+1} - V_j) \quad (2-2)$$

The liquid component balance for component i uses molar fractions of liquid (x_{ji}) and vapor (y_{ji}):

$$\frac{d(M_j x_{ji})}{dt} = (f_{ji} + L_{j-1} x_{j-1,i} - L_j x_{ji}) + (V_{j+1} y_{j+1,i} - V_j y_{ji}) \quad (2-3)$$

Notice the assumption implicit in equation (2-3). The vapor molar holdup of each component is constant, even though the vapor molar fractions are assumed to vary. The changes in total molar holdup can be attributed solely to the liquid of the stage. This assumption is not correct, but because the molar content of the stage is primarily in the liquid, it is often deemed a good assumption. The vapor

molar fractions are allowed to vary as functions of liquid molar fractions. This assumption also allows for the great simplification of obtaining the liquid holdup without explicitly needing to know the flow from liquid to or from the vapor within a stage. The variable V_j now contains this piece of information ($LV_j = V_{j+1} - V_j$). The change in molar holdup of each component as a liquid on a stage (u_{ji}) becomes [24]:

$$\frac{du_{ji}}{dt} = (f_{ji} + L_{j-1} x_{j-1,i} - L_j x_{ji}) + (V_{j+1} y_{j+1,i} - V_j y_{ji}) \quad (2-4)^{GS}$$

$$x_{ji} = \frac{u_{ji}}{\sum_{\forall i} u_{ji}} \quad (2-5)^{GSR}$$

An alternative form of equation (2-4) is derived from equations (2-2) and (2-3) [25]:

$$\frac{dx_{ji}}{dt} = \frac{1}{M_j} \left[f_{ji} - F_j x_{ji} + L_{j-1} (x_{j-1,i} - x_{ji}) + V_{j+1} (y_{j+1,i} - x_{ji}) - V_j (y_{ji} - x_{ji}) \right] \quad (2-6)$$

A more rigorous form of equation (2-4) does not assume constant molar vapor holdup (uv_{ji}):

$$\frac{du_{ji}}{dt} + \frac{duv_{ji}}{dt} = f_{ji} + L_{j-1} x_{j-1,i} - L_j x_{ji} + V_{j+1} y_{j+1,i} - V_j y_{ji} \quad (2-7)^R$$

$$\frac{du_{ji}}{dt} = f_{ji} + L_{j-1} x_{j-1,i} - L_j x_{ji} - LV_{ji} \quad (2-8)^R$$

$$\frac{duv_{ji}}{dt} = V_{j+1} y_{j+1,i} - V_j y_{ji} + LV_{ji} \quad (2-9)^R$$

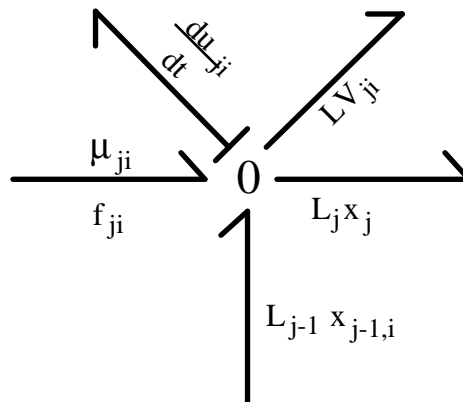


Figure 2.1. Bond graph of liquid mass balance equation (2-8).

In this form, the vapor-liquid equilibrium equations (section 2.4) must provide not the molar fractions y_{ji} , but the actual flow rates of a component from liquid to vapor, LV_{ji} . Very few distillation models consider non-constant vapor holdup [26].

Mass balance is described in a bond graph as a 0-node. Molar flow and chemical potential form a conjugate pair. Equation (2-8) is shown in Figure 2.1 as a collection of inflowing and outflowing bonds. The stroke at the end of the top left bond indicates that the mass-balance is solved for du_{ji}/dt at the 0-node. Solving for the conjugate variable, chemical potential, presents a separate problem.

2.2 Energy balance

There is an overall balance of energy. The energy balance equation closely follows the mass balance equation.

$$\frac{d(\text{Energy holdup})}{dt} = \text{rate of energy coming in} - \text{rate of energy leaving}$$

Except for the condenser and reboiler, the energy coming into or leaving a stage is solely through convection. This takes into account the assumptions of negligible thermal capacitance and an adiabatic column. The equation for the internal energy holdup of a stage (U_j) is similar to equation (2-7):

$$\begin{aligned} \frac{dU_j}{dt} &= \left(U_j^f + \frac{L_{j-1} U_{j-1}^L}{\sum_{\forall i} u_{j-1i}} - \frac{L_j U_j^L}{\sum_{\forall i} u_{ji}} \right) + \left(\frac{V_{j+1} U_{j+1}^V}{\sum_{\forall i} u_{vj+1i}} - \frac{V_j U_j^V}{\sum_{\forall i} u_{vji}} \right) \\ &= \frac{dU_j^L}{dt} + \frac{dU_j^V}{dt} \end{aligned} \quad (2-10)^R$$

Using the assumption of negligible vapor energy holdup, this equation can be simplified to assign all changes in the stage energy to the liquid.

The thermodynamic relationships for internal energy and enthalpy (H) state:

$$\frac{dU}{dt} = T \frac{dS}{dt} - P \frac{dV}{dt} + \sum_{i=1}^c \mu_i \frac{dn_i}{dt} \quad (2-11)$$

$$\frac{dH}{dt} = \frac{dU}{dt} + P \frac{dV}{dt} \quad (2-12)$$

Because the volume of a stage is constant, the change in internal energy of a stage equals the change in enthalpy. Typically, models for distillation columns focus on enthalpy; there are approximations of enthalpy that can be calculated from pressure, temperature, and molar fractions.

One method uses virtual values of the partial molar enthalpies to estimate the enthalpy of the vapor, and a differential equation for the enthalpy of the liquid [4, 27, 28]. Ideal gas enthalpies are found through a polynomial

expansion of the temperature of known coefficients. The actual enthalpy is found by adding to this the departure from ideal enthalpy, as predicted by an equation of state. The virial equation of state is used to calculate the enthalpy departure function for stage j (Ω_j).

$$H_{ji}^V = H_{ji}^{\text{Ideal}} + \Omega_j \quad (2-13)^G$$

$$\Omega_j = \frac{P_j \left(2 - \frac{1}{ZZ_j} \right) \left(T_j \frac{\square B_{mj}}{\square T_j} - B_{mj} \right)}{(2 ZZ_j - 1)} \quad (2-14)^G$$

The partial derivative depends on the mixing functions used to determine the second virial coefficient of the mixture, B_{mj} . The exact equations used for the partial derivative (51 of them) can be found in Appendix B and the 'engder' macro of Appendix D. The equation for the liquid enthalpy becomes:

$$\frac{dH_j^L}{dt} = H_j^f + \frac{L_{j-1} H_{j-1}^L}{\sum_{\forall i} u_{j-1i}} - \frac{L_j H_j^L}{\sum_{\forall i} u_{ji}} + \sum_{\forall i} v_{j+1i} H_{j+1i}^V - \sum_{\forall i} v_{ji} H_{ji}^V \quad (2-15)^{GS}$$

Note the assumption that the difference in the vapor enthalpy flow is credited towards the liquid: the derivative of the enthalpy of the vapor is assumed zero.

Other methods of enthalpy calculation involve various equations of state [29, 30]. Some models use an algebraic equation for the enthalpy balance [25]. Although this form has been shown to be valid [28], it has also been shown less accurate [31].

In bond graph notation, energy and mass are automatically balanced: these equations manifest themselves automatically as 0-nodes and 1-nodes. Instead of dealing with energy or enthalpy in bulk, the components of

thermodynamic energy are considered. The following equations, equation (2-11) restated for one component in a mixture and one form of the Gibbs-Duhem equation, reveal the conjugate pairs that bond graphs look at:

$$\frac{dU_i}{dt} = T \frac{dS_i}{dt} - P \frac{dV_i}{dt} + \mu_i \frac{dn_i}{dt} \quad (2-16)$$

$$\text{Gibbs-Duhem:} \quad \frac{d\mu_i}{dt} n_i = \frac{dP}{dt} V_i - \frac{dT}{dt} S_i \quad (2-17)$$

The corresponding bond graphs contain two new nodes: U_i is a 3 input capacitive element and E_0 is essentially a 3 input 0-node. The use of these nodes will be discussed in the next chapter.

2.3 Hydraulic (pressure and volume flow)

Of all the equations within a distillation column model, the hydraulic equations are the most dependent on the geometry of a particular column, and thus, the most variable. Various types of vapor holes, multiple-pass trays with multiple downcomers, circular flow paths, splash baffles and calming zones before the tray weir, slotted weirs, laminar flow baffles, and various packing arrangements all require special equations to become modeled.

A comprehensive analysis of stage dynamics would have to include the partial derivative continuity equation (Navier-Stokes equation) to adequately

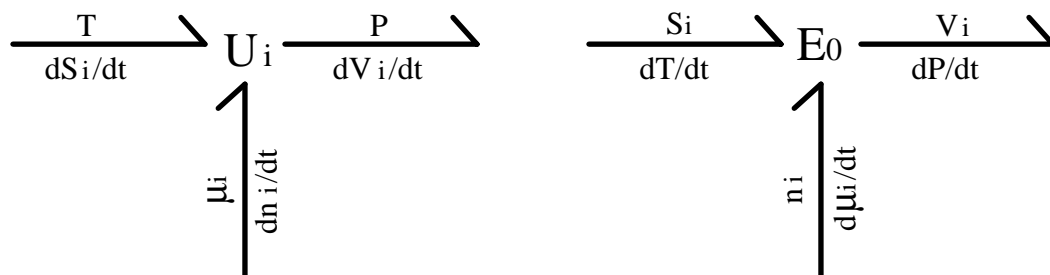


Figure 2.2. Internal energy elements.

describe the interaction of pressure with fluid velocity, viscosity, surface tension, and density of the vapor and liquid as they flow through each other. Bond graphs can be used to describe the continuity equation in fluid flow [32, 33]. For simplicity, flow could be divided into regimes such as spray, froth, emulsion, bubble, and foam. These regimes have been studied and empirical functions created relating various hydrodynamic parameters for each regime [2]. The distillation literature contains many searches for theory and empirical data that accounts for the formation of foam and spray, the flow patterns that form upon and effect the hydraulics of a distillation tray, and the prediction of densities within the different regimes [34]. Yet, such a comprehensive model of the stage plate would require more information about the components than is readily available and contains more information than needed. The large number of untested equations in this type of model suggests more research.

Pressure and volume flow will be determined using Bernoulli's equation [35, 36]:

$$\text{pressure}_1 - \text{pressure}_2 = \frac{1}{2} \rho (\text{velocity}_2^2 - \text{velocity}_1^2) + \rho g (\text{height}_2 - \text{height}_1) \quad (2-18)$$

Bernoulli's equation is essentially balancing the kinetic and potential energy in a flowing fluid. The assumptions used to derive it are constant density, temperature, and molar fractions, as well as perfect transfer of energy (no thermal loss) and steady-state flow. A more complete version of Bernoulli's equation balances more forms of energy and uses length as its dimension [37, 38] :

$$\begin{aligned} \left(J U_1 + z_1 + \frac{P_1}{\rho_1 g} + \frac{v_1^2}{2g} \right) - \left(J U_2 + z_2 + \frac{P_2}{\rho_2 g} + \frac{v_2^2}{2g} \right) \\ = \Delta h_f + \Delta h \end{aligned} \quad (2-19)$$

where J is a conversion factor from heat to mechanical energy and Δh is the external work added to the flow. The term Δh_f is the pressure drop (called head loss when length is the dimension) due to friction. The head loss can be related to velocity of foam (u_f), length of flow path (l_f), hydraulic radius (r_h), and a friction factor (f) [27]:

$$\Delta h_f = \frac{f u_f^2 l_f}{12 g r_h} \quad (2-20)$$

The friction factor is related to the Reynolds number, and is therefore viscosity based. In most instances, this factor is quite small compared to the kinetic and potential energy terms.

Where models in the distillation literature have sought to include the liquid flow through the downcomer and vapor flow through the stage, Bernoulli's equation is used. The nature of the derivation of Bernoulli's equation is evident by examining a more comprehensive equation of motion with mass, velocity and forces.

$$\frac{d(m v)}{dt} = \sum F \quad (2-21)$$

The equation as it stands is suited for a Lagrangian frame of moving solids. The equation needs reforming to be used in a Eulerian fixed frame of flowing fluid, pressure differences and volume flows. This is achieved by dividing each side of

equation (2-21) by area and recasting mass and velocity into density (ρ), volume (V), cross-sectional area (A), and volume flow (Q):

$$\frac{1}{A_0} \frac{d}{dt} \left(\frac{\rho V Q}{A} \right) = \sum P \quad (2-22)$$

Assume equation (2-22) refers to a section of pipe with constant a volume and a fluid with a constant density; only the volume flow and area are left within the derivative. The sum of pressures in this equation is the sum of the pressures at the input and output, the pressure caused by the fluid moving in a gravitational field (potential energy), and any frictional loss pressures. Thus, equation (2-22) becomes

$$\frac{\rho V}{A_0 A^2} (\dot{Q} A - Q \dot{A}) = P_1 - P_2 + \rho g (\text{height}_1 - \text{height}_2) - P_f \quad (2-23)$$

The term A_0 denotes the average cross-sectional area. When the derivative of volume flow is zero, steady-state flow requires the pressure differential to be constant, hence a constant average acceleration through the tube. Part of this pressure differential can be caused by a change in the cross-sectional area of the tube; this is the kinetic energy term of Bernoulli's equation. The derivative of area in equation (2-23) is better formed using the derivative of velocity, acceleration.

$$\begin{aligned} Q &= v A \\ \dot{Q} &= \dot{v} A + v \dot{A} = 0 \\ \dot{A} &= -\frac{A}{v} \dot{v} = -\frac{A^2}{Q} a \end{aligned} \quad (2-24)$$

The kinetic energy term is thus calculated as

$$-\frac{\rho V Q \dot{A}}{A_0 A^2} = \rho \Delta x a = P_{KE} \quad (2-25)$$

$$\frac{d}{dt} P_{KE} = \rho v a \quad (2-25a)$$

where a is the average acceleration through the tube. Equation (2-25a) only makes sense in the Lagrangian sense of a changing Δx ; in the Eulerian sense, the derivative is zero. The actual tube may not be shaped to give a constant acceleration through the tube, but the average acceleration will always be the same as if the acceleration is constant. Acceleration is derived using the traditional method of deriving kinetic energy [35]. The main assumption is movement with constant acceleration.

$$\begin{aligned} a &= \text{constant acceleration} \\ v_2 &= v_1 + a t \quad \square \quad t = \frac{1}{a} (v_2 - v_1) \\ x_2 &= x_1 + v_1 t + \frac{1}{2} a t^2 = x_1 + \frac{1}{a} v_1 (v_2 - v_1) + \frac{1}{2a} (v_2 - v_1)^2 \\ a &= \frac{v_2^2 - v_1^2}{2 \Delta x} = \frac{Q^2}{2 \Delta x} \left(\frac{1}{A_2^2} - \frac{1}{A_1^2} \right) \end{aligned} \quad (2-26)$$

As long as the volume flow is constant, the average acceleration of flow through the tube will equal this constant acceleration. Combining equations (2-23), (2-24), (2-26), a full expression of fluid flow in a tube is realized.

$$\begin{aligned} \frac{\rho V}{A_0^2} \dot{Q} + \frac{\rho Q^2}{2} \left(\frac{1}{A_2^2} - \frac{1}{A_1^2} \right) \\ = P_1 - P_2 + \rho g (\text{height}_1 - \text{height}_2) - P_f \end{aligned} \quad (2-27)$$

Note that the kinetic energy term is of energy stored, not of energy lost. A true energy loss term would change sign with a change in the direction of flow. The second term in equation (2-27) is represented by a KE-element in Figure 2.3;

although it is essentially a resistive element as long as flow remains in one direction, it should not be represented by an R-element [39, 40, 41]. The potential energy term is also an expression of energy stored. The form of equation (2-27) is that of an inertia with various other elements attached:

$$\Delta P + P_{KE} = P_1 - P_2 + P_{PE} - P_f \quad (2-28)$$

$$\Delta P = I \frac{d}{dt} Q = \frac{\rho V}{A_0^2} \dot{Q} \quad (2-28a)$$

$$P_{KE} = \rho \Delta x a = \frac{\rho Q^2}{2} \left(\frac{1}{A_2^2} - \frac{1}{A_1^2} \right) \quad (2-28b)$$

$$P_{PE} = \rho g (\text{height}_1 - \text{height}_2) \quad (2-28c)$$

Thus, a bond graph of this equation, using volume flow as the flow variable and pressure as the effort variable, would center around a 1-node as in Figure 2.3. Note that the potential energy term is not modeled using an energy storage element; any tube used is not likely to be so long as to experience a change in gravitational acceleration. At steady-state, the volume flow and pressures become constant, which converts equation (2-27) into Bernoulli's equation.

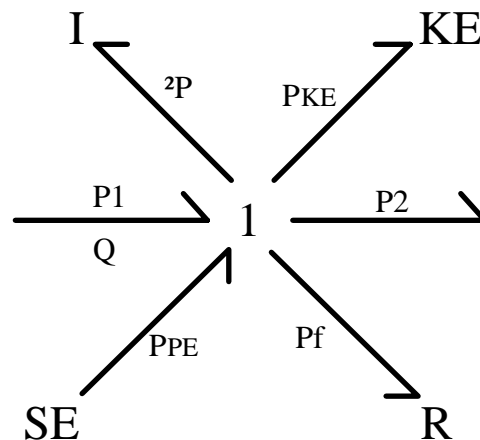


Figure 2.3. Bond graph of fluid flow, equation (2-28).

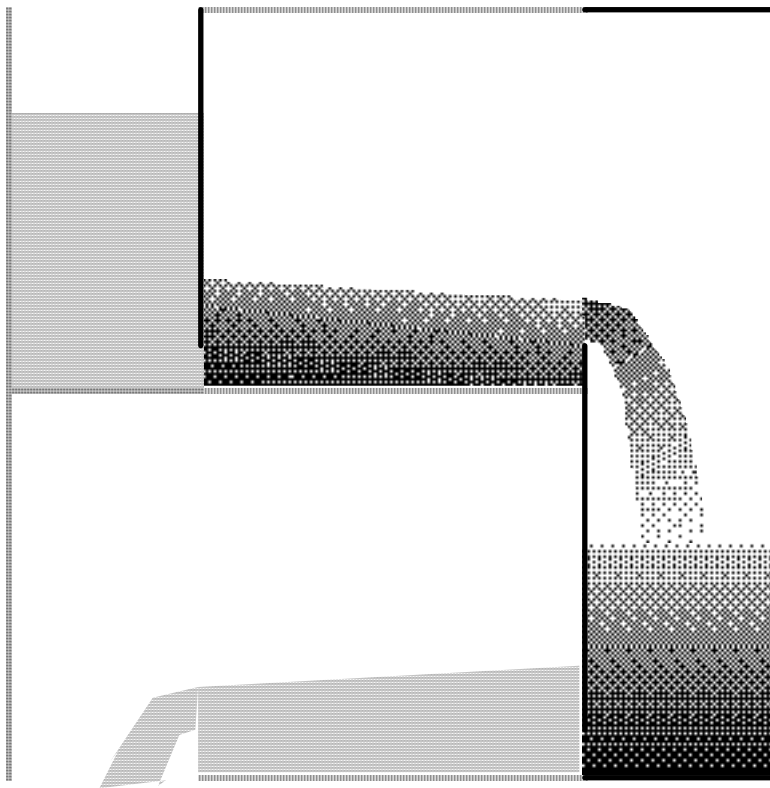


Figure 2.4 The hydraulic variables in a distillation column stage.

Although constant flow is a common assumption, the fluid flows in a distillation column are not always subject to constant pressures. Also, this assumption will lead to an algebraic loop in the vapor flow, depending on how pressure is calculated.

The fluid flow within a distillation column can almost all be modeled using fluid flow in a pipe, equation (2-23). The major difference is that within a distillation column, the flows are not always subject to the constant volume assumptions of tube flow. Hydraulic power flow is considered as the conjugate pair of pressure and volume flow. Referring to Figure 2.4, the hydraulic flow variables are the vapor flow from stage j (QV_j), the liquid flow over the weir

(Q_{s_j}), and the liquid flow leaving the downcomer (Q_{L_j}). The three areas of interest are the foam flow over the weir, the liquid flow through and out of the downcomer, and the vapor flow through the sieve plate.

Consider first the flow through the downcomer. The interaction between liquid and vapor is assumed to have stopped, the foam coming over the weir is quickly reduced to clear liquid. The constriction at the bottom, under the downcomer, limits the flow. The flow is determined by the height difference between the height of liquid in the downcomer (Z_j) and the height of liquid on the next stage plate (h_{j+1}^L , derived later), as well as the pressure differences between the stages. All of these quantities vary dynamically. The height of the liquid in the downcomer is dependent on the flows into and out of the downcomer:

$$\frac{dZ_j}{dt} = \frac{1}{AD} \frac{dV_{dc}}{dt} = \frac{Q_{s_j} - Q_{L_j}}{AD} \quad (2-29)^{SR}$$

The area of the downcomer (AD) is much larger than the area under the downcomer (AUD) through which the liquid flows to the next stage; thus, the velocity of flow is only considered under the downcomer. All but the exiting flow is within the area of the downcomer; thus, the average area is essentially AD . Equation (2-22) can be rephrased in terms of the flow through the downcomer,

$$\frac{\rho_j^L}{A_0} \frac{d}{dt} \left(\frac{V_{dc} Q_{L_j}}{A} \right) = P_j - P_{j+1} + \rho_j^L g (Z_j - h_{j+1}^L) - P_f \quad (2-30)$$

and combined with equation (2-29):

$$\begin{aligned} & \frac{\rho}{A_0^2} \left(\frac{dQL_j}{dt} V_{dc} + (Q_{sj} - QL_j) QL_j \right) + \frac{\rho QL_j^2}{2} \left(\frac{1}{AUD_j^2} - \frac{1}{AD_j^2} \right) \\ & \cong \frac{\rho Z_j}{AD_j} \frac{dQL_j}{dt} + \frac{\rho}{AD_j^2} (Q_{sj} - QL_j) QL_j + \frac{\rho QL_j^2}{2 AUD_j^2} \\ & = P_j - P_{j+1} + \rho g (Z_j - h_{j+1}^L) \end{aligned} \quad (2-31)^{SR}$$

$$\Delta P = \frac{\rho Z_j}{AD_j} \frac{dQL_j}{dt} \quad (2-31a)$$

$$PPE = \rho g (Z_j - h_{j+1}^L) \quad (2-31b)$$

$$P_{dc} = -\frac{\rho}{AD_j^2} (Q_{sj} - QL_j) QL_j + P_j \quad (2-31c)$$

$$PKE = \frac{\rho QL_j^2}{2 AUD_j^2} \quad (2-31d)$$

The kinetic energy term, equation (2-31d), should be immediately compensated for (eliminated) by the expansion of the area through which the liquid flows onto the next stage plate. Instead, the kinetic energy term is kept as an estimate of resistance, as equation (2-20) for resistive head loss does not pertain here. The

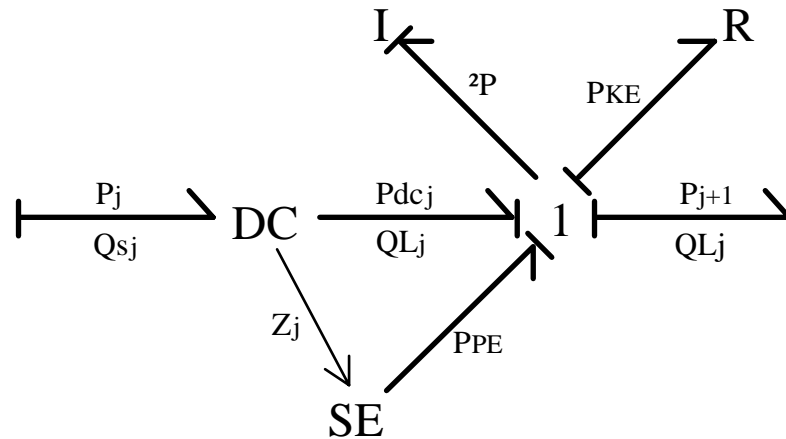


Figure 2.5 Bond graph of downcomer hydraulics, equation (2-31).

bond graph of this equation, Figure 2.5, is quite similar to the bond graph of the hydraulics of a tube, except the change in downcomer volume (dV_{dc}) depends on both the differences in volume flows and pressures. A new element is created to implement this term. The thin arrowed line indicates that the DC element is used to calculate Z_j , equation (2-29), for the potential energy term.

Assuming that the potential energy considerations are the predominant forces on the flow, essentially assuming constant flows, Bernoulli's equation can be used and the volume flow simplifies to

$$Q_{Lj} = C_x A_{UD} \sqrt{2g \left(\frac{P_j - P_{j+1}}{g \rho_j^L} - h_{j+1}^L + Z_j \right)} \quad (2-32)^G$$

Note the inclusion of C_x , accounting for vena contracta effects. Flow through the downcomer is often considered to have negligible dynamics and is omitted from many models. The bond graph of equation (3-32) is similar to Figure 2.5 without the I element or DC element.

For the flow over the weir, the most common equation used is Francis's weir formula, relating the height of foam over the weir (hf_{owj}) to foam volume flow (Q_{fsj}), weir length (L_w), and a vena contracta factor (C_d) [2]:

$$hf_{owj} = \left(\frac{3}{2 C_d \sqrt{2g}} \frac{Q_{fsj}}{L_w} \right)^{\frac{2}{3}} \quad (2-33)$$

The equation assumes the tray and the components are such that the full height of foam on the tray is intact as the fluid flows over the weir (i.e., there is no calming zone). Using relative froth density (ϕ), clear liquid flow (Q_{sj}) can be solved for:

$$\phi = \frac{\rho_j^L}{\rho_{fj}} = \frac{h_j^L}{hf_j} = \frac{Q_{sj}}{Q_{fsj}} = \frac{how_j}{hfow_j}$$

$$Q_{sj} = \frac{2}{3} C_d L_w \sqrt{\frac{2g}{\phi}} (how_j)^{1.5} \quad (2-34)$$

One modification found in the literature is to use a weir constriction factor (F_w) and a foam factor (F_{oam_j}) and solve for the clear liquid height over the weir [1, 27]:

$$F_{oam_j} = \frac{h_j^L}{hw_j + how_j} = \frac{\phi + 1}{2} = f(\text{velocity of vapor})$$

$$how_j = \frac{1.426}{g^{1/3}} F_w \left(\frac{Q_{sj}}{L_w} \right)^{2/3} \quad (2-35)^{GSR}$$

The weir constriction factor modifies the effective weir length much the same as C_d corrects for vena contracta effects. Francis's weir equation or its modification serves as the minimum hydraulics for some models [23, 42]. It can be derived from Bernoulli's equation [2]. Using equation (2-18), choose point 1 to be the top of the foam in the middle of the column and point 2 to be a distance y down from the top of the foam and just over the weir. The pressures are both equal to the stage pressure. Assume the velocity at point 1 is much less than at point 2 and solve for velocity at point 2:

$$v_2 = \sqrt{2gy}$$

The velocity is only a function of depth. Note that at a depth of zero, there is no liquid flowing over the weir. The differential volume flow becomes:

$$dQ_{sj} = dA v = C_d L_w dy \sqrt{2gy}$$

which can be integrated from zero to hf_{owj} to form equation (2-33). The assumption of constant pressure acting on the foam flowing over the weir is probably justified, unless the weir is short enough (as in a column of small diameter) that the flow forms a seal above the downcomer.

In most cases, Francis's formula is worth using. The only quantity to vary dynamically is the height over the weir. The derivation of a dynamic equation for the flow over the weir is similar to that of the flow through the downcomer. Starting with equation (2-30), and using pertinent information for a tray,

$$\frac{\rho_j^L AN}{\phi A_0^2} \left(hf_j \frac{dQ_{fsj}}{dt} + Q_{fsj} \frac{dhf_{owj}}{dt} \right) + \frac{\rho_j^L Q_{fsj}^2}{2 \phi [C_d (hf_{owj} + L_w)]^2} = P_j - P_{j+1} + \rho g y - P_f \quad (2-36)$$

$$\frac{dQ_{fsj}}{dt} = \frac{1}{\phi} \left(\frac{dQ_{sj}}{dt} - Q_{fsj} \frac{d\phi}{dt} \right)$$

The derivative of the height over the weir is not just the difference in volume flows into and out of the tray, but must include the vapor to liquid flow and the feed, as well as the dynamic relative froth density. The height over the weir can be found rather simply as:

$$hf_{owj} = \frac{h_j^L}{\phi} - h_{wj} = \frac{\frac{\sum u_{ji}}{v_i} - AD Z_j}{\bar{\rho}_j^L AN \phi} - h_{wj}$$

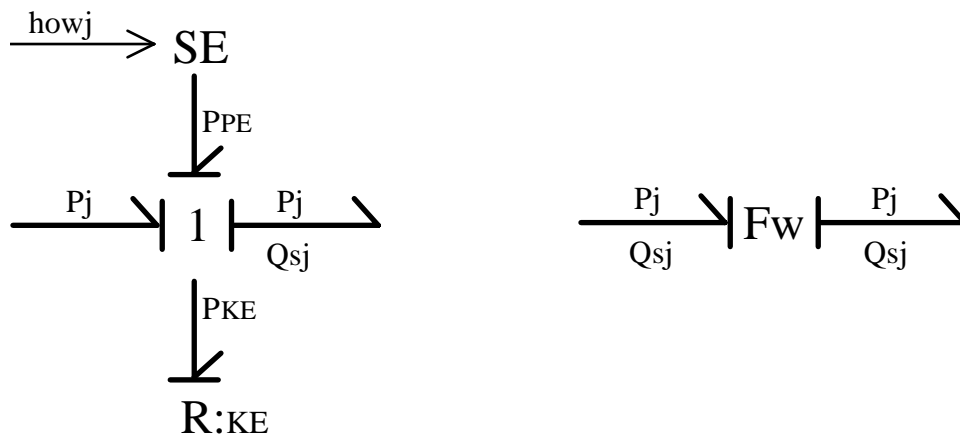
$$\text{how}_j = \frac{h_j^L}{\text{Foam}_j} - \text{hw}_j = \frac{\frac{\sum u_{ji}}{v_i} - \text{AD } Z_j}{\bar{\rho}_j^L \text{AN Foam}_j} - \text{hw}_j \quad (2-37)^{\text{GSR}}$$

The derivative of the height over the weir is not as simple to find. Francis's weir formula will be assumed for use by the models developed.

In terms of bond graphs, the height over the weir represents the volume of fluid on the tray plate. Rearranging equation (2-37) reveals the equation for the tray volume.

$$V_{\text{tray}} = (\text{how}_j + \text{hw}_j) \text{AN} = \frac{\frac{\sum u_{ji}}{v_i} - \text{AD } Z_j}{\text{Foam}_j}$$

Then the flow over the weir is a function of the tray volume. Equation (2-34) can be then represented as in Figure 2.6a, by an effort source of gravity and resistance of kinetic energy. What is not fully conveyed by this graph is that the



Figures 2.6a and 2.6b. Bond graphs of Francis weir formula, equation (2-34).

pressures of both these elements must be equal. The Fw element, shown in Figure 2.6b, encompasses the effort source and the resistance.

Vapor flow through the plate depends on the type of plate. The equations for a sieve tray are developed here. Equations for steady-state flow for bubble cap and valve trays exist [1]. For a sieve plate, the vapor flow is through small holes in the stage plate and is considered incompressible. The area of the holes is significantly smaller than the total area of the plate. The vapor between the stage below and the plate is considered to be well mixed and moving at a much lower velocity. Using equation (2-27) as a starting point, the volume being considered is the volume within the holes of the sieve plate, Vh_j .

$$\begin{aligned} \frac{\rho_{j+1}^V Vh_j}{(C_{vc} AH_j)^2} \frac{dQV_{j+1}}{dt} + \frac{\rho_{j+1}^V QV_{j+1}^2}{2 (C_{vc} AH_j)^2} \\ = P_{j+1} - (P_j + g \rho_j^L h_j^L) - g \rho_{j+1}^V LH_j - P_f \end{aligned} \quad (2-38)$$

$$Vh_j = AH_j LH_j$$

The stage plate is assumed thick enough that vena contracta effects (C_{vc}) are determined within the holes. Rearranging for the derivative, and assuming the vapor potential energy term to be negligible (i.e. $LH_j \ll h_j^L$ and $\rho_{j+1}^V \ll \rho_j^L$), equation (2-38) becomes

$$\frac{dQV_{j+1}}{dt} = \frac{C_{vc}^2 AH_j}{\rho_{j+1}^V LH_j} \left(P_{j+1} - P_j - g \rho_j^L h_j^L - P_f - \frac{\rho_{j+1}^V QV_{j+1}^2}{2 (C_{vc} AH_j)^2} \right) \quad (2-39)^{SR}$$

In this case, the pressure drop due to friction is related to the pressure needed to create bubbles against surface tension (σ) with a diameter equal to the sieve plate hole diameter (D_h) [2].

$$P_f = \frac{4 \sigma}{Dh} \quad (2-40)$$

The assumption of constant forces allows Bernoulli's equation to be used for vapor flow from a stage. Also assuming that the frictional forces are negligible, the vapor flow becomes,

$$QV_{j+1} = C_{vc} A H_j \sqrt{\frac{2}{\rho_{j+1}} (P_{j+1} - P_j - g \rho_j^L h_j^L)} \quad (2-41)^G$$

The distillation models in the literature that include an equation for vapor flow use equation (2-41). The bond graph of vapor flow, equation (2-39), is essentially that of Figure 2.3.

The assumption behind the derivations of these hydraulic equations is that pressure is being specified somewhere. An equation of state can be used for pressure. Unfortunately, the equation of state is usually used to solve for other variables, such as the molar density or compressibility factor. This, of course, leads to algebraic loops. A full hydraulic bond graph of a distillation stage will be developed in Section 3.1.

2.4 Vapor-liquid equilibrium (chemical potential and molar flow)

The equations related to vapor-liquid equilibrium are meant to predict the flow of a component within a stage from vapor to liquid. The relationship between the molar fraction in liquid (x_j) and molar fraction in vapor (y_j) is generally not as simple as described in the example explaining distillation (Section 1.1). Depending on the components and assumptions used, these equations can form a large part of the model. This relationship is the most important within the distillation column model. Levy, *et al.* showed that the

largest time-constants of a distillation model were due to composition dynamics [19]. Ranzi, *et al.*, found that up to 35% of the time in a distillation simulation was taken by vapor-liquid equilibrium calculations [31]. The essential problem of determining this flow is that chemical theory on this point is inadequate: there are no equations for chemical resistance or chemical capacitance to relate chemical potential and molar flow between the liquid and the vapor phases.

Instead of calculating the flow, the traditional method of determining molar content is to assume that after good contact, vapor and liquid reach equilibrium conditions. If equilibrium is assumed within a closed system with a vapor phase and a liquid phase, there are no chemical reactions and pressure, temperature, and especially the total Gibbs free energy are held constant:

$$\frac{dG}{dt} = \sum_{i=1}^c \mu_i^L \frac{dn_i^L}{dt} + \sum_{i=1}^c \mu_i^V \frac{dn_i^V}{dt} = 0$$

In a closed system without reaction, it must also be true that molar flows are equal and opposite:

$$\frac{dn_i^L}{dt} = - \frac{dn_i^V}{dt} \quad (2-42)$$

Thus, the chemical potentials of a component in both liquid and vapor are equal:

$$\mu_i^L = \mu_i^V \quad (2-43)$$

This is the fundamental relationship used to predict multicomponent phase equilibria [37].

Chemical potential is not used in the literature. What follows from equation (2-42) is that at equilibrium, the fugacity of a component in a liquid

equals the fugacity of that component in vapor [4]. Fugacity of a component in a mixture, \hat{f}_i , is defined for a constant temperature:

$$d\mu_i = R T d(\ln(\hat{f}_i)) \quad (2-44a)$$

$$\lim_{P \rightarrow 0} \frac{\hat{f}_i}{x_i P} = 1 \quad (2-44b)$$

If the mixture is a vapor, in an ideal mixture, and the ideal gas law holds, then fugacity becomes the partial pressure of the component. This is evident from the Gibbs-Duhem equation (2-17) combined with ideal mixture (the use of partial pressure), constant temperature, and the ideal gas law.

$$\text{(Gibbs-Duhem)} \quad \frac{d\mu_i}{dt} n_i = \frac{dP_i}{dt} V \quad (2-45)$$

$$\text{(Ideal Gas Law)} \quad V = \frac{n_i R T}{P_i}$$

$$\text{(Fugacity)} \quad \frac{d\mu_i}{dt} = \frac{R T}{P_i} \frac{dP_i}{dt} = R T \frac{d}{dt} \ln(P_i)$$

Essentially, the fugacity of a component is a measure of the partial pressure's deviation from Gibbs-Duhem and Dalton's law (ideal mixture). Partial pressure itself is still used in the traditional model, unqualified by deviations.

Measurement of the actual system pressure does not reveal fugacity, but pressure. Chemical potential, which is not used in the traditional model, is essentially absorbed into fugacity along with any deviations a component may exhibit. In bond graph terminology, these equations suggest a transformer using molar density as the transformation factor.

$$n_i = \bar{p}_i V \quad (2-46)$$

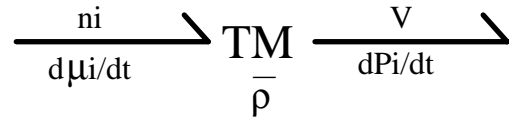


Figure 2.7 Transformer representing chemical to hydraulic power conversion.

$$\frac{d\mu_i}{dt} = \bar{p}_i \frac{dP_i}{dt} = \bar{p}_i \frac{d\hat{f}_i}{dt} \quad (2-47)$$

There are several ways to compute and approximate fugacity, depending on the components used, each involving molar fractions. Thus, a relationship between x_i and y_i is found by equating vapor and liquid fugacities. The general equilibrium equation for this relationship can be stated as:

$$y_i = K_i x_i \quad (2-48)^{GS}$$

where K_i (referred to as the distribution coefficient [30] or K-value) can be a simple or a complex function, depending on what approximations for fugacity are used. The most basic expression for K_i , henceforth referred to as the ideal K-value, is

$$K_i^I = \frac{PS_i}{P} \quad (2-49)^S$$

where PS_i is the vapor pressure (saturation pressure) of component i (a function of temperature only), and P is the total pressure of the system. The ideal K-value is the same as Raoult's law:

$$P y_i = PS_i x_i$$

This equation makes sense; for a pure substance, the equilibrium pressure for two phases is, by definition, the vapor pressure. Thus, in a mixture, the partial pressures of both liquid and vapor should be equal. If the vapor pressure of a substance is twice the system pressure, then the vapor will have twice the molar concentration of the liquid. The implication of this equation is that partial pressure, not chemical potential, is driving molar flow between the phases. As

may be expected, in mixtures, the partial pressures are not uniformly equal for all substances and may serve as a poor model for molar flow. Hence, fugacity has been introduced to replace partial pressures. Nevertheless, the essence of these equations is based on the idea that a difference in partial pressure (fugacity) is driving molar flow between the phases.

For a more detailed expansion, fugacity can be defined in terms of a fugacity coefficient $\hat{\phi}_i$ (measuring the deviation from partial pressure), ideal fugacity coefficient ϕ_i (measuring the deviation from pressure as a pure component), activity coefficient γ_i (measuring the deviation from Dalton's law), ideal fugacity f_i^L , ideal vapor pressure, and pressure [1, 4]:

$$\hat{f}_i^L = \gamma_i^L x_i f_i^L \quad (2-50a)^R$$

$$\hat{f}_i^V = \hat{\phi}_i^V y_i P \quad (2-50b)^R$$

$$f_i^L = P S_i \phi_i^L \quad (2-50c)^R$$

If the substance forms an ideal gas and an ideal mixture and conforms to Gibbs-Duhem, then the fugacity and activity coefficients are one and Raoult's law can be used. Combining these definitions, the relation between the molar fraction of a component in vapor and in liquid can be calculated several ways:

$$y_i = \frac{\gamma_i^L P S_i \phi_i^L}{\hat{\phi}_i^V P} x_i \quad (2-51)$$

$$y_i = \frac{\gamma_i^L K_i^I \phi_i^L}{\hat{\phi}_i^V} x_i \quad (2-52)^G$$

Equations (2-51) and (2-52) are but the start of many various ways in which molar fractions are calculated. Estimating fugacity and its coefficients occupies a substantial segment of the chemical engineering literature. Some methods of

predicting

Error!

The method used by Gallun will serve as proper illustration [24]. Using equation (2-51), we must come up with equations for PS_i , ϕ_i^L , ϕ_i^V , and γ_i^L . The Antoine equation is used to calculate PS_i :

$$\log(PS_i) = A_i + \frac{B_i}{T + C_i} \quad (2-53)^{GR}$$

where T is the only variable. Gallun's equations used for ϕ_i^L were taken from a 1967 monograph by Prausnitz, *et al.*

$$\phi_i^L = \phi_i^S \exp\left(-\frac{\alpha_i^L PS_i}{RT}\right) \quad (2-54)^{GR}$$

$$\phi_i^S = \exp(f_1(T_R) + \omega_i f_2(T_R)) \quad (2-55)^{GR}$$

Temperature is the only variable. To calculate

Error!

$$ZZ = 1 + B_m \bar{p} = \frac{1 + \sqrt{1 + \frac{4 B_m P}{RT}}}{2} = \frac{P V}{n R T} \quad (2-56)^{GR}$$

B_m is the second virial coefficient of the mixture, which must be calculated using the following mixing rules:

$$B_m = \sum_{i=1}^c \sum_{k=1}^c y_i y_k B_{ik} \quad (2-57a)^{GR}$$

$$B_{ik} = \frac{RTCC_{ik} (f_3(T_R) + \omega_{Hi k} f_4(T_R) + f_4(\mu_{R, T_R}) + \eta_{ik} f_6(T_R))}{PCC_{ik}} \quad (2-57b)^{GR}$$

$$T_R = \frac{T}{TCC_{ik}} \quad (2-57c)^{GR}$$

where the symbols here are constants or functions of y_i and T [24]. Then

$\hat{\phi}_i^V$ can be calculated using the following:

$$\ln(\hat{\phi}_i^V) = 2 \bar{\rho}^V \sum_{k=1}^c y_k B_{ik} - \ln(ZZ) \quad (2-58)^{GR}$$

Gallun uses the Wilson equation to calculate γ_i^L . Again, the only system variables that are present are molar fraction (x_k) and temperature (T).

$$\ln(\gamma_i^L) = 1 - \ln\left(\sum_{m=1}^c x_m \Lambda_{im}\right) - \sum_{k=1}^c \frac{x_k \Lambda_{ki}}{\sum_{m=1}^c x_m \Lambda_{km}} \quad (2-59a)^{GR}$$

$$\Lambda_{ik} = \frac{\alpha_k^L}{\alpha_i^L} \exp\left(-\frac{(\lambda_{ik} - \lambda_{ii})}{RT}\right) \quad (2-59b)^{GR}$$

$$\alpha_i^L = \frac{1}{\bar{\rho}_j^L} = f(T) \quad (2-59c)^{GSR}$$

Expanding these equations for all components for every stage, it is easy to understand how these might form a significant portion of a model.

The problem of this method and all methods presented in the above references are that equations for γ_i^L involve x_i and equations for

Error!

Another problem with using vapor-liquid equilibrium equations to find the vapor molar fraction (y_i), is too many equations. Equation (2-48) and the basic definition of molar fractions:

$$1 = \sum_{\forall i} y_i$$

form one more equation than is needed to find the values of the fractions. The system is over-determined and generally is resolved by iterating the value of the temperature until all equations are satisfied. A variation of this method is presented in Section 2.5.

Currently, the only modification to equating liquid and vapor fugacities is the use of an efficiency term. Several definitions have been proposed and developed [2, 46, 47, 48, 49]. The vaporization and modified Murphree plate efficiencies are defined as [4]:

$$E_{ji} = \frac{\hat{f}_i^V}{\hat{f}_i^L} = \frac{y_{ji}}{K_{ji} x_{ji}} \quad (2-60)$$

$$E_{ji}^M = \frac{y_{ji} - y_{j+1i}}{K_{ji} x_{ji} - y_{j+1i}} = \frac{E_{ji} - \frac{y_{j+1i}}{K_{ji} x_{ji}}}{1 - \frac{y_{j+1i}}{K_{ji} x_{ji}}} \quad (2-61)$$

Ideally, the efficiency is one: the vapor and liquid fugacities are equal. Values for modified Murphree efficiency are typically found empirically through some estimate of plate dynamics, but can be derived using film theory, phase resistances, and transfer units for steady-state flows [4]. One theoretical basis for efficiencies is that chemical potential differences are driving molar flows between phases. Using the definition of fugacity, chemical potential differences are modified to become fugacity differences. Efficiencies are mostly used in designing a column to discriminate between the number of ideal trays and number of real trays that are needed.

2.5 Heat (temperature and entropy)

The conjugate pair for heat is entropy flow and temperature. Entropy is not used in traditional models for distillation columns, there can be no bond graph of these equations. Although there are tables of entropy values to be found, they are not extensive enough in terms of substances covered, to be useful. Instead, temperature is found through the over-determined set of vapor-liquid equilibrium equations, described in Section 2.4. Otherwise, the dynamic equation for temperature is typically derived from some function of temperature and time, $f(T_j, t)$:

$$\frac{d}{dt} f(T_j, t) = \frac{\square}{\square T_j} f(T_j, t) \frac{dT_j}{dt} \quad (2-62)^S$$

An appropriate function depends on the model. Because convection is the major source of heat flow, the function should incorporate molar flow.

The dynamic equation for temperature can be derived from the vapor-liquid equilibrium equation. Begin with the basic equations, sum over all i , and then take the derivative:

$$\begin{aligned} y_{ji} &= K_{ji} x_{ji} \\ 1 &= \sum_{i=1}^c y_{ji} = \sum_{i=1}^c K_{ji} x_{ji} \\ 0 &= \sum_{i=1}^c \left(\frac{dK_{ji}}{dt} x_{ji} + K_{ji} \frac{dx_{ji}}{dt} \right) \end{aligned} \quad (2-63)$$

If the ideal K-value is now assumed and the Antoine equation used, then K is a function of P_j and T_j . The derivative of K can be stated:

$$\frac{dK_{ji}}{dt} = \frac{\partial K_{ji}}{\partial T_j} \frac{dT_j}{dt} + \frac{\partial K_{ji}}{\partial P_j} \frac{dP_j}{dt} \quad (2-64a)$$

$$\frac{\partial K_{ji}}{\partial T_j} = B_i K_{ji} (T_j - C_i)^{-2} \ln(10) \quad (2-64b)$$

Now, let the derivative of P_j be zero, combine equations (2-63) and (2-64), and solve for the derivative of T_j :

$$\frac{dT_j}{dt} = - \frac{\sum_{i=1}^c K_{ji} \frac{dx_{ji}}{dt}}{\sum_{i=1}^c B_i K_{ji} (T_j - C_i)^{-2} \ln(10) x_{ji}}$$

Another function used is one for enthalpy, an approximation for enthalpy in liquid as a polynomial function of temperature.

$$H_{ji}^L = a_i + b_i T_j + c_i T_j^2 \quad (2-65)^{GS}$$

Because the liquid enthalpy is calculated using a differential equation (2-15), the derivative of T_j can be found similarly to the derivation above, without having to assume a constant pressure. Again, the key here is that molar flow is the assumed major conveyer of entropy.

Entropy is also flowing from the frictional loss terms of the hydraulic equations, but this is not considered to be a significant source of heat. The real heat flow by conduction occurs in the reboiler and condenser, which will be dealt with in Sections 2.7 and 2.8.

2.6 Equation of state

Ideal	$P = \frac{RT}{v}, \quad v = \frac{V_i}{n_i}$
Virial	$P = \frac{RTZ}{v}, \quad Z = 1 + \frac{B}{v}$
Peng-Robinson	$P = \frac{RT}{(v-b)} - \frac{\alpha a}{v(v+b) + b(v-b)}$ <p>α, a, b are functions of temperature, critical pressure and temperature, and the acentric factor</p>
Incompressible	$v = a + bT + cT^2$

Table 2.1 Equations of state.

An equation relating the steady-state pressure, temperature, volume and number of moles is an equation of state. The equation can serve as a source of behavior of a system. Usually, an equation of state is used to solve for the system pressure of a stage. If the vapor molar holdup is assumed constant, however, the molar volume (molar density) must be calculated from the equation of state. Such a model usually uses Bernoulli's equations to calculate pressure and is forced to either assume values for liquid flow or use iterative methods. The assumption of dynamic equilibrium means the pressure of liquid and vapor are equal.

The equations of state considered are the ideal gas equation, the virial equation of state, and the Peng-Robinson equation of state. Of these equations, only the last one is valid for both liquid and vapor phases. Peng-Robinson does assume that molar volume is known, it can not predict what percentage of the substance is in which phase. Hundreds of equations of state exist [43]; these are considered only as common examples. Also considered is a fluid that does not change volume with a changing pressure, the incompressible fluid. Table 2.1 lists these equations of state. Which equation of state should be used will

Equation of State	$C_s = \frac{dS_i}{dt} / \frac{dT}{dt}$	Assuming (All assume $\frac{dU_i}{dt} = 0$)
Ideal	$\frac{\mu_i n_i}{T^2}$	$\frac{dP}{dt} = \frac{dV_i}{dt} = 0$
	$\frac{P}{T}$	$\frac{dP}{dt} = \frac{dn_i}{dt} = 0$
Virial	$\frac{\mu_i n_i}{T^2}$	$\frac{dZ}{dt} = \frac{dP}{dt} = \frac{dV_i}{dt} = 0$
	$\frac{P}{T}$	$\frac{dZ}{dt} = \frac{dP}{dt} = \frac{dn_i}{dt} = 0$
Peng-Robinson	$\frac{\mu_i R}{T(v-b)} \frac{\square n_i}{\square P}$	$\frac{dP}{dt} = \frac{dV_i}{dt} = 0$
	$\frac{R v P}{V_i(v-b)} \frac{\square n_i}{\square P}$	$\frac{dP}{dt} = \frac{dn_i}{dt} = 0$
	$\frac{\square P}{\square n_i} = \frac{v R T}{(v-b)^2 n_i} - \frac{2 \alpha a v (v+b)}{n_i (v + (\sqrt{2} + 1) b)^2 (v - (\sqrt{2} - 1) b)^2}$	
Incompressible	$-\frac{\mu_i n_i}{V_i T} (b + 2 c T)$	$\frac{dP}{dt} = \frac{dV_i}{dt} = 0$
	$\frac{P n_i}{V_i} (b + 2 c T)$	$\frac{dP}{dt} = \frac{dn_i}{dt} = 0$

Table 2.2 Capacitance of Equation (2-66).

depend on the nature of the distillation components, as well as the information available to compute constants within an equation of state. For instance, the second virial coefficient (B) is detailed in equations (2-57).

Several capacitive relationships can be set up using these equations of state, the internal energy equation and the Gibbs-Duhem equation. The relationships are:

$$\frac{dS_i}{dt} = C_s \frac{dT}{dt} \quad (2-66)$$

Equation of State	$C_v = \frac{dV_i}{dt} / \frac{dP}{dt}$	Assuming
Ideal / Virial	$\frac{V_i^2}{n_i R T}$	$\frac{dT}{dt} = \frac{dn_i}{dt} = 0$
	$\frac{V_i^2 \left(1 - \frac{S_i T}{V_i P}\right)}{S_i T}$	$\frac{d\mu_i}{dt} = \frac{dn_i}{dt} = 0$
Peng-Robinson	$\frac{v V_i R \left(1 - \frac{S_i (v - b)}{V_i R}\right)}{S_i (v - b)}$	$\frac{d\mu_i}{dt} = \frac{dn_i}{dt} = 0$
Incompressible	$\frac{V_i n_i (b + 2 c T)}{S_i}$	$\frac{d\mu_i}{dt} = 0$

Table 2.3 Capacitance of Equation (2-67).

$$\frac{dV_i}{dt} = C_v \frac{dP}{dt} \quad (2-67)$$

$$\frac{dn_i}{dt} = C_n \frac{d\mu_i}{dt} \quad (2-68)$$

The relationships are only true under certain conditions. The values of C_s , C_v , and C_n are shown in Tables 2.2, 2.3 and 2.4 along with the required conditions. Note that none of these conditions are true in a dynamic distillation column. As the equation of state is usually used for pressure calculation, equation (2-67) is usually represented in a bond graph as a C element.

The value of C_n for the ideal gas equation is that used by Oster, *et al.* [50]. In describing the molar flow between phases, only the one for Peng-Robinson is adequate in describing both phases. These relationships can only be used in conjunction with equations that relate chemical potential to molar flow. Unfortunately, as described in Section 2.4, no equations of state nor any other equations exist to provide such a relationship. For instance, equation (2-68) could be used to solve for chemical potential of both the liquid and the vapor in a stage, based on the influx of total moles. The equation can not tell us the flow between the phases because it is only valid for constant volumes. Nor would it make sense to use such a storage element to describe phase flow.

2.7 Condenser and receiver

The condenser and the receiver are separate from the distillation column, though essential for the distillation process. The condenser accepts the vapor rising from the top stage plate and removes a significant amount of heat. The main choice is between total and partial condensers, depending on the type of modeling simplification desired. A total condenser is assumed to remove

Equation of State	$C_n = \frac{dn_i}{dt} / \frac{d\mu_i}{dt}$	Assuming
Ideal	$\frac{n_i}{RT}$	$\frac{dV_i}{dt} = \frac{dT}{dt} = 0$
Virial	$\frac{n_i}{RTZ}$	$\frac{dZ}{dt} = \frac{dV_i}{dt} = \frac{dT}{dt} = 0$
Peng-Robinson	$\frac{n_i}{V_i} \frac{\partial n_i}{\partial P}$	$\frac{dV_i}{dt} = \frac{dT}{dt} = 0$
Incompressible	1	$\frac{dU_i}{dt} = \frac{dV_i}{dt} = \frac{dT}{dt} = 0$

Table 2.4 Capacitance of Equation (2-68).

enough heat to totally condense the vapor, that amount of heat varying with the condition of the vapor flowing in. A partial condenser is assumed to remove a fixed amount of heat, the amount of condensation varying with the condition of the vapor flowing in. The thermal equations and the hydraulic equations developed will be for a total condenser. No change in chemical potential is assumed; phase changes are being driven by entropy flow.

The thermal aspect of the model is power flow due to convection, conduction and heat of vaporization. The vapor is brought up against tubes filled with cooling water. The amount of heat removed is controlled by the flow of cooling water, which in turn is controlled by a valve. Conduction is a function of thermal capacitance and thermal resistance. The thermal equations are of the form,

$$\begin{aligned} \text{heat flow} &= (\text{volume flow}) (\text{heat capacity}) (\Delta\text{Temperature}) \\ &= (\text{heat transfer film coefficient}) (\text{area of heat transfer}) \Delta T \end{aligned}$$

$$\text{change in heat holdup} = (\text{mass}) (\text{specific heat capacity}) \frac{dT}{dt}$$

The mass of the flowing cooling water, the mass of the vapor rising from the top plate, and the mass of the condenser tubes must be considered in these equations. Because total condensation is assumed, the desired variable is the heat flow from vapor (QC). In the bond graph terminology of entropy flow, the above forms can be converted [5].

$$\begin{aligned} \text{entropy flow} &= (\text{volume flow}) (\text{heat capacity}) \Delta T / T \\ &= (\text{heat transfer film coefficient}) (\text{area of heat transfer}) \Delta T / T \end{aligned}$$

$$\text{change in entropy holdup} = (\text{mass}) (\text{specific heat capacity}) \dot{T} / T$$

Specifically, for the condenser described in the dissertation of Gallun [24], the original heat flow equations are:

$$U_{cw} C_{cw} \dot{T}_{wo} = Q_{cw} C_{cw} (T_{wi} - T_{wo}) + U_{wm} A_w (T_{mc} - T_{wo}) \quad (2-69a)^{GS}$$

$$U_{mc} C_{mc} \dot{T}_{mc} = U_{wm} A_w (T_{mc} - T_{wo}) - Q_C \quad (2-69b)^{GS}$$

$$Q_C^3 = \frac{[QV_2]_{REF}}{QV_2} U_{pmo} A_{pc} (T_j - T_{mc})^3 \quad (2-69c)^{GS}$$

The subscripts refer to cooling water (cw), water out (wo), water in (wi), and the mass of the cooling tubes (mc). The equation for the heat flow from the vapor, equation (2-69c), is an empirical approximation from reference values of vapor and heat flow. T_j in this equation is considered to be some average temperature between T_1 (receiver temperature) and T_2 (stage 2 temperature). Unlike pure substances, the distillation mixture will not condense at just one temperature. In terms of entropy flow, these equations become equations (2-70).

$$\dot{S}_{wi} + \Delta\dot{S}_1 = \dot{S}_{mc} + \dot{S}_{wo} \quad (2-70a)^R$$

$$\dot{S}_{mc} + \Delta\dot{S}_2 = Q_C/T_j + \dot{S}_{z1} \quad (2-70b)^R$$

$$\dot{S}_{wi} = Q_{cw} C_{cw} (T_{wo} - T_{wi}) / T_{wo} \quad (2-70c)^R$$

$$\Delta\dot{S}_1 = U_{cw} C_{cw} \dot{T}_{wo} / T_{wo} \quad (2-70d)^R$$

$$\dot{S}_{mc} = U_{wm} A_w (T_{mc} - T_{wo}) / T_{wo} \quad (2-70e)^R$$

$$\Delta\dot{S}_2 = U_{mc} C_{mc} \dot{T}_{mc} / T_{mc} \quad (2-70f)^R$$

$$\dot{S}_{wo} = U_{wm} A_w (T_{mc} - T_{wo})^2 / T_{wo}^2 \quad (2-70g)^R$$

$$Q_C/T_j = U_{pmo} A_{pc} (T_j - T_{mc})/T_j \quad (2-70h)^R$$

$$\dot{S}_{z1} = U_{pmo} A_{pc} (T_j - T_{mc})^2 / (T_{mc} T_j) \quad (2-70i)^R$$

The equation for \dot{S}_{wo} reflects the idea that the power lost in the resistance between the cooling water and the condenser tubes is regained as heat flow into the cooling water. The assumption that $(T_{wo} \gg (T_{mc} - T_{wo}))$ effectively eliminates this term from Gallun's equations (2-69). Figure 2.8 shows the bond graph associated with equations (2-70). The R element, equation (2-70a), in contrast to the RS element, shows that power is lost to convection as the cooling water flows away, and is modulated by the volume flow of cooling water, Q_{cw} . Knowing the heat loss (Q_C), the enthalpy-balance for the receiver becomes a variation of equation (2-15):

$$\frac{dH_1^L}{dt} = - \frac{L_1 H_1^L}{\sum_{\forall i} u_{1i}} + \sum_{\forall i} v_{2i} H_{1+1i}^V - Q_C \quad (2-71)^{GS}$$

The hydraulic aspect of the condenser is the volume flow of vapor entering (Q_V) and the liquid flow leaving. The mass holdup in the condenser is assumed to be constant and at temperatures that vary between T_1 and T_2 . The model assumes a weighted average of T_1 and T_2 . The volume flow of vapor is

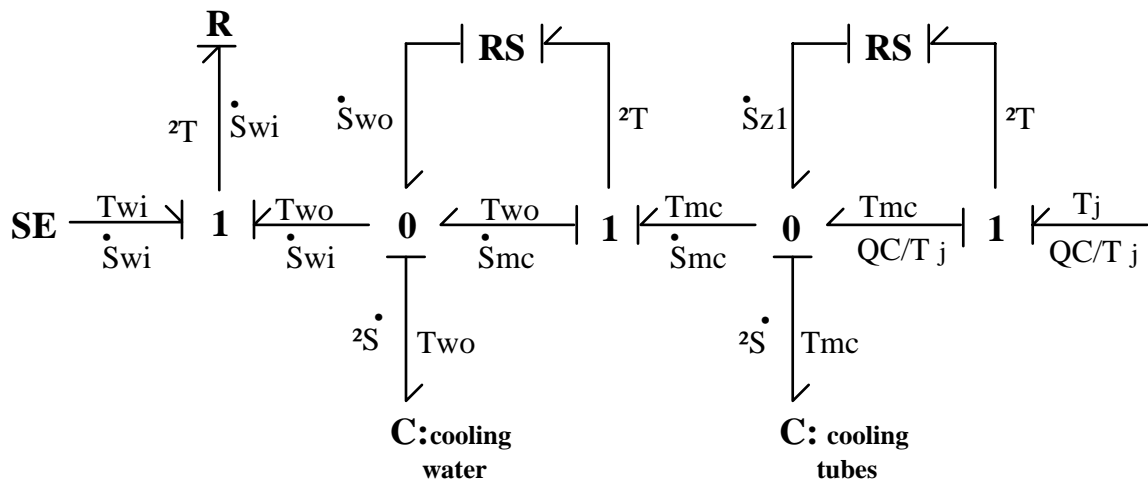


Figure 2.8. The bond graph of the condenser, equations (2-70).

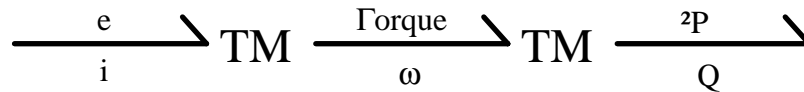


Figure 2.10. Bond graph of pump.

calculated using an empirical estimation based on pressure differences and the vapor's molar density. Also to be considered is the volume flow of cooling water through the cooling tubes, Q_{cw} . The pressures at the inlet and the outlet of these tubes are considered constant and the flow is controlled by means of a valve. Figure 2.9 reveals this simple system.

The hydraulic aspect of the receiver concerns pumps and valves. The receiver is the chamber in which the condensed vapor resides before it gets pumped out. An electric pump is a transformer of electric power to mechanical power to hydraulic power [36]. This is shown in the bond graph of Figure 2.10. The exact nature of the electric power being supplied depends on the pump. A pump is essentially a flow modulated pressure source. Various equations for a pump illustrate this aspect [24, 51]:

$$\Delta P = k_{\text{pump}} \sqrt{Q_{\text{max}} - q} \quad (2-72a)^R$$

$$\Delta P = a + b q + c q^2 \quad (2-72b)^{GS}$$

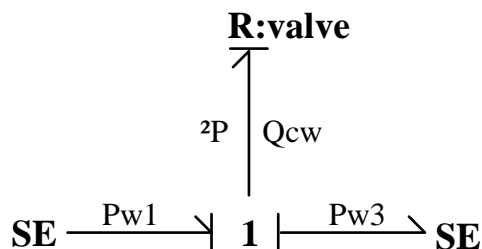


Figure 2.9. Cooling water flow in condenser.

The form of these equations is of a negative resistor. A valve is a hydraulic resistor used to control the flow of the fluid. Equations for a valve include [24, 51, 52]:

$$\Delta P = \frac{k_{\text{valve}}}{2 A^2} q^2 \tag{2-73a)^R}$$

$$\Delta P = a + b q + c q^2 + d q^3 \tag{2-73b)^{GS}}$$

Combining pumps and valves is the essence of hydraulic flow out of the receiver and the base of the column. Fluid flow from the receiver first goes through a pump, then is split into two pipes each containing a control valve. One pipe, containing the reflux, leads to the stage plate below and the other pipe, containing the distillate, leads out of the system. This setup is best shown using a bond graph, Figure 2.11. The effort source on the right is the

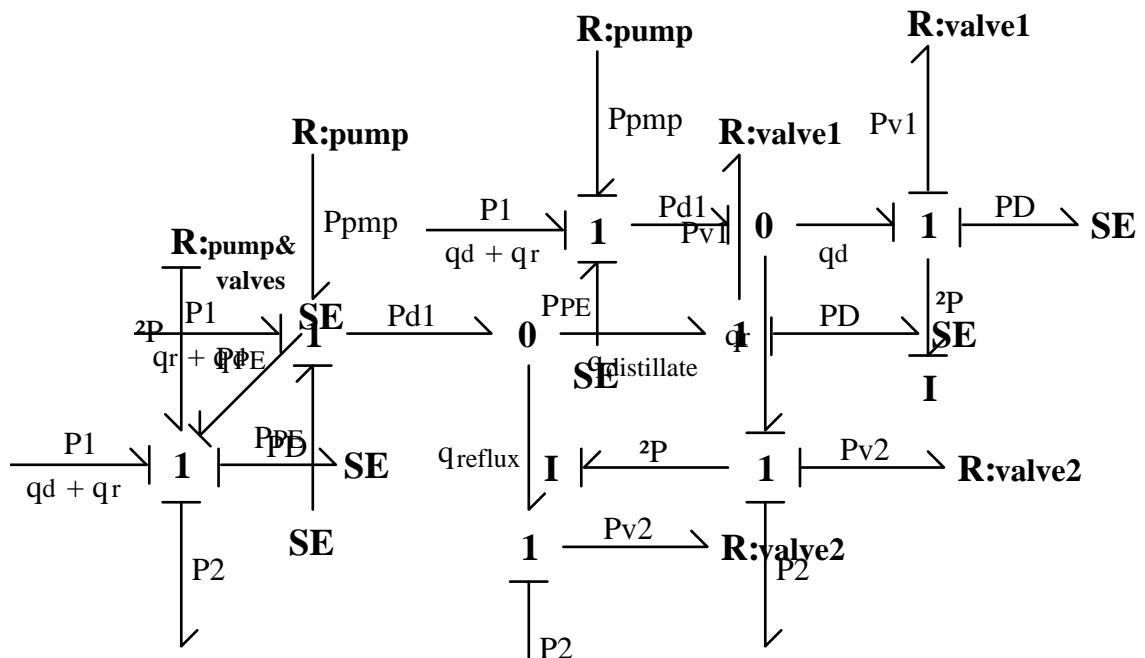


Figure 2.12. Bond graphs of pump and valves without an algebraic loop. a) Bond graph of pump and valves combined into one resistor. b) Bond graph of pump and valves with an algebraic loop. Figure 2.11. Bond graph of pump and valves with an algebraic loop.

pressure increase due to the vertical drop between the base liquid level and the pump. The causality strokes can not be fully assigned because there is a choice of assigning them. Hence, these equations form an algebraic loop. Two ways of breaking this algebraic loop are to combine the resistances or introduce other elements into the system. The valves can be seen as an expression of Bernoulli's equation (Figure 2.3) where there are only the resistive element and the inertial element. Adding these inertial elements to Figure 2.11 will solve the algebraic loop, but this does require a knowledge of the physical dimensions of the piping. The bond graph of Figure 2.11 can thus be solved using bond graph Figure 2.12 a or b. The problem with joining the resistances is that either PD and P2 must be joined somehow (by some average) or the flows must be split somehow. There is no rigorous way to join non-linear resistors along a Y-connection.

2.8 Reboiler

The reboiler infuses heat into and siphons fluid away from the distillation column. The reboiler model is similar to the model for the condenser and receiver. The base of the distillation column contains a pair of outlets; one leading to the reboiler and one out of the system. The reboiler totally vaporizes the fluid entering. Thermal conduction is the driving force of the vaporization. The bottoms are taken out using a pump and valve in series.

The thermal aspects are essentially the same as the condenser. Tubes filled with steam (the steam chamber) transfer heat into the fluid within the reboiler until the fluid vaporizes. A complication exists in that the mass of steam within the steam chamber is not constant because the steam is continually

condensing into water. This provides additional entropy flow from the heat of vaporization. The thermal model for heat of vaporization is expressed in equation (2-74):

$$\begin{aligned} \text{Heat} &= m L^h = S T \\ L^h &= a + b T \quad (\text{empirical estimate}) \\ \frac{d\text{Heat}}{dt} &= \frac{dS}{dt} T = \frac{dm}{dt} (a + b T) \end{aligned} \quad (2-74)$$

If working in enthalpies (H) and tabulated estimates of enthalpies, the model can be altered.

$$\begin{aligned} L^h &= HV(T_{sc}) - hL(T_{sc}) \quad (\text{empirical estimate}) \\ \frac{dH}{dt} &= \frac{dm}{dt} (HV(T_{sc}) - hL(T_{sc})) \end{aligned} \quad (2-75)^{GS}$$

The steam flows from a steam header, which is under constant pressure, through a steam valve, into the steam chamber. Within the steam chamber, the phase change radically alters the volume flow by the change in density. The water flows away under constant pressure. Hydraulically, the effect of the heat of vaporization can be expressed as:

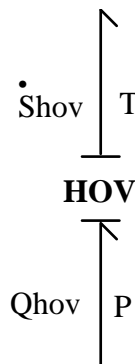


Figure 2.13. HOV element.

$$Q_{hov} = \frac{dm}{dt} \left(\frac{1}{\rho^V} - \frac{1}{\rho^L} \right) \quad (2-76)^R$$

Because the liquid is usually much denser than the vapor, its term can be reasonably dropped from equation (2-76). Together, these equations express a link between thermal and hydraulic power that can be expressed as the HOV element, shown in Figure 2.13. If the HOV element is to behave as other elements, the power in equals the power out:

$$Q_{hov} P = \dot{S}_{hov} T$$

This presents more equations than is evidently needed to determine the flow variables. The problem with these equations are that the chemical power has not been accounted for. A third bond emanates from the HOV element supplying chemical power to the process of condensing. This model does not need to evaluate chemical potential because mass flow is determined by assuming the steam chamber is filled with a constant volume of steam and a constant volume of liquid. Thus, the mass flow of phase change from vapor to liquid is equal to the mass flow into the chamber ($Q_{sh} \rho_{sh}$). The HOV element presented here is based on certain assumptions that do not exist elsewhere in the column: the phase change is due entirely to heat loss and that heat loss is entirely conducted away to the reboiler tubes. Mass flow and chemical potential are not directly calculated or accounted for.

The reboiler and part of the base are shown in the bond graph of Figure 2.14. The entropy flows from the steam header into the steam chamber to the metal of the tubes and into the reboiler chamber. The reboiler chamber is considered to effect the entire base, and so the rightmost 0-nodes of Figure 2.14 show only some of the required bonds. Not shown are the effects of the liquid

and the vapor leaving or coming into the base. Unlike the other valves in the system, the steam valve is modeled as an RS element, rather than just an R element. All valves could be modeled as RS elements, but the hydraulic power flow into thermal power is usually considered negligible. The INC element assumes that the pressure is high enough (as would be typical in a steam header) that the density of the steam

is not dependent on pressure, but on temperature alone. If the steam were not considered incompressible, the INC element would be replaced by a C element

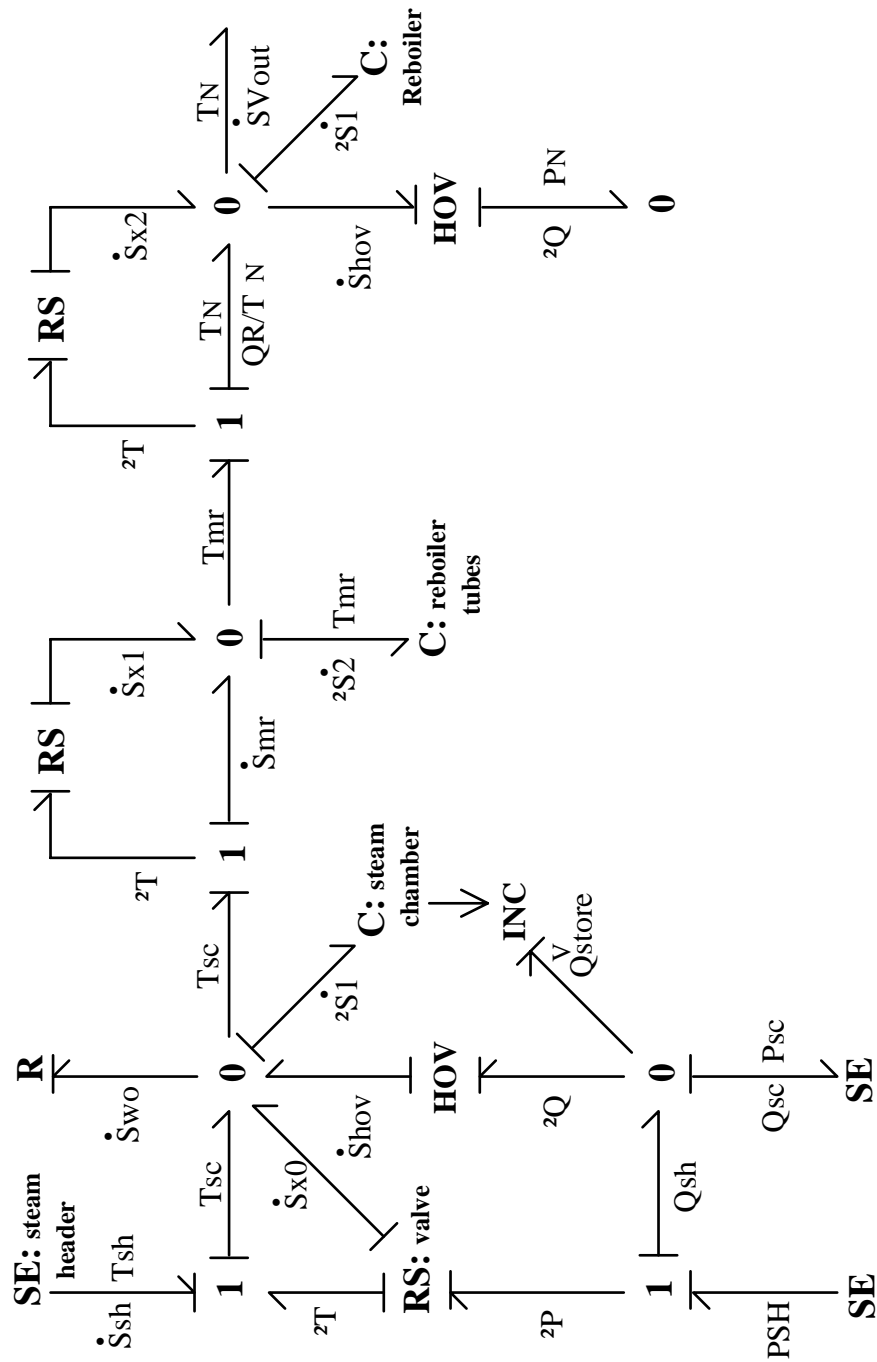


Figure 2.14. Thermal and hydraulic bond graph of reboiler.

(and the pressure could not be held constant by an effort source). The equations related to Figure 2.14 are presented here as equations (2-77).

$$\text{R:} \quad \dot{S}_{wo} = Q_{sc} C_{wo} (T_{sc} - T_{sh}) / T_{sc} \quad (2-77a)^R$$

$$C_{wo} = \rho_w \frac{\square h L_{sc}}{\square T} \quad (2-77b)^R$$

$$\text{RS: valve} \quad \dot{S}_{sh} = Q_{sh} C_{sh} (T_{sh} - T_{sc}) / T_{sc} \quad (2-77c)^R$$

$$\dot{S}_{x0} = \frac{Q_{sh} C_{sh} (T_{sh} - T_{sc})^2}{T_{sc}^2} + \frac{Q_{sh} (P_{SH} - P_{sc})}{T_{sc}} \quad (2-77d)^R$$

$$Q_{sh} = f(P_{SH} - P_{sc}) \quad (2-77e)^R$$

$$\text{HOV:} \quad \dot{S}_{hov} = \frac{Q_{sh} \rho_{sh}}{T_{sc}} (HV_{sc}(T_{sc}) - hL_{sc}(T_{sc})) \quad (2-77f)^R$$

$$\Delta Q = Q_{sh} \rho_{sh} \frac{1}{\rho_{sc}} \quad (2-77g)^R$$

$$\text{C: steam chamber} \quad \dot{T}_{sc} = \frac{\Delta \dot{S}_1 T_{sc}}{V_r C_{sc}} \quad (2-77h)^R$$

$$C_{sc} = \frac{\square \rho_{sc}}{\square T} HV_{sc} + \rho_{sc} \frac{\square HV_{sc}}{\square T} \quad (2-77i)^R$$

$$\text{INC:} \quad Q_{store}^v = \frac{V_r}{\rho_{sc}} \frac{\square \rho_{sc}}{\square T} \dot{T}_{sc} \quad (2-77j)^R$$

$$\text{RS:} \quad \dot{S}_{mr} = \frac{U_s A_s (T_{mr} - T_{sc})}{T_{sc}} \quad (2-77k)^R$$

$$\dot{S}_{x1} = \frac{U_s A_s (T_{mr} - T_{sc})^2}{T_{sc}^2} \quad (2-77l)^R$$

$$\text{C: reboiler tubes} \quad \dot{T}_{mr} = \frac{\Delta \dot{S}_2 T_{mr}}{U_{mr} C_{mr}} \quad (2-77m)^R$$

$$\text{RS:} \quad Q_R = U_{pmr} A_{pmr} (T_{mr} - T_N) \quad (2-77n)^R$$

$$\dot{S}_{x2} = U_{wm} A_w (T_{sc} - T_N)^2 / T_N^2 \quad (2-77o)^R$$

$$\text{HOV:} \quad \dot{S}_{hov} = \frac{Q_{Lin} \rho^L}{T_N} (H_V(T_N) - h_L(T_N)) \quad (2-77p)^R$$

$$\Delta Q = Q_{Lin} \rho^L \left(\frac{1}{\rho^V} - \frac{1}{\rho^L} \right) \quad (2-77q)^R$$

The elements to the rightmost 0-node are only partially shown. The assumption is that the entropy added to the liquid in the reboiler is added to the fluid in the base itself. The enthalpy balance equation for the base becomes a variation of equation (2-15):

$$\frac{dH_N^L}{dt} = \frac{L_{N-1} H_{N-1}^L}{\sum_{\forall i} u_{N-1i}} - \frac{L_N H_N^L}{\sum_{\forall i} u_{Ni}} + Q_R - \sum_{\forall i} v_{Ni} H_{Ni}^V \quad (2-78)^{GS}$$

The pipe under the base of the column also leads away from the system, through a pump and a valve. Just as in the accumulator, the pump and valve in series form an algebraic loop. Either the resistances can be joined or an inertial element may be added to the valve. With only one valve and no Y-junction

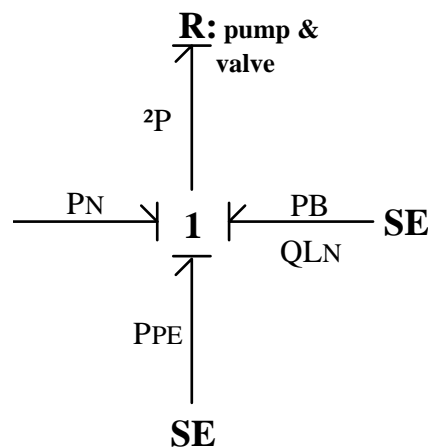


Figure 2.15. Hydraulic bond graph of the base of the column.

splitting the flows, the solution is more straightforward. The “resistance” of the pump and resistance of the valve can be joined directly, as shown in Figure 2.15. The two effort sources represent the constant pressure of the bottoms’ destination (PB), and the pressure drop associated with the height of the liquid in the base and in the pipe below the base.

2.9 Control system

Control of the distillation column can be effected by controlling the valves. Controlling the valves effects the heat transfer and mass flow, as seen in the previous bond graphs of the receiver, condenser, and reboiler. Flow, temperature, and level measurement devices translate measurements into an electrical current. The current is a signal that enters a PI controller. The control signal coming out controls the valve position. To be modeled are the measurement translation, the PI control, and the response of the valve to the control signal.

The k^{th} measurement translation is of the form

$$CI_k = CI_{\min} + B X_k \quad (2-79)^{\text{GSR}}$$

where the constants, CI_{\min} and B , are set to translate a range of measurements (X_k) to a range of current values (CI_k). The PI control consists of comparing the signal to a set point ($CISP_k$) at which the measured value is desired to reside, and outputting a control signal if the signals are not identical.

$$e_k = CI_k - CISP_k \quad (2-80a)^{\text{GSR}}$$

$$u_k = Kp_k e_k + Ki_k \int e_k dt + e_0 \quad (2-80b)^{\text{GSR}}$$

A control signal (u_k) generated by a proportional term and an integral term of the error signal (e_k) is PI control. The response of the valve is of mechanical inertia and damping. The position of the valve (ζ_k) is dependent on the control signal, the velocity of the valve position ($\dot{\zeta}_k$), and the time constant of the valve (τ_{UV_k}).

Error!

The bond graph of this control system, Figure 2.16, assumes that no power is transmitted between the control system and the distillation column. The measurement and position are considered isolated signals to and from the systems. A control system is a manipulation of signals, not of power flows. Thus, the bond graph of the control system, unlike the bond graphs of the physical system, does not enlighten.

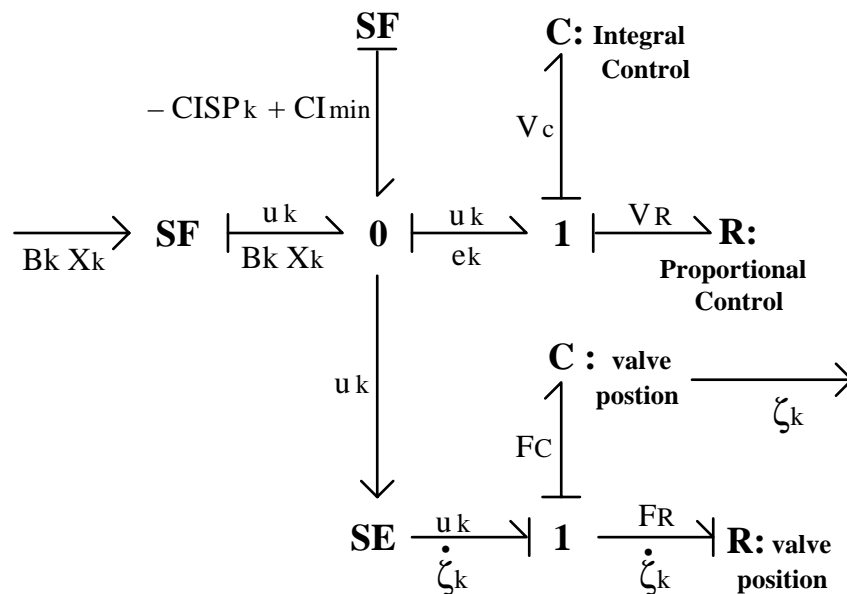


Figure 2.16. Bond graph of PI control of valves.

3.0 MODELING WITH BOND GRAPHS

Assembling the elements of a distillation column into a system is more than just placing the equations together. The elements of a distillation column interact dynamically. Bond graphs of the elements placed together will reveal important aspects of the system. The traditional equations presented in the last chapter were found to be deficient. Bond graphs point to a solution to this deficiency.

3.1 Bond graph representation of the model

Thus far, the elements presented have closely followed the traditional model of a distillation column. Bond graphs reveal the deficiencies that the traditional model hides. Putting together the bond graphs of the previous chapter and grouping them into hydraulic, chemical and thermal, three graphs can be created. They are not complete. What has not been modeled traditionally is the interface between the hydraulic, thermal, and chemical power at the point of liquid and vapor flow interaction. Heat is flowing from the liquid to the vapor in the form of heat of vaporization; heat is being convected along with the fluid and phase flows; heat is being conducted back from the hotter vapor (usually the hotter phase) to the cooler liquid. Chemical potential differences (not pressure differences) are driving phase flow. Volume flow is being driven by pressure and gravity, but is influenced by the source and sink of volumes being generated and shrunk by the phase flow.

The traditional models of hydraulic, vapor-liquid equilibrium and enthalpy balance do not need to present the nature of this interface. Using

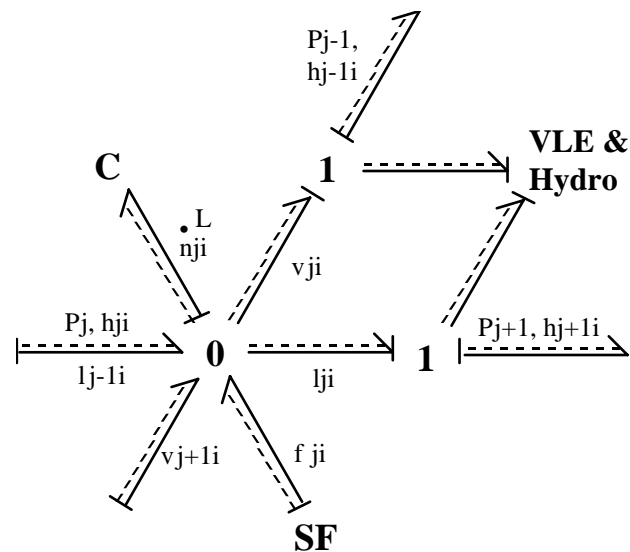


Figure 3.1. Convection bond graph of distillation stage.

equation (2-4) for mass-balance (with its assumption of negligible vapor holdup), the phase flow need never be considered. The energy balance may then be estimated by examining the assumed equilibrium results of phase flow. The hydraulic equations need only be concerned with fluid flow beyond the phase interaction.

The most concise bond graph representation of this traditional model is using the convection bonds of Brown [53]. Figure 3.1 shows such a bond graph. The convection bond combines the forms of power as one bond being driven by molar flow. Entropy, temperature and chemical potential are combined into intensive enthalpy. The VLE & Hydro element is a concise representation of the possible models these equations may use. Depending on the precise model, this element might be best represented by separate elements for the liquid and the vapor flow. The Hydro portion of this element represents the hydraulic flow apart from the vapor-liquid exchange. It could represent flow sources (constant flow) or the entire scope of elements found in Section 2.3 (Figures 3.2 and 3.3

below) that attach to the 1-node for vapor and liquid flow. The VLE portion represents the equations used to determine the vapor molar fractions.

Pseudo-bonds provide another possibility for representing the traditional model, but they will not be considered [54, 55]. The problem with these variants on bond graphs is that they side-step the fundamental strength of bond graphs—revealing power flow and relationships that form a cohesive and rigorous model of a system. These variants do point out the weakness of this fundamental strength; equations and relationships that form a rigorous model may not exist and so can not be bond graphed.

3.1.1 Hydraulic

The hydraulic power equations of liquid and vapor flow show the power flow from one tray to the next. Figures 3.2 and 3.3 are the bond graphs from Section 2.3 that describe these equations.

By themselves, these bond graphs are not complete. A complete hydraulic bond graph for the stage must be able to be replicated and connected together. By the form of these graphs, a 0-node must be added to each in which

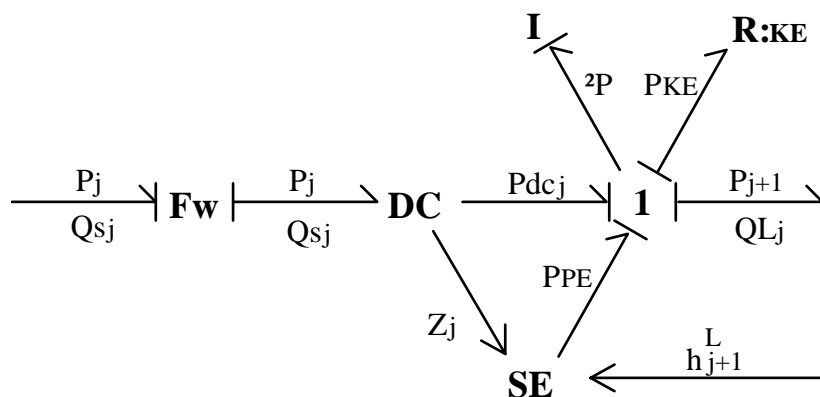


Figure 3.2. Bond graph of liquid hydraulics.

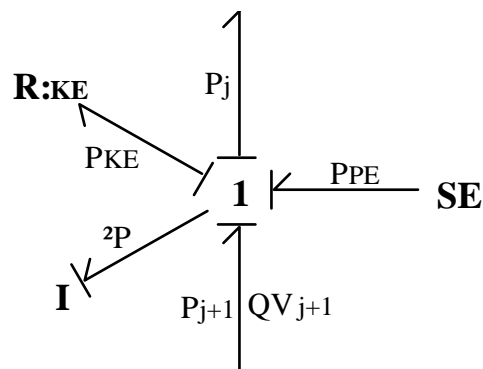


Figure 3.3. Bond graph of vapor hydraulics

the pressure and the liquid tray volume are calculated. From what is known to be happening on the tray, the drastic density transformation of phase change should also be included.

Figure 3.4 shows a possible bond graph configuration that attempts to meet this criteria. The assumption here is that the pressures of liquid and vapor are identical. The HOV element, just as in Section 2.8, attempts to explain the difference in liquid and vapor volume flow. The volume flow is dependent on molar density and

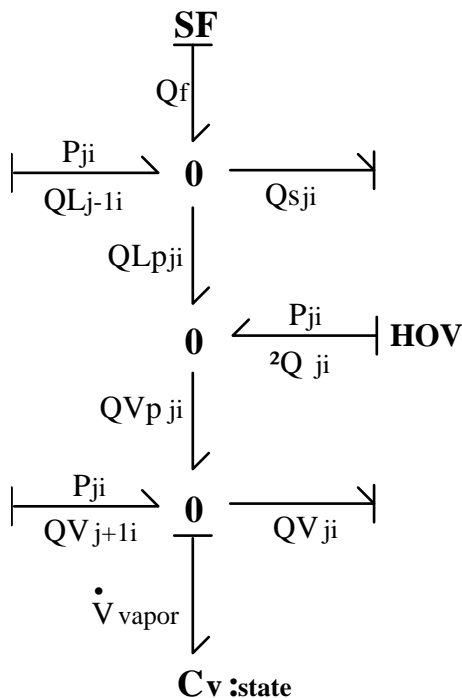


Figure 3.4. Expanded completion to hydraulic bond graph.

molar flow:

$$QLp_{ji} = \frac{LV_{ji}}{\bar{\rho}_j^L} \quad (3-1a)^R$$

$$QVp_{ji} = \frac{LV_{ji}}{\bar{\rho}_j^V} \quad (3-1b)^R$$

$$\Delta Q_{ji} = LV_{ji} \left(\frac{1}{\bar{\rho}_j^V} - \frac{1}{\bar{\rho}_j^L} \right) \quad (3-1c)^R$$

$$= LV_{ji} \left(\frac{RT_j}{P_j} - \frac{1}{\bar{\rho}_j^L} \right) \quad (\text{ideal gas})$$

The HOV element does not relate pressure to volume flow, unless a state equation is used for molar density. Figure 3.4 assumes pressure is calculated with the state equation: the C_v element is the manifestation of a state equation for vapor; see Table 2.3. Power flows out of the HOV element when the flow is from vapor to liquid and into the HOV element when the flow is from liquid to vapor.

Using the traditional method of determining molar flow requires using fugacity. Fugacity can be assumed to be partial pressure, and so fall under the auspices of hydraulics. Fugacity and volume flow may be conjugate variables, but it is certainly not clear whether they form hydraulic power or can be transformed (using a fugacity coefficient) to be joined to the rest of the hydraulic bond graphs. Although it is reasonable to say that chemical potential differences are driving molar flows between phases, fugacity differences will be assumed to be driving volume flow. Efficiencies are essentially the inclusion of a molar flow

resistance. Figure 3.5 shows this additional resistance in which the vapor volume flow is calculated. The exact nature of this resistance as a relation between fugacity and volume flow (or even molar flow) is unknown. The Fug element is used to calculate liquid fugacity; the actual calculation does not express any relation between fugacity and volume flow and so does not represent any real power flow. If the Peng-Robinson equation of state is used, then the Fug element would be changed to a Cv element. The fugacities are not identical to partial pressures and the Cv element would need to be changed to adjust to a change in calculation.

Resistance alone may not be sufficient to describe dynamic vapor-liquid

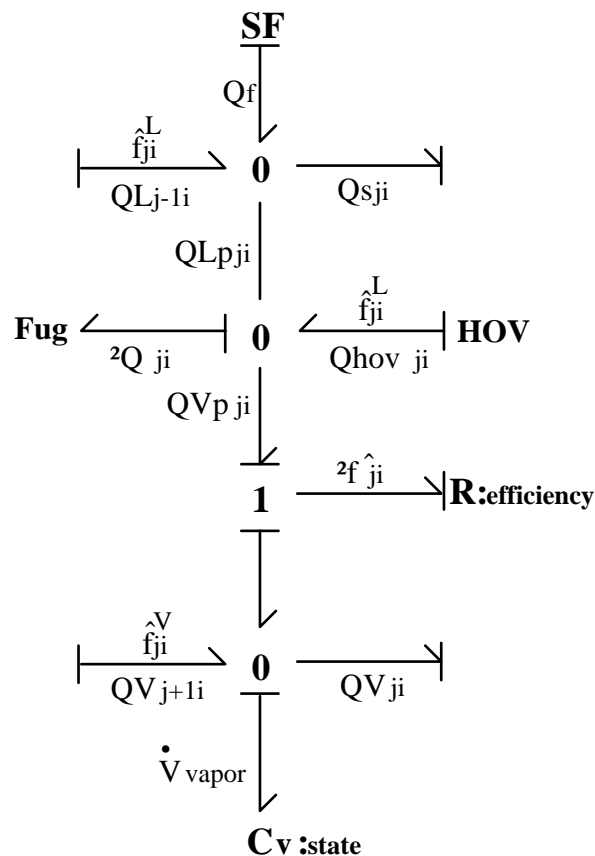


Figure 3.5. Fugacity driven phase flow of traditional model.

flow. Instead, a form for dynamic equations can be assumed. The flow could be modeled as a capacitive and a resistive element sharing a common molar flow:

$$\frac{d\hat{f}_i^C}{dt} = \frac{QVp_{ji}}{C}$$

$$QVp_{ji} = \frac{\hat{f}_i^C - \hat{f}_i^L + \hat{f}_i^V}{R}$$

except, the steady-state flow is now forced to be zero. Although this would allow true chemical power to be used (Figure 2.7), this must be incorrect.

The flow could be instead modeled as an inductive and a resistive element:

$$\frac{dQVp_{ji}}{dt} = \frac{\hat{f}_i^L - \hat{f}_i^V - \hat{f}_i^R}{L}$$

$$\hat{f}_i^R = QVp_{ji} R$$

The transformation to chemical potential is not clear in this case. If fugacity is considered as a variation on chemical potential (as it often is in the literature), then the big assumption of this form is the existence of chemical potential momentum. There is no theoretical basis for chemical potential momentum. If fugacity is considered a variation on partial pressure (as this section has done), then the assumption of this form is of pressure momentum (mass * velocity / area). Conceptually, the nature of the velocity or area of the volume flow between the phases is not clear at all. Essentially, this is the problem of phase changes being driven by partial pressures. This form allows for the elimination of a critical algebraic loop while preserving the extensive collection of thermodynamic data contained in fugacity calculations that is already known.

However, the existence of and finding the values of inductance is quite vague. Obviously, using just the resistance makes sense.

The two forms of Figures 3.4 and 3.5 could be used to complete the hydraulic bond graph. The problem with Figure 3.5, is the uncertain nature of hydraulic resistance and its relation to efficiency. Figure 3.6 shows a bond graph of the complete hydraulic system assuming that chemical potential is used.

Note that there is a slight discrepancy between Figure 3.4 and Figure 3.6. When dealing with the hydraulic flow of the fluids, it is convenient to combine all the components and deal with total volume flow. At the point of molar phase flow (or in a chemical reaction), it is necessary to deal with flows on a component by component basis, as implied by Figure 3.4. The assumption of

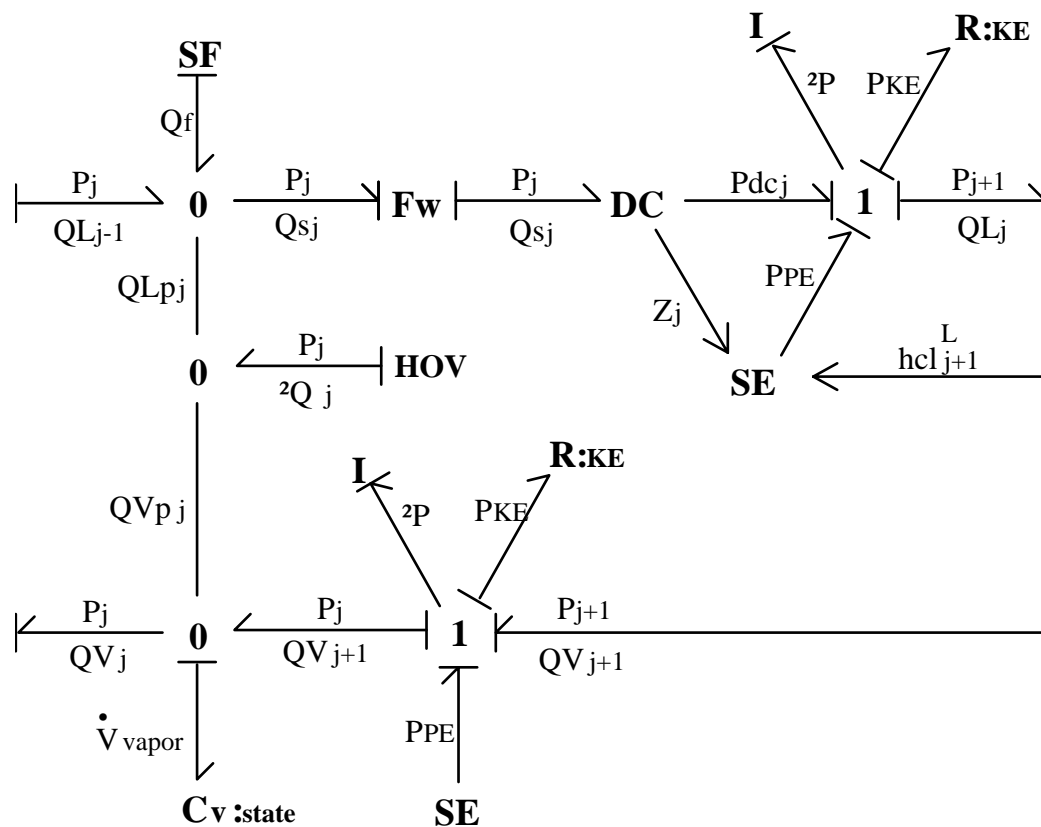


Figure 3.6. Hydraulic bond graph of distillation stage.

Figure 3.6 is that the volume flows computed at each component's HOV element can be simply added together to form the total volume flow. Unless the ideal equation of state is used, it is also important to keep track of the molar fractions to compute pressure (C element) properly.

Also note that the I elements are not necessary to eliminate an algebraic loop. The assumption here is that the equation of state is used to solve for pressure (the C element), the vapor molar density is found by a knowledge of the vapor's volume and molar holdup, and Z_j is found using the DC element. Otherwise, the elimination of the DC, C, and I elements (i.e., the use of the equation of state for molar density in a traditional model) does involve the hydraulic system in an algebraic loop.

3.1.2 Thermal

The traditional thermal and chemical equations for the distillation tray are subsumed into the enthalpy equations. The thermal and chemical power flow is assumed to be entirely dependent on convection outside of the vapor-liquid interaction. Equilibrium conditions justify the use of approximations for the enthalpy of the components.

There are three means of entropy flow between the phases. First, the hotter phase (usually the vapor) conducts entropy to the cooler phase. Second, entropy is convected with the molar flow between the phases. Convection is not necessarily taking place in the same direction as conduction. Third, chemical power and hydraulic power are combining to form the heat of vaporization into or out of thermal power. Thermal power flow can be modeled. Figure 3.7 shows a bond graph of entropy flow. Conduction is assumed to contribute very little heat flow and is not modeled.

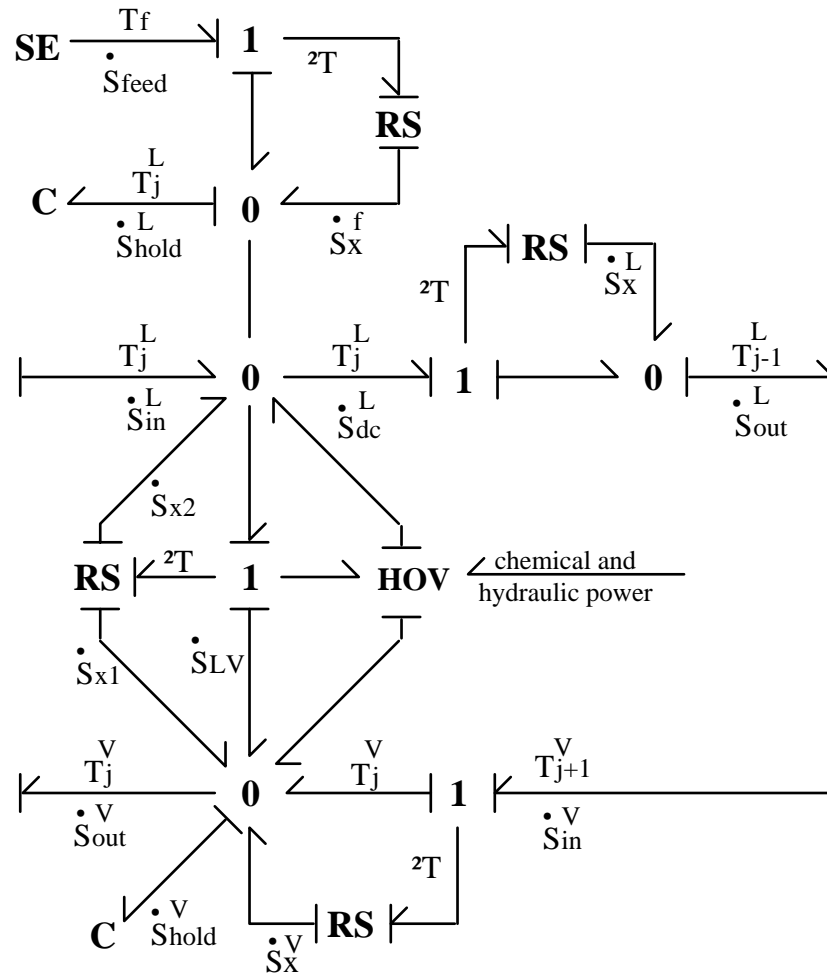


Figure 3.7. Bond graph of thermal power flow.

The C elements represent holdups of enthalpy in the liquid and the vapor. The RS elements are modulated by volume or molar flow: they show convection as the principle means of thermal power flow [5]. The exact equations for these elements relate thermal resistance (R), specific thermal capacitance (c), volume flow (q), and molar density ($\bar{\rho}$) :

$$\text{C element:} \quad \dot{T}_j = \frac{1}{C} \dot{S}_{hold} = \left(\frac{T_j}{c \bar{\rho}} \right) \dot{S}_{hold} \quad (3-2a)^R$$

$$\text{RS element: } \dot{S}_{dc}^L = \frac{1}{R} \Delta T = \left(\frac{C q}{V} \right) \Delta T = \frac{c q \bar{\rho}}{T_{j-1}^L} \Delta T \quad (3-2b)^R$$

$$\dot{S}_x^L = \frac{\dot{S}_{dc}^L \Delta T}{T_{j-1}^L} = \frac{c q \bar{\rho} (\Delta T)^2}{T_{j-1}^L{}^2} \quad (3-2c)^R$$

Equations (3-2b) and (3-2c) refer to the top right RS element. The volume flow in this case is QL_{j-1} . Molar density is used, assuming compatible units for the specific thermal capacitance. The other convection RS elements have similar equations except the one associated with the molar flow. Instead of being modulated by volume flow, molar flow should be used:

$$\dot{S}_{LV} = \frac{1}{R} \Delta T = \left(\frac{C LV_{ji}}{n_{ji}^{LV}} \right) \Delta T = \frac{c LV_{ji}}{T_j^*} \Delta T \quad (3-3a)^R$$

$$T_j^* = \begin{cases} T_j^V & , LV_{ji} > 0 \\ T_j^L & , LV_{ji} < 0 \end{cases} \quad (3-3b)^R$$

$$\dot{S}_{x1} = \text{Error!} \quad (3-3c)^R$$

$$\dot{S}_{x2} = \text{Error!} \quad (3-3d)^R$$

Note that the entropy flows only in the direction of the molar flow.

The exchange of power flow due to heat of vaporization is not as well defined. The model for heat of vaporization assumes a totally reversible process at equilibrium conditions: the liquid and the vapor temperatures are identical and non-varying. Replacing the central 1-node with a 0-node in Figure 3.7 would solve this problem, making the liquid and the vapor temperatures identical, except that the thermal capacities of the liquid and the vapor phases of a substance are not the same. Also, the distillation liquid and vapor might leave

the stage with almost the same temperature, after interacting, but certainly the temperatures are different as they flow through each other. The form of the known model can be described by the following equations.

$$\begin{aligned} \text{Heat} &= n L^h = S T \\ L^h &= a + b T && \text{(empirical estimate)} \\ \frac{d\text{Heat}}{dt} &= \frac{dS}{dt} T = \frac{dn}{dt} (a + b T) && (3-4) \end{aligned}$$

The heat flow is assumed into or out of the entire system. In a distillation stage, the heat flow would presumably be into the vapor. The model is not adaptable to two temperatures. Constant temperature would require the addition of separate temperature regions between vapors and between liquids. The exact nature of the relation between heat of vaporization, hydraulic power, and chemical power is not defined. Thermal and hydraulic power flows from the liquid to the HOV element and then towards the vapor (as thermal power) when the molar flow is from liquid to vapor. Whether the power flow from the liquid is partially thermal (conductive) or entirely chemical is unknown. Power flows from the vapor (as thermal power) into the HOV element and then towards the liquid (as chemical and hydraulic power) when the molar flow is from vapor to liquid. Whether thermal (conductive) power flows to the vapor is unknown.

3.1.3 Chemical

The theoretical inadequacies of the vapor-liquid equilibrium equations have been addressed in the last chapter; they are based on pressure differences rather than chemical potential differences. The only concession to non-equilibrium conditions are efficiencies. Although efficiencies are essentially the inclusion of a molar flow resistance, they do not relate molar flow to chemical potential differences. The true resistance of flow is undoubtedly related to the heat of vaporization as well as the power flow associated with the hydraulic nature of the density transformation.

Assume a fixed-volume closed system of liquid and vapor. The chemical

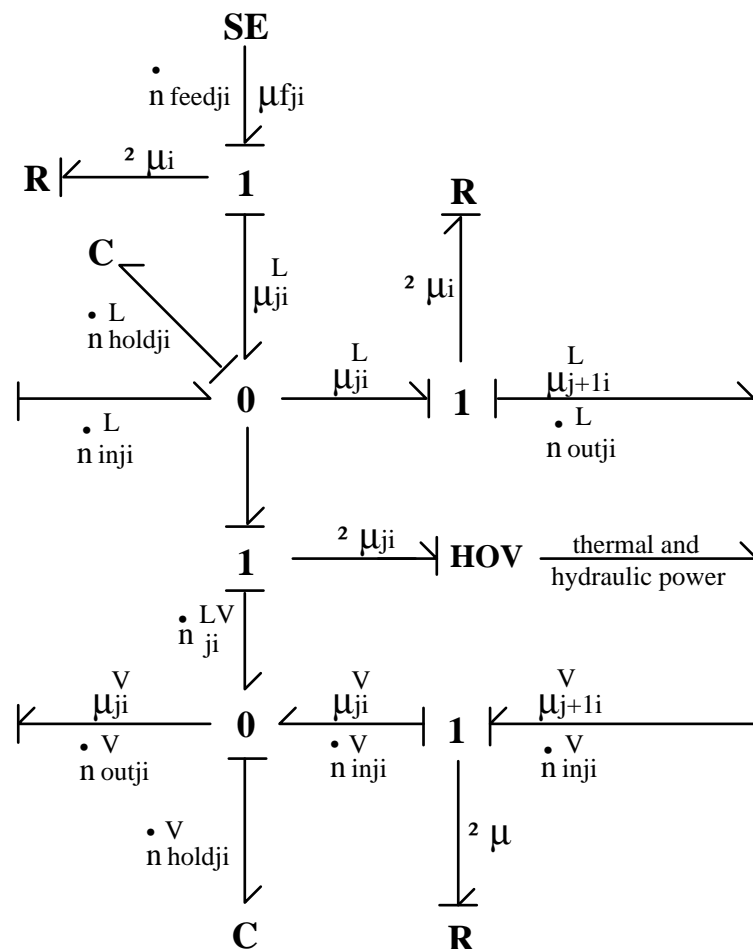


Figure 3.8. Chemical bond graph of distillation stage.

potential of the liquid is higher, so liquid evaporates. The pressure of the system increases. In a traditional view of the system, the vapor pressure is higher than the system pressure and liquid changes to vapor until the two pressures are equal. Entropy flows into vapor as heat of vaporization as well as in convection. The hydraulic power and thermal power can be expressed in terms of the molar flow, but without an explicit relation to chemical potential, entropy flow or pressure, the exact power exchange is unknown.

In terms of creating a theoretically appealing bond graph, molar flow would be driven by chemical potential differences in phase flow and volume flow elsewhere. Figure 3.8 shows a theoretical bond graph of chemical power flow in a distillation column stage. The R elements are expressions of convection and so are modulated by volume flow.

$$\text{R:} \quad \dot{n} = \frac{C_n q}{V} \Delta\mu$$

The form of the R elements is similar to the RS elements of the thermal bond graph, Figure 3.7, except there is no chemical analog to specific thermal capacitance. A better expression for the R element involves molar density:

$$\text{R:} \quad \dot{n} = \bar{\rho}_j q \quad (3-5)^R$$

The C elements are of the form developed in Table 2.4. Equation (3-6) assumes an ideal gas as well as the assumptions of Table 2.4, constant density and temperature.

$$\text{C:} \quad \dot{\mu} = \frac{1}{C_n} \dot{n}_{\text{hold}} = \left(\frac{RT}{n} \right) \dot{n}_{\text{hold}} \quad (3-6)^R$$

Unfortunately, these assumptions are violated by the thermal and the hydraulic C elements, and so equation (3-6) is not necessarily meaningful. The HOV element is an expression of molar flow movement generated by the difference in chemical potential. Its nature is explored in the next section.

3.1.4 Combining hydraulic, thermal, and chemical

The hydraulic, thermal, and chemical systems of a distillation stage are linked. The capacitors of all three bond graphs (Figures 3-6, 3-7, and 3-8) are linked. The hydraulic, thermal, and chemical power of the liquid and the vapor is stored as internal energy. The equations become equations (3-7):

$$\dot{U}_{ji}^L = \dot{S}_{ji}^L T_{ji}^L - \dot{V}_{ji}^L P_{ji}^L + \dot{n}_{\text{hold } ji}^L \mu_{ji}^L \quad (3-7a)$$

$$\dot{U}_{ji}^V = \dot{S}_{ji}^V T_{ji}^V - \dot{V}_{ji}^V P_{ji}^V + \dot{n}_{\text{hold } ji}^V \mu_{ji}^V \quad (3-7b)$$

Hence, the capacitors are special types of the U_i element shown in Figure 2.2. Unfortunately, internal energy on each stage is not held constant except at steady-state and these equations do not add any required information.

The HOV elements of all three bond graphs (Figures 3.6, 3.7, and 3.8) are linked. From the form of the power going in, it is tempting to use the same equation for HOV element as the C element above; unfortunately this does not make sense, as there is no substance to store energy. Also, the flows (through variables) of each input are required to be determined from the HOV element. The form of the HOV element is similar to the E_0 element of Figure 2.2. The link to the hydraulic and the thermal HOV elements requires that the molar flow be determined from chemical potential differences. Assuming no holdup of energy

within the HOV element, then the chemical power should be as large as the sum of thermal and hydraulic power, equation (3-8).

$$LV_{ji} = \frac{\dot{S} \Delta T + P_{Qhov_{ji}}}{\Delta \mu_{ji}} \quad (3-8)$$

The problems with this equation are that the thermal power is not well defined and that both the thermal power and the hydraulic power are dependent on LV_{ji} . This equation will not work here. The exact relationship between molar flow and chemical potential, although not known, can be hypothesized as a resistance, similar to the hydraulic resistance based on efficiencies:

$$LV_{ji} = \frac{\Delta \mu_{ji}}{R} \quad (3-9)^R$$

Unfortunately, the problem with efficiencies arises again; the value of this chemical resistor is not known.

The third link between the systems is the thermal loss. Each of the resistances in the hydraulic and the chemical bond represents power lost to heat. For each R element in the hydraulic and chemical bond graphs, there exists an RS element in the thermal bond graph into which the power flows; the power is not lost. Equation (3-2c) specifies the introduction of this thermal power, and assumes the chemical power and the hydraulic power loss to be negligible. This equation, and all of the equations associated with RS elements, can be modified to include this power.

$$\dot{S}_x^L = \frac{\dot{S}_{dc}^L \Delta T + \dot{n}_{out}^L \Delta \mu + Q_{L_j} P_{KE}}{T_{j-1}}$$

$$= \frac{c Q_{L_j} \bar{\rho} (\Delta T)^2}{T_{j-1}^{L^2}} + \frac{Q_{L_j} \bar{\rho} (\Delta \mu)^2}{R T_{j-1}^{L^2}} + \frac{\rho Q_{L_j}^3}{2 A U D_j^2 T_{j-1}^L} (3-2c_{\text{mod}})^R$$

Thus, the joining together of the three systems into one bond graph can be achieved by picturing only one HOV element, two C elements, and a limited number of 0-nodes and 1-nodes. Figure 3.9 shows a distillation stage as a bond graph. Note the extra 0-nodes; these are added for clarity and collapse with other 0-nodes. The C, HOV, and RS elements represent links between the three power bonds. The 0 and 1-nodes of Figure 3.9 do not link the three types of power bonds, but link all the hydraulic bonds together, the thermal bonds together, and the chemical bonds together.

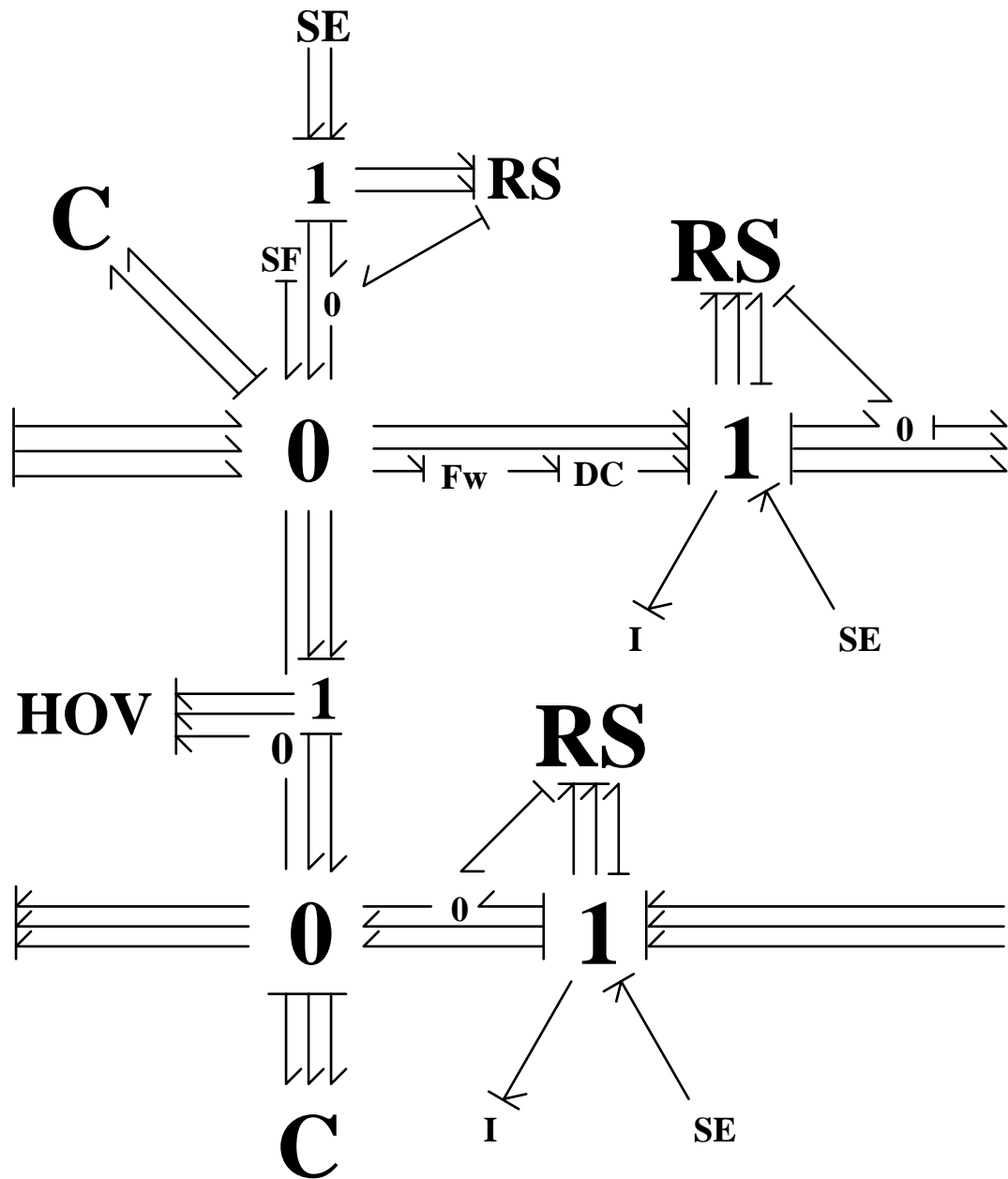


Figure 3.9. Bond graph of distillation stage.

3.2 Hierarchical bond graph representation

A full representation of a distillation column by bond graphs is as daunting as the full representation by the system equations. The components of a distillation tray are separable into three sections for the three areas of fluid flow: the liquid off the tray, the vapor off the tray, and the fluid flow on the tray. Each of these components can be broken down into their hydraulic, thermal, and chemical aspects. Each of these aspects can be broken down into graphs for each chemical component. Section 3.1 details the bond graphs associated with each of these aspects. The complete bond graph, Figure 3.9, obscures the possible differences that may arise with changing columns: various equations of state, fugacity approximations, tray types, or downcomer arrangements. Grouping bond graphs together into one element allows hierarchical bond graphing, reducing the size and increasing intuitive understanding of how the system works.

Figures 3.10, 3.11, and 3.12 show three hierarchical elements that are created by grouping elements and bonds from Figure 3.9. The benefit of this

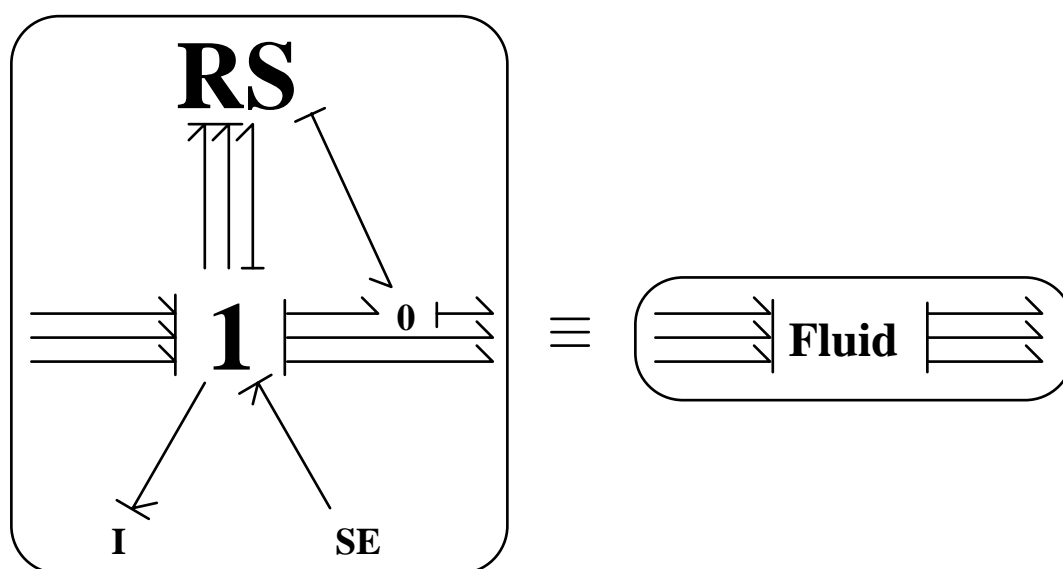


Figure 3.10. Bond graph of fluid flow represented by the Fluid element.

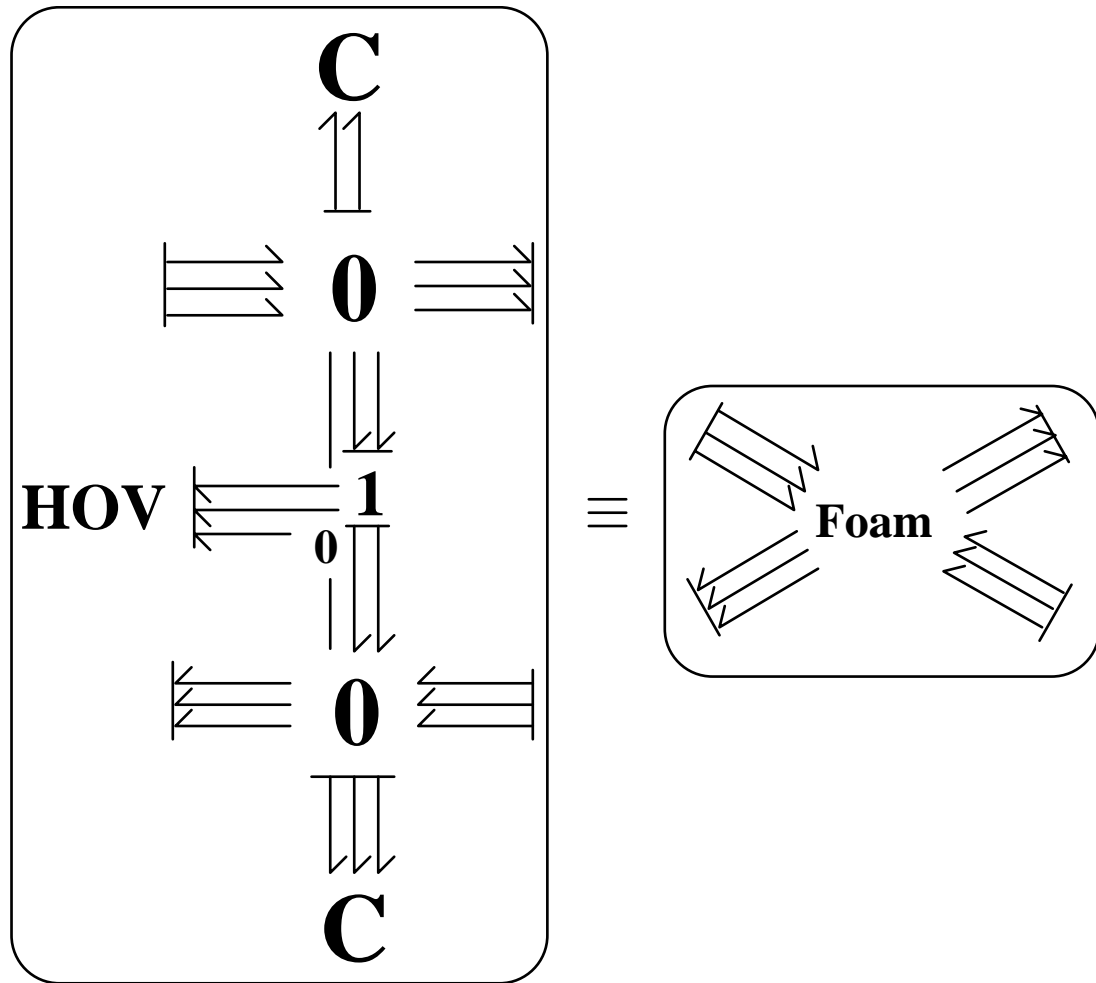


Figure 3.11. Tray bond graph represented by the Foam element.

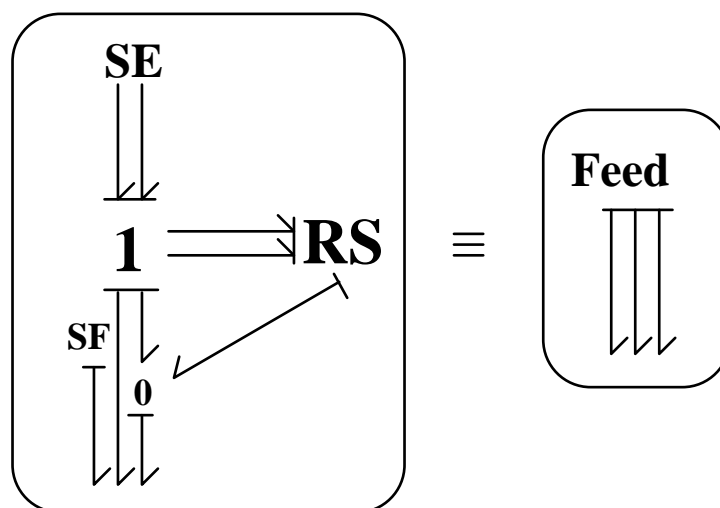


Figure 3.12. Bond graph associated with the feed represented by Feed element.

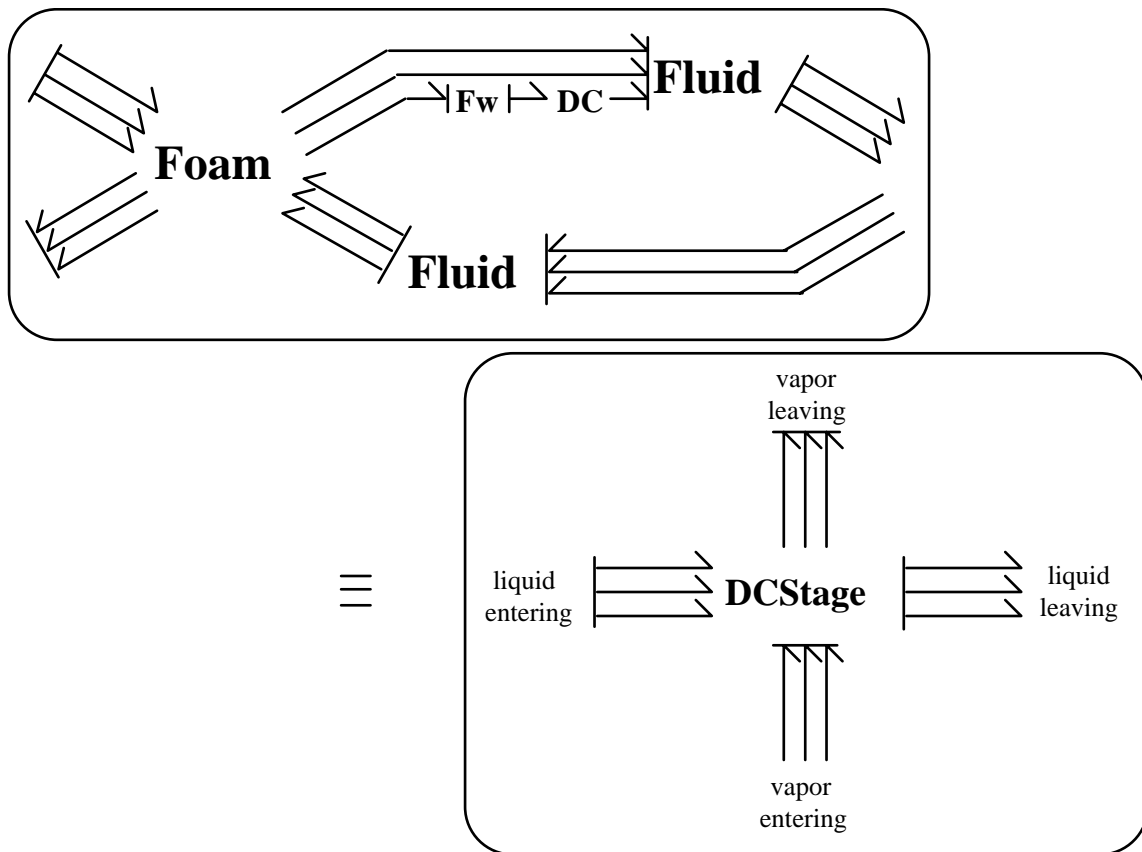


Figure 3.13. Distillation stage bond graph represented by the DCStage element.

type of representation is that the new elements can be reformed into a new representation of a distillation stage, Figure 3.13. The Feed element is not used until Figure 3.17, but could have easily been included into the DCStage element. In Figure 3.14, the Reboiler element is a representation of the bond graph of Figure 2.14. Unlike the reboiler, the influence of the condenser in Figure 3.15 is in more than just the transfer of thermal power. The Condenser element is a representation of the bond graph of Figure 2.8. The Pump & Valve(s) elements are representations of the pump and the valve arrangements of Figures 2.12 and 2.15. Figure 3.17 brings together every element. Because every connection of bonds is the triple bond of thermal, chemical, and hydraulic, the hierarchical bond of Figure 3.15 is used to connect

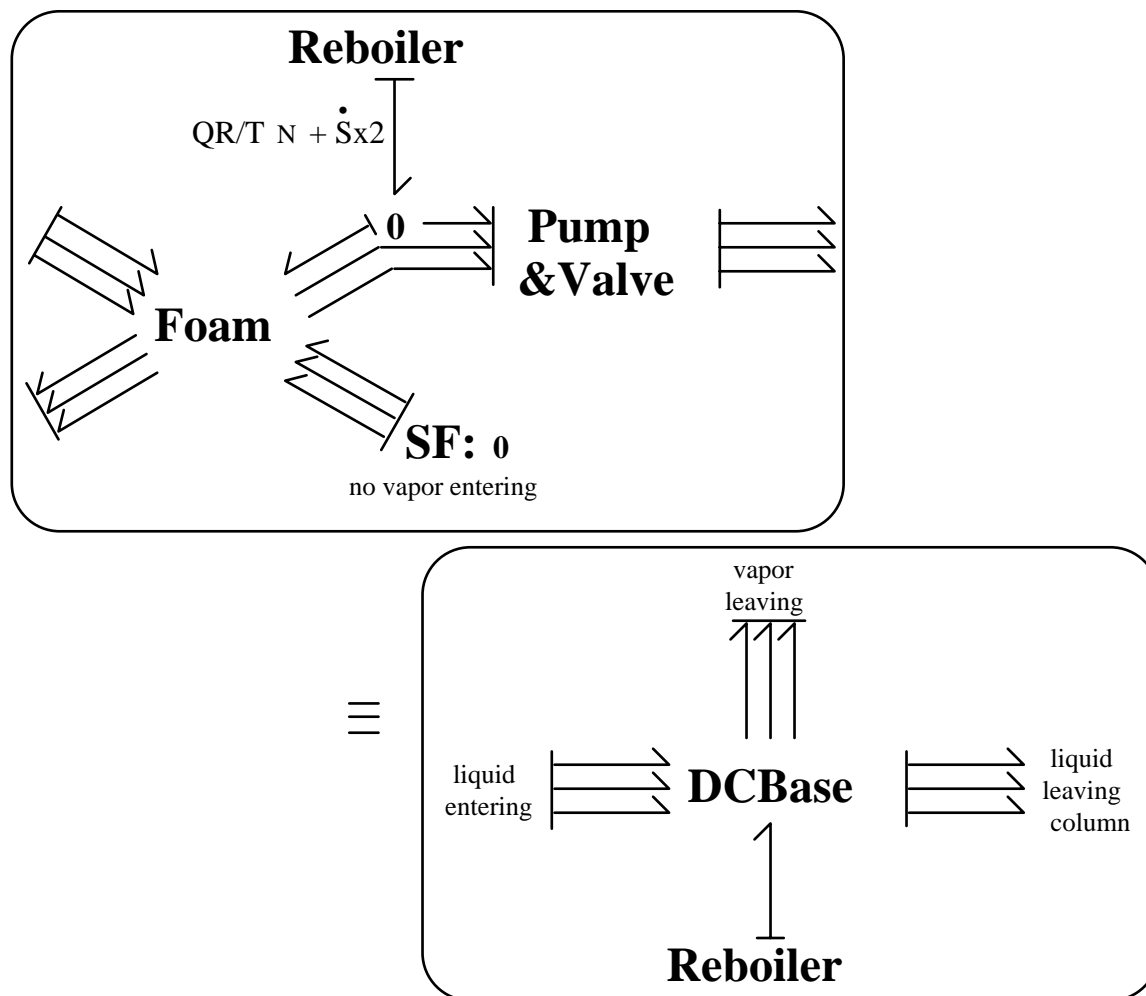


Figure 3.14. Base and reboiler of Figures 2.14 and 2.15 represented by a DCBase element.

the elements. Notice the similarity of Figure 3.17 and that of the drawing of a distillation column, Figure 1.2.

Each element is not necessarily uniquely defined as shown in the previous figures. The hydraulic aspect of a vapor flow, for instance is dependent on the distillation tray used. The I element used in Figure 3.10 and defined by equation (2-28a), applies to downcomers and sieve plates. Other types of downcomers or plates may not require such an element or may require a different definition. Although the internal structure of these elements may

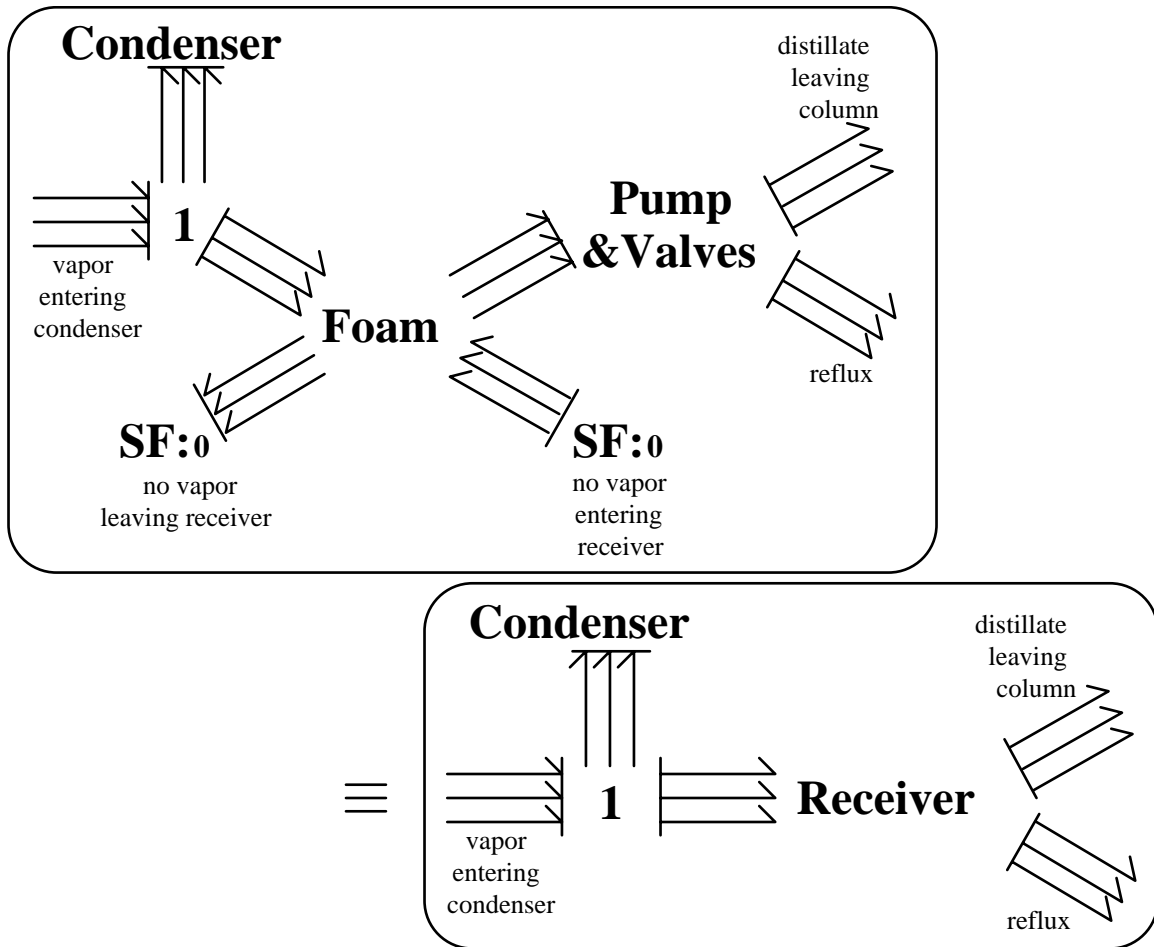


Figure 3.15. Condenser and accumulator of Figures 2.9, 2.12, and 2.13.

differ, the bonds coming out of these elements, if used, are well defined and should not be changed.

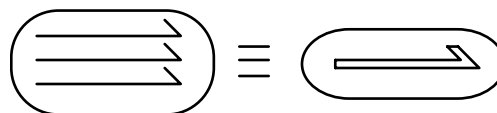


Figure 3.16. Hierarchical bond.

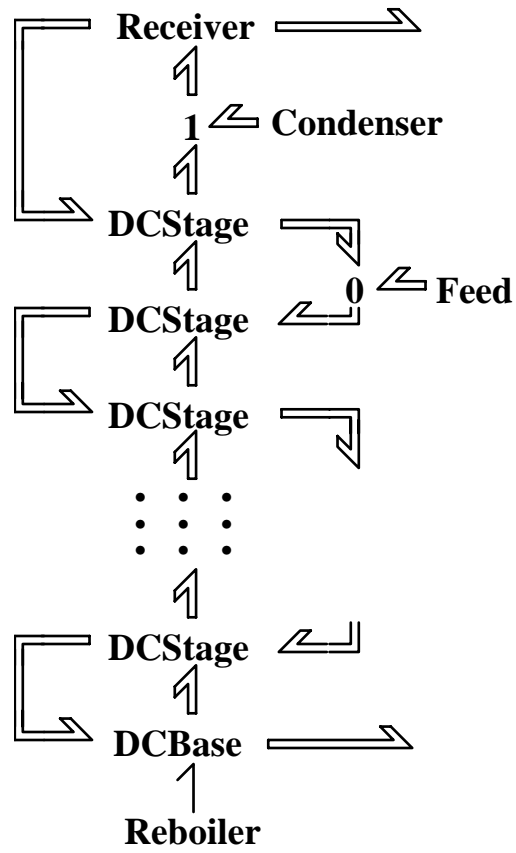


Figure 3.17. Hierarchical bond graph of a distillation column.

4.0 THE DISTILLATION COLUMN AS A SYSTEM

Models for distillation columns range from the simple to the complex. Simple models provide the benefits of easy implementation, short run time, and the possibility of design. Unfortunately, they also tend to be highly inaccurate in their predictions of dynamic behavior (e.g. the start-up period of a column or batch distillation where the contents of the feed changes). Many simple models do not contain any differential equations, and are not solved using simulation. Complex models have the benefits of being more accurate in their dynamics, and thus more reliable in their predictions. Unfortunately, they are harder to implement, take longer to complete a simulation run, are typically proprietary, and contain so many component-dependent details that the full model is seldom published. Complex models, taken as a system of equations, also can contain algebraic loops that limit their usefulness. This chapter examines the historical forms of the system of distillation equations. A specific example is also considered and simulated.

4.1 The early models

The earliest model used in a systematic attempt to design distillation columns was graphical. The McCabe-Thiele method uses a graph of the equilibrium relationship of the component to be distilled, equation (2-48), to determine the number of stages required and the proper reflux ratio [4]. The assumptions of this model are enormous. The method is for designing columns to separate binary mixtures with one feed and a simple equilibrium relationship.

Models for computer simulation purposes arose in the early 1960's [14, 15]. The models concentrated on material-balance including simple equilibrium equations. Meadows included enthalpy-balance equations [15]. Mah, *et al.* admitted that the basic assumptions of distillation models were unrealistic because of a lack of physical knowledge [14], hence the omission of enthalpy-balance was seen as no great loss. Distefano introduced liquid and vapor flow equations based on the mass-balance equations using the assumption of constant liquid volume on each stage [16]. This model is still mentioned as being a rigorous dynamic model by some [56]. Luyben presents the best aspects of these models which serves as the basis for many models, using the assumption of negligible vapor holdup, and obtaining the equations for mass-balance, energy-balance, and dynamic equilibrium [57]. This base model is essentially equations (2-4), (2-15), and (2-48). These three equations form many distillation models [58, 59, 60, 61]. Hydraulic equations are omitted from these models, but Van Winkle [1] and Lockett [2] have presented many empirical and theoretical equations for fluid flow in a distillation column. Gani, *et al.* detail the modern version of this model, including algebraic hydraulic equations and correlations for column problems such as weeping [23]. Simulation of this model requires the iteration of pressure and temperature.

Distillation is considered a mature field within chemical engineering, much has been written on the subject, other models exist. Levy, *et al.* present a model that does not fit the base Luyben model [19]. The model includes an algebraic hydraulic equation for vapor flow, as well as an energy-balance equation using heat capacities and heat of vaporizations, which can be solved for temperature. A search of the literature failed to find this model being used

elsewhere. There are 'rigorous' simulation models that contain only algebraic equations [62, 63]; there are models that attempt to reduce the number of equations by grouping real distillation stages into fewer theoretical stages [64, 65]; there are models that emphasize the possibilities of controlling the distillation process [66, 67, 68]. Today, many chemical system software packages have the ability to design and/or simulate distillation columns [18, 68]. Unfortunately, the systems of equations used are most often proprietary, and so can not be examined. For an extensive list of current distillation models and distillation topics, see [69, 70].

The methods of simulating these models are various: backwards Euler, Newton-Raphson, semi-implicit Runge-Kutta, Adams-Moulton (used in conjunction with other methods), backwards-difference formulas, Gear's method. No purely explicit method can be used because of the algebraic loops that the distillation column models contain [71, 72]. All of the models that consider pressure a variable contain algebraic loops, also known as zero-order causal paths or an index of nilpotency of one [73]. The best numeric method to simulate such systems is Gear's method [74]. A second problem encountered is that chemical systems are typically stiff, the largest eigenvalues of the system are much larger than the smallest eigenvalues. Stiff systems are not simulated well using explicit techniques. Lagar, *et. al.* showed that the stiffness ratio for distillation columns could be as high as one thousand [22]. Gear's method, in particular, simulates stiff systems well, making Gear's method of integration the preferred method in simulating chemical systems.

4.2 The Gallun model

The Gallun model is a complex model of a distillation column, based on the Luyben model, developed by Steven Gallun and published in his dissertation [24]. Not only are equations presented with details, but he compliments this with details of his simulation technique and run. Although the model is detailed, the equations presented are not complete. The complete model, however, can be derived from later publications of his model [27, 28].

The Gallun model describes a 50 stage distillation column with complete condenser, receiver, and reboiler that separates ethanol from a mixture of ethanol, methanol, acetone, and water. There are three feeds and five control valves that control the flow of various fluids. See Figure 4.1 for a diagram of this column. Gallun assumes constant holdup of mass and energy in the vapor stage of a model, allowing for mass and energy balance equations.

The hydraulic equations are derived from the Bernoulli equation for sieve plates and downcomer, equations (2-32), (2-35), and (2-41). The first of these equations is used to solve for liquid flow into the downcomer. Equation (2-35) instead of equation (2-29) is used to solve for the height of the liquid in the downcomer. The flow into and out of the downcomer is assumed identical, even though the volume of the liquid is assumed to vary. The virial equation of state is used to solve for molar density and the compressibility factor (used to calculate fugacity). Pressure is solved for using the Bernoulli equation for vapor flow, equation (2-41). The vapor flow is calculated using the fugacity equations (vapor-liquid equilibrium equations).

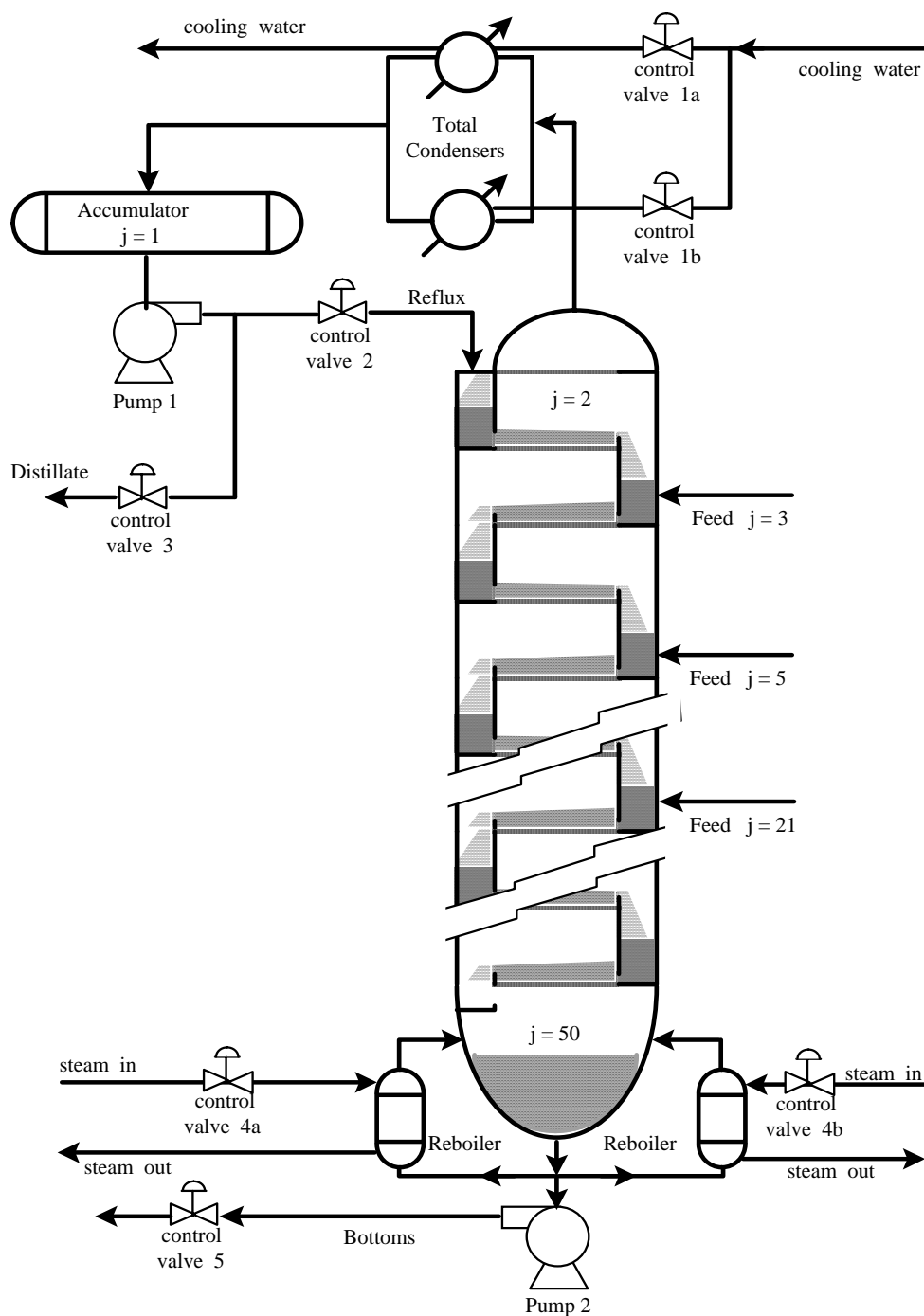


Figure 4.1. The Gallun distillation column.

The vapor-liquid equilibrium equations are listed in equations (2-52) through (2-59). Gallun avoids the over-determined system of these equations by never solving for y_{ji} (except in stage one) . Instead, one modification is done to equation (2-52) for stages 2 through 50:

$$y_{ji} = \frac{v_{ji}}{\sum_{\forall i} v_{ji}} \quad (4-1)^G$$

$$v_{ji} = \frac{\gamma_{ji}^L K_{ji}^I \Phi_{ji}^L}{\hat{\Phi}_{ji}^V} x_{ji} \sum_{\forall i} v_{ji} \quad (4-2)^G$$

The new variable, v_{ji} , is the molar flow rate for component i leaving stage j as a vapor. The sum of all v_{ji} is the total vapor molar flow rate leaving the stage, V_j , and equation (4-1) is certainly valid. These new equations pose a problem besides introducing a new series of algebraic loops (pressure depends on vapor flows depends on fugacities depends on pressure). In this model, there are four components; equation (4-1) can be expanded thus:

$$\begin{bmatrix} y_{j1} - 1 & y_{j1} & y_{j1} & y_{j1} \\ y_{j2} & y_{j2} - 1 & y_{j2} & y_{j2} \\ y_{j3} & y_{j3} & y_{j3} - 1 & y_{j3} \\ y_{j4} & y_{j4} & y_{j4} & y_{j4} - 1 \end{bmatrix} \begin{bmatrix} v_{j1} \\ v_{j2} \\ v_{j3} \\ v_{j4} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad (4-3)$$

The form of this matrix is not particularly perverse until the determinate is evaluated. The determinant of the square matrix is determined:

$$\text{Det} \begin{bmatrix} y_{j1} - 1 & y_{j1} & y_{j1} & y_{j1} \\ y_{j2} & y_{j2} - 1 & y_{j2} & y_{j2} \\ y_{j3} & y_{j3} & y_{j3} - 1 & y_{j3} \\ y_{j4} & y_{j4} & y_{j4} & y_{j4} - 1 \end{bmatrix} = 1 - y_{j1} - y_{j2} - y_{j3} - y_{j4} \quad (4-4)$$

By the definition of molar fractions, the determinate must be zero. The solution (the nullspace) is of the form:

$$\begin{bmatrix} v_{j1} \\ v_{j2} \\ v_{j3} \\ v_{j4} \end{bmatrix} = \begin{bmatrix} y_{j1}/y_{j4} \\ y_{j2}/y_{j4} \\ y_{j3}/y_{j4} \\ 1 \end{bmatrix} \quad (4-5)$$

This merely states that one of the v_i 's is specified elsewhere before the others can be found. The four variables are found through three independent equations. These results make sense; for any concentration of a component, there are an infinite set of rates at which this component might flow away. The reason the equations work is that the system of equations is iterated to a solution. There is only one set of rates that will give the correct concentration in all fifty stages.

The first stage does use vapor molar fractions, there is no vapor flow from the accumulator. Also, there are only 48 stage plates: Bernoulli's equation can only solve for 48 pressures. One other pressure is solved for using the empirical estimate for flow through the condenser, equation (2-69c). The other pressure is solved by iteration with the vapor-liquid equilibrium equations and the equation of state.

Temperature is determined from the enthalpy balance. The method described in Section 2.5, that of differentiating a function of temperature, is not

used. The differential equation for liquid enthalpy holdup is used, the polynomial expansion of temperature estimation of liquid enthalpy holdup is also used. This second equation is essentially solved for temperature by iteration.

The column also includes a control system to ensure optimal performance. Five control variables are controlled using the flow of fluid through the five sets of valves in Figure 4.1. Four of the variables are the temperature in the receiver (T1) controlled by flow of cooling water (Q_{cw}) through valve 1, the reflux flow rate (L1) controlled directly by valve 2, the level of liquid in the receiver (Z1) controlled by the distillate flow through valve 3, and the level of liquid in the base of the column (Z50) controlled by the bottoms flow through valve 5. These four control variables use the PI control strategy presented in Section 2.10, equations (2-79) through (2-81). The fifth controlled variable, the temperature of the 35th stage (T35), is controlled by the flow of steam (Q_{sh}) through valve 4 using a cascaded PI control. For this control, the PI equations are modified to be PI control for the valve, equations (4-6), where the set point is determined by a PI control system of T35, equations (4-7):

$$CI_4 = CI_{\min} + B Q_{sh} \quad (4-6a)^{GSR}$$

$$e_4 = CI_4 - CISP_4 \quad (4-6b)^{GSR}$$

$$u_4 = Kp_4 e_4 + Ki_4 \int e_4 dt + e_0 \quad (4-6c)^{GSR}$$

$$\dot{\zeta}_4 = \frac{u_4 - \zeta_4}{TAUV_4} \quad (4-6d)^{GSR}$$

$$CI_6 = CI_{\min} + B T_M \quad (4-7a)^{GSR}$$

$$e_6 = CI_6 - CISP_6 \quad (4-7b)^{GSR}$$

$$CISP_4 = Kp_6 e_6 + Ki_6 \int e_6 dt + e_0 \quad (4-7c)^{GSR}$$

$$\dot{T}_M = \frac{T_{35} - T_M}{TAUM} \quad (4-7d)^{GSR}$$

Equation (4-7d) represents a temperature measurement device with first order dynamics. The effect is to delay and dampen the effects of the actual temperature on the control system. The effect of all of the equations (4-7) is to delay and dampen the effects of the temperature on the control of the steam valve. With 14 stages between T35 and Qsh, the delay within the control is intended to anticipate the delay within the column.

4.3 Modifying the Gallun model

The Gallun model contains algebraic loops. Algebraic loops can be a problem for simulating. The simulation program Gallun generated for his model was written from scratch into FORTRAN, utilizing Gear's method of integration. Gear's method contains within it a process of iteration to solve algebraic loops. Gallun reported no problems with stability of his simulation routine, though his model does contain dependent equations.

A rigorous elimination of some of the algebraic loops requires knowledge of power flow in phase changes not yet known. Without such knowledge, the loops may be eliminated in a non-rigorous way. Three modifications to Gallun's model will suffice to free the column model of algebraic loops. The hydraulic equations can be made more exact by including the inertial elements and the DC elements. This adds differential equations to the model needed to break the algebraic loops in the liquid flow from the downcomer and allows vapor flow to be calculated from hydraulic equations rather than vapor-liquid equilibrium

equations. Instead of pure Bernoulli's equations, the equations developed in Section 2.3 are used, equations (2-29), (2-31), (2-35), and (2-39). The flow over the weir is not assumed to be the same as the flow out of the downcomer.

The virial equation of state is replaced with the ideal gas equation of state. The virial equation of state is more accurate, but involves vapor molar fractions. In turn, molar fractions depend on pressure, and pressure is found using the equation of state. In Gallun's model, molar fractions depend on vapor flow, vapor flow depends of fugacity, and fugacity requires molar fractions. A more rigorous model would allow the vapor molar fractions and molar density to be calculated from the vapor holdups of each component, as liquid molar fractions are found. This algebraic loop can also be broken by using a simpler equation of state. An additional result of this switch is the reduction in the number of equations. The calculation of the second virial coefficient for a mixture requires a few equations (61 per stage) and the enthalpy departure function (Ω) requires a few more (52 per stage). These are all eliminated by using the ideal gas equation. Molar density is now computed by assuming that the total vapor molar holdup is constant and therefore specified.

The third modification for eliminating algebraic loops is the use of Raoult's law for the vapor-liquid equations. The vapor molar fractions are thus calculated using liquid molar fractions, pressure, and vapor pressure. The use of fugacity and activity coefficients is more accurate, but as long as these are used to calculate the vapor molar fractions, algebraic loops cannot be avoided. A more rigorous model would use chemical potential instead of using partial pressures or fugacities to calculate molar flow between the phases and thus

allowing the virial equation of state to be used. The equations to calculate these coefficients are eliminated (28 per stage).

Two models result from these three changes, a complex model and a simplified model. The complex model incorporates the changes to the hydraulics, includes a non-constant vapor holdup, and must assume a form of resistance for molar flow between the phases. These changes eliminate all of the algebraic loops within the column and retain the thermodynamic and the virial equation calculations, at the expense of having to make up resistance values and create a larger set of equations than Gallun's model. The simplified model incorporates the changes to the hydraulics, uses the ideal gas law, and uses Raoult's law for determining vapor molar fractions. These three changes to Gallun's model eliminate all of the algebraic loops and simplifies the model considerably within the column. Several more algebraic loops exist in the plumbing leading from the reboiler and the receiver. These are solved by combining the resistances of the pump and the valves as described in Sections 2.7 and 2.8. The complex model includes hydraulic inertias, but the exact size and lengths of the pipes are not given and can not be included with any precision.

The last modification to the Gallun model was to reduce the number of stages and feeds in the model. The full number of stages would have created a simple model of about 750 differential equations with several thousand algebraic equations. The number of stages was reduced to nine stages. As the intention of this simulation was not to exactly duplicate the Gallun model (which itself is not based on any real column), but to investigate the form of distillation column models, this reduction was felt to be reasonable. The final

results of all the modifications is a simple distillation column model without algebraic loops, containing 135 differential equations, 697 equations total.

The unmodified Gallun model was coded into the modeling language DYMOLA. DYMOLA has the capability of creating an ACSL program (a simulation language [75]) to simulate a model. Appendix B contains the unmodified Gallun model as presented in his dissertation [24], as well as including details presented in other sources [28, 27]. Appendix B also contains the DYMOLA code for this model as well as DYMOLA's assessment, including a list of algebraic loops within the model.

The simple model was coded into DYMOLA. Debugging of the model had to be conducted iteratively with simulation runs, and so, to facilitate the process, the model was coded into ACSL using only three stages and finally into nine. The nine stage simple model ACSL code is given in Appendix C. It was intended to be recoded into DYMOLA and take advantage of the latest system analysis functions within DYMOLA, but time constraints have not allowed for this. The complex model was also coded into ACSL, but has not been simulated. Appendix D contains the ACSL code for this model.

A third, more rigorous model could be fashioned out of Gallun's model. The bond graph model of a distillation column presented in the previous chapter point to transforming the model into a balance of hydraulic, thermal, and chemical powers. Only the hydraulic power balances have been incorporated into the modified models above. The enthalpy balance equations could be transformed to the thermal bond graph equations. Heat capacities of these substances do exist in chemical tables. The transformation of the

thermodynamic calculations to chemical power balances is not as easily done. Such a third model is left for future work.

4.4 Simulation results

Using fewer stages than the original Gallun model meant different steady-state conditions. Assuming volume flows are about the same, the pressure and the temperature differences between the condenser and the reboiler are greatly reduced. Steady-state conditions were approximated based on material balance equations. The model was first simulated to achieve true steady-state conditions. After this relaxation, initial conditions and controller set-points were modified to begin subsequent simulation runs at steady-state values.

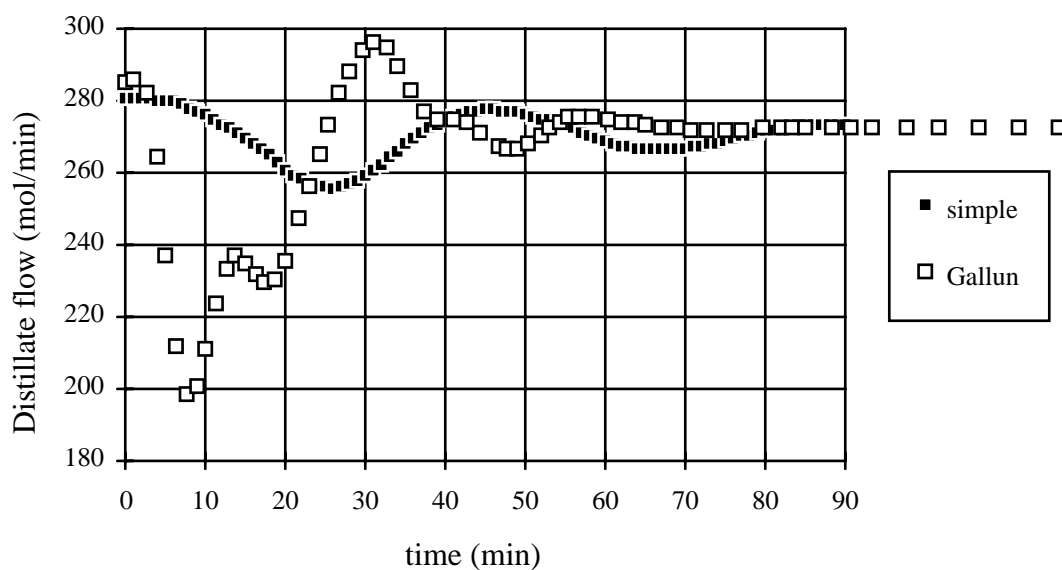


Figure 4.2. Comparison of the distillate flow of Gallun and simple model in experiment one.

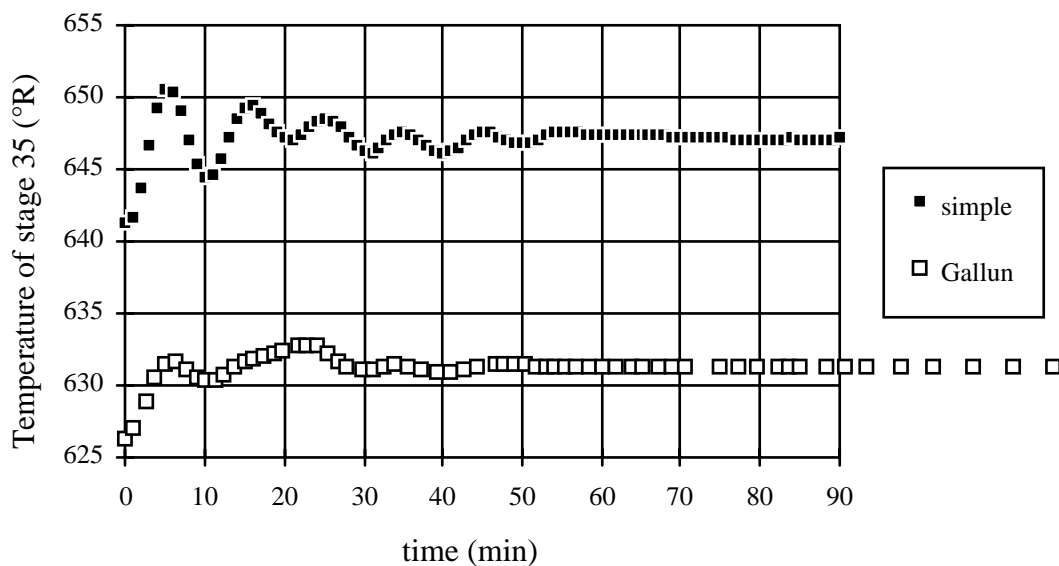


Figure 4.3. Comparison between the stage 35 temperature in Gallun and simple model in experiment one.

The stages in the simple model are not labeled one through nine. In anticipation of expanding the model back to 50 stages, the receiver kept its label 1, the base kept its label 50, the feed stage kept its label 21, and the temperature controlled stage kept its label 35. The nine stages were thus labeled, receiver to base, 1, 2, 3, 4, 5, 21, 35, 49, and 50.

The simple model was simulated under several experiments. The experiments concern changing the set-points of some of the control variables. The original experiment by Gallun was to raise the set temperature of the 35th stage up 5 degrees Rankine. Essentially, such experiments are designed to optimize the settings of the control system, to test the response of the system.

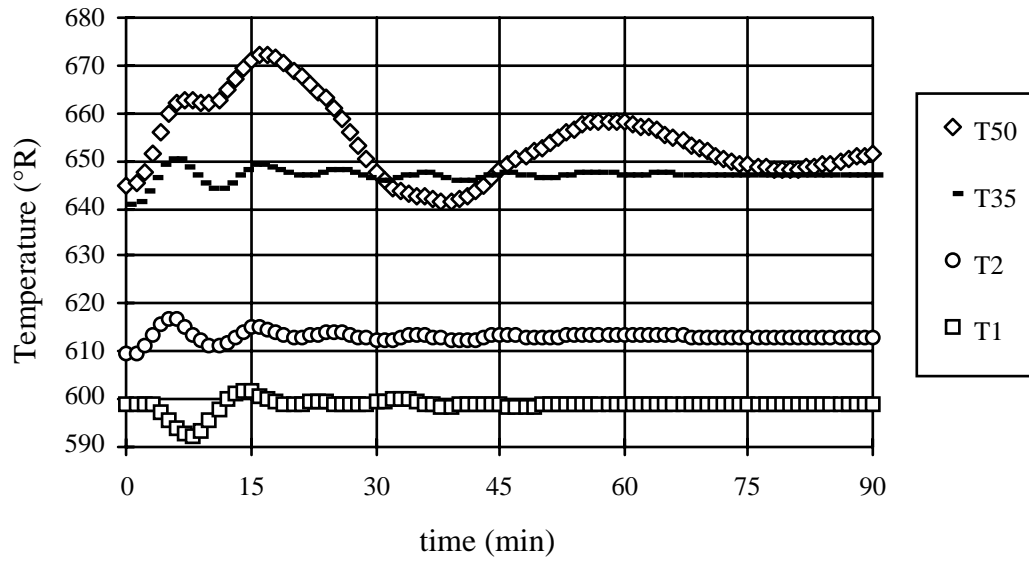


Figure 4.4. Simple model temperature spread for experiment one.

Figures 4.2 through 4.6 show some of the results of this first experiment on both the simple model and Gallun's original simulation [24].

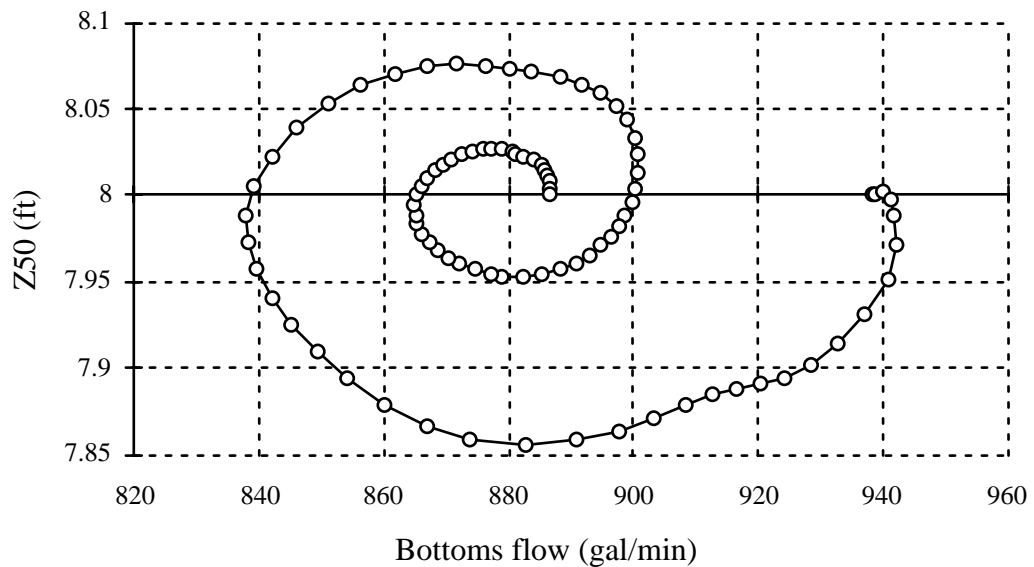


Figure 4.5. Control of base liquid level in simple model in experiment one.

Figure 4.2 shows the distillate flow responding to the change in $CISP_6$. Both the Gallun model and the simple model show a dynamic response such that the distillate flow is reduced by the change. The simple model reveals less overshoot due to the reduced size of the column. Figure 4.3 shows the response of T35 to the change in its set point. Note that in the simple model, only five stages separate stage 1 and stage 35; the reduced temperature differences within the simple model require that the set-point for T35 be much lower than the T35 set-point in the Gallun model. The Gallun model appears to be much less oscillatory, although there is a common 10 minute cycle in the two models. The oscillations can be attributed to the control constants, which are set for a 50-stage column.

Figure 4.4 shows the temperature profile of the simple column, the oscillations in T35 can be seen to be related to the immense temperature swings

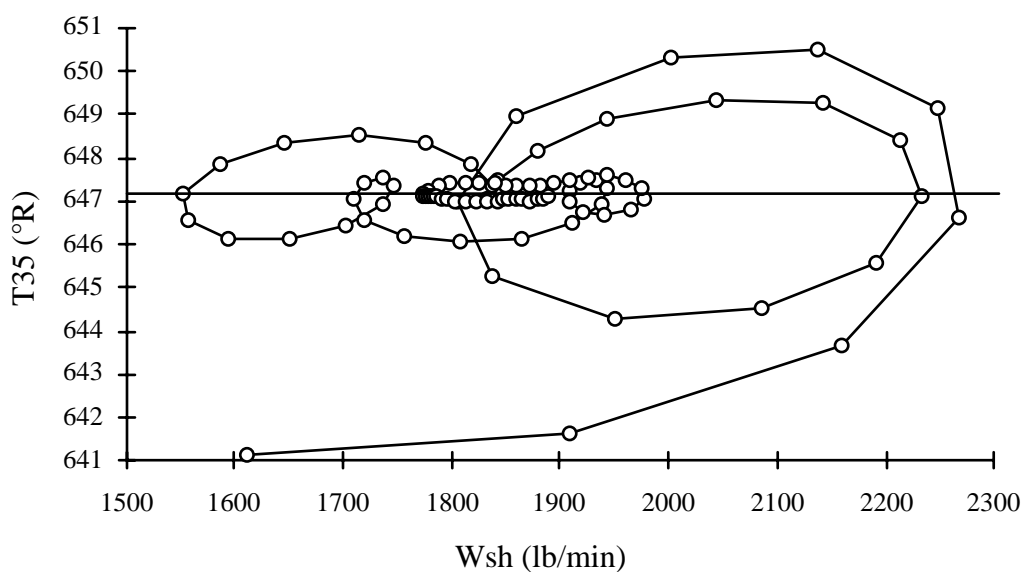


Figure 4.6. Control of T35 using steam flow (Wsh) in the simple model in experiment one.

in the base. Using a better control system, the rise in T50 would be more gradual. Note how T1 and T2 both begin to swing higher at $t=0$, but that the temperature control of T1 immediately tries to compensate.

Figure 4.5 shows the response of another controlled variable, the base liquid level. Here, one can see that the control system slowly works its way to keep the level at 8 feet. The steam flow in the reboiler, W_{sh} , is used to control T35. When the set point is raised from 641.16 to 647.16 °R, W_{sh} increases to raise T35 and decreases to lower T35. This control system, as seen in Figure 4.6, is not as stable or efficient as the base level control.

The second and third experiments are to lower the reference temperature for the 35th stage. As can be seen from Figure 4.7, simply lowering this reference temperature produces an oscillatory system. Experiment three, to determine the source of the instability, lowers the reference temperature as well as adjusting the controller gain values for the temperature and the steam valve

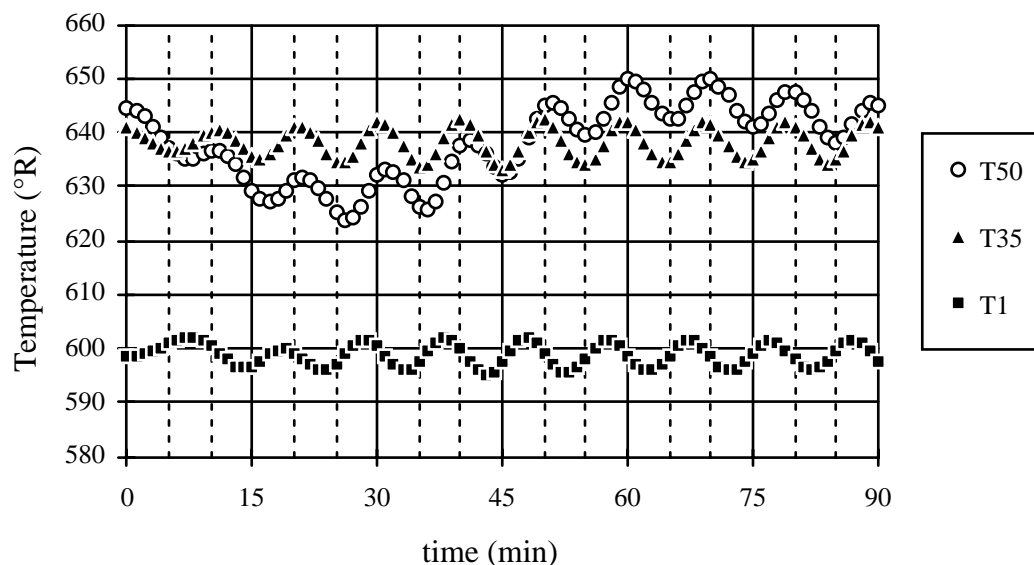


Figure 4.7. Temperature profile of the simple model in experiment two.

control. The adjustments, as seen in Figure 4.8, result in looser control over the temperature. The time constant of the oscillations is smaller, the overshoot is larger, but the system is eventually stabilized without oscillations. What this really points to is this column's need for a more robust control strategy—either the control parameters need optimizing or the control strategy needs the ability to adjust these parameters as the system changes (adaptive control).

The fourth experiment is to reduce the set point of the reflux rate. The reflux rate is kept at 490.135 gallons per minute (reflux ratio of 2.7) by controlling the reflux flow. This experiment changes that value to 400 gallons per minute, effectively increasing the distillate flow. The proportional controller gains for the receiver liquid level and the reflux rate were changed to render this experiment stable. Figure 4.9 plots reflux rate by the distillate rate. The final reflux ratio is 1.6. The composition of the distillate also changes because of this

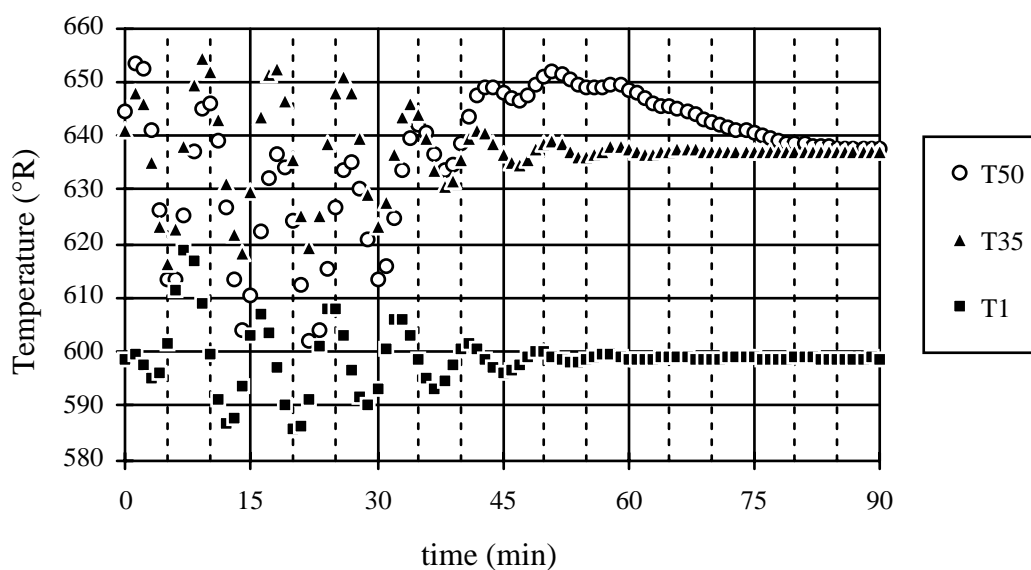


Figure 4.8. Temperature profile of simple model in experiment three (same as experiment two but with controller values modified).

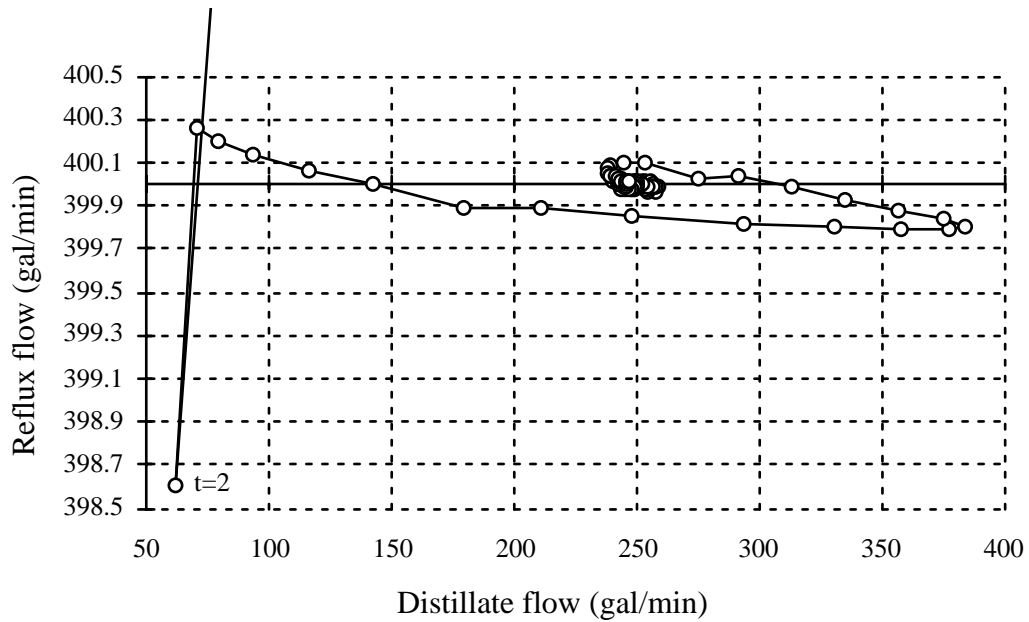


Figure 4.9. Reflux flow control in the simple model in experiment four.

change. As seen in Figure 4.9, the control brought the flow rate within .3 gallons/min. of the new set-point within

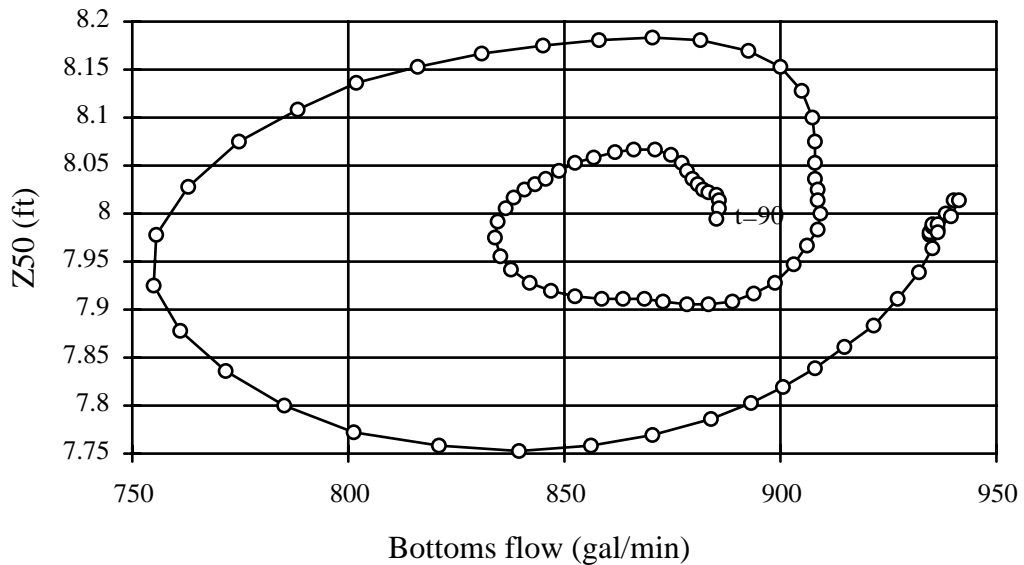


Figure 4.10. Base liquid height control in experiment four.

2 minutes. Obviously, controlling a flow rate directly using a valve results in fast and efficient control. Figure 4.10 shows the base liquid level control working; the bottoms rate reduces to compensate for the increased distillate rate. Note that this experiment effects the level more than the first experiment, Figure 4.5, where only the temperature needed changing.

The fifth and last experiment adjusted the composition of the feed, without changing the temperature or total molar flow of the feed. The feed flow of ethanol was increased as the feed flow of the other components were decreased. Figure 4.11 shows the increase of ethanol in the bottoms product as a result.

These five experiments verified the nature of the equations in the model. Adjusting the various set-points did jolt the model in understandable ways, consistent with the operation of a distillation column. However, the 9-stage

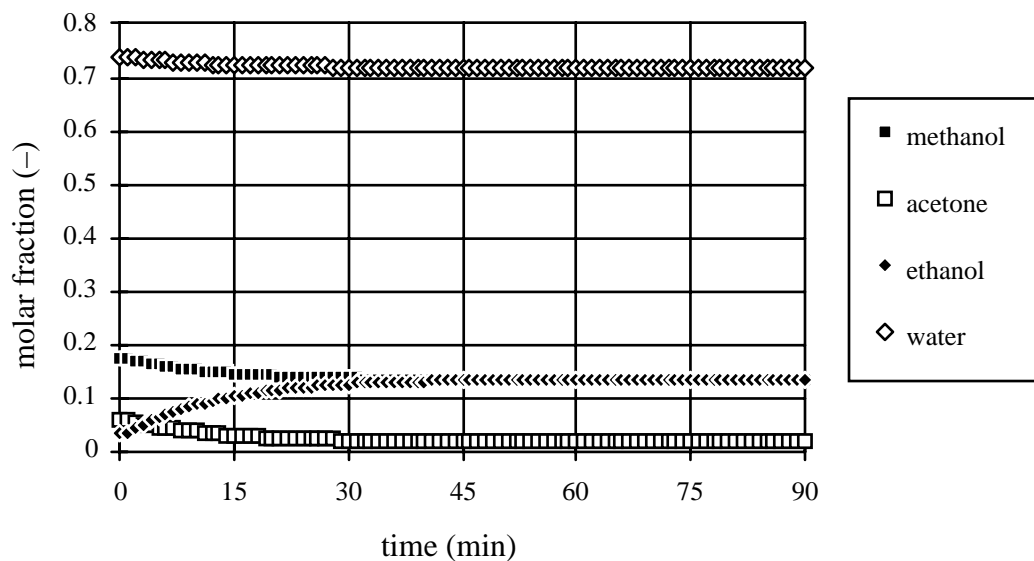


Figure 4.11. Molar fractions of the bottoms product in the simple model with experiment five (changing the composition of the feed).

model is not an adequate substitute for a full 50-stage model in several ways. Most importantly, the simple model did not successfully distill ethanol. Nine stages, one feed, simplified equilibrium equations, and control settings established for a much larger column, combine to defeat the distillation goal. One or more of these factors could possibly be optimized to achieve the proper distillation, perhaps in future work. A fairer comparison to Gallun's model would increase the number of stages and feeds of the simple model.

5.0 CONCLUSION

Distillation columns provide a complex system to model. Previous efforts to model distillation columns have focused on mass and energy balances, not on power balances. These efforts require assumptions of equilibrium and constant vapor holdup of mass and energy. For a rigorous dynamic model of the distillation process, power flow reveals some inadequacies in these models. Modeling using bond graphs have forced some questions about the nature of distillation. The simple model shows that simple models can be constructed without algebraic loops. The complex and bond graph model of the distillation column show the potential in dynamic, rigorous simulation that can be achieved. More needs to be done, both theoretically and in the fundamental research of phase transfer, the basis of distillation.

5.1 Future work in distillation

Only the simplest modification of Gallun's model was simulated. The complex model needs to be simulated, possibly debugged. The simulation results of the complex model will be hard to interpret. Multiple simulation runs will be necessary to determine the role of the molar flow resistances and hydraulic inertias. Both models need to be expanded to 50 stages and 3 feeds for a proper comparison with Gallun's model. These models should also be coded into the modeling program, DYMOLA, to utilize the system analysis features it currently contains. DYMOLA should be able to code an ACSL program that simulates the model in a preordered, and therefore faster, sequence. Once the

power flow between the phases is better understood, a model based on the bond graphs presented in this thesis can be constructed and simulated.

There are other methods of resolving the algebraic loops in Gallun's model. Differentiating the algebraic variables in a loop linearizes their relationship; the loop is broken for these newly formed derivatives by linear means of resolving algebraic loops. For such a large number of equations involved within the algebraic loop of a distillation column, a systematic and computerized application of this method must be applied. DYMOLA, has recently gained the ability to render this, but has not yet been applied to the distillation model. The potential benefit to the Gallun model is limited. The bond graphing of the distillation column has revealed that the algebraic loops are based on fundamental problems within the model.

Further work is needed on individual elements. The hydraulic resistances (including valves) based on kinetic energy are suspect; viscosity plays no part in these terms as they are currently defined. The vapor flow through the sieve plate probably should not assume an incompressible fluid. The variety of elements could be expanded to include the variety of distillation columns, such as elements that describe fluid flow in a packed column. Work on elements will mean adapting current forms of equations to power flows.

The bond graph model of a distillation column developed here, raises many new elements and new questions. The most crucial question is the nature of the molar flow between the phases. The energy-storage element of molar flow and chemical potential needs work. The use of the Peng-Robinson equation of state for a capacitive element, in conjunction with the phase resistances of film theory could result in a viable set of dynamic equations for phase flow. The

problem is that efficiencies based on film theory are not considered to be very accurate; empirically developed efficiencies work much better. These more accurate efficiencies may themselves provide an adequate resistive element for phase flow.

This thesis has tried to focus on macro power flow within a stage as opposed to the micro power flows that sum up to these macro flows. A more rigorous look at a distillation stage shows that pressure, temperature, and chemical potential are not everywhere identical on each stage or within a phase on each stage. The liquid pressure is dependent on the depth of the liquid. The temperature of the vapor is dependent on how far it has traveled through the liquid, the temperature of the liquid is dependent on the distance traveled towards the weir as well as the depth of the liquid. The chemical potential depends on the amount of phase flow already generated. All of these factors affect the phase flow, density, and volume flow. Thus, a more rigorous model of the distillation stage would need to take the form of partial differential equations and, to be bond graphed, would be segmented into many areas of exchange.

5.2 Future work in bond graphs

Bond graphs attempt to model a system using power flows under the assumption that there exist fundamentally similar relationships between power conjugates. The inherent power and weakness of this approach can be seen in the scope of modeling a distillation column. The weakness of bond graphs is that they do not adequately conform to the established forms of distillation equations in use by current models. Modifications to bond graphs, such as

convection bonds, solve this problem, but at the expense of some of the inherent power of the original bond graph. The inherent power of the bond graph is its ability to graphically reveal the system, the ability to show the detailed form of equations used, the ability to encapsulate pieces of the model into sub-models using hierarchical bond graphs, and its demand for explicit details of the system to adequately model the power flows in the system.

Bond graphs have shown some limitations to the traditional distillation models. A choice of assigning causality strokes means algebraic loops within the models. The algebraic loops point to fundamental problems within the system equations. Some of these problems can be fixed immediately by including additional elements, such as the hydraulic inertial elements. Some of these problems can be solved in the type of relationship that is needed, but still require a better understanding of the system, such as phase flow resistances.

The bond graphs also shows ways of expanding the model of a distillation column presented. The addition of heat transfer or sidestreams would expand upon the 0-nodes in the Foam element, similarly to the way the Feed element does. A simple chemical reaction would mean the individual components' molar flow could not simply be added together. The 0-nodes in Figure 3.2 would require an extra molar flow emanating from the node, the flow of one component into another component as the reaction changes the chemical makeup of the mixture. This would require the inclusion of a 1-node and one ChR-element for each chemical reaction [5]. The 1-node connects individual components that are involved in a chemical reaction. Figure 5.1 shows a modification of the bond graph Figure 3.8 of a

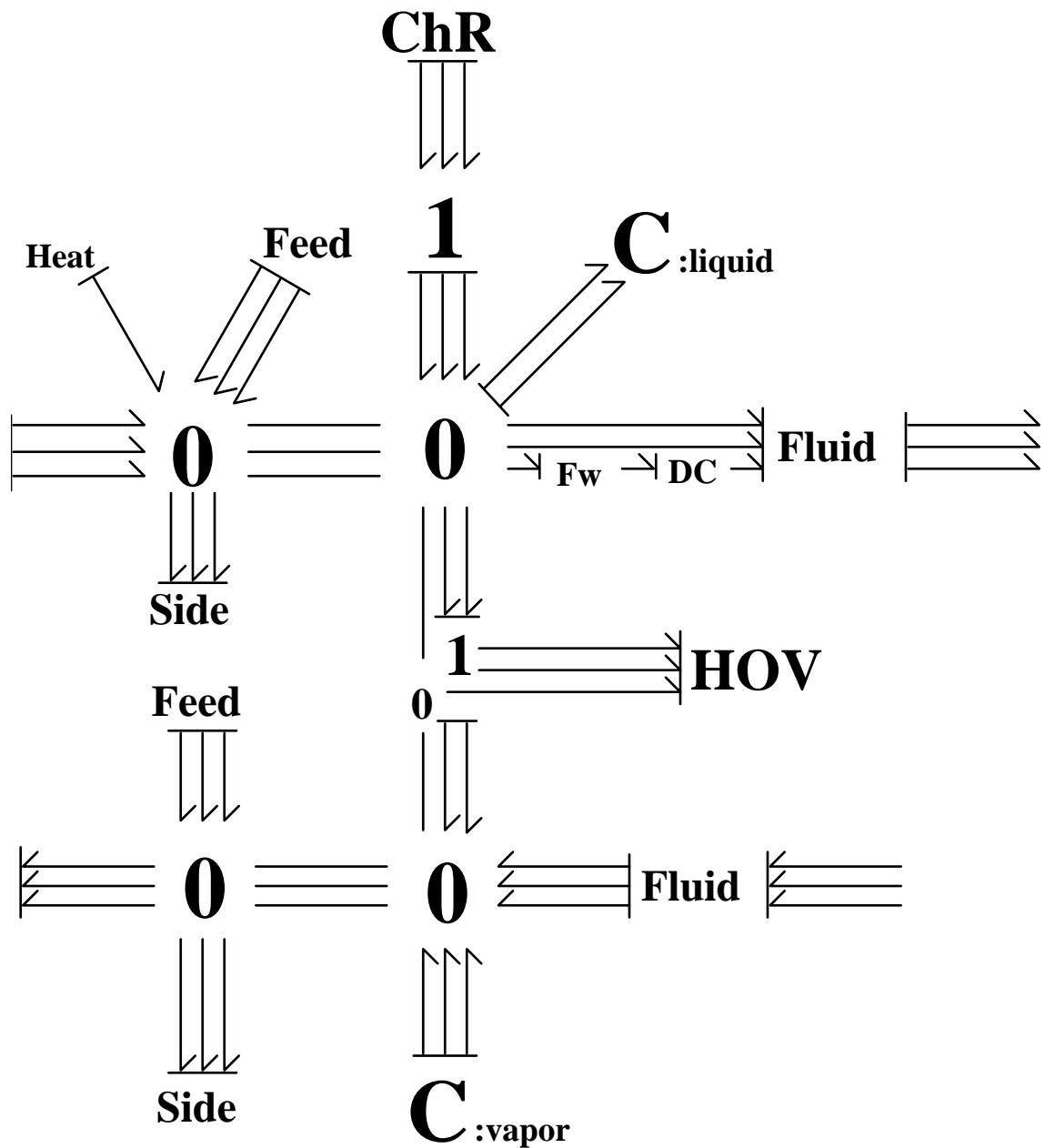


Figure 5.1. A generalized distillation stage.

distillation stage that includes liquid and vapor feed, liquid and vapor sidestreams, a liquid heating element, and one chemical reaction that takes place in the liquid.

The strength of bond graphs—the demand for explicit details of the system—is the major force behind the scope of future work that needs to be done. The traditional model begins and ends with mass and energy balance. While the traditional model has done very well emphasizing those known equations, equilibrium estimates of enthalpy and fugacity, these equations only go so far. A dynamic relationship between the variables in distillation is required for a dynamic model. Bond graphs do balance mass and energy, and attempt to show the dynamic flow of power, in all its forms. Bond graphs, I believe, show the way of future pursuit. The chemical literature shows a lot of continuing interest in developing better equilibrium models. Many chemical systems are stage reactions and could benefit greatly from the modular aspects of bond graphs. The true future of rigorous chemical systems modeling lies in developing loop-free, dynamic, modular models, a future for which the bond graph methodology is well suited.

APPENDIX A: NOTATION

A	area
A_0	average cross-sectional area
AD	cross-sectional area of downcomer (constant)
AH	total area of holes in the sieve plate (constant)
A_i, B_i, C_i	coefficients that depend on component i
AN	nominal area of stage plate (constant)
A_{pc}	area of heat transfer from condensing mixture to condenser tubes (constant)
A_{pmr}	area for boiling heat transfer in the reboiler (constant)
A_s	area for steam condensation in the reboiler steam chamber (constant)
AUD	area of opening under the downcomer, below downcomer apron (constant)
A_w	Area for heat transfer from cooling water to tubes (constant)
B_{ik}	second virial cross-coefficient of components i and k
B_{mj}	second virial coefficient of the vapor mixture on stage j
C	compliance element in bond graph
c	number of components in mixture
C_{cw}	cooling water heat capacity
CI_k	input to k^{th} controller
$CISP_k$	set point (reference value) of k^{th} controller
C_{mc}	heat capacity of condenser tubes (constant)
C_{mr}	heat capacity of reboiler tubes (constant)

C_{sh}	heat capacity of steam in steam header
C_{wo}	heat capacity of water in steam chamber
C_x, C_d, C_{vc}	vena contracta factors
D_h	diameter of holes in the sieve plate (constant)
e	generic effort variable
E_{ji}	vaporization plate efficiency
E_{ji}^M	modified Murphree plate efficiency
e_k	error signal in the k^{th} controller
f	generic flow variable
f	subscript – friction
f	superscript – feed
f_1, f_2, \dots, f_6	mixing functions
\hat{f}_i	fugacity of component i in mixture
f_i	ideal fugacity of component i
F_j	total molar liquid feed rate on stage j
f_{ji}	molar liquid feed rate of component i on stage j
$Foam_j$	foam factor on stage j
F_w	weir constriction factor
G	Gibbs free energy
g	acceleration due to gravity (constant)
Δh	head loss (pressure drop)
H_j^f	enthalpy flow from feed onto stage j
hf_j	height of foam on the stage j tray
$hfow_j$	height of foam above the weir on stage j tray
H_j	enthalpy holdup on stage j

h_j^L	height of clear liquid on the stage j tray
h_{Lsc}	enthalpy of water in steam chamber (function of T_{sc})
h_{owj}	height of clear liquid above the weir on stage j tray
H_{Vsc}	enthalpy of steam in steam chamber (function of T_{sc})
h_{wj}	height of weir of stage j (constant)
I	inertial element in bond graph
i	subscript – denotes i^{th} component of mixture
J	conversion factor from heat to mechanical energy
j	subscript – denotes j^{th} stage
K_i	K-value (distribution coefficient) of component i
K_i^I	ideal K-value of component i
K_{ik}	integral constant of the k^{th} PI controller
K_{pk}	proportion constant of the k^{th} PI controller
L	superscript – liquid
L^h	heat of vaporization per unit mass (function of temperature)
LH_j	length of holes in (thickness of) sieve plate of stage j (constant)
L_j	liquid molar flow rate from the j^{th} distillation stage
l_{ji}	liquid molar flow rate of the i^{th} component from the j^{th} stage
LV_{ji}	molar flow rate from liquid to vapor of component i on stage j
L_w	weir length (constant)
M	molar holdup

N	number of stages in distillation column, as a subscript it denotes the base of the column
n_{ji}	molar holdup of component i on stage j
P	pressure
PB	pressure outside distillation column to which bottoms flow (constant)
PCC_{ik}	cross-critical pressure of components i and k (constants)
PC_i	critical pressure of component i (constant)
PD	pressure outside system to which distillate flows (constant)
Pdc	pressure due to changes in the downcomer liquid height
Psc	pressure in steam chamber of reboiler
PSH	pressure in steam header (constant)
PS_i	ideal vapor pressure of component i (function of temperature)
Q, q	volume flow
QC	heat flow from vapor into the condenser
Qcw	volume flow of cooling water in condenser
Qfs_j	foam volume flow over the tray weir of stage j
QL_j	liquid volume flow leaving the downcomer of stage j
QR	heat flow into liquid from the reboiler
Qsc	volume flow of water leaving steam chamber
Qsh	volume flow of steam from the steam header
Qs_j	liquid volume flow over the tray weir of stage j
QV_j	vapor volume flow from stage j
R	ideal gas constant

R	resistive element in bond graph
RS	resistive-source element in bond graph
S	entropy
SE	effort source element in bond graph
SF	flow source element in bond graph
T	temperature
t	time
TAUV _k	time constant of the k th control valve (constants)
TCC _{ik}	cross-critical temperature of components i and k (constants)
TC _i	critical temperature of component i (constants)
T _M	temperature reading of measurement device used on stage

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T _{mc}	temperature of mass of cooling tubes in condenser
T _{mr}	temperature of mass of reboiler tubes
T _R	reduced temperature (T/TC)
T _{sc}	temperature of steam in steam chamber
T _{sh}	temperature of steam in steam header (constant)
T _{wi}	temperature of cooling water coming into condenser tubes
T _{wo}	temperature of cooling water leaving condenser tubes
U _{cw}	mass of cooling water in condenser tubes
U _j ^f	internal power flow from the feed on stage j
U _j	internal energy holdup on stage j
u _{ji}	molar liquid holdup of component i on stage j
u _k	output signal of the k th controller
U _{mc}	mass of condenser tubes (constant)

U_{mr}	mass of metal in the reboiler (constant)
U_{pmo}	reference heat transfer film coefficient between distillation mixture and condenser tubes (constant)
U_{pmr}	boiling film coefficient in reboiler (constant)
U_s	reboiler steam side condensing film coefficient (constant)
u_{vji}	molar vapor holdup of component i on stage j
U_{wm}	reference heat transfer film coefficient between cooling water and condenser tube wall (constant)
V	superscript - vapor
V	volume
v	velocity
V_{dc}	volume of liquid in downcomer of stage j
V_{hj}	Volume of holes in sieve plate of stage j (constant)
V_j	vapor molar flow rate from stage j
v_{ji}	vapor molar flow rate for component i from stage j
V_r	volume of steam chamber (constant)
x_i	molar fraction of component i in liquid mixture
y_i	molar fraction of component i in vapor mixture
z	height
Z_j	height of clear liquid in downcomer of stage j
Z_N	height of clear liquid in base of column, stage N
ZT_j	distance between stage plate j and stage plate $j+1$ (constant)
ZZ_j	compressibility factor
$\hat{\alpha}$	molar volume of mixture

α_i	molar volume of component i
γ_i	activity coefficient of component i
ζ_k	position of the k th control valve
η_{ik}	cross self-interaction parameters (constants)
$\lambda_{ik} - \lambda_{ii}$	Wilson coefficients (constants)
μ	chemical potential
μ_R	mixture reduced dipole moment (constants)
ρ	mass density
$\bar{\rho}$	molar density, moles per unit volume
σ	surface tension
$\hat{\Phi}_i$	fugacity coefficient of component i in mixture
φ_i	ideal fugacity coefficient of component i
ϕ	relative froth density
ω_{Hik}	cross-acentric factor of the first homograph of components i and k (constants)
ω_i	acentric factor of component i (constant)
Ω_j	enthalpy departure function (from ideal gas) for stage j

APPENDIX B: GALLUN'S DISTILLATION COLUMN

B.1 The equations of the model.

–for $j=[1,50]$ and $i=[1,4]$ unless otherwise stated.

Energy Balance Equations:

$$\begin{aligned}
 0 &= \text{Hf}(1) + v(2,1)*\text{HV}(2,1) + v(2,2)*\text{HV}(2,2) + v(2,3)*\text{HV}(2,3) + v(2,4)*\text{HV}(2,4) - (1 + \\
 &\quad R)*L(1)*E(1)/(R * (u(1,1) + u(1,2) + u(1,3) + u(1,4))) - \text{QC} - \text{der}(E(1)) \\
 0 &= \text{Hf}(j) + L(j-1)*E(j-1)/((u(j-1,1) + u(j-1,2) + u(j-1,3) + u(j-1,4)) - L(j)*E(j)/((u(j,1) + u(j,2) + u(j,3) + \\
 &\quad u(j,4)) + v(j+1,1)*\text{HV}(j+1,1) - v(j,1)*\text{HV}(j,1) + v(j+1,2)*\text{HV}(j+1,2) - v(j,2)*\text{HV}(j,2) + \\
 &\quad v(j+1,3)*\text{HV}(j+1,3) - v(j,3)*\text{HV}(j,3) + v(j+1,4)*\text{HV}(j+1,4) - v(j,4)*\text{HV}(j,4) - \text{der}(E(j)) \\
 &\quad \text{–for } j=[2,49] \\
 0 &= \text{Hf}(50) + L(49)*E(49)/(u(49,1) + u(49,2) + u(49,3) + u(49,4)) - L(50)*E(50)/((u(50,1) + u(50,2) + \\
 &\quad u(50,3) + u(50,4)) - v(50,1)*\text{HV}(50,1) - v(50,2)*\text{HV}(50,2) - v(50,3)*\text{HV}(50,3) - v(50,4)*\text{HV}(50,4) \\
 &\quad + \text{QR} - \text{der}(E(50)) \\
 0 &= u(j,1)*hL(j,1) + u(j,2)*hL(j,2) + u(j,3)*hL(j,3) + u(j,4)*hL(j,4) + - E(j) \\
 hL(j,i) &= hL\text{COEF}(1,i) + hL\text{COEF}(2,i)*T(j) + hL\text{COEF}(3,i)*T(j)**2 \\
 \text{HV}(j,i) &= \text{H0}(j,i) + \text{OMEGA}(j) \\
 \text{H0}(j,i) &= \text{HVCOEF}(1,i) + \text{HVCOEF}(2,i)*T(j) + \text{HVCOEF}(3,i)*T(j)**2 + \text{HVCOEF}(4,i)*T(j)**3 + \\
 &\quad \text{HVCOEF}(5,i)*T(j)**4 \\
 \text{OMEGA}(j) &= (2 - 1/\text{ZZ}(j))*P(j)/(2*\text{ZZ}(j) - 1) * (\text{TK}(j)*\text{dBm}(j) - \text{Bm}(j)) \\
 \text{dBm}(j) &= (v(j,1)*v(j,1)*\text{dB11}(j) + v(j,1)*v(j,2)*\text{dB12}(j) + v(j,1)*v(j,3)*\text{dB13}(j) + v(j,1)*v(j,4)*\text{dB14}(j) + \\
 &\quad v(j,2)*v(j,1)*\text{dB21}(j) + v(j,2)*v(j,2)*\text{dB22}(j) + v(j,2)*v(j,3)*\text{dB23}(j) + v(j,2)*v(j,4)*\text{dB24}(j) + \\
 &\quad v(j,3)*v(j,1)*\text{dB31}(j) + v(j,3)*v(j,2)*\text{dB32}(j) + v(j,3)*v(j,3)*\text{dB33}(j) + v(j,3)*v(j,4)*\text{dB34}(j) + \\
 &\quad v(j,4)*v(j,1)*\text{dB41}(j) + v(j,4)*v(j,2)*\text{dB42}(j) + v(j,4)*v(j,3)*\text{dB43}(j) + v(j,4)*v(j,4)*\text{dB44}(j))/(v(j,1) \\
 &\quad + v(j,2) + v(j,3) + v(j,4))**2 \\
 \text{dB11}(j) &= \text{RR}(1)*\text{TCC}(1,1)/\text{PCC}(1,1)*(df311(j) + wH(1,1)*df411(j) + df511(j) + \text{ETTA}(1,1)*df611(j)) \\
 \text{dB12}(j) &= \text{RR}(1)*\text{TCC}(1,2)/\text{PCC}(1,2)*(df312(j) + wH(1,2)*df412(j) + df512(j) + \text{ETTA}(1,2)*df612(j)) \\
 \text{dB13}(j) &= \text{RR}(1)*\text{TCC}(1,3)/\text{PCC}(1,3)*(df313(j) + wH(1,3)*df413(j) + df513(j) + \text{ETTA}(1,3)*df613(j)) \\
 \text{dB14}(j) &= \text{RR}(1)*\text{TCC}(1,4)/\text{PCC}(1,4)*(df314(j) + wH(1,4)*df414(j) + df514(j) + \text{ETTA}(1,4)*df614(j)) \\
 \text{dB21}(j) &= \text{dB12} \\
 \text{dB22}(j) &= \text{RR}(1)*\text{TCC}(2,2)/\text{PCC}(2,2)*(df322(j) + wH(2,2)*df422(j) + df522(j) + \text{ETTA}(2,2)*df622(j)) \\
 \text{dB23}(j) &= \text{RR}(1)*\text{TCC}(2,3)/\text{PCC}(2,3)*(df323(j) + wH(2,3)*df423(j) + df523(j) + \text{ETTA}(2,3)*df623(j)) \\
 \text{dB24}(j) &= \text{RR}(1)*\text{TCC}(2,4)/\text{PCC}(2,4)*(df324(j) + wH(2,4)*df424(j) + df524(j) + \text{ETTA}(2,4)*df624(j)) \\
 \text{dB31}(j) &= \text{dB13}(j) \\
 \text{dB32}(j) &= \text{dB32}(j) \\
 \text{dB33}(j) &= \text{RR}(1)*\text{TCC}(3,3)/\text{PCC}(3,3)*(df333(j) + wH(3,3)*df433(j) + df533(j) + \text{ETTA}(3,3)*df633(j)) \\
 \text{dB34}(j) &= \text{RR}(1)*\text{TCC}(3,4)/\text{PCC}(3,4)*(df334(j) + wH(3,4)*df434(j) + df534(j) + \text{ETTA}(3,4)*df634(j)) \\
 \text{dB41}(j) &= \text{dB14}(j) \\
 \text{dB42}(j) &= \text{dB24}(j) \\
 \text{dB43}(j) &= \text{dB34}(j) \\
 \text{dB44}(j) &= \text{RR}(1)*\text{TCC}(4,4)/\text{PCC}(4,4)*(df344(j) + wH(4,4)*df444(j) + df544(j) + \text{ETTA}(4,4)*df644(j)) \\
 \text{df311}(j) &= -0.330*\text{TCC}(1,1)/\text{TK}(j)**2 + 0.1385*\text{TCC}(1,1)**2/\text{TK}(j)**3 + \\
 &\quad 0.0121*\text{TCC}(1,1)**3/\text{TK}(j)**4
 \end{aligned}$$

$$\begin{aligned}
df312(j) &= -0.330*TCC(1,2)/TK(j)**2 + 0.1385*TCC(1,2)**2/TK(j)**3 + \\
&\quad 0.0121*TCC(1,2)**3/TK(j)**4 \\
df313(j) &= -0.330*TCC(1,1)/TK(j)**2 + 0.1385*TCC(1,3)**2/TK(j)**3 + \\
&\quad 0.0121*TCC(1,3)**3/TK(j)**4 \\
df314(j) &= -0.330*TCC(1,4)/TK(j)**2 + 0.1385*TCC(1,4)**2/TK(j)**3 + \\
&\quad 0.0121*TCC(1,4)**3/TK(j)**4 \\
df322(j) &= -0.330*TCC(2,2)/TK(j)**2 + 0.1385*TCC(2,2)**2/TK(j)**3 + \\
&\quad 0.0121*TCC(2,2)**3/TK(j)**4 \\
df323(j) &= -0.330*TCC(2,3)/TK(j)**2 + 0.1385*TCC(2,3)**2/TK(j)**3 + \\
&\quad 0.0121*TCC(2,3)**3/TK(j)**4 \\
df324(j) &= -0.330*TCC(2,4)/TK(j)**2 + 0.1385*TCC(2,4)**2/TK(j)**3 + \\
&\quad 0.0121*TCC(2,4)**3/TK(j)**4 \\
df333(j) &= -0.330*TCC(3,3)/TK(j)**2 + 0.1385*TCC(3,3)**2/TK(j)**3 + \\
&\quad 0.0121*TCC(3,3)**3/TK(j)**4 \\
df334(j) &= -0.330*TCC(3,4)/TK(j)**2 + 0.1385*TCC(3,4)**2/TK(j)**3 + \\
&\quad 0.0121*TCC(3,4)**3/TK(j)**4 \\
df344(j) &= -0.330*TCC(4,4)/TK(j)**2 + 0.1385*TCC(4,4)**2/TK(j)**3 + \\
&\quad 0.0121*TCC(4,4)**3/TK(j)**4 \\
df411(j) &= -0.4600*TCC(1,1)/TK(j)**2 + 0.5000*TCC(1,1)/TK(j)**3 + 0.0970*TCC(1,1)**3/TK(j)**4 \\
&\quad + 0.0073*TCC(1,1)**8/TK(j)**9 \\
df412(j) &= -0.4600*TCC(1,2)/TK(j)**2 + 0.5000*TCC(1,2)/TK(j)**3 + 0.0970*TCC(1,2)**3/TK(j)**4 \\
&\quad + 0.0073*TCC(1,2)**8/TK(j)**9 \\
df413(j) &= -0.4600*TCC(1,3)/TK(j)**2 + 0.5000*TCC(1,3)/TK(j)**3 + 0.0970*TCC(1,3)**3/TK(j)**4 \\
&\quad + 0.0073*TCC(1,3)**8/TK(j)**9 \\
df414(j) &= -0.4600*TCC(1,4)/TK(j)**2 + 0.5000*TCC(1,4)/TK(j)**3 + 0.0970*TCC(1,4)**3/TK(j)**4 \\
&\quad + 0.0073*TCC(1,4)**8/TK(j)**9 \\
df422(j) &= -0.4600*TCC(2,2)/TK(j)**2 + 0.5000*TCC(2,2)/TK(j)**3 + 0.0970*TCC(2,2)**3/TK(j)**4 \\
&\quad + 0.0073*TCC(2,2)**8/TK(j)**9 \\
df423(j) &= -0.4600*TCC(2,3)/TK(j)**2 + 0.5000*TCC(2,3)/TK(j)**3 + 0.0970*TCC(2,3)**3/TK(j)**4 \\
&\quad + 0.0073*TCC(2,3)**8/TK(j)**9 \\
df424(j) &= -0.4600*TCC(2,4)/TK(j)**2 + 0.5000*TCC(2,4)/TK(j)**3 + 0.0970*TCC(2,4)**3/TK(j)**4 \\
&\quad + 0.0073*TCC(2,4)**8/TK(j)**9 \\
df433(j) &= -0.4600*TCC(3,3)/TK(j)**2 + 0.5000*TCC(3,3)/TK(j)**3 + 0.0970*TCC(3,3)**3/TK(j)**4 \\
&\quad + 0.0073*TCC(3,3)**8/TK(j)**9 \\
df434(j) &= -0.4600*TCC(3,4)/TK(j)**2 + 0.5000*TCC(3,4)/TK(j)**3 + 0.0970*TCC(3,4)**3/TK(j)**4 \\
&\quad + 0.0073*TCC(3,4)**8/TK(j)**9 \\
df444(j) &= -0.4600*TCC(4,4)/TK(j)**2 + 0.5000*TCC(4,4)/TK(j)**3 + 0.0970*TCC(4,4)**3/TK(j)**4 \\
&\quad + 0.0073*TCC(4,4)**8/TK(j)**9 \\
df511(j) &= (5.769770 - 6.181427*MUR(1,1) + 2.283270*MUR(1,1)**2 - 0.2649074*MUR(1,1)**3) \\
&\quad *TCC(1,1)/TK(j)**2 \\
df512(j) &= (5.769770 - 6.181427*MUR(1,2) + 2.283270*MUR(1,2)**2 - 0.2649074*MUR(1,2)**3) \\
&\quad *TCC(1,2)/TK(j)**2 \\
df513(j) &= (5.769770 - 6.181427*MUR(1,3) + 2.283270*MUR(1,3)**2 - 0.2649074*MUR(1,3)**3) \\
&\quad *TCC(1,3)/TK(j)**2 \\
df514(j) &= (5.769770 - 6.181427*MUR(1,4) + 2.283270*MUR(1,4)**2 - 0.2649074*MUR(1,4)**3) \\
&\quad *TCC(1,4)/TK(j)**2 \\
df522(j) &= (5.769770 - 6.181427*MUR(2,2) + 2.283270*MUR(2,2)**2 - 0.2649074*MUR(2,2)**3) \\
&\quad *TCC(2,2)/TK(j)**2
\end{aligned}$$

$$\begin{aligned}
df523(j) &= (5.769770 - 6.181427*MUR(2,3) + 2.283270*MUR(2,3)**2 - 0.2649074*MUR(2,3)**3) \\
&\quad *TCC(2,3)/TK(j)**2 \\
df524(j) &= (5.769770 - 6.181427*MUR(2,4) + 2.283270*MUR(2,4)**2 - 0.2649074*MUR(2,4)**3) \\
&\quad *TCC(2,4)/TK(j)**2 \\
df533(j) &= (5.769770 - 6.181427*MUR(3,3) + 2.283270*MUR(3,3)**2 - 0.2649074*MUR(3,3)**3) \\
&\quad *TCC(3,3)/TK(j)**2 \\
df534(j) &= (5.769770 - 6.181427*MUR(3,4) + 2.283270*MUR(3,4)**2 - 0.2649074*MUR(3,4)**3) \\
&\quad *TCC(3,4)/TK(j)**2 \\
df544(j) &= (5.769770 - 6.181427*MUR(4,4) + 2.283270*MUR(4,4)**2 - 0.2649074*MUR(4,4)**3) \\
&\quad *TCC(4,4)/TK(j)**2 \\
df611(j) &= 101.49*EXP(-6.6*TK(j)/TCC(1,1)) \\
df612(j) &= 101.49*EXP(-6.6*TK(j)/TCC(1,2)) \\
df613(j) &= 101.49*EXP(-6.6*TK(j)/TCC(1,3)) \\
df614(j) &= 101.49*EXP(-6.6*TK(j)/TCC(1,4)) \\
df622(j) &= 101.49*EXP(-6.6*TK(j)/TCC(2,2)) \\
df623(j) &= 101.49*EXP(-6.6*TK(j)/TCC(2,3)) \\
df624(j) &= 101.49*EXP(-6.6*TK(j)/TCC(2,4)) \\
df633(j) &= 101.49*EXP(-6.6*TK(j)/TCC(3,3)) \\
df634(j) &= 101.49*EXP(-6.6*TK(j)/TCC(3,4)) \\
df644(j) &= 101.49*EXP(-6.6*TK(j)/TCC(4,4))
\end{aligned}$$

Material Balance Equations:

$$\begin{aligned}
0 &= f(1,i) - (1 + R)*L(1)*u(1,i)/(R * (u(1,1) + u(1,2) + u(1,3) + u(1,4))) + v(2,i) - \text{der}(u(1,i)) \\
&\quad - \text{for } i=[1,4] \\
0 &= f(j,i) + L(j-1)*u(j-1,i)/(u(j-1,1) + u(j-1,2) + u(j-1,3) + u(j-1,4)) - L(j)*u(j,i)/(u(j,1) + u(j,2) + u(j,3) \\
&\quad + u(j,4)) - v(j,i) + v(j+1,i) - \text{der}(u(j,i)) \\
&\quad - \text{for } i=[1,4], j=[2,49] \\
0 &= f(50,i) + L(49)*u(49,i)/(u(49,1) + u(49,2) + u(49,3) + u(49,4)) - L(50)*u(50,i)/(u(50,1) + u(50,2) \\
&\quad + u(50,3) + u(50,4)) - v(50,i) - \text{der}(u(50,i)) \\
&\quad - \text{for } i=[1,4]
\end{aligned}$$

Equilibrium Equations:

$$\begin{aligned}
0 &= Y(1,i)*PHIV(1,i)/(Y(1,1) + Y(1,2) + Y(1,3) + Y(1,4)) - u(1,i)*GAM(1,i)*K(1,i)*PHIOL(j,i)/(u(1,1) \\
&\quad + u(1,2) + u(1,3) + u(1,4)) \\
0 &= Y(1,1) + Y(1,2) + Y(1,3) + Y(1,4) - 1.0 \\
0 &= v(j,i)*PHIV(j,i)/(v(j,1) + v(j,2) + v(j,3) + v(j,4)) - u(j,i)*GAM(j,i)*K(j,i)*PHIOL(j,i)/(u(j,1) + \\
&\quad u(j,2) + u(j,3) + u(j,4)) \\
&\quad - j=[2,50] \\
K(j,i) &= PS(j,i)/P(j) \\
GAM(j,i) &= (EXP(1 - u(j,1)*LAMB(j,1,i)/(u(j,1)*LAMB(j,1,1) + u(j,1)*LAMB(j,1,2) + \\
&\quad u(j,1)*LAMB(j,1,3) + u(j,1)*LAMB(j,1,4)) + u(j,2)*LAMB(j,2,i)/(u(j,2)*LAMB(j,2,1) + \\
&\quad u(j,2)*LAMB(j,2,2) + u(j,2)*LAMB(j,2,3) + u(j,2)*LAMB(j,2,4)) + \\
&\quad u(j,3)*LAMB(j,3,i)/(u(j,3)*LAMB(j,3,1) + u(j,3)*LAMB(j,3,2) + u(j,3)*LAMB(j,3,3) + \\
&\quad u(j,3)*LAMB(j,3,4)) + u(j,4)*LAMB(j,4,i)/(u(j,4)*LAMB(j,4,1) + u(j,4)*LAMB(j,4,2) + \\
&\quad u(j,4)*LAMB(j,4,3) + u(j,4)*LAMB(j,4,4))) * HOLD(j)/(u(j,1)*LAMB(j,1,i) + u(j,2)*LAMB(j,2,i) \\
&\quad + u(j,3)*LAMB(j,3,i) + u(j,4)*LAMB(j,4,i)) \\
LAMB(j,i,k) &= ALPH(j,k)/ALPH(j,i) * EXP(WLAMB(k,i)/(RR(4)*T(j)))
\end{aligned}$$

$$\begin{aligned}
& \text{ALPH}(j,i) = \text{MV}(1,i) + \text{MV}(2,i)*\text{T}(j) + \text{MV}(3,i)*\text{T}(j)**2 \\
& \text{PHIS}(j,i) = \text{EXP}(f1(j,i) + f2(j,i) + \text{WW}(i)) \\
& \text{TR}(j,i) = \text{T}(j)/\text{TC}(i) \\
& \quad \text{note that TR has the dimension of [Rankine/Kelvin]} \\
& f1(j,i) = -3.5021358 + \text{TR}(j,i)*(5.6085595 + \text{TR}(j,i)*(-3.076574 + \text{TR}(j,i)*0.57335015)) \\
& f2(j,i) = -3.7690418 + \text{TR}(j,i)*(4.3538729 + \text{TR}(j,i)*(0.3166137 + \text{TR}(j,i)*(0.12666184 + \text{TR}(j,i)*(- \\
& \quad 1.1662283 + \text{TR}(j,i)*(-0.10665730 + \text{TR}(j,i)*(0.12147436 + \text{TR}(j,i)*(0.18927037 + \\
& \quad \text{TR}(j,i)*(0.14936906 + \text{TR}(j,i)*(0.024364816 + \text{TR}(j,i)*(-0.068603516 + \text{TR}(j,i)*(-0.015172164 + \\
& \quad \text{TR}(j,i)*0.012089114)))))))))) \\
& \text{PHIOL}(j,i) = \text{PHIS}(j,i)*\text{EXP}(-\text{ALPH}(j,i)*\text{PS}(j,i)/(\text{RR}(2)*\text{TK}(j))) \\
& \text{Bm}(j) = (v(j,1)*(v(j,1)*\text{B}(j,1,1) + v(j,2)*\text{B}(j,1,2) + v(j,3)*\text{B}(j,1,3) + v(j,4)*\text{B}(j,1,4)) + \\
& \quad v(j,2)*(v(j,1)*\text{B}(j,2,1) + v(j,2)*\text{B}(j,2,2) + v(j,3)*\text{B}(j,2,3) + v(j,4)*\text{B}(j,2,4)) + v(j,3)*(v(j,1)*\text{B}(j,3,1) + \\
& \quad v(j,2)*\text{B}(j,3,2) + v(j,3)*\text{B}(j,3,3) + v(j,4)*\text{B}(j,3,4)) + v(j,4)*(v(j,1)*\text{B}(j,4,1) + v(j,2)*\text{B}(j,4,2) + \\
& \quad v(j,3)*\text{B}(j,4,3) + v(j,4)*\text{B}(j,4,4)))/(v(j,1) + v(j,2) + v(j,3) + v(j,4))**2 \\
& \text{TRR}(j,i,k) = \text{TK}(j)/\text{TCC}(i,k) \\
& \text{PC}(j,i,k)*\text{B}(j,i,k)/(\text{RR}()*\text{TCC}(i,k)) = f3(j,i,k) + \text{wH}(i,k)*f4(j,i,k) \\
& f3(j,i,k) = 0.1445 - 0.330/\text{TRR}(j,i,k) - 0.1385/(\text{TRR}(j,i,k)**2) - 0.0121/(\text{TRR}(j,i,k)**3) \\
& f4(j,i,k) = 0.073 + 0.46/\text{TRR}(j,i,k) - 0.5/(\text{TRR}(j,i,k)**2) - 0.097/(\text{TRR}(j,i,k)**3) - \\
& \quad 0.0073/(\text{TRR}(j,i,k)**8) \\
& f5(j,i,k) = -5.237220 + 5.665807*\text{MUR}(i,k) - 2.133816*\text{MUR}(i,k)**2 + 0.2525373*\text{MUR}(i,k)**3 + \\
& \quad (5.769770 - 6.181427*\text{MUR}(i,k) + 2.283270*\text{MUR}(i,k)**2 - 0.2649074*\text{MUR}(i,k)**3)/\text{TRR}(j,i,k) \\
& f6(j,i,k) = \text{EXP}(4.62 - 6.6*\text{TRR}(j,i,k)) \\
& \text{TCC}(i,k) = \text{SQRT}(\text{TC}(i)*\text{TC}(k)) \\
& \text{PCC}(i,k) = 4*\text{TCC}(i,k)*(\text{PC}(i)*\text{VC}(i)/\text{TC}(i) + \text{PC}(k)*\text{VC}(k)/\text{TC}(k))/(\text{VC}(i)**0.33 + \text{VC}(k)**0.33)**3 \\
& \text{MUR}(i,k) = \ln(10**5 * \text{MU}(i)*\text{MU}(k)*\text{PCC}(i,k)/(\text{TCC}(i,k)**2)) \\
& \text{PHIV}(j,i) = \exp(2*(v(j,1)*\text{B}(j,i,1) + v(j,2)*\text{B}(j,i,2) + v(j,3)*\text{B}(j,i,3) + v(j,4)*\text{B}(j,i,4))/(\text{Vm}(j)*(v(j,1) + \\
& \quad v(j,2) + v(j,3) + v(j,4)))) - \text{ZZ}(j) \\
& \text{TK}(j) = 5.0*\text{T}(j)/9.0 \\
& \text{ZZ}(j) = (1. + \text{SQRT}(1. + 4*\text{Bm}(j)*\text{P}(j)/(\text{RR}(3)*\text{TK}(j))))/2.0 \\
& \text{Vm}(j) = \text{Bm}(j)/(\text{ZZ}(j) - 1) \\
& \text{PS}(j,i) = \text{ALOG10}(\text{ANT}(1,i) - (\text{ANT}(2,i)/(\text{ANT}(3,i) + (\text{TK}(j) - 273.15))))
\end{aligned}$$

Pressure Drop Equations:

$$\begin{aligned}
& 0 = \text{P}(1) - \text{P}(2) - (v(2,1) + v(2,2) + v(2,3) + v(2,4))**2 * \text{RHMV}(2)*\text{REF1} \\
& \text{REF1} = (760 - 787.09)/(105.8752**2 * 0.002549852) \\
& 0 = \text{P}(j) - \text{P}(j-1) - g*760*\text{RHOL}(j-1)/(gc*14.696*1728.0) * (\text{HO}(j-1) + \text{HCTR}(j-1)) \\
& \quad \text{— for } j=[3,50] \\
& \text{H0}(j) = 0.186*(\text{UH}(j)/\text{CD}(j))**2 * \text{RHOV}(j+1)/\text{RHOL}(j) \\
& \quad \text{— for } j=[2,49] \\
& \text{HCTR}(j) = \text{FOAM}(j)*(0.4896*(\text{QL}(j)/\text{LW})**0.67 + \text{HW}) \\
& \quad \text{— for } j=[2,49] \\
& \text{QL}(j) = 7.48*L(j)/\text{RHML}(j) \\
& \text{UVA}(j) = (v(j,1) + v(j,2) + v(j,3) + v(j,4))/(\text{AN}*\text{RHMV}(j)*60) \\
& \quad \text{— for } j=[2,49] \\
& \text{FVA}(j) = \text{UVA}(j)*\text{SQRT}(\text{RHOV}(j)) \\
& \quad \text{— for } j=[2,49] \\
& \text{FOAM}(j) = 1 - 0.372192*\text{FVA}(j)**0.177709 \\
& \quad \text{— for } j=[2,49]
\end{aligned}$$

$$\begin{aligned}
UH &= (v(j+1,1) + v(j+1,2) + v(j+1,3) + v(j+1,4)) / (AH(j) * RHMV(j+1) * 60) \\
&\text{--for } j=[2,49] \\
0 &= P(j) - P(j+1) + g * 760 / (gc * 14.696 * 1728) * ((12 * Z(j) - HHUD(j)) * RHOL(j) - \\
&\quad HCTR(j+1) * RHOL(j+1)) \\
&\text{--for } j=[2,49] \\
HHUD(j) &= 0.000003 * (QL / AUD) ** 2 \\
&\text{--for } j=[2,49] \\
0 &= (u(j,1) + u(j,2) + u(j,3) + u(j,4)) - HOLD(j) \\
&\text{--for } j=[2,49] \\
HOLD(j) &= RHML(j) * (HCTR(j) * AA / 12.0 + Z(j) * AD) \\
&\text{--for } j=[2,49] \\
0 &= (u(1,1) + u(1,2) + u(1,3) + u(1,4)) - RHML(1) * VOLREC \\
VOLREC &= LR * ((\pi / 2.0 + ASIN(2 * Z(1) / DR - 1)) * (DR / 2.0) ** 2 + (Z(1) - DR / 2.0) * (Z(1) * DR - \\
&\quad Z(1) ** 2) ** 0.5) \\
0 &= (u(50,1) + u(50,2) + u(50,3) + u(50,4)) - RHML(50) * VOLBTW \\
VOLBTW &= 100 + \pi * Z(50) * DTT ** 2 / 4
\end{aligned}$$

Condenser and Receiver Equations:

$$\begin{aligned}
0 &= Q_{cw} * C_{cw} * (T_{wi} - T_{wo}) * 8.34 + U_{wmo} / 60 * A_w * (T_{mc} - T_{wo}) * (Q_{cw} / Q_{cwo}) ** 1.8 - \\
&\quad U_{cw} * C_{cw} * \text{der}(T_{wo}) \\
0 &= 105.8752 / (v(2,1) + v(2,2) + v(2,3) + v(2,4)) * (U_{pmo} / 60 * A_{pc} * ((1 - \text{ALPHA}) * T(2) + \\
&\quad \text{ALPHA} * T(1) - T_{mc}) ** 3 - Q_C ** 3 \\
0 &= Q_C - U_{wmo} / 60 * (Q_{cs} / Q_{cwo}) ** 1.8 * A_w * (T_{mc} - T_{wo}) - U_{mc} * C_{mc} * \text{der}(T_{mc}) \\
0 &= (P_{w1} - P_{w3} - \text{REF2} * (Q_{cw} / Q_{cwo}) ** 1.8) * CV1 ** 2 - (Q_{cw} / 2) ** 2 \\
\text{REF2} &= 9 \\
0 &= P_{d1} - P_{s1} - \text{HEAD1} \\
\text{HEAD1} &= 9.870927E1 - 9.794161E-3 * (q_1 + q_2) - 1.95175E-6 * (q_1 + q_2) ** 2 - 1.954559E-9 * (q_1 + q_2) ** 3 \\
0 &= q_1 * RHML(1) - L(1) * 7.481 \\
0 &= R * q_2 - q_1 \\
0 &= q_1 ** 2 * RHOL(1) / 62.4 - CV2 ** 2 * (P_{d1} * RHOL(1) * g / (144 * gc) - P(2) * 14.696 / 760) \\
0 &= q_2 ** 2 * RHOL(1) / 62.4 - CV3 ** 2 * (P_{d1} * RHOL(1) * g / (144 * gc) - P_D * 14.696 / 760) \\
0 &= RHOL(1) * (P_{s1} - Z(1) - Z_C) - P(1) * 14.696 * 144 * gc / (760 * g)
\end{aligned}$$

Reboiler and Tower Base Equations:

$$\begin{aligned}
0 &= U_s * A_s / 60 * (T_{sc} - T_{mr}) - Q_R - U_{mr} * C_{mr} * \text{der}(T_{mr}) \\
0 &= U_{pmr} * A_{pmr} / 60 * (T_{mr} - T(50)) - Q_R \\
0 &= P_{s2} - (P(50) * 14.696 * 144 * g / (760 * gc * RHOL(50)) + Z(50) + Z_B) \\
0 &= q_{50} * RHML(50) - L(50) * 7.481 \\
0 &= (P_{d2} * RHOL(50) * g / (144 * gc) - P_B) * CV5 ** 2 - q_{50} ** 2 * RHOL(50) / 62.4 \\
0 &= PSH * CS4 / 60 - W_{sh} / 2 * (1 + 0.00065 * (T_{SH} - T_{SAT})) \\
0 &= W_{sc} - W_{sh} + V_r * \text{der}(RH_{sc}) \\
0 &= RH_{sc} - RH_{osc} \\
RH_{osc} &= 1.031951E-2 + 1.427797E1 * T_{sc} + 0.9414444 * T_{sc} ** 2 + 2.048037 * T_{sc} ** 3 + 5.956991 * T_{sc} ** 4 \\
0 &= W_{sh} * H_{SH} - W_{sc} * h_{LSC} - U_s * A_s / 60 * (T_{sc} - T_{mr}) - \text{der}(E_s) \\
h_{LSC} &= -1.6029E2 + 8.06427E-2 * T_{sc} + 7.361453E-5 * T_{sc} ** 2 + 1.501012E-6 * T_{sc} ** 3 - 9.9964334E- \\
&\quad 10 * T_{sc} ** 4 \\
0 &= V_r * RH_{sc} * HV_{sc} - E_s
\end{aligned}$$

$$\text{HVSC} = 5.448738\text{E}2 + 8.039637\text{E}-1 \cdot \text{Tsc} + 1.931794\text{E}-3 \cdot \text{Tsc}^{**2} - 3.938661\text{E}-6 \cdot \text{Tsc}^{**3} + 1.907853\text{E}-9 \cdot \text{Tsc}^{**4}$$

$$0 = \text{Pd2} - \text{Ps2} - \text{HEAD2}$$

$$\text{HEAD2} = 9.152028\text{E}1 - 6.584299\text{E}-2 \cdot \text{q}(50) + 7.533832\text{E}-5 \cdot \text{q}(50)^{**2} - 4.300139\text{E}-8 \cdot \text{q}(50)^{**3}$$

Valve equations

$$\text{CV1} = \text{CV1CO}(2, \text{ZETA1}) + \text{CV1CO}(3, \text{ZETA1}) \cdot (\text{ZETA1} - \text{CV1CO}(1, \text{ZETA1})) + \text{CV1CO}(4, \text{ZETA1}) \cdot (\text{ZETA1} - \text{CV1CO}(1, \text{ZETA1}))^{**2} + \text{CV1CO}(5, \text{ZETA1}) \cdot (\text{ZETA1} + \text{CV1CO}(1, \text{ZETA1}))^{**3}$$

$$\text{CV2} = \text{CV2CO}(2, \text{ZETA2}) + \text{CV2CO}(3, \text{ZETA2}) \cdot (\text{ZETA2} - \text{CV2CO}(1, \text{ZETA2})) + \text{CV2CO}(4, \text{ZETA2}) \cdot (\text{ZETA2} - \text{CV2CO}(1, \text{ZETA2}))^{**2} + \text{CV2CO}(5, \text{ZETA2}) \cdot (\text{ZETA2} + \text{CV2CO}(1, \text{ZETA2}))^{**3}$$

$$\text{CV3} = \text{CV3CO}(2, \text{ZETA3}) + \text{CV3CO}(3, \text{ZETA3}) \cdot (\text{ZETA3} - \text{CV3CO}(1, \text{ZETA3})) + \text{CV3CO}(4, \text{ZETA3}) \cdot (\text{ZETA3} - \text{CV3CO}(1, \text{ZETA3}))^{**2} + \text{CV3CO}(5, \text{ZETA3}) \cdot (\text{ZETA3} + \text{CV3CO}(1, \text{ZETA3}))^{**3}$$

$$\text{CS4} = \text{CS4CO}(2, \text{ZETA4}) + \text{CS4CO}(3, \text{ZETA4}) \cdot (\text{ZETA4} - \text{CS4CO}(1, \text{ZETA4})) + \text{CS4CO}(4, \text{ZETA4}) \cdot (\text{ZETA4} - \text{CS4CO}(1, \text{ZETA4}))^{**2} + \text{CS4CO}(5, \text{ZETA4}) \cdot (\text{ZETA4} + \text{CS4CO}(1, \text{ZETA4}))^{**3}$$

$$\text{CV5} = \text{CV5CO}(2, \text{ZETA5}) + \text{CV5CO}(3, \text{ZETA5}) \cdot (\text{ZETA5} - \text{CV5CO}(1, \text{ZETA5})) + \text{CV5CO}(4, \text{ZETA5}) \cdot (\text{ZETA5} - \text{CV5CO}(1, \text{ZETA5}))^{**2} + \text{CV5CO}(5, \text{ZETA5}) \cdot (\text{ZETA5} + \text{CV5CO}(1, \text{ZETA5}))^{**3}$$

Control Equations:

$$0 = \text{CI1} + 12.0 - 0.032 \cdot \text{P}(1)$$

$$0 = \text{CO1} - \text{XKC1} \cdot (\text{CI1} - \text{CISP1} + \text{I1} / \text{TAUI1})$$

$$0 = \text{CI1} - \text{CISP1} - \text{der}(\text{I1})$$

$$0 = -0.25 + 0.0625 \cdot \text{CO1} - \text{ZETA1} - \text{TAUV1} \cdot \text{der}(\text{ZETA1})$$

$$0 = \text{CI2} - 4.0 - (\text{q1} / 200)^{**2}$$

$$0 = \text{CO2} - \text{XKC2} \cdot (\text{CISP2} - \text{CI2} + \text{I2} / \text{TAUI2})$$

$$0 = \text{CISP2} - \text{CI2} - \text{der}(\text{I2})$$

$$0 = -0.25 + 0.0625 \cdot \text{CO2} - \text{ZETA2} - \text{TAUV2} \cdot \text{der}(\text{ZETA2})$$

$$0 = \text{CI3} - 4.0 - 1.6 \cdot \text{Z}(1)$$

$$0 = \text{CO3} - \text{XKC3} \cdot (\text{CI3} - \text{CISP3} + \text{I3} / \text{TAUI3})$$

$$0 = \text{CI3} - \text{CISP3} - \text{der}(\text{I3})$$

$$0 = -0.25 + 0.0625 \cdot \text{CO3} - \text{ZETA3} - \text{TAUV3} \cdot \text{der}(\text{ZETA3})$$

$$0 = \text{CI5} + 20.0 - 4 \cdot \text{Z}(50)$$

$$0 = \text{CO5} - \text{XKC5} \cdot (\text{CI5} - \text{CISP5} + \text{I5} / \text{TAUI5})$$

$$0 = \text{CI5} - \text{CISP5} - \text{der}(\text{I5})$$

$$0 = -0.25 + 0.0625 \cdot \text{CO5} - \text{ZETA5} - \text{TAUV5} \cdot \text{der}(\text{ZETA5})$$

$$0 = \text{CI4} - 4.0 - 16 \cdot (\text{Wsh} / 3000)^{**2}$$

$$0 = \text{CO4} - \text{XKC4} \cdot (\text{CO4} - \text{CI4} + \text{I4} / \text{TAUI4})$$

$$0 = \text{CO4} - \text{CI4} - \text{der}(\text{I4})$$

$$0 = -0.25 + 0.0625 \cdot \text{CO4} - \text{ZETA4} - \text{TAUV4} \cdot \text{der}(\text{ZETA4})$$

$$0 = \text{T}(35) - \text{TM} - \text{TAUM} \cdot \text{der}(\text{TM})$$

$$0 = \text{CO6} - \text{XKC6} \cdot (\text{CISP6} - \text{CI6} + \text{I6} / \text{TAUI6})$$

$$0 = \text{CISP6} - \text{CI6} - \text{der}(\text{I6})$$

$$0 = \text{CI6} + 236 - 0.4 \cdot \text{TM}$$

Forcing Functions:

$f(3,1) = 0.0$	$f(3,2) = 0.0$	$f(3,3) = 0.0$	$f(3,4) = 5.0$
$f(5,1) = 25.0$	$f(5,2) = 0.5$	$f(5,3) = 5.0$	$f(5,4) = 197.5$
$f(21,1) = 65.0$	$f(21,2) = 25.0$	$f(21,3) = 5.0$	$f(21,4) = 5.0$
$f(j \neq 3,5,21, i) = 0$			
$Hf(3) = 6118.898$	$Hf(5) = 513543.3$	$Hf(21) = 146509.6$	$Hf(j \neq 3,5,21) = 0$
$Twi = 545$	$Pw1 = 60$	$Pw3 = 35$	$PD = 40$
$PB = 30$	$TSH = 960.0$	$PSH = 255.0$	$HVSH = 1262.8$
$TSAT = 862.7$			
$CISP1 = 12.32$	$CISP2 = 10.0058$	$CISP3 = 8.8$	$CISP5 = 12.0$
$CISP6 = 14.49044 \rightarrow 15.49044$			

Constant Functions(see tables of Appendix C):

$ANT(n,i) = \dots$	$CVkCO(a,Zeta) = \dots$	$ETTA(i,k) = \dots$
$hLCOEF(n,i) = \dots$	$HVCOEF(n,i) = \dots$	$MU(i) = \dots$
$PC(i) = \dots$	$TC(i) = \dots$	$VC(i) = \dots$
$wH(i,k) = \dots$		

Constants:

$AA=141.372$	$AD=17.6715$	$ALPHA=0.2$
$AN=141.372$	$Apc=16022.16$	$Apmr=3361.826$
$As=3844.168$	$AT=176.714$	$AUD=0.908375$
$Aw=13940.0$	$Ccw=1.0$	$Cmc=0.12$
$Cmr=0.12$	$DH=0.1875$	$DR=10.0$
$DTT=15.0$	$g=32.0898$	$gc=g$ (Newton's second law conversion factor.)
$HSH=1262.8$	$HW=1.0$	$HWSP=1.25$
$LR=16.0$	$LW=130.806$	$LWSP=149.0$
$P1P2R=27.09$	$PB=30$	$PD=40$
$pii=3.14159$	$PSH=255.0$	$Pw2Pw3=9.0$
$Pw3=35$	$Qcwo=8653.0$	$RHO2VR=0.002549852$
$Sv2IR=105.8752$	$TAUM=0.20$	$TT=0.09375$
$Ucw=17160.0$	$Umc=45000.0$	$Umr=11000.0$
$Upmo=213.0$	$Upmr=300.0$	$Us=1000.0$
$Uwmo=1250.0$	$Vr=68.83$	$ZB=10.0$
$ZC=5.0$		

Initial Steady-State Values:

$CI1 = 12.32$	$CI2 = 10.006$	$CI3 = 8.800$	$CI4 = 7.239$	$CI5 = 12.000$
$CI6 = 14.491$	$CO1 = 11.589$	$CO2 = 13.834$	$CO3 = 10.191$	$CO4 = 15.076$
$CO5 = 9.428$	$CO6 = 7.239$	$Es = 10443.20$	$I1 = 23.179$	$I2 = 5.534$

I3 = 6.948	I4 = 25.127	I5 = 18.857	I6 = 8.687	Pd1 = 135.33
Pd2 = 132.31	Ps1 = 44.89	Ps2 = 71.21	q1 = 490.14	q2 = 196.01
q50 = 923.47	QC = 1122967.0	Qcw = 5338.92	QR = 1360293	R = 2.5
TM = 626.22	Tmc = 579.44	Tmr = 726.17	Tsc = 747.4	Two = 570.22
Wsh = 1349.84	ZETA1 = 0.47433	ZETA2 = 0.61463	ZETA3 = 0.38692	ZETA4 = 0.69228
ZETA5 = 0.33928				

B.2 DYMOLA code of Gallun's model

There is no guarantee that the equations are bug-free, only that the form of these equations are correct. Note that the equations of Appendix B.1 are mostly used as they were given. DYMOLA will solve for the appropriate variable. The following code is broken into submodels (model types) and so can be used for any number of stages and feeds. The final assemblage of the submodels, model distGh, is for a 3 stage distillation column.

```
{Dymola version of Gallun's Distillation Column-distGh.dym}
{with one modification: 3 stages instead of 50}
{The number of non-trivial equations is      715}
{The number of unknown variables is        726}

{----Energy Balance Equations:}
model type engder
  cut dB(dBmj, dB11, dB12, dB13, dB14, dB22, dB23, dB24, ->
      dB33, dB34, dB44)
  cut vji(vj1, vj2, vj3, vj4, sumvj)
  cut T(Tj, TKj)

  local  df311, df312, df313, df314, df322, df323, df324, ->
      df333, df334, df344, df411, df412, df413, df414, ->
      df422, df423, df424, df433, df434, df444, ->
      df511, df512, df513, df514, df522, df523, df524, ->
      df533, df534, df544, df611, df612, df613, df614, ->
      df622, df623, df624, df633, df634, df644

  dBmj = (vj1*vj1*dB11 + vj1*vj2*dB12 ->
      + vj1*vj3*dB13 + vj1*vj4*dB14 ->
      + vj2*vj1*dB12 + vj2*vj2*dB22 ->
      + vj2*vj3*dB23 + vj2*vj4*dB24 ->
      + vj3*vj1*dB13 + vj3*vj2*dB23 ->
      + vj3*vj3*dB33 + vj3*vj4*dB34 ->
      + vj4*vj1*dB14 + vj4*vj2*dB24 ->
      + vj4*vj3*dB34 + vj4*vj4*dB44)/sumvj**2

  dB11 = RR(1)*TCC(1,1)/PCC(1,1)*(df311 + wH(1,1)*df411 ->
      + df511 + ETТА(1,1)*df611)
  dB12 = RR(1)*TCC(1,2)/PCC(1,2)*(df312 + wH(1,2)*df412 ->
      + df512 + ETТА(1,2)*df612)
  dB13 = RR(1)*TCC(1,3)/PCC(1,3)*(df313 + wH(1,3)*df413 ->
      + df513 + ETТА(1,3)*df613)
  dB14 = RR(1)*TCC(1,4)/PCC(1,4)*(df314 + wH(1,4)*df414 ->
      + df514 + ETТА(1,4)*df614)

  dB22 = RR(1)*TCC(2,2)/PCC(2,2)*(df322 + wH(2,2)*df422 ->
      + df522 + ETТА(2,2)*df622)
  dB23 = RR(1)*TCC(2,3)/PCC(2,3)*(df323 + wH(2,3)*df423 ->
      + df523 + ETТА(2,3)*df623)
```



```

dB24 = RR(1)*TCC(2,4)/PCC(2,4)*(df324 + wH(2,4)*df424 ->
+ df524 + ETTA(2,4)*df624)
dB33 = RR(1)*TCC(3,3)/PCC(3,3)*(df333 + wH(3,3)*df433 ->
+ df533 + ETTA(3,3)*df633)
dB34 = RR(1)*TCC(3,4)/PCC(3,4)*(df334 + wH(3,4)*df434 ->
+ df534 + ETTA(3,4)*df634)
dB44 = RR(1)*TCC(4,4)/PCC(4,4)*(df344 + wH(4,4)*df444 ->
+ df544 + ETTA(4,4)*df644)

df311 = -0.330*TCC(1,1)/TKj**2 + 0.1385*TCC(1,1)**2/TKj**3 ->
+ 0.0121*TCC(1,1)**3/TKj**4
df312 = -0.330*TCC(1,2)/TKj**2 + 0.1385*TCC(1,2)**2/TKj**3 ->
+ 0.0121*TCC(1,2)**3/TKj**4
df313 = -0.330*TCC(1,1)/TKj**2 + 0.1385*TCC(1,3)**2/TKj**3 ->
+ 0.0121*TCC(1,3)**3/TKj**4
df314 = -0.330*TCC(1,4)/TKj**2 + 0.1385*TCC(1,4)**2/TKj**3 ->
+ 0.0121*TCC(1,4)**3/TKj**4

df322 = -0.330*TCC(2,2)/TKj**2 + 0.1385*TCC(2,2)**2/TKj**3 ->
+ 0.0121*TCC(2,2)**3/TKj**4
df323 = -0.330*TCC(2,3)/TKj**2 + 0.1385*TCC(2,3)**2/TKj**3 ->
+ 0.0121*TCC(2,3)**3/TKj**4
df324 = -0.330*TCC(2,4)/TKj**2 + 0.1385*TCC(2,4)**2/TKj**3 ->
+ 0.0121*TCC(2,4)**3/TKj**4

df333 = -0.330*TCC(3,3)/TKj**2 + 0.1385*TCC(3,3)**2/TKj**3 ->
+ 0.0121*TCC(3,3)**3/TKj**4
df334 = -0.330*TCC(3,4)/TKj**2 + 0.1385*TCC(3,4)**2/TKj**3 ->
+ 0.0121*TCC(3,4)**3/TKj**4

df344 = -0.330*TCC(4,4)/TKj**2 + 0.1385*TCC(4,4)**2/TKj**3 ->
+ 0.0121*TCC(4,4)**3/TKj**4

df411 = - 0.4600*TCC(1,1)/TKj**2 ->
+ 0.5000*TCC(1,1)/TKj**3 ->
+ 0.0970*TCC(1,1)**3/TKj**4 ->
+ 0.0073*TCC(1,1)**8/TKj**9 ->
df412 = - 0.4600*TCC(1,2)/TKj**2 ->
+ 0.5000*TCC(1,2)/TKj**3 ->
+ 0.0970*TCC(1,2)**3/TKj**4 ->
+ 0.0073*TCC(1,2)**8/TKj**9 ->
df413 = - 0.4600*TCC(1,3)/TKj**2 ->
+ 0.5000*TCC(1,3)/TKj**3 ->
+ 0.0970*TCC(1,3)**3/TKj**4 ->
+ 0.0073*TCC(1,3)**8/TKj**9 ->
df414 = - 0.4600*TCC(1,4)/TKj**2 ->
+ 0.5000*TCC(1,4)/TKj**3 ->
+ 0.0970*TCC(1,4)**3/TKj**4 ->
+ 0.0073*TCC(1,4)**8/TKj**9 ->

df422 = - 0.4600*TCC(2,2)/TKj**2 ->
+ 0.5000*TCC(2,2)/TKj**3 ->
+ 0.0970*TCC(2,2)**3/TKj**4 ->
+ 0.0073*TCC(2,2)**8/TKj**9 ->
df423 = - 0.4600*TCC(2,3)/TKj**2 ->
+ 0.5000*TCC(2,3)/TKj**3 ->
+ 0.0970*TCC(2,3)**3/TKj**4 ->
+ 0.0073*TCC(2,3)**8/TKj**9 ->
df424 = - 0.4600*TCC(2,4)/TKj**2 ->
+ 0.5000*TCC(2,4)/TKj**3 ->
+ 0.0970*TCC(2,4)**3/TKj**4 ->

```

```

+ 0.0073*TCC(2,4)**8/TKj**9

df433 = - 0.4600*TCC(3,3)/TKj**2 ->
+ 0.5000*TCC(3,3)/TKj**3 ->
+ 0.0970*TCC(3,3)**3/TKj**4 ->
+ 0.0073*TCC(3,3)**8/TKj**9
df434 = - 0.4600*TCC(3,4)/TKj**2 ->
+ 0.5000*TCC(3,4)/TKj**3 ->
+ 0.0970*TCC(3,4)**3/TKj**4 ->
+ 0.0073*TCC(3,4)**8/TKj**9

df444 = - 0.4600*TCC(4,4)/TKj**2 ->
+ 0.5000*TCC(4,4)/TKj**3 ->
+ 0.0970*TCC(4,4)**3/TKj**4 ->
+ 0.0073*TCC(4,4)**8/TKj**9

df511 = (5.769770 - 6.181427*MUR(1,1) ->
+ 2.283270*MUR(1,1)**2 ->
- 0.2649074*MUR(1,1)**3) *TCC(1,1)/TKj**2
df512 = (5.769770 - 6.181427*MUR(1,2) ->
+ 2.283270*MUR(1,2)**2 ->
- 0.2649074*MUR(1,2)**3) *TCC(1,2)/TKj**2
df513 = (5.769770 - 6.181427*MUR(1,3) ->
+ 2.283270*MUR(1,3)**2 ->
- 0.2649074*MUR(1,3)**3) *TCC(1,3)/TKj**2
df514 = (5.769770 - 6.181427*MUR(1,4) ->
+ 2.283270*MUR(1,4)**2 ->
- 0.2649074*MUR(1,4)**3) *TCC(1,4)/TKj**2

df522 = (5.769770 - 6.181427*MUR(2,2) ->
+ 2.283270*MUR(2,2)**2 ->
- 0.2649074*MUR(2,2)**3) *TCC(2,2)/TKj**2
df523 = (5.769770 - 6.181427*MUR(2,3) ->
+ 2.283270*MUR(2,3)**2 ->
- 0.2649074*MUR(2,3)**3) *TCC(2,3)/TKj**2
df524 = (5.769770 - 6.181427*MUR(2,4) ->
+ 2.283270*MUR(2,4)**2 ->
- 0.2649074*MUR(2,4)**3) *TCC(2,4)/TKj**2

df533 = (5.769770 - 6.181427*MUR(3,3) ->
+ 2.283270*MUR(3,3)**2 ->
- 0.2649074*MUR(3,3)**3) *TCC(3,3)/TKj**2
df534 = (5.769770 - 6.181427*MUR(3,4) ->
+ 2.283270*MUR(3,4)**2 ->
- 0.2649074*MUR(3,4)**3) *TCC(3,4)/TKj**2

df544 = (5.769770 - 6.181427*MUR(4,4) ->
+ 2.283270*MUR(4,4)**2 ->
- 0.2649074*MUR(4,4)**3) *TCC(4,4)/TKj**2

df611 = 101.49*EXP(-6.6*TKj/TCC(1,1))
df612 = 101.49*EXP(-6.6*TKj/TCC(1,2))
df613 = 101.49*EXP(-6.6*TKj/TCC(1,3))
df614 = 101.49*EXP(-6.6*TKj/TCC(1,4))

df622 = 101.49*EXP(-6.6*TKj/TCC(2,2))
df623 = 101.49*EXP(-6.6*TKj/TCC(2,3))
df624 = 101.49*EXP(-6.6*TKj/TCC(2,4))

df633 = 101.49*EXP(-6.6*TKj/TCC(3,3))
df634 = 101.49*EXP(-6.6*TKj/TCC(3,4))

```

```

df644 = 101.49*EXP(-6.6*TKj/TCC(4,4))
end

model type engb1
terminal R, QC, Ej, Pj, Lj

cut eql1(ZZj, Bmj)
cut uji(uj1, uj2, uj3, uj4, HLDPj)
cut HVjpi(HVjp1, HVjp2, HVjp3, HVjp4)
cut vjpi(vjp1, vjp2, vjp3, vjp4, sumvjp)
cut T(Tj, TKj)

local hLj1, hLj2, hLj3, hLj4
terminal Hfj

0 = Hfj + vjp1*HVjp1 + vjp2*HVjp2 + vjp3*HVjp3+vjp4*HVjp4 - (1 + -
>
    R)*Lj*Ej/(R * HLDPj) - QC - der(Ej)

0 = uj1*hLj1 + uj2*hLj2 + uj3*hLj3 + uj4*hLj4 - Ej

hLj1 = hLCO(1,1) + hLCO(2,1)*Tj + hLCO(3,1)*Tj**2
hLj2 = hLCO(1,2) + hLCO(2,2)*Tj + hLCO(3,2)*Tj**2
hLj3 = hLCO(1,3) + hLCO(2,3)*Tj + hLCO(3,3)*Tj**2
hLj4 = hLCO(1,4) + hLCO(2,4)*Tj + hLCO(3,4)*Tj**2
end

model type engbj
submodel engder

terminal Ej, Pj, Lj, Ljm, Ejm

cut eql1(ZZj, Bmj)
cut uji(uj1, uj2, uj3, uj4, HLDPj)
cut ujmi(ujm1, ujm2, ujm3, ujm4, HLDPjm)
cut HVji(HVj1, HVj2, HVj3, HVj4)
cut HVjpi(HVjp1, HVjp2, HVjp3, HVjp4)
cut vji(vj1, vj2, vj3, vj4, sumvji)
cut vjpi(vjp1, vjp2, vjp3, vjp4, sumvjp)
cut T(Tj, TKj)
cut dB(dBmj, dB11, dB12, dB13, dB14, dB22, dB23, dB24, ->
    dB33, dB34, dB44)

local hLj1, hLj2, hLj3, hLj4, OMEGAj, H0j1, H0j2, H0j3, H0j4

terminal Hfj

connect engder:dB at dB
connect engder:T at T
connect engder:vji at vji

0 = Hfj + Ljm*Ejm/HLDPjm - Lj*Ej/HLDPj + vjp1*HVjp1 - vj1*HVj1 + -
>
    vjp2*HVjp2 - vj2*HVj2 + vjp3*HVjp3 - vj3*HVj3 + vjp4*HVjp4 - -
>
    vj4*HVj4 - der(Ej)

0 = uj1*hLj1 + uj2*hLj2 + uj3*hLj3 + uj4*hLj4 - Ej

```

```

hLj1 = hLCO(1,1) + hLCO(2,1)*Tj + hLCO(3,1)*Tj**2
hLj2 = hLCO(1,2) + hLCO(2,2)*Tj + hLCO(3,2)*Tj**2
hLj3 = hLCO(1,3) + hLCO(2,3)*Tj + hLCO(3,3)*Tj**2
hLj4 = hLCO(1,4) + hLCO(2,4)*Tj + hLCO(3,4)*Tj**2

HVj1 = H0j1 + OMEGAj
HVj2 = H0j2 + OMEGAj
HVj3 = H0j3 + OMEGAj
HVj4 = H0j4 + OMEGAj

H0j1 = HVCO(1,1)+HVCO(2,1)*Tj+HVCO(3,1)*Tj**2+HVCO(4,1)*Tj**3+ ->
HVCO(5,1)*Tj**4
H0j2 = HVCO(1,2)+HVCO(2,2)*Tj+HVCO(3,2)*Tj**2+HVCO(4,2)*Tj**3+ ->
HVCO(5,2)*Tj**4
H0j3 = HVCO(1,3)+HVCO(2,3)*Tj+HVCO(3,3)*Tj**2+HVCO(4,3)*Tj**3+ ->
HVCO(5,3)*Tj**4
H0j4 = HVCO(1,4)+HVCO(2,4)*Tj+HVCO(3,4)*Tj**2+HVCO(4,4)*Tj**3+ ->
HVCO(5,4)*Tj**4

OMEGAj = (2 - 1/ZZj)*Pj/(2*ZZj -1) * (TKj*dBmj - Bmj)
end

model type engbN
submodel engder
terminal Ej, Pj, Lj, Ljm, Ejm, QR

cut eql1(ZZj, Bmj)
cut uji(uj1, uj2, uj3, uj4, HLDpj)
cut ujmi(ujm1, ujm2, ujm3, ujm4, HLDpj)
cut HVji(HVj1, HVj2, HVj3, HVj4)
cut vji(vj1, vj2, vj3, vj4, sumvj)
cut T(Tj, TKj)
cut dB(dBmj, dB11, dB12, dB13, dB14, dB22, dB23, dB24, ->
dB33, dB34, dB44)

local hLj1, hLj2, hLj3, hLj4, OMEGAj, H0j1, H0j2, H0j3, H0j4

terminal Hfj

connect engder:dB at dB
connect engder:T at T
connect engder:vji at vji

0 = Hfj + Ljm*Ejm/HLDpj - Lj*Ej/HLDpj - vj1*HVj1 - vj2*HVj2 - ->
vj3*HVj3 - vj4*HVj4 + QR - der(Ej)

0 = uj1*hLj1 + uj2*hLj2 + uj3*hLj3 + uj4*hLj4 - Ej

hLj1 = hLCO(1,1) + hLCO(2,1)*Tj + hLCO(3,1)*Tj**2
hLj2 = hLCO(1,2) + hLCO(2,2)*Tj + hLCO(3,2)*Tj**2
hLj3 = hLCO(1,3) + hLCO(2,3)*Tj + hLCO(3,3)*Tj**2
hLj4 = hLCO(1,4) + hLCO(2,4)*Tj + hLCO(3,4)*Tj**2

HVj1 = H0j1 + OMEGAj
HVj2 = H0j2 + OMEGAj
HVj3 = H0j3 + OMEGAj
HVj4 = H0j4 + OMEGAj

H0j1 = HVCO(1,1) +HVCO(2,1)*Tj +HVCO(3,1)*Tj**2+HVCO(4,1)*Tj**3+ -
>
HVCO(5,1)*Tj**4

```

```

H0j2 = HVCO(1,2) +HVCO(2,2)*Tj+HVCO(3,2)*Tj**2+HVCO(4,2)*Tj**3 + -
>
      HVCO(5,2)*Tj**4
H0j3 = HVCO(1,3) +HVCO(2,3)*Tj+HVCO(3,3)*Tj**2+HVCO(4,3)*Tj**3 + -
>
      HVCO(5,3)*Tj**4
H0j4 = HVCO(1,4) + HVCO(2,4)*Tj+HVCO(3,4)*Tj**2+HVCO(4,4)*Tj**3+ -
>
      HVCO(5,4)*Tj**4

OMEGAj = (2 - 1/ZZj)*Pj/(2*ZZj -1) * (TKj*dBmj - Bmj)
end

{----Material Balance Equations:}
model type matb1
  cut uji(uj1, uj2, uj3, uj4, HLDP1)
  cut vjpi(vjp1, vjp2, vjp3, vjp4, sumvjp)
  terminal R, Lj

  terminal fj1, fj2, fj3, fj4

  0 = fj1 - (1 + R)*Lj*uj1/(R * HLDP1) + vjp1 - der(uj1)
  0 = fj2 - (1 + R)*Lj*uj2/(R * HLDP1) + vjp2 - der(uj2)
  0 = fj3 - (1 + R)*Lj*uj3/(R * HLDP1) + vjp3 - der(uj3)
  0 = fj4 - (1 + R)*Lj*uj4/(R * HLDP1) + vjp4 - der(uj4)
  HLDP1 = uj1 + uj2 + uj3 + uj4
end

model type matbj
  cut uji(uj1, uj2, uj3, uj4, HLDPj)
  cut ujmi(ujm1, ujm2, ujm3, ujm4, HLDPjm)
  cut vji(vj1, vj2, vj3, vj4, sumvj)
  cut vjpi(vjp1, vjp2, vjp3, vjp4, sumvjp)
  terminal Lj, Ljm

  terminal fj1, fj2, fj3, fj4

  0 = fj1 + Ljm*ujm1/HLDPjm - Lj*uj1/HLDPj - vj1 + vjp1 - der(uj1)
  0 = fj2 + Ljm*ujm2/HLDPjm - Lj*uj2/HLDPj - vj2 + vjp2 - der(uj2)
  0 = fj3 + Ljm*ujm3/HLDPjm - Lj*uj3/HLDPj - vj3 + vjp3 - der(uj3)
  0 = fj4 + Ljm*ujm4/HLDPjm - Lj*uj4/HLDPj - vj4 + vjp4 - der(uj4)
  HLDPj = uj1 + uj2 + uj3 + uj4
end

model type matbN
  cut uji(uj1, uj2, uj3, uj4, HLDPj)
  cut ujmi(ujm1, ujm2, ujm3, ujm4, HLDPjm)
  cut vji(vj1, vj2, vj3, vj4, sumvj)
  terminal Lj, Ljm

  terminal fj1, fj2, fj3, fj4

  0 = fj1 + Ljm*ujm1/HLDPjm - Lj*uj1/HLDPj - vj1 - der(uj1)
  0 = fj2 + Ljm*ujm2/HLDPjm - Lj*uj2/HLDPj - vj2 - der(uj2)
  0 = fj3 + Ljm*ujm3/HLDPjm - Lj*uj3/HLDPj - vj3 - der(uj3)
  0 = fj4 + Ljm*ujm4/HLDPjm - Lj*uj4/HLDPj - vj4 - der(uj4)
  HLDPj = uj1 + uj2 + uj3 + uj4
end

{----Equilibrium Equations:}
model type eqlcom

```

```

cut eqlc(LMBjik, ALPHji, ALPHjk, Bjik)
cut T(Tj, TKj)

local TRRjik, f3jik, f4jik, f5jik, f6jik

parameter i, k

constant RR1 = 1.314, RR2=62361.0, RR3=555.0 RR4=1.987

LMBjik = ALPHjk/ALPHji * EXP(WLMB(i,k)/(RR4*Tj))

TRRjik = TKj/TCC(i,k)

PCC(i,k)*Bjik/(RR4*TCC(i,k)) = f3jik + wH(i,k)*f4jik + f5jik + ->
    ETTA(i,k)*f6jik

f3jik = 0.1445 - 0.330/TRRjik - 0.1385/(TRRjik**2) - ->
    0.0121/(TRRjik**3)
f4jik = 0.073 + 0.46/TRRjik - 0.5/(TRRjik**2) -0.097/(TRRjik**3) -
>
    - 0.0073/(TRRjik**8)
f5jik = -5.237220 + 5.665807*MUR(i,k) - 2.133816*MUR(i,k)**2 + ->
    0.2525373*MUR(i,k)**3 + (5.769770 - 6.181427*MUR(i,k) + ->
    2.283270*MUR(i,k)**2 - 0.2649074*MUR(i,k)**3)/TRRjik
f6jik = EXP(4.62 - 6.6*TRRjik)
end

model type eqlbm1
submodel (eqlcom) eqlc11(i = 1, k = 1), eqlc12(i = 1, k = 2), ->
    eqlc13(i=1, k=3), eqlc14(i=1, k=4), eqlc21(i=2, k=1), ->
    eqlc22(i=2, k=2), eqlc23(i=2, k=3), eqlc24(i=2, k=4), ->
    eqlc31(i=3, k=1), eqlc32(i=3, k=2), eqlc33(i=3, k=3), ->
    eqlc34(i=3, k=4), eqlc41(i=4, k=1), eqlc42(i=4, k=2), ->
    eqlc43(i = 4, k = 3), eqlc44(i = 4, k = 4)

cut uji(uj1, uj2, uj3, uj4, HLDPj)
cut Yji(Y11, Y12, Y13, Y14, sumvj)
cut T(Tj,TKj)
cut eql1(ZZj, Bmj)
cut eql2(Kj1, Kj2, Kj3 ,Kj4)
cut eql11(LMBj11, ALPHj1, ALPHj1, Bj11)
cut eql12(LMBj12, ALPHj1, ALPHj2, Bj12)
cut eql13(LMBj13, ALPHj1, ALPHj3, Bj13)
cut eql14(LMBj14, ALPHj1, ALPHj4, Bj14)
cut eql21(LMBj21, ALPHj2, ALPHj1, Bj21)
cut eql22(LMBj22, ALPHj2, ALPHj2, Bj22)
cut eql23(LMBj23, ALPHj2, ALPHj3, Bj23)
cut eql24(LMBj24, ALPHj2, ALPHj4, Bj24)
cut eql31(LMBj31, ALPHj3, ALPHj1, Bj31)
cut eql32(LMBj32, ALPHj3, ALPHj2, Bj32)
cut eql33(LMBj33, ALPHj3, ALPHj3, Bj33)
cut eql34(LMBj34, ALPHj3, ALPHj4, Bj34)
cut eql41(LMBj41, ALPHj4, ALPHj1, Bj41)
cut eql42(LMBj42, ALPHj4, ALPHj2, Bj42)
cut eql43(LMBj43, ALPHj4, ALPHj3, Bj43)
cut eql44(LMBj44, ALPHj4, ALPHj4, Bj44)
terminal Pj

local Vmj, PHIVj1, PHIVj2, PHIVj3, PHIVj4, GAMj1, GAMj2, GAMj3, ->
    GAMj4, PHILj1, PSj1, PHISj1, f1j1, f2j1, TRj1, ->
    PHILj2, PSj2, PHISj2, f1j2, f2j2, TRj2, ->

```

PHILj3, PSj3, PHISj3, f1j3, f2j3, TRj3, ->
 PHILj4, PSj4, PHISj4, f1j4, f2j4, TRj4

parameter RR1 = 1.314, RR2=62361.0, RR3=555.0, RR4=1.987

connect eq1c11:q1c at eq111
 connect eq1c12:q1c at eq112
 connect eq1c13:q1c at eq113
 connect eq1c14:q1c at eq114
 connect eq1c21:q1c at eq121
 connect eq1c22:q1c at eq122
 connect eq1c23:q1c at eq123
 connect eq1c24:q1c at eq124
 connect eq1c31:q1c at eq131
 connect eq1c32:q1c at eq132
 connect eq1c33:q1c at eq133
 connect eq1c34:q1c at eq134
 connect eq1c41:q1c at eq141
 connect eq1c42:q1c at eq142
 connect eq1c43:q1c at eq143
 connect eq1c44:q1c at eq144
 connect eq1c11:T at T
 connect eq1c12:T at T
 connect eq1c13:T at T
 connect eq1c14:T at T
 connect eq1c21:T at T
 connect eq1c22:T at T
 connect eq1c23:T at T
 connect eq1c24:T at T
 connect eq1c31:T at T
 connect eq1c32:T at T
 connect eq1c33:T at T
 connect eq1c34:T at T
 connect eq1c41:T at T
 connect eq1c42:T at T
 connect eq1c43:T at T
 connect eq1c44:T at T

0 = Y11*PHIVj1 - uj1*GAMj1*Kj1*PHILj1/HLDPj
 0 = Y12*PHIVj2 - uj2*GAMj2*Kj2*PHILj2/HLDPj
 0 = Y13*PHIVj3 - uj3*GAMj3*Kj3*PHILj3/HLDPj
 0 = Y14*PHIVj4 - uj4*GAMj4*Kj4*PHILj4/HLDPj

Y11 + Y12 + Y13 + Y14 = 1
 sumvj = Y11 + Y12 + Y13 + Y14

Kj1 = PSj1/Pj

GAMj1 = EXP(1 - uj1*LMBj11/(uj1*LMBj11 + uj1*LMBj12 + uj1*LMBj13 -

>

+ uj1*LMBj14) + uj2*LMBj21/(uj2*LMBj21 + uj2*LMBj22 + ->
 uj2*LMBj23 + uj2*LMBj24) + uj3*LMBj31/(uj3*LMBj31 + ->
 uj3*LMBj32 + uj3*LMBj33 + uj3*LMBj34) + ->
 uj4*LMBj41/(uj4*LMBj41 + uj4*LMBj42 + uj4*LMBj43 + ->
 uj4*LMBj44)) * HLDPj/(uj1*LMBj11 + uj2*LMBj21 +uj3*LMBj31 + -

>

uj4*LMBj41)

ALPHj1 = MV(1,1) + MV(2,1)*Tj + MV(3,1)*Tj**2

PHISj1 = EXP(f1j1 + f2j1 + WW(1))

TRj1 = Tj/TC(1)

f1j1 = -3.5021358 + TRj1*(5.6085595 + TRj1*(-3.076574 + ->
 TRj1*0.57335015))

```

f2j1 = -3.7690418 + TRj1*( 4.3538729 + TRj1*( 0.3166137 + TRj1*( -
>
0.12666184 + TRj1*(-1.1662283 + TRj1*(-0.10665730 + TRj1*( ->
0.12147436 + TRj1*( 0.18927037 + TRj1*(0.14936906 + ->
TRj1*(0.024364816 + TRj1*(-0.068603516 + TRj1*(-0.015172164 ->
+ TRj1*0.012089114)))))))))
PHILj1 = PHISj1*EXP(-ALPHj1*PSj1/(RR2*TKj))
PHIVj1 = exp(2*(Y11*Bj11 + Y12*Bj12 + Y13*Bj13 + ->
Y14*Bj14)/(Vmj*(Y11 + Y12 + Y13 + Y14)) ) - ZZj
PSj1 = ALOG10(ANT(1,1) - (ANT(2,1)/(ANT(3,1) + (TKj - 273.15))))
{-----}
Kj2 = PSj2/Pj
GAMj2 = EXP(1 - uj1*LMBj12/(uj1*LMBj11 + uj1*LMBj12 +uj1*LMBj13 -
>
+ uj1*LMBj14) + uj2*LMBj22/(uj2*LMBj21 + uj2*LMBj22 + ->
uj2*LMBj23 + uj2*LMBj24) + uj3*LMBj32/(uj3*LMBj31 + ->
uj3*LMBj32 + uj3*LMBj33 + uj3*LMBj34) + ->
uj4*LMBj42/(uj4*LMBj41 + uj4*LMBj42 + uj4*LMBj43 + ->
uj4*LMBj44)) * HLDpj/(uj1*LMBj12 + uj2*LMBj22 +uj3*LMBj32 + -
>
uj4*LMBj42)
ALPHj2 = MV(1,2) + MV(2,2)*Tj + MV(3,2)*Tj**2
PHISj2 = EXP(f1j2 + f2j2 + WW(2))
TRj2 = TKj/TC(2)
f1j2 = -3.5021358 + TRj2*( 5.6085595 + TRj2*(-3.076574 + ->
TRj2*0.57335015))
f2j2 = -3.7690418 + TRj2*( 4.3538729 + TRj2*( 0.3166137 + TRj2*( -
>
0.12666184 + TRj2*(-1.1662283 + TRj2*(-0.10665730 + TRj2*( ->
0.12147436 + TRj2*( 0.18927037 + TRj2*(0.14936906 + ->
TRj2*(0.024364816 + TRj2*(-0.068603516 + TRj2*(-0.015172164 ->
+ TRj2*0.012089114)))))))))
PHILj2 = PHISj2*EXP(-ALPHj2*PSj2/(RR2*TKj))
PHIVj2 = exp(2*(Y11*Bj21 + Y12*Bj22 + Y13*Bj23 + ->
Y14*Bj24)/(Vmj*(Y11 + Y12 + Y13 + Y14)) ) - ZZj
PSj2 = ALOG10(ANT(1,2) - (ANT(2,2)/(ANT(3,2) + (TKj - 273.15))))
{-----}
Kj3 = PSj3/Pj
GAMj3 = EXP(1 - uj1*LMBj13/(uj1*LMBj11 + uj1*LMBj12 +uj1*LMBj13 -
>
+ uj1*LMBj14) + uj2*LMBj23/(uj2*LMBj21 + uj2*LMBj22 + ->
uj2*LMBj23 + uj2*LMBj24) + uj3*LMBj33/(uj3*LMBj31 + ->
uj3*LMBj32 + uj3*LMBj33 + uj3*LMBj34) + ->
uj4*LMBj43/(uj4*LMBj41 + uj4*LMBj42 + uj4*LMBj43 + ->
uj4*LMBj44)) * HLDpj/(uj1*LMBj13 + uj2*LMBj23 +uj3*LMBj33 + -
>
uj4*LMBj43)
ALPHj3 = MV(1,3) + MV(2,3)*Tj + MV(3,3)*Tj**2
PHISj3 = EXP(f1j3 + f2j3 + WW(3))
TRj3 = TKj/TC(3)
f1j3 = -3.5021358 + TRj3*( 5.6085595 + TRj3*(-3.076574 + ->
TRj3*0.57335015))
f2j3 = -3.7690418 + TRj3*( 4.3538729 + TRj3*( 0.3166137 + TRj3*( -
>
0.12666184 + TRj3*(-1.1662283 + TRj3*(-0.10665730 + TRj3*( ->
0.12147436 + TRj3*( 0.18927037 + TRj3*(0.14936906 + ->
TRj3*(0.024364816 + TRj3*(-0.068603516 + TRj3*(-0.015172164 ->
+ TRj3*0.012089114)))))))))
PHILj3 = PHISj3*EXP(-ALPHj3*PSj3/(RR2*TKj))
PHIVj3 = exp(2*(Y11*Bj31 + Y12*Bj32 + Y13*Bj33 + ->
Y14*Bj34)/(Vmj*(Y11 + Y12 + Y13 + Y14)) ) - ZZj

```



```

PSj3 = ALOG10 (ANT(1,3) - (ANT(2,3)/(ANT(3,3) + (TKj - 273.15))))
{-----}
Kj4 = PSj4/Pj
GAMj4 = EXP(1 - ujl*LMBj14/(ujl*LMBj11 + ujl*LMBj12 +ujl*LMBj13 -
>
+ ujl*LMBj14) + uj2*LMBj24/(uj2*LMBj21 + uj2*LMBj22 + ->
uj2*LMBj23 + uj2*LMBj24) + uj3*LMBj34/(uj3*LMBj31 + ->
uj3*LMBj32 + uj3*LMBj33 + uj3*LMBj34) + ->
uj4*LMBj44/(uj4*LMBj41 + uj4*LMBj42 + uj4*LMBj43 + ->
uj4*LMBj44)) * HLDpj/(ujl*LMBj14 + uj2*LMBj24 +uj3*LMBj34 + -
>
uj4*LMBj44)
ALPHj4 = MV(1,4) + MV(2,4)*Tj + MV(3,4)*Tj**2
PHISj4 = EXP(f1j4 + f2j4 + WW(4))
TRj4 = TKj/TC(4)
f1j4 = -3.5021358 + TRj4*( 5.6085595 + TRj4*(-3.076574 + ->
TRj4*0.57335015))
f2j4 = -3.7690418 + TRj4*( 4.3538729 + TRj4*( 0.3166137 + TRj4*( -
>
0.12666184 + TRj4*(-1.1662283 + TRj4*(-0.10665730 + TRj4*( ->
0.12147436 + TRj4*( 0.18927037 + TRj4*(0.14936906 + ->
TRj4*(0.024364816 + TRj4*(-0.068603516 + TRj4*(-0.015172164 ->
+ TRj4*0.012089114)))))))))
PHILj4 = PHISj4*EXP(-ALPHj4*PSj4/(RR2*TKj))
PHIVj4 = exp(2*(Y11*Bj41 + Y12*Bj42 + Y13*Bj43 + ->
Y14*Bj44)/(Vmj*(Y11 + Y12 + Y13 + Y14)) ) - ZZj
PSj4 = ALOG10 (ANT(1,4) - (ANT(2,4)/(ANT(3,4) + (TKj - 273.15))))
{-----}
Bmj = ( Y11*(Y11*Bj11 + Y12*Bj12 + Y13*Bj13 + Y14*Bj14) + ->
Y12*(Y11*Bj21 + Y12*Bj22 + Y13*Bj23 + Y14*Bj24) + ->
Y13*(Y11*Bj31 + Y12*Bj32 + Y13*Bj33 + Y14*Bj34) + ->
Y14*(Y11*Bj41 + Y12*Bj42 + Y13*Bj43 + Y14*Bj44))/(Y11 + Y12 ->
+ Y13 + Y14)**2
TKj = 5.0*Tj/9.0
ZZj = (1. + SQRT(1. + 4*Bmj*Pj/(RR3*TKj)))/2.0
Vmj = Bmj/(ZZj - 1)
end

model type eqlbm
submodel (eqlcom) eqlc11(i = 1, k = 1), eqlc12(i = 1, k = 2), ->
eqlc13(i=1, k=3), eqlc14(i= 1, k = 4), eqlc21(i = 2, k = 1), -
>
eqlc22(i=2, k=2), eqlc23(i= 2, k = 3), eqlc24(i = 2, k = 4), -
>
eqlc31(i=3, k=1), eqlc32(i= 3, k = 2), eqlc33(i = 3, k = 3), -
>
eqlc34(i=3, k=4), eqlc41(i= 4, k = 1), eqlc42(i = 4, k = 2), -
>
eqlc43(i = 4, k = 3), eqlc44(i = 4, k = 4)

cut uji(uj1, uj2, uj3, uj4, HLDpj)
cut T(Tj,TKj)
cut vji(vj1, vj2, vj3, vj4, sumvj)
cut eql1(ZZj, Bmj)
cut eql2(Kj1, Kj2, Kj3 ,Kj4)
cut eql11(LMBj11, ALPHj1, ALPHj1, Bj11)
cut eql12(LMBj12, ALPHj1, ALPHj2, Bj12)
cut eql13(LMBj13, ALPHj1, ALPHj3, Bj13)
cut eql14(LMBj14, ALPHj1, ALPHj4, Bj14)
cut eql21(LMBj21, ALPHj2, ALPHj1, Bj21)
cut eql22(LMBj22, ALPHj2, ALPHj2, Bj22)

```

```

cut eql23(LMBj23, ALPHj2, ALPHj3, Bj23)
cut eql24(LMBj24, ALPHj2, ALPHj4, Bj24)
cut eql31(LMBj31, ALPHj3, ALPHj1, Bj31)
cut eql32(LMBj32, ALPHj3, ALPHj2, Bj32)
cut eql33(LMBj33, ALPHj3, ALPHj3, Bj33)
cut eql34(LMBj34, ALPHj3, ALPHj4, Bj34)
cut eql41(LMBj41, ALPHj4, ALPHj1, Bj41)
cut eql42(LMBj42, ALPHj4, ALPHj2, Bj42)
cut eql43(LMBj43, ALPHj4, ALPHj3, Bj43)
cut eql44(LMBj44, ALPHj4, ALPHj4, Bj44)

```

```
terminal Pj, Vmj
```

```

local PHIVj1, PHIVj2, PHIVj3, PHIVj4, GAMj1, GAMj2, GAMj3, ->
    GAMj4, PHILj1, PSj1, PHISj1, f1j1, f2j1, TRj1, ->
    PHILj2, PSj2, PHISj2, f1j2, f2j2, TRj2, ->
    PHILj3, PSj3, PHISj3, f1j3, f2j3, TRj3, ->
    PHILj4, PSj4, PHISj4, f1j4, f2j4, TRj4

```

```
parameter RR1 = 1.314, RR2=62361.0, RR3=555.0, RR4=1.987
```

```

connect eqlc11:q1c at eql11
connect eqlc12:q1c at eql12
connect eqlc13:q1c at eql13
connect eqlc14:q1c at eql14
connect eqlc21:q1c at eql21
connect eqlc22:q1c at eql22
connect eqlc23:q1c at eql23
connect eqlc24:q1c at eql24
connect eqlc31:q1c at eql31
connect eqlc32:q1c at eql32
connect eqlc33:q1c at eql33
connect eqlc34:q1c at eql34
connect eqlc41:q1c at eql41
connect eqlc42:q1c at eql42
connect eqlc43:q1c at eql43
connect eqlc44:q1c at eql44
connect eqlc11:T at T
connect eqlc12:T at T
connect eqlc13:T at T
connect eqlc14:T at T
connect eqlc21:T at T
connect eqlc22:T at T
connect eqlc23:T at T
connect eqlc24:T at T
connect eqlc31:T at T
connect eqlc32:T at T
connect eqlc33:T at T
connect eqlc34:T at T
connect eqlc41:T at T
connect eqlc42:T at T
connect eqlc43:T at T
connect eqlc44:T at T

```

```

0 = vj1*PHIVj1/(vj1 + vj2 + vj3 + vj4) - ->
    uj1*GAMj1*Kj1*PHILj1/HLDPj

```

```
Kj1 = PSj1/Pj
```

```

GAMj1 = EXP(1 - uj1*LMBj11/(uj1*LMBj11 + uj1*LMBj12 +uj1*LMBj13 -
>
    + uj1*LMBj14) + uj2*LMBj21/(uj2*LMBj21 + uj2*LMBj22 + ->

```

```

uj2*LMBj23 + uj2*LMBj24) + uj3*LMBj31/(uj3*LMBj31 + ->
uj3*LMBj32 + uj3*LMBj33 + uj3*LMBj34) + ->
uj4*LMBj41/(uj4*LMBj41 + uj4*LMBj42 + uj4*LMBj43 + ->
uj4*LMBj44)) * HLDPj/(uj1*LMBj11 + uj2*LMBj21 +uj3*LMBj31 + -
>
uj4*LMBj41)
ALPHj1 = MV(1,1) + MV(2,1)*Tj + MV(3,1)*Tj**2
PHISj1 = EXP(f1j1 + f2j1 + WW(1))
TRj1 = Tj/TC(1)
f1j1 = -3.5021358 + TRj1*( 5.6085595 + TRj1*(-3.076574 + ->
TRj1*0.57335015))
f2j1 = -3.7690418 + TRj1*( 4.3538729 + TRj1*( 0.3166137 + TRj1*( -
>
0.12666184 + TRj1*(-1.1662283 + TRj1*(-0.10665730 + TRj1*( ->
0.12147436 + TRj1*( 0.18927037 + TRj1*(0.14936906 + ->
TRj1*(0.024364816 + TRj1*(-0.068603516 + TRj1*(-0.015172164 ->
+ TRj1*0.012089114)))))))))
PHILj1 = PHISj1*EXP(-ALPHj1*PSj1/(RR2*TKj))
PHIVj1 = exp(2*(vj1*Bj11 + vj2*Bj12 + vj3*Bj13 + ->
vj4*Bj14)/(Vmj*(vj1 + vj2 + vj3 + vj4)) ) - ZZj
PSj1 = ALOG10(ANT(1,1) - (ANT(2,1)/(ANT(3,1) + (TKj - 273.15))))
{-----}
0 = vj2*PHIVj2/(vj1 + vj2 + vj3 + vj4) - ->
uj2*GAMj2*Kj2*PHILj2/HLDPj

Kj2 = PSj2/Pj
GAMj2 = EXP(1 - uj1*LMBj12/(uj1*LMBj11 + uj1*LMBj12 +uj1*LMBj13 -
>
+ uj1*LMBj14) + uj2*LMBj22/(uj2*LMBj21 + uj2*LMBj22 + ->
uj2*LMBj23 + uj2*LMBj24) + uj3*LMBj32/(uj3*LMBj31 + ->
uj3*LMBj32 + uj3*LMBj33 + uj3*LMBj34) + ->
uj4*LMBj42/(uj4*LMBj41 + uj4*LMBj42 + uj4*LMBj43 + ->
uj4*LMBj44)) * HLDPj/(uj1*LMBj12 + uj2*LMBj22 +uj3*LMBj32 + -
>
uj4*LMBj42)
ALPHj2 = MV(1,2) + MV(2,2)*Tj + MV(3,2)*Tj**2
PHISj2 = EXP(f1j2 + f2j2 + WW(2))
TRj2 = TKj/TC(2)
f1j2 = -3.5021358 + TRj2*( 5.6085595 + TRj2*(-3.076574 + ->
TRj2*0.57335015))
f2j2 = -3.7690418 + TRj2*( 4.3538729 + TRj2*( 0.3166137 + TRj2*( -
>
0.12666184 + TRj2*(-1.1662283 + TRj2*(-0.10665730 + TRj2*( ->
0.12147436 + TRj2*( 0.18927037 + TRj2*(0.14936906 + ->
TRj2*(0.024364816 + TRj2*(-0.068603516 + TRj2*(-0.015172164 ->
+ TRj2*0.012089114)))))))))
PHILj2 = PHISj2*EXP(-ALPHj2*PSj2/(RR2*TKj))
PHIVj2 = exp(2*(vj1*Bj21 + vj2*Bj22 + vj3*Bj23 + ->
vj4*Bj24)/(Vmj*(vj1 + vj2 + vj3 + vj4)) ) - ZZj
PSj2 = ALOG10(ANT(1,2) - (ANT(2,2)/(ANT(3,2) + (TKj - 273.15))))
{-----}
0 = vj3*PHIVj3/(vj1 + vj2 + vj3 + vj4) - ->
uj3*GAMj3*Kj3*PHILj3/HLDPj

Kj3 = PSj3/Pj
GAMj3 = EXP(1 - uj1*LMBj13/(uj1*LMBj11 + uj1*LMBj12 +uj1*LMBj13 -
>
+ uj1*LMBj14) + uj2*LMBj23/(uj2*LMBj21 + uj2*LMBj22 + ->
uj2*LMBj23 + uj2*LMBj24) + uj3*LMBj33/(uj3*LMBj31 + ->
uj3*LMBj32 + uj3*LMBj33 + uj3*LMBj34) + ->
uj4*LMBj43/(uj4*LMBj41 + uj4*LMBj42 + uj4*LMBj43 + ->

```

```

uj4*LMBj44)) * HLDPj/(uj1*LMBj13 + uj2*LMBj23 +uj3*LMBj33 + -
>
uj4*LMBj43)
ALPHj3 = MV(1,3) + MV(2,3)*Tj + MV(3,3)*Tj**2
PHISj3 = EXP(f1j3 + f2j3 + WW(3))
TRj3 = TKj/TC(3)
f1j3 = -3.5021358 + TRj3*( 5.6085595 + TRj3*(-3.076574 + ->
TRj3*0.57335015))
f2j3 = -3.7690418 + TRj3*( 4.3538729 + TRj3*( 0.3166137 + TRj3*( -
>
0.12666184 + TRj3*(-1.1662283 + TRj3*(-0.10665730 + TRj3*( ->
0.12147436 + TRj3*( 0.18927037 + TRj3*(0.14936906 + ->
TRj3*(0.024364816 + TRj3*(-0.068603516 + TRj3*(-0.015172164 ->
+ TRj3*0.012089114)))))))))
PHILj3 = PHISj3*EXP(-ALPHj3*PSj3/(RR2*TKj))
PHIVj3 = exp(2*(vj1*Bj31 + vj2*Bj32 + vj3*Bj33 + ->
vj4*Bj34)/(Vmj*(vj1 + vj2 + vj3 + vj4)) ) - ZZj

PSj3 = ALOG10(ANT(1,3) - (ANT(2,3)/(ANT(3,3) + (TKj - 273.15))))
{-----}
0 = vj4*PHIVj4/(vj1 + vj2 + vj3 + vj4) - ->
uj4*GAMj4*Kj4*PHILj4/HLDPj

Kj4 = PSj4/Pj
GAMj4 = EXP(1 - uj1*LMBj14/(uj1*LMBj11 + uj1*LMBj12 +uj1*LMBj13 -
>
+ uj1*LMBj14) + uj2*LMBj24/(uj2*LMBj21 + uj2*LMBj22 + ->
uj2*LMBj23 + uj2*LMBj24) + uj3*LMBj34/(uj3*LMBj31 + ->
uj3*LMBj32 + uj3*LMBj33 + uj3*LMBj34) + ->
uj4*LMBj44/(uj4*LMBj41 + uj4*LMBj42 + uj4*LMBj43 + ->
uj4*LMBj44)) * HLDPj/(uj1*LMBj14 + uj2*LMBj24 +uj3*LMBj34 + -
>
uj4*LMBj44)
ALPHj4 = MV(1,4) + MV(2,4)*Tj + MV(3,4)*Tj**2
PHISj4 = EXP(f1j4 + f2j4 + WW(4))
TRj4 = TKj/TC(4)
f1j4 = -3.5021358 + TRj4*( 5.6085595 + TRj4*(-3.076574 + ->
TRj4*0.57335015))
f2j4 = -3.7690418 + TRj4*( 4.3538729 + TRj4*( 0.3166137 + TRj4*( -
>
0.12666184 + TRj4*(-1.1662283 + TRj4*(-0.10665730 + TRj4*( ->
0.12147436 + TRj4*( 0.18927037 + TRj4*(0.14936906 + ->
TRj4*(0.024364816 + TRj4*(-0.068603516 + TRj4*(-0.015172164 ->
+ TRj4*0.012089114)))))))))
PHILj4 = PHISj4*EXP(-ALPHj4*PSj4/(RR2*TKj))
PHIVj4 = exp(2*(vj1*Bj41 + vj2*Bj42 + vj3*Bj43 + ->
vj4*Bj44)/(Vmj*(vj1 + vj2 + vj3 + vj4)) ) - ZZj
PSj4 = ALOG10(ANT(1,4) - (ANT(2,4)/(ANT(3,4) + (TKj - 273.15))))
{-----}
Bmj = ( vj1*(vj1*Bj11 + vj2*Bj12 + vj3*Bj13 + vj4*Bj14) + ->
vj2*(vj1*Bj21 + vj2*Bj22 + vj3*Bj23 + vj4*Bj24) + ->
vj3*(vj1*Bj31 + vj2*Bj32 + vj3*Bj33 + vj4*Bj34) + ->
vj4*(vj1*Bj41 + vj2*Bj42 + vj3*Bj43 + vj4*Bj44))/(vj1 + vj2 ->
+ vj3 + vj4)**2

TKj = 5.0*Tj/9.0
sumvj = vj1 + vj2 + vj3 + vj4
ZZj = (1. + SQRT(1. + 4*Bmj*Pj/(RR3*TKj)))/2.0
Vmj = Bmj/(ZZj - 1)
end

```

```

{----Pressure Drop Equations:}
model type pres1
  terminal P1, P2, RHMV2, RHML1, Z1
  cut uji(uj1, uj2, uj3, uj4, HLDpj)
  cut vjpi(v21, v22, v23, v24, sumvjp)

  local VOLREC

  parameter REF1 = 0.947775644, LR=16.0, pii=3.141592653, DR=10.0

  0 = P1 - P2 - sumvjp**2 * RHMV2*REF1
  0 = HLDpj - RHML1*VOLREC

  VOLREC = LR*((pii/2.0 + ASIN(2*Z1/DR - 1)) *(DR/2.0)**2 + (Z1 - ->
    DR/2.0)*(Z1*DR - Z1**2)**0.5)
end

model type presj
  terminal Pj, Pjp, RHOLj, RHOLjp, RHOVj, RHOVjp, Lj, RHMVj, RHMVjp, -
  >
    Zj, HCTRj, HCTRjp, Vmj
  cut uji(uj1, uj2, uj3, uj4, HLDpj)
  cut vji(vj1, vj2, vj3, vj4, sumvj)
  cut vjpi(vjp1, vjp2, vjp3, vjp4, sumvjp)

  local HOj, FOAMj, QLj, FVAj, UVAj, UHj, HLUdj, RHMLj, HOLDj

  terminal CDj, AHj
  {AN = AA ???????}
  parameter gc=32.17, g=32.0898, LW=130.806, HW=1.0, AN=141.372, ->
    AUD=0.908375, AA=141.372, AD=17.6715

  RHMVj = 1/Vmj
  0 = Pjp - Pj - g*760*RHOLj/(gc*14.696*1728.0) * (HOj + HCTRj)

  HOj = 0.186*(UHj/CDj)**2 * RHOVjp/RHOLj
  HCTRj = FOAMj*(0.4896*(QLj/LW)**0.67 + HW)
  QLj = 7.48*Lj/RHMLj
  UVAj = sumvj/(AN*RHMVj*60)
  FVAj = UVAj*SQRT(RHOVj)
  FOAMj = 1 - 0.372192*FVAj**0.177709
  UHj = sumvjp/(AHj*RHMVjp*60)
  0 = Pj - Pjp + g*760/(gc*14.696*1728) * ((12*Zj - HLUdj)*RHOLj - -
  >
    HCTRjp*RHOLjp)
  HLUdj = 0.000003*(QLj/AUD)**2
  0 = HLDpj - HOLDj
  HOLDj = RHMLj*(HCTRj*AA/12.0 + Zj*AD)
end

model type presN
  terminal Z50, RHML50, q50, HCTRj, RHMVj, RHOVj, Vmj
  cut uji(uj1, uj2, uj3, uj4, HLDpj)
  cut vji(vj1, vj2, vj3, vj4, sumvj)

  local VOLBTW, FOAMj, UVAj, FVAj

  parameter AN=141.372, LW=130.806, HW=1.0, pii=3.141592653, ->
    DTT=15.0

  RHMVj = 1/Vmj

```

```

0 = HLDpj - RHML50*VOLBTW
VOLBTW = 100 + pi*Z50*DTT**2/4
HCTRj = FOAMj*(0.4896*(q50/LW)**0.67 + HW)
UVAj = sumvj/(AN*RHMvj*60)
FVAj = UVAj*SQRT(RHOvj)
FOAMj = 1 - 0.372192*FVAj**0.177709
end

{----Condenser and Receiver Equations:}
model type condsr
terminal QC, L1, RHML1, R, P2, Z1, P1, q1
cut T(T1,TK1)
cut Tp(T2,TK2)
cut vjpi(v21, v22, v23, v24, sumvj)
cut contr1(CV1, CV2, CV3)

local HEAD1, Pd1, Ps1, q2, Qcw, Tmc, Two, RHOL1
parameter ALPHA=0.2 , Apc=16022.16, Aw=13940.0,Ccw=1.0,Cmc=0.12, -
>
g=32.0898, gc=32.17, PD=40.0, Pw1=60, Pw3=35.0, REF2 = 9.0, ->
Qcwo=8653.0, Twi=545, Umc=45000.0, Upmo=213.0, Uwmo=1250.0, ->
ZC=5.0, Ucw=17160.0

0 = Qcw*Ccw*(Twi - Two)*8.34 + Uwmo/60 * Aw*(Tmc - ->
Two)*(Qcw/Qcwo)**1.8 - Ucw*Ccw*der(Two)
0 = 105.8752/(v21 + v22 + v23 + v24) * (Upmo/60 * Apc*((1-->
ALPHA)*T2 + ALPHA*T1 - Tmc))**3 - QC**3
0 = QC - Uwmo/60 * (Qcw/Qcwo)**1.8 * Aw*(Tmc - Two) - ->
Umc*Cmc*der(Tmc)
0 = (Pw1 - Pw3 - REF2*(Qcw/Qcwo)**1.8)*CV1**2 - (Qcw/2)**2
0 = Pd1 - Ps1 - HEAD1

HEAD1 = 9.870927E1 - 9.794161E-3*(q1 + q2) - 1.95175E-6*(q1 + ->
q2)**2 - 1.954559E-9*(q1 + q2)**3

0 = q1*RHML1 - L1*7.481
0 = R*q2 - q1
0 = q1**2 * RHOL1/62.4 - CV2**2 * (Pd1*RHOL1*g/(144*gc) - ->
P2*14.696/760)
0 = q2**2 * RHOL1/62.4 - CV3**2 * (Pd1*RHOL1*g/(144*gc) - ->
PD*14.696/760)
0 = RHOL1*(Ps1 - Z1 - ZC) - P1*14.696*144*gc/(760*g)
end

{----Reboiler and Tower Base Equations:}
model type reboil
terminal QR, P50, RHOL50, Z50, RHML50, L50, Wsh, q50
cut T(T50,TK50)
cut contr2(CS4, CV5)

local Tsc, Tmr,Ps2, Pd2, RHsc, RHOSC, hLSC, Es, HVSC, HEAD2, Wsc
parameter Apmr=3361.826, As=3844.168, Cmr=0.12, g=32.0898, ->
gc=32.17, HSH=1262.8, PB=30.0, PSH=255.0, TSH=960.0, ->
TSAT=862.7, Umr=11000.0, Upmr=300.0, Us=1000.0, Vr=68.83, ->
ZB=10.0

0 = Us*As/60 * (Tsc - Tmr) - QR - Umr*Cmr*der(Tmr)
0 = Upmr*Apmr/60 * (Tmr - T50) - QR

```

```

0 = Ps2 - (P50*14.696*144*g/(760*gc*RHOL50) + Z50 + ZB)
0 = q50*RHML50 - L50*7.481
0 = (Pd2*RHOL50*g/(144*gc) - PB) * CV5**2 - q50**2*RHOL50/62.4
0 = PSH*CS4/60 - Wsh/2 * (1 + 0.00065*(TSH - TSAT))
0 = Wsc - Wsh + Vr*der(RHsc)
0 = RHsc - RHOSC
RHOSC = 1.031951E-2 + 1.427797E1*Tsc/610 + 0.9414444*(Tsc/610)**2 -
>
+ 2.048037*(Tsc/610)**3 + 5.956991*(Tsc/610)**4

0 = Wsh*HSH - Wsc*hLSC - Us*As/60 * (Tsc - Tmr) - der(Es)

hLSC = -1.6029E2 + 8.06427E-2*Tsc + 7.361453E-5*Tsc**2 + ->
1.501012E-6*Tsc**3 - 9.9964334E-10*Tsc**4
0 = Vr*RHsc*HVSC - Es
HVSC = 5.448738E2 + 8.039637E-1*Tsc + 1.931794E-3*Tsc**2 - ->
3.938661E-6*Tsc**3 + 1.907853E-9*Tsc**4

0 = Pd2 - Ps2 - HEAD2
HEAD2 = 9.152028E1 - 6.584299E-2*q50 + 7.533832E-5*q50**2 - ->
4.300139E-8*q50**3
end

{----Control Equations}
model type contrl
cut contr1(CV1, CV2, CV3)
cut contr2(CS4, CV5)
cut T(T35, TK35)
terminal P1, q1, Z1, Z50, Wsh

local CI1, CI2, CI3, CI4, CI5, CI6, CO1, CO2,CO3,CO4, CO5, CO6, -
>
I1, I2, I3, I4, I5, I6, TM, ZETA1, ZETA2, ZETA3, ZETA4, ->
ZETA5

parameter TAUM=0.20

CV1 = CV1CO(2,ZETA1) + CV1CO(3,ZETA1)*( ZETA1 ->
- CV1CO(1,ZETA1)) + CV1CO(4,ZETA1)*( ZETA1 ->
- CV1CO(1,ZETA1))**2 ->
+ CV1CO(5,ZETA1)*(ZETA1 - CV1CO(1,ZETA1))**3
CV2 = CV2CO(2,ZETA2) + CV2CO(3,ZETA2)*( ZETA2 ->
- CV2CO(1,ZETA2)) + CV2CO(4,ZETA2)*( ZETA2 ->
- CV2CO(1,ZETA2))**2 ->
+ CV2CO(5,ZETA2)*(ZETA2 - CV2CO(1,ZETA2))**3
CV3 = CV3CO(2,ZETA3) + CV3CO(3,ZETA3)*( ZETA3 ->
- CV3CO(1,ZETA3)) + CV3CO(4,ZETA3)*( ZETA3 ->
- CV3CO(1,ZETA3))**2 ->
+ CV3CO(5,ZETA3)*(ZETA3 - CV3CO(1,ZETA3))**3
CS4 = CSCO(2,ZETA4) + CSCO(3,ZETA4)*(ZETA4 ->
- CSCO(1,ZETA4)) + CSCO(4,ZETA4)*(ZETA4 ->
- CSCO(1,ZETA4))**2 + CSCO(5,ZETA4)*(ZETA4 ->
- CSCO(1,ZETA4))**3
CV5 = CV5CO(2,ZETA5) + CV5CO(3,ZETA5)*(ZETA5 ->
- CV5CO(1,ZETA5)) + CV5CO(4,ZETA5)*(ZETA5 ->
- CV5CO(1,ZETA5))**2 + CV5CO(5,ZETA5)*(ZETA5 ->
- CV5CO(1,ZETA5))**3

0 = CI1 + 12.0 - 0.032*P1
0 = CO1 - XKC(1)*(CI1 - CISP(1) + I1/TAUI(1))
0 = CI1 - CISP(1) - der(I1)

```

```

0 = -0.25 + 0.0625*CO1 - ZETA1 - TAUUV(1)*der(ZETA1)
0 = CI2 - 4.0 - (q1/200)**2
0 = CO2 - XKC(2)*(CISP(2) - CI2 + I2/TAUI(2))
0 = CISP(2) - CI2 - der(I2)
0 = -0.25 + 0.0625*CO2 - ZETA2 - TAUUV(2)*der(ZETA2)
0 = CI3 - 4.0 - 1.6*Z1
0 = CO3 - XKC(3)*(CI3 - CISP(3) + I3/TAUI(3))
0 = CI3 - CISP(3) - der(I3)
0 = -0.25 + 0.0625*CO3 - ZETA3 - TAUUV(3)*der(ZETA3)
0 = CI5 + 20.0 - 4*Z50
0 = CO5 - XKC(5)*(CI5 - CISP(5) + I5/TAUI(5))
0 = CI5 - CISP(5) - der(I5)
0 = -0.25 + 0.0625*CO5 - ZETA5 - TAUUV(5)*der(ZETA5)
0 = CI4 - 4.0 - 16*(Wsh/3000)**2
0 = CO4 - XKC(4)*(CO4 - CI4 + I4/TAUI(4))
0 = CO4 - CI4 - der(I4)
0 = -0.25 + 0.0625*CO4 - ZETA4 - TAUUV(4)*der(ZETA4)
0 = T35 - TM - TAUM*der(TM)
0 = CO6 - XKC(6)*(CISP(6) - CI6 + I6/TAUI(6))
0 = CISP(6) - CI6 - der(I6)
0 = CI6 + 236 - 0.4*TM
end

```

```

model type stageG
  submodel engbj
  submodel matbj
  submodel eqlbm
  submodel presj
  cut uji(uj1, uj2, uj3, uj4, HLDPj)
  cut ujmi(ujm1, ujm2, ujm3, ujm4, HLDPjm)
  cut T(Tj, TKj)
  cut HVji(HVj1, HVj2, HVj3, HVj4)
  cut HVjpi(HVjp1, HVjp2, HVjp3, HVjp4)
  cut vji(vj1, vj2, vj3, vj4, sumvj)
  cut vjpi(vjp1, vjp2, vjp3, vjp4, sumvjp)
  cut sup(Pjp, RHOLjp, RHOVjp, RHMVjp, HCTRjp)
  cut stup(Pj, RHOLj, RHOVj, RHMVj, HCTRj)
  cut stgup[sup, HVjpi, vjpi]
  cut stgupp[stup, HVji, vji]
  cut sdn(Ljm, Ejm)
  cut stdn(Lj, Ej)
  cut stgdn[sdn, ujmi]
  cut stgdnn[stdn, uji]

  parameter Hfj, fj1, fj2, fj3, fj4, CDj, AHj

  connect engbj:eql1 at eqlbm:eql1
  connect engbj:uji at matbj:uji
  connect eqlbm:uji at matbj:uji
  connect presj:uji at matbj:uji
  connect matbj:uji at uji
  connect engbj:ujmi at ujmi
  connect matbj:ujmi at ujmi
  connect engbj:HVji at HVji
  connect engbj:HVjpi at HVjpi
  connect engbj:vji at eqlbm:vji
  connect matbj:vji at eqlbm:vji
  connect presj:vji at eqlbm:vji
  connect eqlbm:vji at vji
  connect engbj:vjpi at matbj:vjpi
  connect presj:vjpi at matbj:vjpi

```



```

connect matbj:vjpi at vjpi
connect engbj:T at eqlbm:T
connect engbj:T at T

engbj.Hfj = Hfj
matbj.fj1 = fj1
matbj.fj2 = fj2
matbj.fj3 = fj3
matbj.fj4 = fj4
presj.CDj = CDj
presj.AHj = AHj
engbj.Ej = Ej
presj.Pj = Pj
engbj.Pj = presj.Pj
eqlbm.Pj = presj.Pj
engbj.Lj = matbj.Lj
engbj.Lj = Lj
presj.Lj = Lj
engbj.Ljm = matbj.Ljm
engbj.Ljm = Ljm
engbj.Ejm = Ejm
presj.RHOLj = RHOLj
presj.RHOLjp = RHOLjp
presj.RHOVj = RHOVj
presj.RHOVjp = RHOVjp
presj.RHMVj = RHMVj
presj.RHMVjp = RHMVjp
presj.HCTRj = HCTRj
presj.HCTRjp = HCTRjp
eqlbm.Vmj = presj.Vmj
end

model type condG
submodel engb1
submodel matb1
submodel eqlbm1
submodel pres1
submodel condsr
cut T(Tj,TKj)
cut Tp(Tjp,TKj)
cut vji(vj1, vj2, vj3, vj4, sumvj)
cut vjpi(vjp1, vjp2, vjp3, vjp4, sumvj)
cut uji(uj1, uj2, uj3, uj4, HLDpj)
cut contr1(CV1, CV2, CV3)
cut HVjpi(HVjp1, HVjp2, HVjp3, HVjp4)
cut sup(Pjp, RHOLjp, RHOVjp, RHMVjp, HCTRjp)
cut stgup[sup, HVjpi, vjpi]
cut stdn(Lj, Ej)
cut stgdnn[stdn, uji]

terminal q1, P1, Z1
parameter Hfj=0, fj1=0, fj2=0, fj3=0, fj4=0

connect engb1:q1 at eqlbm1:q1
connect engb1:uji at matb1:uji
connect eqlbm1:uji at matb1:uji
connect pres1:uji at matb1:uji
connect matb1:uji at uji
connect engb1:HVjpi at HVjpi
connect eqlbm1:Yji at vji
connect engb1:vjpi at vjpi

```

```

connect matbl:vjpi at vjpi
connect pres1:vjpi at vjpi
connect condsr:vjpi at vjpi
connect engbl:T at eqlbm1:T
connect condsr:T at eqlbm1:T
connect condsr:Tp at Tp
connect condsr:contr1 at contr1

engbl.Hfj = Hfj
matbl.fj1 = fj1
matbl.fj2 = fj2
matbl.fj3 = fj3
matbl.fj4 = fj4
engbl.R = condsr.R
matbl.R = condsr.R
engbl.QC = condsr.QC
engbl.Ej = Ej
engbl.Pj = pres1.P1
eqlbm1.Pj = pres1.P1
condsr.P1 = pres1.P1
pres1.P1 = P1
engbl.Lj = matbl.Lj
condsr.L1 = matbl.Lj
matbl.Lj = Lj
pres1.P2 = Pjp
condsr.P2 = Pjp
pres1.RH MV2 = RHM Vjp
pres1.RH ML1 = condsr.RH ML1
pres1.Z1 = condsr.Z1
condsr.Z1 = Z1
condsr.q1 = q1
end

model type reboG
submodel engbN
submodel matbN
submodel eqlbm
submodel presN
submodel reboil
cut uji(uj1, uj2, uj3, uj4, HLD Pj)
cut ujmi(ujm1, ujm2, ujm3, ujm4, HLD Pjm)
cut HVji(HVj1, HVj2, HVj3, HVj4)
cut vji(vj1, vj2, vj3, vj4, sumvj)
cut stup(Pj, RHOLj, RHOVj, RHM Vj, HCTRj)
cut stgupp[stup, HVji, vji]
cut sdn(Ljm, Ejm)
cut stgdn[sdn, ujmi]
cut contr2(CS4, CV5)

terminal Z50, Wsh
parameter Hfj=0, fj1=0, fj2=0, fj3=0, fj4=0

connect engbN:eql1 at eqlbm:eql1
connect engbN:uji at uji
connect eqlbm:uji at uji
connect presN:uji at uji
connect matbN:uji at uji
connect engbN:ujmi at ujmi
connect matbN:ujmi at ujmi
connect engbN:HVji at HVji
connect engbN:vji at eqlbm:vji

```

```

connect matbN:vji at eqlbm:vji
connect presN:vji at vji
connect eqlbm:vji at vji
connect engbN:T at eqlbm:T
connect reboil:T at eqlbm:T
connect reboil:contr2 at contr2

engbN.Hfj = Hfj
matbN.fj1 = fj1
matbN.fj2 = fj2
matbN.fj3 = fj3
matbN.fj4 = fj4
engbN.Pj = Pj
reboil.P50 = Pj
eqlbm.Pj = Pj
engbN.Lj = matbN.Lj
reboil.L50 = matbN.Lj
engbN.Ljm = Ljm
matbN.Ljm = Ljm
engbN.Ejm = Ejm
engbN.QR = reboil.QR
presN.Z50 = Z50
reboil.Z50 = Z50
presN.RHML50 = reboil.RHML50
reboil.RHOL50 = RHOLj
reboil.Wsh = Wsh
presN.q50 = reboil.q50
presN.HCTRj = HCTRj
presN.RHMOVj = RHMVj
presN.RHOVj = RHOVj
eqlbm.Vmj = presN.Vmj
end

model distGh
{converting this model to 50 stages would mean adding 47 more }
{      stageG submodels and 94  more connections between the stages}

submodel (stageG) stag35(513543.3, 25.0, 0.5, ->
    5.0, 197.5, 0.72, 13.0)
submodel reboG(0.0, 0.0, 0.0, 0.0, 0.0)
submodel condG(0.0, 0.0, 0.0, 0.0, 0.0)
submodel contr1

connect contr1:T at stag35:T
connect condG:Tp at stag35:T
connect contr1:contr2 at reboG:contr2
connect contr1:contr1 at condG:contr1

contr1.P1 = condG.P1
contr1.q1 = condG.q1
contr1.Z1 = condG.Z1
contr1.Z50 = reboG.Z50
contr1.Wsh = reboG.Wsh

connect condG:stgdnn at stag35:stgdn
connect stag35:stgdnn at reboG:stgdn

connect reboG:stgupp at stag35:stgup
connect stag35:stgupp at condG:stgup
end

```

```
{-----end of distGh.dym-----  
}
```

B.3 DYMOLA assessment of Gallun's model

The number of non-trivial equations is 715

The number of unknown variables is 726

Singular problem.

Unassigned variables:

stag35::engbj.derEj	L1	T35
reboG::engbN.derEj	L35	T50
stag35::matbj.deruj2	RHOL50	RHOL50
reboG::matbN.deruj1	L50	RHMOV50
condG::condsr.Qcw	rearrange	
reboG::reboil.derRHsc	New	
stag35.RHOLj	RHOL35	RHOL35
stag35.RHOVj	RHOV35	RHOV35
condG.Tj	T1	T1
condG.Z1	RHOL1	RHOL1
reboG.RHOVj	RHOV50	RHOV50
reboG.Z50	New (RHOL50)	RHMOV35

Redundant equations:

reboG::reboil $HVSC = 5.448738E2 + 8.039637E-1 * Tsc + 1.931794E-3 * Tsc^{**2} - 3.938661E-6 * Tsc^{**3} + 1.907853E-9 * Tsc^{**4}$

System of 5 equations. Unknown variables:

condG::condsr.T2
 stag35::engbj.hLj1
 stag35::engbj.hLj2
 stag35::engbj.hLj3
 stag35::engbj.hLj4

-stag35::engbj $hLj1 = hLCO(1,1) + hLCO(2,1) * [condG::condsr.T2] + hLCO(3,1) * [condG::condsr.T2]^{**2}$
 - $0 = stag35::matbj.uj1 * [hLj1] + stag35::matbj.uj2 * hLj2 + stag35::matbj.uj3 * hLj3 + stag35::matbj.uj4 * hLj4 - Ej$
 - $[hLj2] = hLCO(1,2) + hLCO(2,2) * condG::condsr.T2 + hLCO(3,2) * condG::condsr.T2^{**2}$
 - $[hLj3] = hLCO(1,3) + hLCO(2,3) * condG::condsr.T2 + hLCO(3,3) * condG::condsr.T2^{**2}$
 - $[hLj4] = hLCO(1,4) + hLCO(2,4) * condG::condsr.T2 + hLCO(3,4) * condG::condsr.T2^{**2}$

End of system of equations.

System of equations is nonlinear.

System of 5 equations. Unknown variables:

condG::condsr.T1
 condG::engb1.hLj1
 condG::engb1.hLj2

condG::engb1.hLj3

condG::engb1.hLj4

-condG::engb1 hLj1 = hLCO(1,1) + hLCO(2,1)*[condG::condsr.T1] +
 hLCO(3,1)*[condG::condsr.T1]**2
 - 0 = condG::matb1.uj1*[hLj1] + condG::matb1.uj2*hLj2 +
 condG::matb1.uj3*hLj3 + condG::matb1.uj4*hLj4 - Ej
 - [hLj2] = hLCO(1,2) + hLCO(2,2)*condG::condsr.T1 +
 hLCO(3,2)*condG::condsr.T1**2
 - [hLj3] = hLCO(1,3) + hLCO(2,3)*condG::condsr.T1 +
 hLCO(3,3)*condG::condsr.T1**2
 - [hLj4] = hLCO(1,4) + hLCO(2,4)*condG::condsr.T1 +
 hLCO(3,4)*condG::condsr.T1**2
 End of system of equations.
 System of equations is nonlinear.

System of 16 equations. Unknown variables:

condG.P1

condG::engb1.ZZj

PHIVj4

Y14

PHIVj3

Y13

PHIVj2

Y12

Y11

PHIVj1

Vmj

condG::engb1.Bmj

Kj1

Kj2

Kj3

Kj4

- condG::engb1.ZZj = (1 + SQRT(1 + 4*condG::engb1.Bmj*[
 condG.P1]/(RR3*condG::condsr.TK1)))/2
 - PHIVj4 = exp(2*(Y11*eqlc41.Bjik + Y12*eqlc42.Bjik +
 Y13*eqlc43.Bjik + Y14*eqlc44.Bjik)/(Vmj*(Y11 + Y12 + Y13 + Y14))) - [
 condG::engb1.ZZj]
 - 0 = Y14*[PHIVj4] - condG::matb1.uj4*GAMj4*Kj4*PHILj4/
 condG::pres1.HLDPj
 - PHIVj3 = exp(2*(Y11*eqlc31.Bjik + Y12*eqlc32.Bjik +
 Y13*eqlc33.Bjik + [Y14]*eqlc34.Bjik)/(Vmj*(Y11 + Y12 + Y13 + [Y14]
)) - condG::engb1.ZZj
 - 0 = Y13*[PHIVj3] - condG::matb1.uj3*GAMj3*Kj3*PHILj3/
 condG::pres1.HLDPj
 - PHIVj2 = exp(2*(Y11*eqlc21.Bjik + Y12*eqlc22.Bjik + [
 Y13]*eqlc23.Bjik + Y14*eqlc24.Bjik)/(Vmj*(Y11 + Y12 + [Y13] + Y14))) -
 condG::engb1.ZZj

- $0 = Y12*[PHIVj2] - \text{condG}::\text{matb1.uj2}*GAMj2*Kj2*PHILj2/$
 $\text{condG}::\text{pres1.HLDPj}$

- $Y11 + [Y12] + Y13 + Y14 = 1$

- $0 = [Y11]*PHIVj1 - \text{condG}::\text{matb1.uj1}*GAMj1*Kj1*PHILj1/$
 $\text{condG}::\text{pres1.HLDPj}$

- $[PHIVj1] = \exp(2*(Y11*eq1c11.Bjik + Y12*eq1c12.Bjik +$
 $Y13*eq1c13.Bjik + Y14*eq1c14.Bjik)/(Vmj*(Y11 + Y12 + Y13 + Y14))) -$
 $\text{condG}::\text{engb1.ZZj}$

- $[Vmj] = \text{condG}::\text{engb1.Bmj}/(\text{condG}::\text{engb1.ZZj} - 1)$

- $[\text{condG}::\text{engb1.Bmj}] = (Y11*(Y11*eq1c11.Bjik + Y12*$
 $eq1c12.Bjik + Y13*eq1c13.Bjik + Y14*eq1c14.Bjik) + Y12*(Y11*eq1c21.$
 $Bjik + Y12*eq1c22.Bjik + Y13*eq1c23.Bjik + Y14*eq1c24.Bjik) + Y13*($
 $Y11*eq1c31.Bjik + Y12*eq1c32.Bjik + Y13*eq1c33.Bjik + Y14*eq1c34.Bjik$
 $) + Y14*(Y11*eq1c41.Bjik + Y12*eq1c42.Bjik + Y13*eq1c43.Bjik + Y14*$
 $eq1c44.Bjik))/(Y11 + Y12 + Y13 + Y14)**2$

- $[Kj1] = PSj1/\text{condG.P1}$

- $[Kj2] = PSj2/\text{condG.P1}$

- $[Kj3] = PSj3/\text{condG.P1}$

- $[Kj4] = PSj4/\text{condG.P1}$

End of system of equations.
System of equations is nonlinear.

System of 18 equations. Unknown variables:

stag35::presj.vj1
PHIVj1
stag35::presj.vj2
PHIVj2
stag35::presj.vj3
PHIVj3
stag35::presj.vj4
PHIVj4
stag35::presj.Vmj
stag35::engbj.Bmj
stag35::engbj.ZZj
stag35.Pj
stag35::presj.sumvj
stag35.RHMVj
Kj4
Kj3
Kj2
Kj1

- $0 = [\text{stag35}::\text{presj.vj1}]*PHIVj1/([\text{stag35}::\text{presj.vj1}] +$
 $\text{stag35}::\text{presj.vj2} + \text{stag35}::\text{presj.vj3} + \text{stag35}::\text{presj.vj4}) - \text{stag35}::$
 $\text{matbj.uj1}*GAMj1*Kj1*PHILj1/\text{stag35}::\text{presj.HLDPj}$

- $[PHIVj1] = \exp(2*(\text{stag35}::\text{presj.vj1}*eq1c11.Bjik +$
 $\text{stag35}::\text{presj.vj2}*eq1c12.Bjik + \text{stag35}::\text{presj.vj3}*eq1c13.Bjik + \text{stag35}::$
 $\text{presj.vj4}*eq1c14.Bjik)/(\text{stag35}::\text{presj.Vmj}*(\text{stag35}::\text{presj.vj1} + \text{stag35}::$
 $\text{presj.vj2} + \text{stag35}::\text{presj.vj3} + \text{stag35}::\text{presj.vj4}))) - \text{stag35}::\text{engbj.}$

$$\begin{aligned}
& \text{ZZj} \\
- & \quad 0 = [\text{stag35}::\text{presj.vj2}] * \text{PHIVj2} / (\text{stag35}::\text{presj.vj1} + [\text{stag35}::\text{presj.vj2}] + \text{stag35}::\text{presj.vj3} + \text{stag35}::\text{presj.vj4}) - \text{stag35}::\text{matbj.uj2} * \text{GAMj2} * \text{Kj2} * \text{PHILj2} / \text{stag35}::\text{presj.HLDPj} \\
- & \quad [\text{PHIVj2}] = \exp(2 * (\text{stag35}::\text{presj.vj1} * \text{eqlc21.Bjik} + \text{stag35}::\text{presj.vj2} * \text{eqlc22.Bjik} + \text{stag35}::\text{presj.vj3} * \text{eqlc23.Bjik} + \text{stag35}::\text{presj.vj4} * \text{eqlc24.Bjik}) / (\text{stag35}::\text{presj.Vmj} * (\text{stag35}::\text{presj.vj1} + \text{stag35}::\text{presj.vj2} + \text{stag35}::\text{presj.vj3} + \text{stag35}::\text{presj.vj4}))) - \text{stag35}::\text{engbj.} \\
& \text{ZZj} \\
- & \quad 0 = [\text{stag35}::\text{presj.vj3}] * \text{PHIVj3} / (\text{stag35}::\text{presj.vj1} + \text{stag35}::\text{presj.vj2} + [\text{stag35}::\text{presj.vj3}] + \text{stag35}::\text{presj.vj4}) - \text{stag35}::\text{matbj.uj3} * \text{GAMj3} * \text{Kj3} * \text{PHILj3} / \text{stag35}::\text{presj.HLDPj} \\
- & \quad [\text{PHIVj3}] = \exp(2 * (\text{stag35}::\text{presj.vj1} * \text{eqlc31.Bjik} + \text{stag35}::\text{presj.vj2} * \text{eqlc32.Bjik} + \text{stag35}::\text{presj.vj3} * \text{eqlc33.Bjik} + \text{stag35}::\text{presj.vj4} * \text{eqlc34.Bjik}) / (\text{stag35}::\text{presj.Vmj} * (\text{stag35}::\text{presj.vj1} + \text{stag35}::\text{presj.vj2} + \text{stag35}::\text{presj.vj3} + \text{stag35}::\text{presj.vj4}))) - \text{stag35}::\text{engbj.} \\
& \text{ZZj} \\
- & \quad 0 = [\text{stag35}::\text{presj.vj4}] * \text{PHIVj4} / (\text{stag35}::\text{presj.vj1} + \text{stag35}::\text{presj.vj2} + \text{stag35}::\text{presj.vj3} + [\text{stag35}::\text{presj.vj4}]) - \text{stag35}::\text{matbj.uj4} * \text{GAMj4} * \text{Kj4} * \text{PHILj4} / \text{stag35}::\text{presj.HLDPj} \\
- & \quad [\text{PHIVj4}] = \exp(2 * (\text{stag35}::\text{presj.vj1} * \text{eqlc41.Bjik} + \text{stag35}::\text{presj.vj2} * \text{eqlc42.Bjik} + \text{stag35}::\text{presj.vj3} * \text{eqlc43.Bjik} + \text{stag35}::\text{presj.vj4} * \text{eqlc44.Bjik}) / (\text{stag35}::\text{presj.Vmj} * (\text{stag35}::\text{presj.vj1} + \text{stag35}::\text{presj.vj2} + \text{stag35}::\text{presj.vj3} + \text{stag35}::\text{presj.vj4}))) - \text{stag35}::\text{engbj.} \\
& \text{ZZj} \\
- & \quad [\text{stag35}::\text{presj.Vmj}] = \text{stag35}::\text{engbj.Bmj} / (\text{stag35}::\text{engbj.ZZj} - 1) \\
- & \quad [\text{stag35}::\text{engbj.Bmj}] = (\text{stag35}::\text{presj.vj1} * (\text{stag35}::\text{presj.vj1} * \text{eqlc11.Bjik} + \text{stag35}::\text{presj.vj2} * \text{eqlc12.Bjik} + \text{stag35}::\text{presj.vj3} * \text{eqlc13.Bjik} + \text{stag35}::\text{presj.vj4} * \text{eqlc14.Bjik}) + \text{stag35}::\text{presj.vj2} * (\text{stag35}::\text{presj.vj1} * \text{eqlc21.Bjik} + \text{stag35}::\text{presj.vj2} * \text{eqlc22.Bjik} + \text{stag35}::\text{presj.vj3} * \text{eqlc23.Bjik} + \text{stag35}::\text{presj.vj4} * \text{eqlc24.Bjik}) + \text{stag35}::\text{presj.vj3} * (\text{stag35}::\text{presj.vj1} * \text{eqlc31.Bjik} + \text{stag35}::\text{presj.vj2} * \text{eqlc32.Bjik} + \text{stag35}::\text{presj.vj3} * \text{eqlc33.Bjik} + \text{stag35}::\text{presj.vj4} * \text{eqlc34.Bjik}) + \text{stag35}::\text{presj.vj4} * (\text{stag35}::\text{presj.vj1} * \text{eqlc41.Bjik} + \text{stag35}::\text{presj.vj2} * \text{eqlc42.Bjik} + \text{stag35}::\text{presj.vj3} * \text{eqlc43.Bjik} + \text{stag35}::\text{presj.vj4} * \text{eqlc44.Bjik})) / (\text{stag35}::\text{presj.vj1} + \text{stag35}::\text{presj.vj2} + \text{stag35}::\text{presj.vj3} + \text{stag35}::\text{presj.vj4}) ** 2 \\
- & \quad [\text{stag35}::\text{engbj.ZZj}] = (1 + \text{SQRT}(1 + 4 * \text{stag35}::\text{engbj.Bmj} * \text{stag35.Pj} / (\text{RR3} * \text{condG}::\text{condsr.TK2}))) / 2 \\
- \text{condG}::\text{pres1} & \quad 0 = \text{condG.P1} - [\text{stag35.Pj}] - \text{stag35}::\text{presj.sumvj} ** 2 * \text{stag35.RHMOVj} * \text{REF1} \\
- \text{stag35}::\text{eqlbm} & \quad [\text{stag35}::\text{presj.sumvj}] = \text{stag35}::\text{presj.vj1} + \text{stag35}::\text{presj.vj2} + \text{stag35}::\text{presj.vj3} + \text{stag35}::\text{presj.vj4} \\
- \text{stag35}::\text{presj} & \quad [\text{stag35.RHMOVj}] = 1 / \text{Vmj} \\
- \text{stag35}::\text{eqlbm} & \quad [\text{Kj4}] = \text{PSj4} / \text{stag35.Pj} \\
- & \quad [\text{Kj3}] = \text{PSj3} / \text{stag35.Pj} \\
- & \quad [\text{Kj2}] = \text{PSj2} / \text{stag35.Pj} \\
- & \quad [\text{Kj1}] = \text{PSj1} / \text{stag35.Pj}
\end{aligned}$$

End of system of equations.
System of equations is nonlinear.

System of 5 equations. Unknown variables:

reboG::reboil.T50
reboG::engbN.hLj1
reboG::engbN.hLj2
reboG::engbN.hLj3
reboG::engbN.hLj4

-reboG::engbN hLj1 = hLCO(1,1) + hLCO(2,1)*[reboG::reboil.T50] +
 hLCO(3,1)*[reboG::reboil.T50]**2
- 0 = reboG::matbN.uj1*[hLj1] + reboG::matbN.uj2*hLj2 +
 reboG::matbN.uj3*hLj3 + reboG::matbN.uj4*hLj4 - Ej
- [hLj2] = hLCO(1,2) + hLCO(2,2)*reboG::reboil.T50 +
 hLCO(3,2)*reboG::reboil.T50**2
- [hLj3] = hLCO(1,3) + hLCO(2,3)*reboG::reboil.T50 +
 hLCO(3,3)*reboG::reboil.T50**2
- [hLj4] = hLCO(1,4) + hLCO(2,4)*reboG::reboil.T50 +
 hLCO(3,4)*reboG::reboil.T50**2

End of system of equations.
System of equations is nonlinear.

****NOTE** how this system of equations includes variables from all stages**

System of 26 equations. Unknown variables:

condG.Lj
stag35.Lj
reboG::matbN.Lj
reboG::matbN.vj1
reboG::eqlbm.PHIVj1
reboG::matbN.vj2
reboG::matbN.vj3
reboG::eqlbm.PHIVj3
reboG::matbN.vj4
reboG::eqlbm.PHIVj4
reboG::presN.Vmj
reboG::engbN.Bmj
reboG::engbN.ZZj
reboG::eqlbm.PHIVj2
reboG::eqlbm.Kj2
reboG.Pj
reboG::eqlbm.Kj4
reboG::eqlbm.Kj3
reboG::eqlbm.Kj1
reboG::engbN.HVj1
reboG::engbN.OMEGAj
reboG::engbN::engder.dBmj
reboG::matbN.sumvj

reboG::engbN.HVj2
 reboG::engbN.HVj3
 reboG::engbN.HVj4

-stag35::engbj 0 = stag35.Hfj + [condG.Lj]*condG::engb1.Ej/condG::
 pres1.HLDPj - stag35.Lj*Ej/stag35::presj.HLDPj + reboG::matbN.vj1*reboG::
 engbN.HVj1 - stag35::presj.vj1*HVj1 + reboG::matbN.vj2*reboG::engbN.
 HVj2 - stag35::presj.vj2*HVj2 + reboG::matbN.vj3*reboG::engbN.HVj3 -
 stag35::presj.vj3*HVj3 + reboG::matbN.vj4*reboG::engbN.HVj4 - stag35::
 presj.vj4*HVj4 - derEj

-reboG::engbN 0 = reboG.Hfj + [stag35.Lj]*stag35::engbj.Ej/stag35::
 presj.HLDPj - reboG::matbN.Lj*Ej/reboG::matbN.HLDPj - reboG::matbN.
 vj1*HVj1 - reboG::matbN.vj2*HVj2 - reboG::matbN.vj3*HVj3 - reboG::matbN.
 vj4*HVj4 + reboG::reboil.QR - derEj

-reboG::matbN 0 = reboG.fj1 + stag35.Lj*stag35::matbj.uj1/stag35::
 presj.HLDPj - [Lj]*uj1/HLDPj - vj1 - deruj1

-reboG::eqlbm 0 = [reboG::matbN.vj1]*PHIVj1/([reboG::matbN.vj1] +
 reboG::matbN.vj2 + reboG::matbN.vj3 + reboG::matbN.vj4) - reboG::matbN.
 uj1*GAMj1*Kj1*PHILj1/reboG::matbN.HLDPj

- [PHIVj1] = exp(2*(reboG::matbN.vj1*eqlc11.Bjik +
 reboG::matbN.vj2*eqlc12.Bjik + reboG::matbN.vj3*eqlc13.Bjik + reboG::
 matbN.vj4*eqlc14.Bjik)/(reboG::presN.Vmj*(reboG::matbN.vj1 + reboG::
 matbN.vj2 + reboG::matbN.vj3 + reboG::matbN.vj4))) - reboG::engbN.ZZj

-stag35::matbj 0 = stag35.fj2 + condG.Lj*condG::matb1.uj2/condG::
 pres1.HLDPj - stag35.Lj*uj2/stag35::presj.HLDPj - stag35::presj.vj2 + [
 reboG::matbN.vj2] - deruj2

-reboG::eqlbm 0 = [reboG::matbN.vj3]*PHIVj3/(reboG::matbN.vj1 +
 reboG::matbN.vj2 + [reboG::matbN.vj3] + reboG::matbN.vj4) - reboG::
 matbN.uj3*GAMj3*Kj3*PHILj3/reboG::matbN.HLDPj

- [PHIVj3] = exp(2*(reboG::matbN.vj1*eqlc31.Bjik +
 reboG::matbN.vj2*eqlc32.Bjik + reboG::matbN.vj3*eqlc33.Bjik + reboG::
 matbN.vj4*eqlc34.Bjik)/(reboG::presN.Vmj*(reboG::matbN.vj1 + reboG::
 matbN.vj2 + reboG::matbN.vj3 + reboG::matbN.vj4))) - reboG::engbN.ZZj

- 0 = [reboG::matbN.vj4]*PHIVj4/(reboG::matbN.vj1 +
 reboG::matbN.vj2 + reboG::matbN.vj3 + [reboG::matbN.vj4]) - reboG::
 matbN.uj4*GAMj4*Kj4*PHILj4/reboG::matbN.HLDPj

- [PHIVj4] = exp(2*(reboG::matbN.vj1*eqlc41.Bjik +
 reboG::matbN.vj2*eqlc42.Bjik + reboG::matbN.vj3*eqlc43.Bjik + reboG::
 matbN.vj4*eqlc44.Bjik)/(reboG::presN.Vmj*(reboG::matbN.vj1 + reboG::
 matbN.vj2 + reboG::matbN.vj3 + reboG::matbN.vj4))) - reboG::engbN.ZZj

- [reboG::presN.Vmj] = reboG::engbN.Bmj/(reboG::engbN.
 ZZj - 1)

- [reboG::engbN.Bmj] = (reboG::matbN.vj1*(reboG::matbN.
 vj1*eqlc11.Bjik + reboG::matbN.vj2*eqlc12.Bjik + reboG::matbN.vj3*eqlc13.
 Bjik + reboG::matbN.vj4*eqlc14.Bjik) + reboG::matbN.vj2*(reboG::matbN.
 vj1*eqlc21.Bjik + reboG::matbN.vj2*eqlc22.Bjik + reboG::matbN.vj3*eqlc23.
 Bjik + reboG::matbN.vj4*eqlc24.Bjik) + reboG::matbN.vj3*(reboG::matbN.
 vj1*eqlc31.Bjik + reboG::matbN.vj2*eqlc32.Bjik + reboG::matbN.vj3*eqlc33.
 Bjik + reboG::matbN.vj4*eqlc34.Bjik) + reboG::matbN.vj4*(reboG::matbN.

$$\frac{vj1*eq1c41.Bjik + reboG::matbN.vj2*eq1c42.Bjik + reboG::matbN.vj3*eq1c43.Bjik + reboG::matbN.vj4*eq1c44.Bjik)}{(reboG::matbN.vj1 + reboG::matbN.vj2 + reboG::matbN.vj3 + reboG::matbN.vj4)**2}$$

$$- PHIVj2 = \exp(2*(reboG::matbN.vj1*eq1c21.Bjik + reboG::matbN.vj2*eq1c22.Bjik + reboG::matbN.vj3*eq1c23.Bjik + reboG::matbN.vj4*eq1c24.Bjik)/(reboG::presN.Vmj*(reboG::matbN.vj1 + reboG::matbN.vj2 + reboG::matbN.vj3 + reboG::matbN.vj4))) - [reboG::engbN.ZZj]$$

$$- 0 = reboG::matbN.vj2*[PHIVj2]/(reboG::matbN.vj1 + reboG::matbN.vj2 + reboG::matbN.vj3 + reboG::matbN.vj4) - reboG::matbN.uj2*GAMj2*Kj2*PHILj2/reboG::matbN.HLDPj$$

$$- [Kj2] = PSj2/reboG.Pj$$

$$- reboG::engbN.ZZj = (1 + \text{SQRT}(1 + 4*reboG::engbN.Bmj*[reboG.Pj]/(RR3*reboG::reboil.TK50))))/2$$

$$- [Kj4] = PSj4/reboG.Pj$$

$$- [Kj3] = PSj3/reboG.Pj$$

$$- [Kj1] = PSj1/reboG.Pj$$

$$-reboG::engbN [HVj1] = H0j1 + OMEGAj$$

$$- [OMEGAj] = (2 - 1/ZZj)*reboG.Pj/(2*ZZj - 1)*(reboG::reboil.TK50*engder.dBmj - Bmj)$$

$$-reboG::engbN::engder [dBmj] = (reboG::matbN.vj1*reboG::matbN.vj1*dB11 + reboG::matbN.vj1*reboG::matbN.vj2*dB12 + reboG::matbN.vj1*reboG::matbN.vj3*dB13 + reboG::matbN.vj1*reboG::matbN.vj4*dB14 + reboG::matbN.vj2*reboG::matbN.vj1*dB12 + reboG::matbN.vj2*reboG::matbN.vj2*dB22 + reboG::matbN.vj2*reboG::matbN.vj3*dB23 + reboG::matbN.vj2*reboG::matbN.vj4*dB24 + reboG::matbN.vj3*reboG::matbN.vj1*dB13 + reboG::matbN.vj3*reboG::matbN.vj2*dB23 + reboG::matbN.vj3*reboG::matbN.vj3*dB33 + reboG::matbN.vj3*reboG::matbN.vj4*dB34 + reboG::matbN.vj4*reboG::matbN.vj1*dB14 + reboG::matbN.vj4*reboG::matbN.vj2*dB24 + reboG::matbN.vj4*reboG::matbN.vj3*dB34 + reboG::matbN.vj4*reboG::matbN.vj4*dB44)/reboG::matbN.sumvj**2$$

$$-reboG::eq1bm [reboG::matbN.sumvj] = reboG::matbN.vj1 + reboG::matbN.vj2 + reboG::matbN.vj3 + reboG::matbN.vj4$$

$$-reboG::engbN [HVj2] = H0j2 + OMEGAj$$

$$- [HVj3] = H0j3 + OMEGAj$$

$$- [HVj4] = H0j4 + OMEGAj$$

End of system of equations.
System of equations is nonlinear.

System of 5 equations. Unknown variables:

condG::condsr.q2

condG::condsr.RHOL1

condG::condsr.Pd1

condG::condsr.Ps1

condG::condsr.HEAD1

-condG::condsr $0 = [q2]**2*RHOL1/62.4 - \text{contrl.CV3**2}*(Pd1*RHOL1*g/(144*gc) - PD*14.696/760)$

- $0 = \text{condG.q1**2}[RHOL1]/62.4 - \text{contrl.CV2**2}*(Pd1*[RHOL1]*g/(144*gc) - \text{stag35.Pj*14.696/760})$

- $0 = [Pd1] - Ps1 - HEAD1$
 - $0 = RHOL1 * ([Ps1] - condG.Z1 - ZC) - condG.P1 * 14.696 * 144 * gc / (760 * g)$
 - $[HEAD1] = 9.870927E1 - 9.794161E-3 * (condG.q1 + q2) - 1.95175E-6 * (condG.q1 + q2) ** 2 - 1.954559E-9 * (condG.q1 + q2) ** 3$
 End of system of equations.
 System of equations is nonlinear.

System of 3 equations. Unknown variables:

reboG.RHOLj
 reboG::reboil.Pd2
 reboG::reboil.Ps2

-reboG::reboil $0 = (Pd2 * [reboG.RHOLj] * g / (144 * gc) - PB) * contrl.CV5 ** 2 - q50 ** 2 * [reboG.RHOLj] / 62.4$
 - $0 = [Pd2] - Ps2 - HEAD2$
 - $0 = [Ps2] - (reboG.Pj * 14.696 * 144 * g / (760 * gc * reboG.RHOLj) + reboG.Z50 + ZB)$
 End of system of equations.
 System of equations is nonlinear.

System of 6 equations. Unknown variables:

stag35::presj.Pjp
 stag35.HCTRj
 stag35::presj.QLj
 stag35::presj.RHMLj
 stag35::presj.Zj
 stag35::presj.HLUDj

-stag35::presj $0 = [Pjp] - stag35.Pj - g * 760 * stag35.RHOLj / (gc * 14.696 * 1728.0) * (HOj + stag35.HCTRj)$
 - $[stag35.HCTRj] = FOAMj * (0.4896 * (QLj / LW) ** 0.67 + HW)$
 - $[QLj] = 7.48 * stag35.Lj / RHMLj$
 - $HOLDj = [RHMLj] * (stag35.HCTRj * AA / 12.0 + Zj * AD)$
 - $0 = stag35.Pj - Pjp + g * 760 / (gc * 14.696 * 1728) * ((12 * [Zj] - HLUDj) * stag35.RHOLj - reboG.HCTRj * reboG.RHOLj)$
 - $[HLUDj] = 0.000003 * (QLj / AUD) ** 2$
 End of system of equations.
 System of equations is nonlinear.

APPENDIX C: ACSL CODE FOR SIMPLE DISTILLATION

COLUMN MODEL

```

PROGRAM ACSL simplified distillation -- distsim.csl 6/10/92
"Contains distgbh.dym 3/30/92 with alternate eqlbm"
"3 stages (3,5,21) added 4/3/92"
"large scale simplification of l-v eqlbm and vapor flow, elimination"
"  of virial equation as eq of state, 9 stages used "
"  (1,2,3,4,5,21,35,49,50), elimination of all "
"  algebraic loops."
"Because of the use of submodels (MACROs), a full 50 stage model would"
"  nearly require additional stage(...) statements in the DERIVATIVE"
"  section of this program. "

"-----Variable and constant definition-----"
" AA Active area of sieve plate. Constant. (ft2)"
" AD Downcomer crosssectional area. Constant. (ft2)"
" AH(j) Area of holes in sieve plate j. Constants. (ft2)"
" ailg=2 Gear's method of integration "
" ALPHA Factor to account for temperature drop across condenser. "
" Constant. (ft2)"
" ALPHji Molar volume of component i in the liquid phase of "
" stage j. (cm3/gmol)"
" AN Nominal Area of sieve plate. Constant. (ft2)"
" ANT(a,i) Antoine constants A,B,C for component i. Constants"
" Apc Area of condensation heat transfer in the condenser.
Constant. (ft2)"
" Apmr Area of boiling heat transfer in the reboiler. Constant. "
" (ft2)"
" As Area of steam condensation in the reboiler. Constant. (ft2)"
" AT Tower corss sectional area. Constant. (ft2)"
" AUD Area under downcomer. Constant. (ft2)"
" Aw Area of heat transfer from cooling water to condenser tube wall.
Constant. (ft2)"
" Ccw Cooling water heat capacity. Constant. (BTU/lb °R)"
" Cdd Vena contracta coefficient for flow over wier. (-)"
" CIk kth controller input. (mA/min)"
" cinterval communication interval "
" CISPk kth controller set point translated to (mA/min)"
" Cmc Heat capacity of condenser tubes. Constant. (BTU/lb °R)"
" Cmr Heat capacity of reboiler tubes. Constant. (BTU/lb °R)"
" COk kth controller output to valves. (mA/min)"
" CS4 Control valve position for steam flow (valve 4). (in2/hr)"
" Csc Heat capacity of steam in reboiler tubes. (BTU/lb °R)"
" CSCO Coefficients used to determine CS4."
" CVkCO coefficients used to determine CVk"
" Cvc Vena contracta coefficient for a circular hole. (-)"
" CVk kth control valve position for liquid flow. (gal/min
 $\sqrt{\text{lb/in}^2}$  )"
" Cx Vena contract coefficient for flow from downcomer. (-)"
" DH Sieve plate hole diameter. Constant."

```

" dQVj Total change in vapor flow through sieve plate. (ft²)"

" DR Diameter of the distillate receiver. Constant. (ft)"

" DTT Tower diameter. Constant. (ft)"

" Ej Holdup of enthalpy in liquid phase of stage j. (BTU)"

" ETTA(i,k) Cross self-interaction parameter. Constants. (-)"

" EVj Enthalpy of vapor flow leaving stage j. (BTU/min)"

" F Feed rate. Constants. (mol/min)"

" FOAMj Froth density correction factor. (-)"

" FVAj Factor related to kinetic energy of vapor leaving stage j. "

" (ft. $\sqrt{\text{lb}/\text{ft}^3}$ /sec)"

" g Acceleration of gravity. Constant. (ft/min²)"

" HCTRj Equivalent height of clear liquid on the sieve plate "

" of stage j. (ft)"

" Hf Enthalpy of the feed to stage j. constant. (BTU/min)"

" hLCO(i) Coefficients to determine enthalpy of liquid, hLji."

" HLDPj Total liquid mass on stage j. (mol)"

" hLji Partial molar enthalpy of component i in liquid phase "

" of stage j. (BTU/mol)"

" hLSC Enthalpy of saturated condensate (water) leaving the "

" reboiler. (BTU/lb)"

" hLSCO Coefficients used to determine hLSC."

" howj Height of foam over the wier on stage plate j. (ft)"

" HSH Enthalpy in the steam header. Constant. (BTU/lb)"

" HVCO Vapor enthalpy coefficients used for HVji. Constants"

" HVji Partial molar enthalpy of component i in vapor phase of "

" stage j. In this model, ideal gas is assumed. (BTU/mol)"

" HVSC Enthalpy of saturated steam in the reboiler. (BTU/lb)"

" HVSCO coefficients for HVSC."

" HW Height of the weir of sieve plate j. Constant. (in)"

" HWSP Height of the weir of the seal pan (stage 50). "

" Constant (in)"

" Ik Sum of the integral of the error and the steady-state bias "

" for contoller k. (mA)"

" jm postscript denoting stage j-1"

" jp postscript denoting stage j+1"

" Kji Ideal equilibrium ratio (K-value) for component i on stage j."

" LH Thickness of sieve plate. Constant. (ft)"

" Lj Total molar flow rate of liquid leaving stage j. (mol/min)"

" LR Length of the receiver. constant. (ft)"

" Lspj Total molar flow rate of liquid leaving seal pan. (mol/min)"

" LW Length of the weir of sieve plates. Constant. (in)"

" LWSP Length of the seal pan weir. (in)"

" merror relative error of state variables"

" MOL Molecular weight of component i. Constants. (lb/mol)"

" MOLV Weighted average of vapor molecular weight. (lb/mol)"

" MV Molar volume coefficients for liquid. "

" nsteps initial # of steps per cint "

" PB Pressure downstream of bottom product control valve. "

" Constant. (lb/in²)"

" PC Critical pressure for component i. Constants. (atm)"

" PCC Cross critical pressure of components i and k. constants. "

" (atm)"

" PD Pressure downstream of overhead product control valve. "

" Constant. (lb/in²)"

" Pd1 Discharge pressure of pump 1"

" Pd2 Discharge pressure of pump 2"

" Pj Pressure of stage j (lb/in²)"

" PDD Average of PD and P2 "

" pii π "
 " Pke Pressure drop across sieve plate due to kinetic energy of vapor. (lb/in²)"
 " Ps1 Suction pressure of pump 1"
 " Ps2 Suction pressure of pump 2"
 " PSH Steam pressure upsteam of steam control valve. (lb/in²)"
 " PSji Saturation pressure (vapor pressure) of liquid phase of component i as predicted by Antone's equation. (mmHg)"
 " PUD Pressure drop under the downcomer. (ft)"
 " Pw1 Cooling tower pressure upstream of control valve. Constant. (lb/in²)"
 " Pw2Pw3 Reference pressure drop across condenser. (lb/in²)"
 " Pw3 Cooling water pressure downstream of condenser. (lb/in²)"
 " q1 Volume flow of reflux. (gal/min)"
 " q2 Volume flow of overhead product (distillate). (gal/min)"
 " QC Condenser duty, heat flow to condenser. (BTU/min)"
 " Qcw Volume flow of cooling water. (gal/min)"
 " Qcwo Reference volume flow of cooling water. (gal/min)"
 " QLj Volume flow of liquid leaving stage j. (ft³/min)"
 " QR Reboiler duty, heat flow from reboiler. (BTU/min)"
 " Qsj Volume flow of liquid over the weir of stage j. (ft³/min)"
 " R Reflux ratio."
 " RECVOL(Zj) Receiver volume function. (ft³)"
 " REF2 Reference pressure drop across condenser. (lb/in²)"
 " REF3 Reference pressure drop across condenser divided by the product of vapor molar flow into the condenser and vapor mass density. Constant. (ft min²/mol)"
 " RHMLj Molar density of liquid of stage j. (mol/ft³)"
 " RHMVj Molar density of vapor of stage j. (mol/ft³)"
 " RHOLj Mass density of liquid of stage j. (lb/ft³)"
 " RHOSC Mass density of saturated steam in the reboiler. (mol/ft³)"
 " RHOSCO Coefficients used to determine RHOSC."
 " RHOVj Mass density of vapor of stage j. (lb/ft³)"
 " RR Gas constant. (Various units, depending on use)"
 " SP Set Points of the 5 variables controlled: P1(mmHg), q2(gal/min), Z1(ft), (), Z50(ft), T35(R)"
 " sumvj Molar vapor flow leaving stage j. (mol/min)"
 " TAUI time constants of Integrator in 6 PI controllers, constants. (min)"
 " TAUM time constant of the temperature sensor. (min)"
 " TAUV time constants of 6 control Valves, constants. (min)"
 " TC Critical temperature of component i. (°R)"
 " TCC Cross-critical temperature of component i. (°R)"
 " Tj Temperature of liquid and vapor leaving stage j. (°R)"
 " TKj Temperature in Kelvin."
 " Tmc Temperature of condenser tubes. (°R)"
 " Tmr Temperature of reboiler tubes. (°R)"
 " tmx Max time of simulation (min.)"
 " TR Reduced temperature, except is has funny dimensions. (°R/°K)"
 " TRR Reduced temperature. (-)"
 " TSAT Saturated temperature of steam at header pressure. Constant. (°R)"
 " Tsc Temperature of steam in reboiler tubes. (°R)"
 " TSH Temperature of super-heated steam in the steam header. Constant. (°R)"
 " TT Sieve plate thickness. Constant. (in)"

```

" Twi      Temperature of cooling water entering condenser. Constant.
           (°R) "
" Two      Temperature of cooling water leaving condenser. (°R) "
" Ucw      Holdup of cooling water in condenser. Constant. (lb) "
" UHj      Velocity of vapor in the holes of the stage j sieve plate. "
           (ft/sec) "
" uji      Molar holdup of component i liquid of stage j. (mol) "
" Umc      Mass of tube metal in condenser. Constant. (lb) "
" Umr      Mass of tube metal in reboiler. Constant. (lb) "
" Upmo     Reference heat transfer film coefficient between process "
           and condenser tube wall. Constant. (BTU/hr ft2 °R) "
" Upmr     Boiling film coefficient in reboiler. Constant. "
           (BTU/hr ft2 °R) "
" Us       Reboiler steam side condensing film coefficient. Constant. "
           (BTU/hr ft2 °R) "
" UVj      Molar vapor holdup on stage j. Constants. (mol) "
" UVAj     Velocity of vapor leaving stage j. (ft/sec) "
" Uwmo     Reference heat transfer film coefficient between cooling "
           water and condenser tube wall. Constant. (BTU/hr ft2 °R) "
" VC       Critical volume of component i. Constants. (cm3/gmol) "
" Vdc      Volume of liquid in stage j downcomer. (ft3) "
" vji      Molar flow of component i from stage j as vapor. (mol/min) "
" VOLBTW   Volume of liquid in the tower base. (ft3) "
" VOLREC   Volume of liquid in the receiver. (ft3) "
" Vr       Volume of steam side of reboiler. (ft3) "
" Wsh      Steam flow to the reboiler. (lb/min) "
" X,Y,Z    Intermediate values used to determine Pd1. "
" XKC      proportional gain in 6 PI controllers, constants "
" Yji      Molar fraction of component i in vapor. (-) "
" ZB       Vertical distance from column base to pump 2. Constant. (ft) "
" ZC       Vertical distance from bottom of receiver to pump 1. Constant.
           (ft) "
" ZETAk    kth control valve position. (mA) "
" Zj       Height of equivalent clear liquid in the downcomer of stage j.
           (ft) "

```

```

"-----ACSL program control variables"

```

```

tmx = 60.0
cinterval cint=1.0
algorithm ailg=2
nsteps nstps=1000
mininterval mint=0.0001
maxterval maxt=5.0
merror u22=1.E-5, T1=1.E-7, T50=1.E-7, z97377=1.E-3,Z98533=1.E-3, ...
      Z98827=1.E-3, Z99121=1.E-3, E1=7.E-7, E2=8.E-6, E3=9.E-6, ...
      E4=8.E-6, E5=5.E-6, E21=5.E-6 ,E35=5.E-6, E49=7.E-6

```

```

"-----Initial Values"

```

```

constant E01=903324.0, E02=70279.2, E03=74348.1, ...
      E04=98215., E05=250686, E021=251678., ...
      E035=249803., E049=267101., E050=9950470.
constant T01=598.770, T02=609.211, T03=616.34, ...
      T04=627.371, T05=639.640, T021=640.197, ...
      T035=641.159, T049=643.617, T050=644.693
constant Z01=3.0, Z02=.374189, Z03=.331997, ...
      Z04=.455558, Z05=1.09806, Z021=1.08924, ...

```



```

Z035=1.06254, Z049=1.13209, Z050=8.
constant Qs01=65.518, Qs02=59.4878, Qs03=51.2026, ...
  Qs04=42.4723, Qs05=194.664, Qs021=193.908, ...
  Qs035=191.331, Qs049=185.191, Qs050=169.196
constant how02=.0941719, how03=.0814453, ...
  how04=.0709429, how05=.206904, how021=.20602, ...
  how035=.204584, how049=.200172, how050=.184973
constant hcl02=.105436, hcl03=.0977002, ...
  hcl04=.0914545, hcl05=.172059, hcl021=.171555, ...
  hcl035=.170726, hcl049=.168104
constant u101=221.458, u201=126.773, u301=8.33504, ...
  u401=8.26399, ...
  u102=16.2189, u202=6.96898, u302=1.06823, u402=2.47162, ...
  u103=14.3473, u203=5.37857, u303=1.38011, u403=6.51095, ...
  u104=13.3136, u204=4.96873, u304=1.6149, u404=14.9326, ...
  u105=20.8692, u205=7.96256, u305=3.00135, u405=53.5029, ...
  u1021=20.8436, u2021=7.79217, u3021=3.03287, u4021=53.7695, ...
  u1035=20.382, u2035=7.37883, u3035=3.06659, u4035=54.2729, ...
  u1049=19.8538, u2049=6.89401, u3049=3.26108, u4049=59.5047, ...
  u1050=582.659, u2050=190.483, u3050=112.989, u4050=2496.92
constant ...
  v102=62.737, v202=35.9139, v302=2.36122, v402=2.34108, ...
  v103=61.8336, v203=28.9926, v303=3.59338, v403=7.46932, ...
  v104=53.9779, v204=23.5895, v304=4.19821, v404=17.4251, ...
  v105=43.2344, v205=19.5179, v305=3.82395, v405=30.0847, ...
  v1021=44.5776, v2021=19.6452, v3021=3.99251, v4021=31.1786, ...
  v1035=44.3349, v2035=18.839, v3035=4.11403, v4035=32.0323, ...
  v1049=42.4142, v2049=17.0497, v3049=4.28344, v4049=34.6156, ...
  v1050=35.5974, v2050=13.3416, v3050=4.41514, v4050=44.5073

constant I01=22.8315, I02=4.93478, I03=7.16095, I04=26.2638, ...
  I05=33.5039, I06=10.3385, ...
  ZET01=.463481, ZET02=.521059, ZET03=.406421, ...
  ZET04=0.734895, ZET05=.796989

constant Tmc0=579.767, Two0=566.222, ...
  Tmr0=739.522, Tsc0=764.402, Tm0=641.159

"-----controller set-points, gains, time-constants"
TABLE SP, 1, 6 /...
  1,2,3,4,5,6, 760, 490.135, 3.0, 0.0, 8.0, 641.161/
TABLE KKC,1,6/...
  1,2,3,4,5,6,...
  1.5, 0.25, 1.1, 0.15, 0.5, 0.5/
TABLE TAUI,1,6/...
  1,2,3,4,5,6,...
  3.0, 0.1, 0.75, 0.25, 1.0, 0.6/
TABLE TAUV,1,6/...
  1,2,3,4,5,6,...
  0.15, 0.15, 0.15, 0.2, 0.15, 0.15/

" Twi changed from 545.---6/5/92"
INITIAL
Constant...
AA=141.372 , AD=17.6715 , ALPHA=0.2 , AN=141.372 , ...
Apc=16022.16 , Apmr=3361.826 , As=3844.168 , AT=176.714 , ...
AUD=0.908375 , Aw=13940.0 , Ccw=1.0 , Cmc=0.12 , ...
Cmr=0.12 , Cvc = .65, Cx = .58, DH=0.1875, DR=10.0 , ...
DTT=15.0 , g = 115523.24, HSH=1262.8 , HW=1.0 , ...
HWSP=1.25 , LH = 0.0078125, LR=16.0 , LW=130.806 , ...
LWSP=149.0 , PB=30 , PD=40 , pii=3.14159 , ...

```

```

PSH=255.0 , Pw1=60 , Pw2Pw3=9.0 , Pw3=35 , Qcwo=8653.0 , ...
REF1 = 0.947775644, REF2 = 9.0, REF3=2.9659168, ...
RHO2VR=0.002549852, sumv1 = 1.0, Sv2IR=105.8752 , ...
TAUM=0.20 , TSAT=862.7 , TSH=960.0 , TT=0.09375 , ...
Twi=530. , Ucw=17160.0 , Umc=45000.0 , Umr=11000.0 , ...
Upmo=213.0 , Upmr=300.0 , Us=1000.0 , Uwmo=1250.0 , ...
Vr=68.83 , ZB=10.0 , ZC=5.0

```

"gravitational acceleration, g, in ft/min**2"

"-----controller set points (in mA.) "

```

CISP1 = 0.032*SP(1.0) - 12.0
CISP2 = (SP(2.0)/200)**2 + 4.0
CISP3 = 4.0 + 1.6*SP(3.0)
CISP5 = -20.0 + 4*SP(5.0)
CISP6 = 0.4*SP(6.0) - 236.

```

"-----coefficients "

TABLE MV, 2, 3, 4 /...

```

1,2,3, 1,2,3,4,...
0.6451094E2, -0.1095359 , 0.1195526E-3,...
0.5686523E2, 0.468039E-2, 0.5094978E-4,...
0.5370027E2, -0.1728176E-1, 0.493820E-4,...
0.2288676E2, -0.2023121E-1, 0.2115899E-4/

```

TABLE HVCO, 2, 5, 4/...

```

1, 2, 3, 4, 5, 1, 2, 3, 4,...
0.1174119E5, 0.7121495E1, 0.5579442E-2, ...
-0.450617E-6, -0.2091904E-10,...
0.867332E4, 0.4735799E1, 0.1452860E-1,...
-0.1121397E-5, -0.2018173E-9,...
0.106486E5, 0.7515997E1, 0.1151360E-1,...
-.01682096E-5, 0.9036333E-10,...
0.1545871E5, 0.8022526E1, -0.4745722E-3,...
0.6878047E-6, -0.1439752E-9/

```

TABLE hLCO, 2, 3, 4/...

```

1, 2, 3, 1, 2, 3, 4,...
-0.3119436E4, -4.145198, 0.2131106E-1, ...
-0.115334E5, 0.1770348E2, 0.1166435E-1, ...
0.4046348E3, -0.2410286E2, 0.472823E-1, ...
-0.87838059E4, 0.175845E2, 0.3651369E-3/

```

TABLE ANT, 2, 3, 4/...

```

1,2,3, 1,2,3,4,...
7.87863, 1.47311E3, 2.3E2,...
7.02447, 1.16E3, 2.24E2,...
8.04494, 1.5543E3, 2.2265E2,...
7.96681, 1.66821E3,2.28E2/

```

TABLE WLMB,2,4,4/...

```

1,2,3,4, 1,2,3,4,...
0.0, 0.66408E3, 0.59844E3, 0.20530E3,...
-0.21495E3, 0.0, 0.38170E2, 0.43964E3,...
0.51139E3, 0.41896E3, 0.0, 0.38230E3,...
0.48216E3, 0.140549E3, 0.95549E3, 0.0/

```

TABLE RHOSCO, 1, 5/...

```

1,2,3,4,5,...
1.031951E-2, 1.427797E1, 0.9414444, 2.048037, 5.956991/

```

TABLE hLSCO, 1, 5/...

```

1,2,3,4,5,...
-1.6029E2, 8.06427E-2, 7.361453E-5, 1.501012E-6,...
-9.9964334E-10/

```

TABLE HVSCO, 1, 5/...

```

1,2,3,4,5,...

```

5.448738E2, 8.039637E-1, 1.931794E-3, -3.938661E-6, ...
1.907853E-9/
TABLE HEDCO, 2, 4, 2/...
1, 2, 3, 4, 1, 2, ...
9.870927E1, -9.794161E-3, -1.95175E-6, -1.954559E-9, ...
9.152028E1, -6.584299E-2, 7.533832E-5, -4.300139E-8/
TABLE CV1CO, 2, 5, 20/...
1, 2, 3, 4, 5, ...
0.0, 0.099, 0.1, 0.19, 0.2, 0.29, 0.3, 0.39, 0.4, 0.49, ...
0.5, 0.59, 0.6, 0.69, 0.7, 0.79, 0.8, 0.89, 0.9, 1.0, ...
0.0, 0.0, 0.6759999E2, -0.6691973E3, 0.6691969E4, ...
0.0, 0.0, 0.6759999E2, -0.6691973E3, 0.6691969E4, ...
0.1, 0.676E1, 0.1345197E3, -0.1167920E4, 0.8667223E4, ...
0.1, 0.676E1, 0.1345197E3, -0.1167920E4, 0.8667223E4, ...
0.2, 0.5810001E2, 0.9598074E3, -7506973E4, 0.8598887E5, ...
0.2, 0.5810001E2, 0.9598074E3, -7506973E4, 0.8598887E5, ...
0.3, 0.165E3, .2038081E4, -0.768066E4, 0.8299831E5, ...
0.3, 0.165E3, .2038081E4, -0.768066E4, 0.8299831E5, ...
0.4, 0.375E3, 0.2991901E4, -0.6826715E4, 0.4807690E5, ...
0.4, 0.375E3, 0.2991901E4, -0.6826715E4, 0.4807690E5, ...
0.5, 0.654E3, 0.3068865E4, -0.5726895E4, 0.6382414E4, ...
0.5, 0.654E3, 0.3068865E4, -0.5726895E4, 0.6382414E4, ...
0.6, 0.91E3, 0.2114958E4, -0.2852868E5, 0.2237909E6, ...
0.6, 0.91E3, 0.2114958E4, -0.2852868E5, 0.2237909E6, ...
0.7, 0.106E4, 0.3122954E4, 0.1411841E5, -0.9347956E5, ...
0.7, 0.106E4, 0.3122954E4, 0.1411841E5, -0.9347956E5, ...
0.8, 0.142E4, 0.3142248E4, -0.2419347E5, 0.1177098E6, ...
0.8, 0.142E4, 0.3142248E4, -0.2419347E5, 0.1177098E6, ...
0.9, 0.161E4, 0.1834851E4, -0.6969128E3, 0.3484387E4, ...
0.9, 0.161E4, 0.1834851E4, -0.6969128E3, 0.3484387E4/
TABLE CV2CO, 2, 5, 20/...
1, 2, 3, 4, 5, ...
0.0, 0.099, 0.1, 0.19, 0.2, 0.29, 0.3, 0.39, 0.4, 0.49, ...
0.5, 0.59, 0.6, 0.69, 0.7, 0.79, 0.8, 0.89, 0.9, 1.0, ...
0.0, 0.0, 0.6759999E2, -0.6691973E3, 0.6691969E4, ...
0.0, 0.0, 0.6759999E2, -0.6691973E3, 0.6691969E4, ...
0.1, 0.676E1, 0.1345197E3, -0.1167920E4, 0.8667223E4, ...
0.1, 0.676E1, 0.1345197E3, -0.1167920E4, 0.8667223E4, ...
0.2, 0.172E2, 0.1609525E3, -0.5040024E3, 0.5344770E4, ...
0.2, 0.172E2, 0.1609525E3, -0.5040024E3, 0.5344770E4, ...
0.3, 0.3360001E2, 0.2204954E3, -0.1038741E4, 0.8337859E4, ...
0.3, 0.3360001E2, 0.2204954E3, -0.1038741E4, 0.8337859E4, ...
0.4, 0.5360001E2, 0.2628831E3, -0.9942312E3, 0.8153996E4, ...
0.4, 0.5360001E2, 0.2628831E3, -0.9942312E3, 0.8153996E4, ...
0.5, 0.7810001E2, 0.3086567E3, -0.1381982E4, 0.1085412E5, ...
0.5, 0.7810001E2, 0.3086567E3, -0.1381982E4, 0.1085412E5, ...
0.6, 0.106E3, 0.3578840E3, -0.1145935E4, 0.8670914E4, ...
0.6, 0.106E3, 0.3578840E3, -0.1145935E4, 0.8670914E4, ...
0.7, 0.139E3, 0.3888247E3, -0.1526535E4, 0.1038285E5, ...
0.7, 0.139E3, 0.3888247E3, -0.1526535E4, 0.1038285E5, ...
0.8, 0.173E3, 0.3950034E3, -0.6824436E3, 0.2324071E4, ...
0.8, 0.173E3, 0.3950034E3, -0.6824436E3, 0.2324071E4, ...
0.9, 0.208E3, 0.3282368E3, -0.1564725E4, 0.7823613E4, ...
0.9, 0.208E3, 0.3282368E3, -0.1564725E4, 0.7823613E4/
TABLE CV3CO, 2, 5, 20/...
1, 2, 3, 4, 5, ...
0.0, 0.099, 0.1, 0.19, 0.2, 0.29, 0.3, 0.39, 0.4, 0.49, ...
0.5, 0.59, 0.6, 0.69, 0.7, 0.79, 0.8, 0.89, 0.9, 1.0, ...
0.0, 0.0, 0.6689999E2, -0.17743E3, 0.1742997E4, ...
0.0, 0.0, 0.6689999E2, -0.17743E3, 0.1742997E4, ...
0.1, 0.669E1, 0.8432991E2, -0.8532524E3, 0.5009532E4, ...

0.1, 0.669E1, 0.8432991E2, -0.8532524E3, 0.5009532E4, ...
 0.2, 0.116E2, 0.6396542E2, -0.3343521E3, 0.3846974E4, ...
 0.2, 0.116E2, 0.6396542E2, -0.3343521E3, 0.3846974E4, ...
 0.3, 0.185E2, 0.1125043E3, -0.6310693E3, 0.6060258E4, ...
 0.3, 0.185E2, 0.1125043E3, -0.6310693E3, 0.6060258E4, ...
 0.4, 0.295E2, 0.1680985E3, -0.9577654E3, 0.9167789E4, ...
 0.4, 0.295E2, 0.1680985E3, -0.9577654E3, 0.9167789E4, ...
 0.5, 0.4589999E2, 0.2515793E3, -0.132549E4, 0.1269696E5, ...
 0.5, 0.4589999E2, 0.2515793E3, -0.132549E4, 0.1269696E5, ...
 0.6, 0.705E2, 0.3673904E3, -0.1754303E4, 0.1630397E5, ...
 0.6, 0.705E2, 0.3673904E3, -0.1754303E4, 0.1630397E5, ...
 0.7, 0.106E3, 0.5056489E3, -0.2605563E4, 0.2349071E5, ...
 0.7, 0.106E3, 0.5056489E3, -0.2605563E4, 0.2349071E5, ...
 0.8, 0.154E3, 0.6892578E3, -0.2990246E4, 0.2697664E5, ...
 0.8, 0.154E3, 0.6892578E3, -0.2990246E4, 0.2697664E5, ...
 0.9, 0.22E3, 0.9005083E3, -0.1210117E4, 0.6050512E4, ...
 0.9, 0.22E3, 0.9005083E3, -0.1210117E4, 0.6050512E4/

TABLE CV5CO, 2, 5, 20/...

1,2,3,4,5, ...
 0.0, 0.099, 0.1, 0.19, 0.2, 0.29, 0.3, 0.39, 0.4, 0.49, ...
 0.5, 0.59, 0.6, 0.69, 0.7, 0.79, 0.8, 0.89, 0.9, 1.0, ...
 0.0, 0.0, 0.463E3, -0.3610995E4, 0.3610991E5, ...
 0.0, 0.0, 0.463E3, -0.3610995E4, 0.3610991E5, ...
 0.1, 0.463E2, 0.8240989E3, -0.5206883E4, 0.3035894E5, ...
 0.1, 0.463E2, 0.8240989E3, -0.5206883E4, 0.3035894E5, ...
 0.2, 0.107E3, 0.6934902E3, -0.1574331E4, 0.1039425E5, ...
 0.2, 0.107E3, 0.6934902E3, -0.1574331E4, 0.1039425E5, ...
 0.3, 0.171E3, 0.6904519E3, -0.2672921E4, 0.1468400E5, ...
 0.3, 0.171E3, 0.6904519E3, -0.2672921E4, 0.1468400E5, ...
 0.4, 0.228E3, 0.5963877E3, -0.2192055E4, 0.1328175E5, ...
 0.4, 0.228E3, 0.5963877E3, -0.2192055E4, 0.1328175E5, ...
 0.5, 0.279E3, 0.5564294E3, -0.1604116E4, 0.8398187E4, ...
 0.5, 0.279E3, 0.5564294E3, -0.1604116E4, 0.8398187E4, ...
 0.6, 0.327E3, 0.4875520E3, -0.1870622E4, 0.9950992E4, ...
 0.6, 0.327E3, 0.4875520E3, -0.1870622E4, 0.9950992E4, ...
 0.7, 0.367E3, 0.4119575E3, -0.4696677E3, -0.1499096E4, ...
 0.7, 0.367E3, 0.4119575E3, -0.4696677E3, -0.1499096E4, ...
 0.8, 0.402E3, 0.2730510E3, -0.1572119E4, 0.6416082E4, ...
 0.8, 0.402E3, 0.2730510E3, -0.1572119E4, 0.6416082E4, ...
 0.9, 0.42E3, 0.1511098E3, -0.4221873E3, 0.2110922E4, ...
 0.9, 0.42E3, 0.1511098E3, -0.4221873E3, 0.2110922E4/

TABLE CSCO, 2, 5, 20/...

1,2,3,4,5, ...
 0.0, 0.099, 0.1, 0.19, 0.2, 0.29, 0.3, 0.39, 0.4, 0.49, ...
 0.5, 0.59, 0.6, 0.69, 0.7, 0.79, 0.8, 0.89, 0.9, 1.0, ...
 0.0, 0.0, 0.112E3, -0.280999E3, 0.2809984, ...
 0.0, 0.0, 0.112E3, -0.280999E3, 0.2809984, ...
 0.1, 0.193E2, 0.9875446E2, -0.6029138E3, 0.6653684E4, ...
 0.1, 0.193E2, 0.9875446E2, -0.6029138E3, 0.6653684E4, ...
 0.2, 0.193E2, 0.9875446E2, -0.6029138E3, 0.6653684E4, ...
 0.2, 0.193E2, 0.9875446E2, -0.6029138E3, 0.6653684E4, ...
 0.3, 0.298E2, 0.1777826E3, -0.8587102E3, 0.8508832E4, ...
 0.3, 0.298E2, 0.1777826E3, -0.8587102E3, 0.8508832E4, ...
 0.4, 0.475E2, 0.2613057E3, -0.1764654E4, 0.1651596E5, ...
 0.4, 0.475E2, 0.2613057E3, -0.1764654E4, 0.1651596E5, ...
 0.5, 0.725E2, 0.4038538E3, -0.2260444E4, 0.2271903E5, ...
 0.5, 0.725E2, 0.4038538E3, -0.2260444E4, 0.2271903E5, ...
 0.6, 0.133E3, 0.6333362E3, -0.2353483E4, 0.2220118E5, ...
 0.6, 0.133E3, 0.6333362E3, -0.2353483E4, 0.2220118E5, ...
 0.7, 0.175E3, 0.8286753E3, -0.2622047E4, 0.1935291E5, ...
 0.7, 0.175E3, 0.8286753E3, -0.2622047E4, 0.1935291E5, ...

```

0.8, 0.251E3, 0.8848535E3, -0.6906321E3, -0.4579047E4,...
0.8, 0.251E3, 0.8848535E3, -0.6906321E3, -0.4579047E4,...
0.9, 0.328E3, 0.6093555E3, -0.4187094E4, 0.2093548E5,...
0.9, 0.328E3, 0.6093555E3, -0.4187094E4, 0.2093548E5/
"-----Physical constants "
TABLE PCC, 2, 4, 4/...
  1,2,3,4, 1,2,3,4,...
  78.5, 59.6, 70.0, 127.8,...
  59.6, 46.6, 54.0, 93.5,...
  70.0, 54.0, 63.0, 111.9,...
  127.8, 93.5, 111.9, 218.3/
TABLE TCC, 2, 4, 4/...
  1,2,3,4, 1,2,3,4,...
  513.2, 510.9, 514.1, 576.4,...
  510.9, 508.7, 512.3, 573.9,...
  514.1, 512.3, 516.0, 578.0,...
  576.4, 573.9, 578.0, 647.4/
TABLE TC,1,4/...
  1,2,3,4,...
  513.2, 508.7, 516.0, 647.4/
TABLE PC,1,4/...
  1,2,3,4,...
  78.5, 46.6, 63.0, 218.3/
TABLE VC,1,4/...
  1,2,3,4,...
  118.0, 213.5, 161.3, 55.2/
TABLE WW,1,4/...
  1,2,3,4,...
  0.557, 0.309, 0.637, 0.344/
TABLE WWH,1,4/...
  1,2,3,4,...
  0.105, 0.187, 0.152, 0.010/
TABLE MU,1,4/...
  1,2,3,4,...
  1.66, 2.88, 1.69, 1.83/
TABLE ETTA, 2,4,4/...
  1,2,3,4, 1,2,3,4,...
  1.21, 0.605, 1.155, 0.605,...
  0.605, 0.0, 0.55, 0.0,...
  1.155, 0.55, 1.1, 0.55,...
  0.605, 0.0, 0.55, 0.0/
TABLE MUR, 2, 4, 4/...
  1,2,3,4, 1,2,3,4,...
  4.408, 4.693, 4.308, 4.761,...
  4.693, 5.006, 4.607, 5.008,...
  4.308, 4.607, 4.213, 4.640,...
  4.761, 5.008, 4.640, 5.161/
TABLE WH, 2, 4, 4/...
  1,2,3,4, 1,2,3,4,...
  0.105, 0.146, 0.1285, 0.0575,...
  0.146, 0.187, 0.1695, 0.0985,...
  0.1285, 0.1695, 0.152, 0.081,...
  0.0575, 0.0985, 0.081, 0.01/
TABLE MOL, 1, 4/...
  1,2,3,4,...
  32.04,58.08,46.07,18.016/
"-----Column constants and forcing functions "
TABLE AH, 1, 4/...
  1,3,4,50,...
  18,18,13,13/
TABLE CD, 1, 4/...

```

```

1, 3, 4, 50,...
0.75, 0.75, 0.72, 0.72/
TABLE F, 2, 10, 4/...
1,2,3,4,5,6,20,21,22,50,...
1,2,3,4,...
0., 0., 0., 0., 65.25, 0.,0., .0, 0., 0., ...
0., 0., 0., 0., 25.5, 0., 0., .0, 0., 0., ...
0., 0., 0., 0., 10.0, 0., 0., .0, 0., 0., ...
0., 0., 0., 0., 207.5, 0., 0., .0, 0., 0./
TABLE Hf, 1, 10/...
1,2,3,4,5,6,20,21,22,50,...
0.0, 0.0, 0.0, 0.0, 868000., 0.0, ...
0.0, 0.0, 0.0, 0.0/
"-----Receiver liquid height to volume function"
TABLE RECVOL, 1, 27/...
0.0,2.12692,5.99764,10.9848,16.8604,23.4904,42.8183,...
65.4004,90.6624,118.2,178.918,245.674,317.069,391.969,...
469.392,548.452,628.319,708.185,787.245,864.668,939.568,...
1010.96,1077.72,1138.44,1191.24,1233.15,1256.64,...
0.0,0.1,0.2,0.3,0.4,0.5,0.75,1.0,1.25,1.5,2.0,2.5,3.0,...
3.5,4.0,4.5,5.0,5.5,6.0,6.5,7.0,7.5,8.0,8.5,9.0,9.5,10.0/

"UV(1) changed from 2.1557724"
TABLE UV, 1, 9/...
1,2,3,4,5,21,35,49,50,...
2.15, 2.00531, 1.9955679, 1.965454, 1.8892558, ...
1.9032513, 1.91708, 1.92265, 2.0345702/

"-----Gas Constant in atm*ft**3/lBmol*K, cm**3*mmHg/gmol*K,"
" ft**3*mmHg/lBmol*R, cal/gmol*K, lb*ft**3/ft**2*lBmol*R"
TABLE RR, 1, 5/...
1,2,3,4,5,...
1.314, 62361.0, 555.0, 1.987, 1545.0/

"-----Energy models-----"
MACRO engb1(Tj, TKj, R, QC, Ej, Lj, HLDPj, EVjp, ...
uj1, uj2, uj3, uj4, duj1,duj2,duj3,duj4, J)

MACRO Redefine Ejdot, jj, dTj, hLj1,hLj2,hLj3,hLj4

jj = J/1.0
Ejdot = Hf(jj) + EVjp - (1 + R)*Lj*Ej/(R * HLDPj) - QC
Ej = INTEG(Ejdot, E0&J)

hLj1 = hLCO(1.0,1.0) + hLCO(2.0,1.0)*Tj + hLCO(3.0,1.0)*Tj**2
hLj2 = hLCO(1.0,2.0) + hLCO(2.0,2.0)*Tj + hLCO(3.0,2.0)*Tj**2
hLj3 = hLCO(1.0,3.0) + hLCO(2.0,3.0)*Tj + hLCO(3.0,3.0)*Tj**2
hLj4 = hLCO(1.0,4.0) + hLCO(2.0,4.0)*Tj + hLCO(3.0,4.0)*Tj**2

Tj = INTEG(dTj, T0&J)
TKj = 5.0*Tj/9.0
dTj = (Ejdot - hLj1*duj1 - hLj2*duj2 - hLj3*duj3 - hLj4*duj4)/ ...
((hLCO(2.0,1.0) + 2*hLCO(3.0,1.0)*Tj)*uj1 ...
+ (hLCO(2.0,2.0) + 2*hLCO(3.0,2.0)*Tj)*uj2 ...
+ (hLCO(2.0,3.0) + 2*hLCO(3.0,3.0)*Tj)*uj3 ...
+ (hLCO(2.0,4.0) + 2*hLCO(3.0,4.0)*Tj)*uj4)

MACRO END

MACRO engbj(Ej, Lj, Ljm, Ejm,uj1, uj2, uj3, uj4, ...

```

```

HLDPj, HLDPjm, duj1,duj2,duj3,duj4, EVj,EVjp, ...
vj1,vj2,vj3,vj4,sumvj, Tj, TKj, J)

MACRO Redefine Ejdot,jj, dTj, hLj1,hLj2,hLj3,hLj4, ...
    HVj1,HVj2,HVj3,HVj4

jj = J/1.0
Ejdot = Hf(jj) + Ljm*Ejm/HLDPjm - Lj*Ej/HLDPj + ...
    EVjp - EVj
Ej = INTEG(Ejdot, E0&J)

HVj1 = HVCO(1.0,1.0) + HVCO(2.0,1.0)*Tj + HVCO(3.0,1.0)*Tj**2 +
...
    HVCO(4.0,1.0)*Tj**3 + HVCO(5.0,1.0)*Tj**4
HVj2 = HVCO(1.0,2.0) + HVCO(2.0,2.0)*Tj + HVCO(3.0,2.0)*Tj**2 +
...
    HVCO(4.0,2.0)*Tj**3 + HVCO(5.0,2.0)*Tj**4
HVj3 = HVCO(1.0,3.0) + HVCO(2.0,3.0)*Tj + HVCO(3.0,3.0)*Tj**2 +
...
    HVCO(4.0,3.0)*Tj**3 + HVCO(5.0,3.0)*Tj**4
HVj4 = HVCO(1.0,4.0) + HVCO(2.0,4.0)*Tj + HVCO(3.0,4.0)*Tj**2 +
...
    HVCO(4.0,4.0)*Tj**3 + HVCO(5.0,4.0)*Tj**4

hLj1 = hLCO(1.0,1.0) + hLCO(2.0,1.0)*Tj + hLCO(3.0,1.0)*Tj**2
hLj2 = hLCO(1.0,2.0) + hLCO(2.0,2.0)*Tj + hLCO(3.0,2.0)*Tj**2
    HVCO(4.0,1.0)*Tj**3 + HVCO(5.0,1.0)*Tj**4
HVj2 = HVCO(1.0,2.0) + HVCO(2.0,2.0)*Tj + HVCO(3.0,2.0)*Tj**2 +
...
    HVCO(4.0,2.0)*Tj**3 + HVCO(5.0,2.0)*Tj**4
HVj3 = HVCO(1.0,3.0) + HVCO(2.0,3.0)*Tj + HVCO(3.0,3.0)*Tj**2 +
...
    HVCO(4.0,3.0)*Tj**3 + HVCO(5.0,3.0)*Tj**4
HVj4 = HVCO(1.0,4.0) + HVCO(2.0,4.0)*Tj + HVCO(3.0,4.0)*Tj**2 +
...
    HVCO(4.0,4.0)*Tj**3 + HVCO(5.0,4.0)*Tj**4

hLj1 = hLCO(1.0,1.0) + hLCO(2.0,1.0)*Tj + hLCO(3.0,1.0)*Tj**2
hLj2 = hLCO(1.0,2.0) + hLCO(2.0,2.0)*Tj + hLCO(3.0,2.0)*Tj**2
hLj3 = hLCO(1.0,3.0) + hLCO(2.0,3.0)*Tj + hLCO(3.0,3.0)*Tj**2
hLj4 = hLCO(1.0,4.0) + hLCO(2.0,4.0)*Tj + hLCO(3.0,4.0)*Tj**2

EVj = vj1*HVj1 + vj2*HVj2 + vj3*HVj3 + vj4*HVj4

Tj = INTEG(dTj, T0&J)
TKj = 5.0*Tj/9.0
dTj = (Ejdot - hLj1*duj1 - hLj2*duj2 - hLj3*duj3 - hLj4*duj4)/ ...
    ((hLCO(2.0,1.0) + 2*hLCO(3.0,1.0)*Tj)*uj1 ...
    + (hLCO(2.0,2.0) + 2*hLCO(3.0,2.0)*Tj)*uj2 ...
    + (hLCO(2.0,3.0) + 2*hLCO(3.0,3.0)*Tj)*uj3 ...
    + (hLCO(2.0,4.0) + 2*hLCO(3.0,4.0)*Tj)*uj4)

MACRO END

"-----Material-balance models-----"

MACRO matb1(uj1, uj2, uj3, uj4, HLDP1, ...
    vjp1, vjp2, vjp3, vjp4, sumvjp, ...
    duj1,duj2,duj3,duj4, R, Lj, J)

MACRO Redefine jj

```

```

jj = J/1.0

duj1 = f(jj,1.0) - (1 + R)*Lj*uj1/(R * HLDP1) + vjp1
uj1 = INTEG(duj1, u10&J)
duj2 = f(jj,2.0) - (1 + R)*Lj*uj2/(R * HLDP1) + vjp2
uj2 = INTEG(duj2, u20&J)
duj3 = f(jj,3.0) - (1 + R)*Lj*uj3/(R * HLDP1) + vjp3
uj3 = INTEG(duj3, u30&J)
duj4 = f(jj,4.0) - (1 + R)*Lj*uj4/(R * HLDP1) + vjp4
uj4 = INTEG(duj4, u40&J)
HLDP1 = uj1 + uj2 + uj3 + uj4

MACRO END

MACRO matbj(uj1, uj2, uj3, uj4, HLDPj,ujm1,ujm2, ujm3, ujm4, ...
          HLDPjm,vj1, vj2, vj3, vj4, sumvj, ...
          vjp1, vjp2, vjp3, vjp4, sumvjp, Lj, Ljm, ...
          duj1, duj2, duj3, duj4, J)

MACRO Redefine jj

jj = J*1.0/1.0

duj1 = f(jj,1.0) + Ljm*ujm1/HLDPjm - Lj*uj1/HLDPj - vj1 + vjp1
uj1 = INTEG(duj1, u10&J)
duj2 = f(jj,2.0) + Ljm*ujm2/HLDPjm - Lj*uj2/HLDPj - vj2 + vjp2
uj2 = INTEG(duj2, u20&J)
duj3 = f(jj,3.0) + Ljm*ujm3/HLDPjm - Lj*uj3/HLDPj - vj3 + vjp3
uj3 = INTEG(duj3, u30&J)
duj4 = f(jj,4.0) + Ljm*ujm4/HLDPjm - Lj*uj4/HLDPj - vj4 + vjp4
uj4 = INTEG(duj4, u40&J)
HLDPj = uj1 + uj2 + uj3 + uj4
MACRO END

MACRO matbN(uj1, uj2, uj3, uj4, HLDPj,ujm1,ujm2, ujm3, ujm4, ...
          HLDPjm,vj1, vj2, vj3, vj4, sumvj, ...
          duj1, duj2, duj3, duj4, Lj, Ljm, J)

MACRO Redefine jj

jj = J*1.0/1.0
duj1 = f(jj,1.0) + Ljm*ujm1/HLDPjm - Lj*uj1/HLDPj - vj1
uj1 = INTEG(duj1, u10&J)
duj2 = f(jj,2.0) + Ljm*ujm2/HLDPjm - Lj*uj2/HLDPj - vj2
uj2 = INTEG(duj2, u20&J)
duj3 = f(jj,3.0) + Ljm*ujm3/HLDPjm - Lj*uj3/HLDPj - vj3
uj3 = INTEG(duj3, u30&J)
duj4 = f(jj,4.0) + Ljm*ujm4/HLDPjm - Lj*uj4/HLDPj - vj4
uj4 = INTEG(duj4, u40&J)
HLDPj = uj1 + uj2 + uj3 + uj4
MACRO END

"-----pressure models-----"

MACRO pres1(Pj, Pjp, Z1, RHMLj, HLDPj, sumvjp, Tj, ...
          vjp1,vjp2,vjp3,vjp4, Yjp1,Yjp2,Yjp3,Yjp4, J)

MACRO Redefine VOLREC, RHMVj, efl1, efl2, efl3, efl4,dP

Pj = RR(5.0)*Tj*RHMVj
RHMVj = UV(1.0)/(1256.6 - VOLREC)

```



```

VOLREC = HLDPj/RHMLj
Z1 = RECVOL(VOLREC)

dP = Pjp - Pj
sumvjp = SIGN(1.0,dP)*SQRT(ABS(dP)/(RHMVj*REF3))
" vjp1 = IMPL(v102, 1.0, 7, efl1, Yjp1*sumvjp , 0.5) "
" vjp2 = IMPL(v202, 1.0, 7, efl2, Yjp2*sumvjp , 0.5) "
" vjp3 = IMPL(v302, 1.0, 7, efl3, Yjp3*sumvjp , 0.5) "
" vjp4 = IMPL(v402, 1.0, 7, efl4, Yjp4*sumvjp , 0.5) "

vjp1 = Yjp1*sumvjp
vjp2 = Yjp2*sumvjp
vjp3 = Yjp3*sumvjp
vjp4 = Yjp4*sumvjp

MACRO END

MACRO presj(Pj, Pjp, Lj, Ljm, HCTRj, HCTRjp, ...
  RHOVj, RHMVj, RHMLj, RHOLj, RHOVjp, RHMVjp, ...
  HLDPj, sumvj, vjp1,vjp2,vjp3,vjp4,sumvjp, ...
  Yjp1,Yjp2,Yjp3,Yjp4, Yj1,Yj2,Yj3,Yj4, Tj, Zj, ...
  duj1,duj2,duj3,duj4, Jp,J)

MACRO Redefine HOj, FOAMj, QLj, FVAj, UVAj, UHj, HLUdj, ...
  MOLV, HOLDj, jj, dPdc, Pdc, dVdc, ...
  Vdc, dhow, howj, PUD, Qs, dQs, Cdd, dHLDPj, dQVjp, ...
  dvjp, dZj, QQs, Pke, dHCL

jj = J/1.0
RHMVj = UV(jj)/(883.57 - HLDPj/RHMLj)
MOLV = Yj1*MOL(1.0) + Yj2*MOL(2.0) + Yj3*MOL(3.0) + ...
  Yj4*MOL(4.0)
RHOVj = MOLV*RHMVj
Pj = RR(5.0)*Tj*RHMVj

" HCTRj = FOAMj*(howj + HW/12) "
dHCL = (dHLDPj/RHMLj - dVdc)/AN
HCTRj = INTEG(dHCL, hc10&J)

FOAMj = 1 - 0.372192*FVAj**0.177709
FVAj = UVAj*SQRT(RHOVj)
UVAj = sumvj/(AN*RHMVj*60)

" UHj = sumvjp/(AH(jj)*RHMVjp) "
" --HOj-- POj = (UHj/CD(jj))**2 * RHOVjp/(2*g) "
Pke = RHOVjp*(sumvjp/(RHMVjp*AH(jj)*Cvc)**2)/(2*g)
dQVjp = Cvc**2*AH(jj)*(Pjp - Pj - HCTRj*RHOLj - Pke)/(RHOVj*LH)
dvjp = dQVjp*RHMVjp
vjp1 = INTEG(Yjp1*dvjp, V10&Jp)
vjp2 = INTEG(Yjp2*dvjp, V20&Jp)
vjp3 = INTEG(Yjp3*dvjp, V30&Jp)
vjp4 = INTEG(Yjp4*dvjp, V40&Jp)
sumvjp = vjp1 + vjp2 + vjp3 + vjp4

" -----downcomer hydrolic capacitance"
" dPdc = RHOLj*dZj "
" Pdc = INTEG(dPdc, (Zj*RHOLj)) "
dVdc = dZj * AD
dZj = (Qs - QLj)/AD
Vdc = Zj * AD
Zj = INTEG(dZj,Z0&J)

```

```

"      --note that flows are allowed to become negative"
QLj = Cx*AUD*SIGN(1.0,PUD)*SQRT(2*g*ABS(PUD))
PUD = (Pj - Pjp)/RHOLj - HCTRjp + Zj
Lj = QLj*RHMLj

"      -----wier equations"
dQs = Cdd*LW*dhow*SIGN(1.0,howj)*SQRT(2*g*ABS(howj))/12.0
QQs = INTEG(dQs, Qs0&J )
Qs = FCNSW(howj, 0.0, 0.0, QQs)
Cdd = (1.368*(1.01 + .0063*(Qs*(12/LW)**2.5)))*1.5
dhow = (dHLDpj/RHMLj - dVdc)/(AN*FOAMj)
dHLDpj = duj1 + duj2 + duj3 + duj4
howj = INTEG(dhow, how0&J )
MACRO END

"-----Liquid-Vapor equilibrium model-----"
MACRO eql(uj1, uj2, uj3, uj4, HLDpj,Tj,TKj, ...
  Pj, Yj1, Yj2, Yj3, Yj4, RHMLj, RHOLj, J)

  MACRO Redefine PSj1, PSj2, PSj3, PSj4, Kj1, Kj2, Kj3 ,Kj4, ...
    ALPHj1, ALPHj2, ALPHj3, ALPHj4,sumK

  Yj1 = uj1*Kj1/sumK
  Yj2 = uj2*Kj2/sumK
  Yj3 = uj3*Kj3/sumK
  Yj4 = uj4*Kj4/sumK

  sumK = uj1*Kj1 + uj2*Kj2 + uj3*Kj3 + uj4*Kj4

  Kj1 = PSj1/Pj

  ALPHj1 = MV(1.0,1.0) + MV(2.0,1.0)*Tj + MV(3.0,1.0)*Tj**2
  PSj1 = 2.7855*10.**(ANT(1.0,1.0) - (ANT(2.0,1.0)/(ANT(3.0,1.0) +
...
    (TKj - 273.15))))
  "-----"
  Kj2 = PSj2/Pj
  ALPHj2 = MV(1.0,2.0) + MV(2.0,2.0)*Tj + MV(3.0,2.0)*Tj**2
  PSj2 = 2.7855*10.**(ANT(1.0,2.0) - (ANT(2.0,2.0)/(ANT(3.0,2.0) +
...
    (TKj - 273.15))))
  "-----"
  Kj3 = PSj3/Pj
  ALPHj3 = MV(1.0,3.0) + MV(2.0,3.0)*Tj + MV(3.0,3.0)*Tj**2
  PSj3 = 2.7855*10.**(ANT(1.0,3.0) - (ANT(2.0,3.0)/(ANT(3.0,3.0) +
...
    (TKj - 273.15))))
  "-----"
  Kj4 = PSj4/Pj
  ALPHj4 = MV(1.0,4.0) + MV(2.0,4.0)*Tj + MV(3.0,4.0)*Tj**2
  PSj4 = 2.7855*10.**(ANT(1.0,4.0) - (ANT(2.0,4.0)/(ANT(3.0,4.0) +
...
    (TKj - 273.15))))
  "-----"
  RHMLj = 62.43*HLDpj/(ALPHj1*uj1 +ALPHj2*uj2 + ...
    ALPHj3*uj3 + ALPHj4*uj4)
  RHOLj = 62.43*HLDpj/(ALPHj1*uj1/MOL(1.0) + ...
    ALPHj2*uj2/MOL(2.0) + ALPHj3*uj3/MOL(3.0) + ...
    ALPHj4*uj4/MOL(4.0))
MACRO END

```

```

"-----condenser and receiver model-----"
MACRO condsr(QC, L1, RHMLj, R, Pjp, Z1, Pj, q1, q2, RHOL1, ...
    T1,T2, sumvjp,CV1, CV2, CV3)

    "Redefine Tmc,Two,Qcw"
    MACRO Redefine Pd1, Ps1, ...
        Z, Y, X, PDD

    Two = INTEG(((Qcw*Ccw*(Twi - Two)*8.34 + Uwmo/60 * Aw*(Tmc - ...
        Two)*(Qcw/Qcwo)**1.8 )/(Ucw*Ccw)), Two0)
    QC = (105.8752/(sumvjp))**0.33 *(Upmo/60 * Apc*( ...
        (1-ALPHA)*T2 + ALPHA*T1 - Tmc))
    Tmc = INTEG(((QC - Uwmo/60 * (Qcw/Qcwo)**1.8 * Aw*(Tmc - Two)) ...
        /(Umc*Cmc)), Tmc0)
    Qcw = ((Pw1 - Pw3)*CV1**2/(0.25 + ...
        REF2*CV1**2/Qcwo**1.8))**0.5157507757

    PDD = (Pjp/144 *CV2**2/(CV2**2 + CV3**2) + ...
        PD*RHOL1/144 *CV3**2/(CV2**2 + CV3**2))
    Ps1 = Z1 + ZC + Pj/RHOL1
    q1 = SQRT(ABS(CV2**2 *(Pd1 - Pj/144)))
    R = q1/q2
    q2 = SQRT(ABS(CV3**2 * (Pd1 - PD*RHOL1/144)))
    L1 = q1*RHMLj/7.481

    Z = -0.00540862*RHOL1/144 *(CV2 + CV3)
    Y = 97.4907*RHOL1/144 + Ps1*RHOL1/144 + PDD*7.08247E-6 *RHOL1 ...
        *(CV2 + CV3)**2/144
    X = -7.08247E-6 *RHOL1/144 *(CV2 + CV3)**2 - 1.0
    Pd1 = (Z**2 - 2*X*Y + Z*SQRT(Z**2 - 4*X*(Y + X*PDD))) ...
        /(2*X**2)

MACRO END

"-----reboiler model-----"
MACRO reboil(HCTRj, QR, P50, Z50, q50,L50, Ljm, Lspj, ...
    Wsh, RHOVj, RHMVj, RHMLj, RHOL50, ...
    HLDpj, Yj1, Yj2, Yj3, Yj4, T50, CS4, CV5, J)

    MACRO Redefine Tsc, Tmr, Ps2, Pd2, RHOSC, hLSC, HVSC, ...
        VOLBTW, MOLV, dHVSC, FVAj, Csc, dRHOSC, ...
        dhow, howj, dQs, Qs, Qsj, Cdd

"-----pressure---"

    RHMVj = UV(50.0)/(2297.290 - Z50*176.715)
    MOLV = Yj1*MOL(1.0) + Yj2*MOL(2.0) + Yj3*MOL(3.0) + ...
        Yj4*MOL(4.0)
    RHOVj = MOLV*RHMVj
    VOLBTW = 100 + pii*Z50*DTT**2/4

    HCTRj = howj + HWSP/12
    dhow = (Ljm/RHMLj - Qs)/11.01
    howj = INTEG(dhow, how0&J )
    dQs = Cdd*149.0*dhow*SIGN(1.0,howj)*SQRT(2*g*ABS(howj))/12.0
    Qs = INTEG(dQs, Qs0&J )
    Qsj = FCNSW(howj, 0.0, 0.0, QQs)
    Cdd = (1.368*(1.01 + .0063*(Qs*(12/LSPW)**2.5)))*1.5

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Lspj = Qs*RHMLj

Z50 = 4/(pii*DTT**2)*(HLDPj/RHMLj - 100)
P50 = RR(5.0)*T50*RHMVj

"-----reboiler enthalpy balance and pump pressures----"
Tmr = INTEG(((Us*As/60 * (Tsc - Tmr) - QR)/(Umr*Cmr)), ...
  Tmr0)
Tsc = INTEG(((Wsh*(HSH - hLSC) - Us*As/60 * (Tsc - Tmr)) ...
  /(Csc*Vr*RHOSC - hLSC*dRHOSC*Vr)), Tsc0)
Csc = dHVSC + HVSC*dRHOSC/RHOSC
QR = Upmr*Apmr/60 * (Tmr - T50)
q50 = (0.0156369 - SQRT((0.0156369)**2 - 4*(-2.7865E-5 - ...
  144/(62.4*CV5**2)) * (70.3698 - HP)))/(2* ...
  (-2.7865E-5 - 144/(62.4*CV5**2)))
HP = PB*144/RHOL50 - Ps2
L50 = q50*RHMLj/7.481
Wsh = 2*PSH*CS4/(60*(1.0 + 0.00065*(TSH - TSAT)))
RHOSC = 1.031951E-2 + 1.427797E1*Tsc/610 + 0.9414444* ...
  (Tsc/610)**2 ...
  + 2.048037*(Tsc/610)**3 + 5.956991*(Tsc/610)**4
dRHOSC = ( RHOSCO(2.0) + 2*RHOSCO(3.0)*Tsc/610 + 3*RHOSCO(4.0) ...
  *(Tsc/610)**2 + 4*RHOSCO(5.0)*(Tsc/610)**3 )/610
hLSC = -1.6029E2 + 8.06427E-2*Tsc + 7.361453E-5*Tsc**2 + ...
  1.501012E-6*Tsc**3 - 9.9964334E-10*Tsc**4
dHVSC = 8.039637E-1 + 2*1.931794E-3*Tsc - 3*3.938661E-6* ...
  Tsc**2 + 4*1.907853E-9 * Tsc**3
HVSC = 5.448738E2 + 8.039637E-1*Tsc + 1.931794E-3*Tsc**2 - ...
  3.938661E-6*Tsc**3 + 1.907853E-9*Tsc**4
Ps2 = P50/RHOL50 + Z50 + ZB
MACRO END

"-----Controllers model-----"

MACRO contrl(CV1, CV2, CV3, CS4, CV5, ...
  T35, TK35, Pj, q1, Z1, Z50, Wsh)

MACRO Redefine CI1, CI2, CI3, CI4, CI5, CI6, CO1, CO2, CO3, ...
  CO4, CO5, CO6, I2, I3, I4, I5, I6, TM, ZETA2, ...
  ZETA3, ZETA4, ZETA5, dzETA1, dzETA2, dzETA3, dzETA5

CV1 = CV1CO(2.0,ZETA1) + CV1CO(3.0,ZETA1)*( ZETA1 ...
  - CV1CO(1.0,ZETA1)) + CV1CO(4.0,ZETA1)*( ZETA1 ...
  - CV1CO(1.0,ZETA1))**2 ...
  + CV1CO(5.0,ZETA1)*(ZETA1 - CV1CO(1.0,ZETA1))**3
CV2 = CV2CO(2.0,ZETA2) + CV2CO(3.0,ZETA2)*( ZETA2 ...
  - CV2CO(1.0,ZETA2)) + CV2CO(4.0,ZETA2)*( ZETA2 ...
  - CV2CO(1.0,ZETA2))**2 ...
  + CV2CO(5.0,ZETA2)*(ZETA2 - CV2CO(1.0,ZETA2))**3
CV3 = CV3CO(2.0,ZETA3) + CV3CO(3.0,ZETA3)*( ZETA3 ...
  - CV3CO(1.0,ZETA3)) + CV3CO(4.0,ZETA3)*( ZETA3 ...
  - CV3CO(1.0,ZETA3))**2 ...
  + CV3CO(5.0,ZETA3)*(ZETA3 - CV3CO(1.0,ZETA3))**3
CS4 = CSCO(2.0,ZETA4) + CSCO(3.0,ZETA4)*(ZETA4 ...
  - CSCO(1.0,ZETA4)) + CSCO(4.0,ZETA4)*(ZETA4 ...
  - CSCO(1.0,ZETA4))**2 + CSCO(5.0,ZETA4)*(ZETA4 ...
  - CSCO(1.0,ZETA4))**3
CV5 = CV5CO(2.0,ZETA5) + CV5CO(3.0,ZETA5)*(ZETA5 ...
  - CV5CO(1.0,ZETA5)) + CV5CO(4.0,ZETA5)*(ZETA5 ...
  - CV5CO(1.0,ZETA5))**2 + CV5CO(5.0,ZETA5)*(ZETA5 ...
  - CV5CO(1.0,ZETA5))**3

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```

Pbob = Pj/2.7855
CI1 = 0.032*Pbob - 12.0
I1 = INTEG(CI1 - CISP1, I01)
CO1 = XKC(1.0)*(CI1 - CISP1 + I1/TAUI(1.0))
ZETA1 = INTEG(dZETA1, ZET01)
dZETA1 = (-0.25 + 0.0625*CO1 - ZETA1)/TAUV(1.0)

CI2 = (q1/200)**2 + 4.0
I2 = INTEG(CISP2 - CI2, I02)
CO2 = XKC(2.0)*(-CI2 + CISP2 + I2/TAUI(2.0))
ZETA2 = INTEG(dZETA2, ZET02)
dZETA2 = (-0.25 + 0.0625*CO2 - ZETA2)/TAUV(2.0)

CI3 = 4.0 + 1.6*Z1
I3 = INTEG(CI3 - CISP3, I03)
CO3 = XKC(3.0)*(CI3 - CISP3 + I3/TAUI(3.0))
ZETA3 = INTEG(dZETA3, ZET03)
dZETA3 = (-0.25 + 0.0625*CO3 - ZETA3)/TAUV(3.0)

CI5 = -20.0 + 4*Z50
I5 = INTEG(CI5 - CISP5, I05)
CO5 = XKC(5.0)*(CI5 - CISP5 + I5/TAUI(5.0))
ZETA5 = INTEG(dZETA5, ZET05)
dZETA5 = (-0.25 + 0.0625*CO5 - ZETA5)/TAUV(5.0)

CI4 = 4 + 16*(Wsh/3000)**2
I4 = INTEG(CO6 - CI4, I04)
CO4 = XKC(4.0)*(CO6 - CI4 + I4/TAUI(4.0))
ZETA4 = INTEG((-0.25 + 0.0625*CO4 - ZETA4)/TAUV(4.0), ...
ZET04)
TM = INTEG((T35 - TM)/TAUM, TM0)
CI6 = 0.4*TM - 236.
CO6 = XKC(6.0)*(CISP6 - CI6 + I6/TAUI(6.0))
I6 = INTEG(CISP6 - CI6, I06)
MACRO END

"-----stage 1 model-----"
MACRO cond(Tj,Tjp, vjp1, vjp2, vjp3, vjp4, sumvjp, ...
Yjp1, Yjp2, Yjp3, Yjp4, uj1, uj2, uj3, uj4, HLDpj,...
CV1, CV2, CV3, EVjp, ...
RHOLj, RHMLjp, RHOVjp, RHMVjp, ...
Pj, Pjp, HCTRjp, Lj, Ej, q1,dist, R, Zj)

"-----Redefine QC"
MACRO Redefine TKj, RHMLj, Yj1,Yj2,Yj3,Yj4, ...
duj1, duj2, duj3, duj4

engbl(Tj, TKj, R, QC, Ej, Lj, HLDpj, EVjp, ...
uj1, uj2, uj3, uj4, duj1,duj2,duj3,duj4, 1)
matbl(uj1, uj2, uj3, uj4, HLDpj, ...
vjp1, vjp2, vjp3, vjp4, sumvjp, ...
duj1, duj2, duj3, duj4, R, Lj, 1)
eql(uj1, uj2, uj3, uj4, HLDpj,Tj,TKj, ...
Pj, Yj1, Yj2, Yj3, Yj4, RHMLj, RHOLj, 1)
pres1(Pj, Pjp, Zj, RHMLj, HLDpj, sumvjp, Tj, ...
vjp1,vjp2,vjp3,vjp4,Yjp1,Yjp2,Yjp3,Yjp4, 1)
conds(QC, Lj, RHMLj, R, Pjp, Zj, Pj, q1, dist, RHOLj, ...
Tj,Tjp, sumvjp,CV1, CV2, CV3)
MACRO END

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```

"-----stage 2-49 model-----"
MACRO stage(uj1, uj2, uj3, uj4, HLDPj,ujm1, ujm2, ujm3, ujm4, ...
  HLDPjm,Tj, TKj,EVj,EVjp, ...
  vj1, vj2, vj3, vj4, sumvj,vjp1, vjp2, vjp3, vjp4, ...
  sumvjp, Yjp1, Yjp2, Yjp3, Yjp4, Yj1, Yj2, Yj3, Yj4,...
  RHOLj, RHOVj, RHMVj, RHMLj, RHOVjp, RHMVjp, ...
  Zj, Pjp, HCTRjp,Pj, HCTRj,Ljm, Ejm,Lj, Ej, Jp,J)

MACRO Redefine duj1, duj2, duj3, duj4

  eql(uj1, uj2, uj3, uj4, HLDPj,Tj,TKj, ...
    Pj, Yj1, Yj2, Yj3, Yj4, RHMLj, RHOLj, J)
  matbj(uj1, uj2, uj3, uj4, HLDPj,ujm1,ujm2, ujm3, ujm4, ...
    HLDPjm,vj1, vj2, vj3, vj4, sumvj, ...
    vjp1, vjp2, vjp3, vjp4, sumvjp, Lj, Ljm, ...
    duj1, duj2, duj3, duj4, J)
  engbj(Ej, Lj, Ljm, Ejm,uj1, uj2, uj3, uj4, ...
    HLDPj, HLDPjm, duj1,duj2,duj3,duj4, EVj,EVjp, ...
    vj1,vj2,vj3,vj4,sumvj, Tj, TKj, J)
  presj(Pj, Pjp, Lj, Ljm, HCTRj, HCTRjp, ...
    RHOVj, RHMVj, RHMLj, RHOLj, RHOVjp, RHMVjp, ...
    HLDPj, sumvj, vjp1,vjp2,vjp3,vjp4,sumvjp, ...
    Yjp1,Yjp2,Yjp3,Yjp4, Yj1,Yj2,Yj3,Yj4, Tj, Zj, ...
    duj1,duj2,duj3,duj4, Jp,J)
MACRO END

"-----stage 50 model-----"
MACRO rebo(uj1, uj2, uj3, uj4, HLDPj,ujm1, ujm2, ujm3, ujm4, ...
  HLDPjm, EVj, vj1, vj2, vj3, vj4, sumvj, ...
  Yj1, Yj2, Yj3, Yj4, RHOLj, RHOVj, RHMVj,Pj, ...
  HCTRj,Ljm, Ejm,CS4, CV5, Zj, Wsh, bot,Lj, Tj, J)

MACRO Redefine QR, RHMLj, TKj, Lqj,duj1, duj2, duj3, duj4

  engbN(Lj, Ljm, Ejm, QR,uj1, uj2, uj3, uj4, ...
    HLDPj, HLDPjm, duj1,duj2,duj3,duj4, EVj, ...
    vj1, vj2, vj3, vj4,Tj, TKj, J)
  matbN(uj1, uj2, uj3, uj4, HLDPj,ujm1,ujm2, ujm3, ujm4, ...
    HLDPjm,vj1, vj2, vj3, vj4, sumvj, ...
    duj1, duj2, duj3, duj4, Lj, Lqj, J)
  eql(uj1, uj2, uj3, uj4, HLDPj,Tj,TKj, ...
    Pj, Yj1, Yj2, Yj3, Yj4, RHMLj, RHOLj, J)
  reboil(HCTRj, QR, Pj, Zj, bot,Lj, Ljm, Lqj,...
    Wsh, RHOVj, RHMVj, RHMLj, RHOLj, ...
    HLDPj, Yj1, Yj2, Yj3, Yj4, Tj, CS4, CV5, J)
MACRO END

  END    $" of INITIAL"
"-----"
DYNAMIC
DERIVATIVE

cond(T1, T2, v21, v22, v23, v24, sumv2, ...
  Y21, Y22, Y23, Y24, u11, u12, u13, u14, HLDP1,...
  CV1, CV2, CV3, EV2, ...
  RHOL1, RHML2, RHOV2, RHMV2, ...
  P1, P2, HCTR2, L1, E1, q1,dist, R,Z1)

stage(u21, u22, u23, u24, HLDP2,u11, u12, u13, u14, ...
  HLDP1,T2, TK2, EV2,EV3 , ...

```

```

v21, v22, v23, v24, sumv2,v31, v32, v33, v34, ...
sumv3, Y31, Y32, Y33, Y34, Y21, Y22, Y23, Y24,...
RHOL2,RHOV2, RHMV2, RHML2, RHOV3, RHMV3, ...
Z2,P3, HCTR3,P2, HCTR2,L1, E1,L2, E2, 3,2)
stage(u31, u32, u33, u34, HLDP3,u21, u22, u23, u24, ...
HLDP2,T3, TK3, EV3,EV4 , ...
v31, v32, v33, v34, sumv3,v41, v42, v43, v44, ...
sumv4, Y41, Y42, Y43, Y44, Y31, Y32, Y33, Y34,...
RHOL3,RHOV3, RHMV3, RHML3, RHOV4, RHMV4, ...
Z3,P4, HCTR4,P3, HCTR3,L2, E2,L3, E3, 4,3)
stage(u41, u42, u43, u44, HLDP4,u31, u32, u33, u34, ...
HLDP3,T4,TK4, EV4, EV5 ,...
v41, v42, v43, v44, sumv4,v51, v52, v53, v54, ...
sumv5, Y51, Y52, Y53, Y54, Y41, Y42, Y43, Y44,...
RHOL4, RHOV4, RHMV4, RHML4, RHOV5, RHMV5, ...
Z4,P5, HCTR5,P4, HCTR4,L3, E3,L4, E4, 5,4)

stage(u51, u52, u53, u54, HLDP5,u41, u42, u43, u44, ...
HLDP4,T5,TK5, EV5, EV21 ,...
v51, v52, v53, v54, sumv5,v211, v212, v213, v214, ...
sumv21, Y211, Y212, Y213, Y214, Y51, Y52, Y53, Y54,...
RHOL5, RHOV5, RHMV5, RHML5, RHOV21, RHMV21, ...
Z5,P21, HCTR21,P5, HCTR5,L4, E4,L5, E5, 21,5)
stage(u211, u212, u213, u214, HLDP21,u51, u52, u53, u54, ...
HLDP5,T21,TK21, EV21, EV35 ,...
v211, v212, v213, v214, sumv21,v351, v352, v353, v354, ...
sumv35, Y351, Y352, Y353, Y354, Y211, Y212, Y213, Y214,...
RHOL21, RHOV21, RHMV21, RHML21, RHOV35, RHMV35, ...
Z21,P35, HCTR35,P21, HCTR21,L5, E5,L21, E21,35, 21)
stage(u351, u352, u353, u354, HLDP35,u211, u212, u213, u214, ...
HLDP21,T35,TK35, EV35, EV49, ...
v351,v352,v353,v354,sumv35, v491,v492,v493, v494, ...
sumv49, Y491, Y492, Y493, Y494, Y351,Y352, Y353, Y354,...
RHOL35,RHOV35, RHMV35, RHML35, RHOV49, RHMV49, ...
Z35,P49, HCTR49,P35, HCTR35,L21, E21,L35, E35, 49,35)
stage(u491, u492, u493, u494, HLDP49,u351, u352, u353, u354, ...
HLDP35,T49,TK49, EV49, EV50 , ...
v491, v492, v493, v494, sumv49,v501, v502, v503, v504, ...
sumv50, Y501, Y502, Y503, Y504, Y491, Y492, Y493, Y494,...
RHOL49,RHOV49, RHMV49, RHML49, RHOV50, RHMV50, ...
Z49,P50, HCTR50,P49, HCTR49,L35, E35,L49, E49, 50,49)

rebo(u501, u502, u503, u504, HLDP50,u491, u492, u493, u494, ...
HLDP49, EV50, v501,v502,v503,v504,sumv50, ...
Y501, Y502, Y503, Y504, RHOL50, RHOV50, RHMV50,P50, ...
HCTR50,L49, E49,CS4, CV5, Z50, Wsh,bot, L50, T50, 50)

contrl(CV1, CV2, CV3, CS4, CV5, ...
T35, TK35, P1, q1, Z1, Z50, Wsh)

END $ "of DERIVATIVE"
Termt(t .ge.tmx)
END $ "of DYNAMIC"
END $"of Program distsim.csl"

```

APPENDIX D: ACSL CODE FOR COMPLEX DISTILLATION COLUMN MODEL

This code was only run in sections, never as a whole, as it was too big. The molar flow is calculated by using the method suggested by Figure 3.5, except that the efficiency resistance values have to be guessed at.

```
PROGRAM ACSL complex distillation -- distcom.csl
"Contains distsim.csl 5/20/92 but with changes back to Gallun"
"Altered to include virial equation of state, which required "
"  non-constant vapor molar holdup, which required "
"  calculation of liquid-to-vapor flow, which required "
"  imagination (LVji is based on theorized R). "
"  The complete Gallun fugacity equations are used, but without "
"  algebraic loops. The complete Gallun virtual vapor enthalpy "
"  equations are used. 9 stages used as in distsim.csl. "
"Yet to be altered is the assumption of constant energy vapor holdup"
"  which would require heat of vaporization details. "
"Does not run (does translate, compile and link) because of access "
"  privilege violations (i.e. not enough memory). Note that the "
"  executable file of distcom is more than 3 times the size of the "
"  executable file of distsim. "

"-----program control variables"
tmx = 10.0
cinterval cint=1.0
algorithm ailg=2
nsteps nstps=1000
mininterval mint=0.00001
maxterval maxt=5.0
merror u22=1.E-5, E1=1.E-7, T2=1.E-6, E2=1.E-6, T3=1.E-7, ...
      E3=1.E-6, T4=1.E-7, E4=1.E-6, T5=1.E-7, E5=1.E-6, ...
      T21=1.E-7, E21=1.E-6, T50=1.E-7, ...
      Qs3=1.E-3, Qs4=1.E-3, Qs5=1.E-3, Qs50=1.E-3, ...
      Qs2=1.E-3, Qs21=1.E-3, Qs35=1.E-3, Qs49=1.E-3

"-----Initial Values"

constant E01=888778., E02=70563.8, E03=22500.3, ...
      E04=20082.5, E05=254095., E021=254407., ...
      E035=255363., E049=275502., E050=1.04314E7
constant T01=599., T02=609.948, T03=617.824, ...
      T04=629.117, T05=640.4, T021=641.168, ...
      T035=642.161, T049=644.67, T050=651.331
constant P01=2117., P02=2192.5, P03=2203.7, ...
      P04=2213.3, P05=2226.1, P021=2244.7, ...
      P035=2263.1, P049=2281.3, P050=2299.2
constant L01=75.3482, L02=73.9229, L03=63.7142, ...
      L04=60.3716, L05=380.301, L021=374.943, ...
      L035=379.537, L049=379.043, L050=278.111
constant Z01=3.0, Z02=.3846, Z03=.3158, ...
      Z04=.4398, Z05=1.1086, Z021=1.0948, ...
      Z035=1.0752, Z049=1.1532, Z050=8.
constant Qs01=65.518, Qs02=59.4972, Qs03=45.3983, ...
      Qs04=36.4225, Qs05=194.938, Qs021=193.481, ...
      Qs035=191.355, Qs049=185.339, Qs050=168.596
```



```

constant how02=.0923, how03=.07707, how04=.06655, how05=.20362, ...
      how021=.2026, how035=.20111, how049=.19688, how050=.18483
constant u101=221.596, u201=126.272, u301=8.38675, u401=8.38675, ...
      u102=16.3432, u202=7.00848, u302=1.08277, u402=2.51991, ...
      u103=13.8607, u203=5.04879, u303=1.38213, u403=6.63553, ...
      u104=12.5007, u204=4.42564, u304=1.62497, u404=15.4035, ...
      u105=20.9044, u205=7.94464, u305=3.02323, u405=53.8308, ...
      u1021=20.8149, u2021=7.74166, u3021=3.04893, u4021=54.0149, ...
      u1035=20.4257, u2035=7.34855, u3035=3.09519, u4035=54.6731, ...
      u1049=20.0008, u2049=6.86185, u3049=3.28681, u4049=60.135, ...
      u1050=574.262, u2050=183.052, u3050=112.714, u4050=2527.614
constant uv101=1.30802, uv201=.75050, uv301=0.042886, ...
      uv401=0.042886, ...
      uv102=1.25504, uv202=0.71517, uv302=0.0475, ...
      uv402=0.0475, ...
      uv103=1.21071, uv203=0.56874, uv303=0.07024, uv403=0.14588, ...
      uv104=1.07025, uv204=0.46873, uv304=0.08298, uv404=0.34336, ...
      uv105=0.84613, uv205=0.38213, uv305=0.074752, uv405=0.58609, ...
      uv1021=0.85364, uv2021=0.37631, uv3021=0.07650, ...
      uv4021=.59697, ...
      uv1035=0.85569, uv2035=0.36361, uv3035=0.07933, ...
      uv4035=0.61844, ...
      uv1049=0.82964, uv2049=0.3333, uv3049=0.0835, ...
      uv4049=0.67621, ...
      uv1050=0.74581, uv2050=0.27694, uv3050=0.088916, ...
      uv4050=0.90691
constant V02=105.487, V03=104.062, V04=93.8535, V05=90.5108, ...
      V021=102.19, V035=101.833, V049=101.427, V050=102.23

constant LV101=0., LV201=0., LV301=0., LV401=0., ...
      LV102=.9683, LV202=6.8715, LV302=-1.23652, LV402=-5.17789, ...
      LV103=12.0247, LV203=7.2746, LV303=-0.30083, LV403=-8.7899, ...
      LV104=10.5706, LV204=4.0775, LV304=0.38116, LV404=-11.6866, ...
      LV105=-5.2853, LV205=-1.885, LV305=-0.52613, LV405=-3.9825, ...
      LV1021=0.3947, LV2021=0.8999, LV3021=-0.11441, LV4021=-0.823, ...
      LV1035=1.7418, LV2035=1.7496, LV3035=-.2031, LV4035=-2.8822, ...
      LV1049=6.6555, LV2049=3.796, LV3049=-0.06587, LV4049=-9.8906, ...
      LV1050=37.0355, LV2050=13.7452, LV3050=4.49227, LV4050=45.6589

constant I01=23.17856, I02=4.868, I03=7.26471, I04=26.7935, ...
      I05=31.3931, I06=11.142628, ...
      ZET01=.47433, ZET02=.510625, ZET03=.415932, ...
      ZET04=0.754757, ZET05=.726259

constant Tmc0=579.441, Two0=566.204, ...
      Tmr0=751.405, Tsc0=777.66, TMO=642.223
Rf = 30.0

"-----controller set-points, gains, time-constants"
TABLE SP, 1, 6 /...
      1,2,3,4,5,6,      760., 490.135, 3.0, 0.0, 8.0, 642.223/
CISP1 = 0.032*SP(1.0) - 12.0
CISP2 = (SP(2.0)/200)**2 + 4.0
CISP3 = 4.0 + 1.6*SP(3.0)
CISP5 = -20.0 + 4*SP(5.0)
CISP6 = 0.4*SP(6.0) - 232.
" TABLE CISP, 1, 6 /... "
"      1,2,3,4,5,6,... "
"      12.32, 10.0058, 8.8, 0, 12.0, 24.889/"
TABLE XKC,1,6/...
      1,2,3,4,5,6,...

```

```

1.5, 0.25, 1.1, 0.15, 0.5, 0.5/
TABLE TAUI,1,6/...
1,2,3,4,5,6,...
3.0, 0.1, 0.75, 0.25, 1.0, 0.6/
TABLE TAUV,1,6/...
1,2,3,4,5,6,...
0.15, 0.15, 0.15, 0.2, 0.15, 0.15/
"-----coefficients "
TABLE MV, 2, 3, 4 /...
1,2,3, 1,2,3,4,...
0.6451094E2, -0.1095359 , 0.1195526E-3,...
0.5686523E2, 0.468039E-2, 0.5094978E-4,...
0.5370027E2, -0.1728176E-1, 0.493820E-4,...
0.2288676E2, -0.2023121E-1, 0.2115899E-4/
TABLE HVCO, 2, 5, 4/...
1, 2, 3, 4, 5, 1, 2, 3, 4,...
0.1174119E5, 0.7121495E1, 0.5579442E-2, ...
-0.450617E-6, -0.2091904E-10,...
0.867332E4, 0.4735799E1, 0.1452860E-1,...
-0.1121397E-5, -0.2018173E-9,...
0.106486E5, 0.7515997E1, 0.1151360E-1,...
-.01682096E-5, 0.9036333E-10,...
0.1545871E5, 0.8022526E1, -0.4745722E-3,...
0.6878047E-6, -0.1439752E-9/
TABLE hLCO, 2, 3, 4/...
1, 2, 3, 1, 2, 3, 4,...
-0.3119436E4, -4.145198, 0.2131106E-1, ...
-0.115334E5, 0.1770348E2, 0.1166435E-1, ...
0.4046348E3, -0.2410286E2, 0.472823E-1, ...
-0.87838059E4, 0.175845E2, 0.3651369E-3/
TABLE ANT, 2, 3, 4/...
1,2,3, 1,2,3,4,...
7.87863, 1.47311E3, 2.3E2,...
7.02447, 1.16E3, 2.24E2,...
8.04494, 1.5543E3, 2.2265E2,...
7.96681, 1.66821E3,2.28E2/
TABLE WLMB,2,4,4/...
1,2,3,4, 1,2,3,4,...
0.0, 0.66408E3, 0.59844E3, 0.20530E3,...
-0.21495E3, 0.0, 0.38170E2, 0.43964E3,...
0.51139E3, 0.41896E3, 0.0, 0.38230E3,...
0.48216E3, 0.140549E3, 0.95549E3, 0.0/
TABLE RHOSCO, 1, 5/...
1,2,3,4,5,...
1.031951E-2, 1.427797E1, 0.9414444, 2.048037, 5.956991/
TABLE hLSCO, 1, 5/...
1,2,3,4,5,...
-1.6029E2, 8.06427E-2, 7.361453E-5, 1.501012E-6,...
-9.9964334E-10/
TABLE HVSCO, 1, 5/...
1,2,3,4,5,...
5.448738E2, 8.039637E-1, 1.931794E-3, -3.938661E-6,...
1.907853E-9/
TABLE HEDCO, 2,4,2/...
1,2,3,4, 1,2,...
9.870927E1, -9.794161E-3, -1.95175E-6, -1.954559E-9,...
9.152028E1, -6.584299E-2, 7.533832E-5, -4.300139E-8/
TABLE CV1CO , 2, 5, 20/...
1,2,3,4,5,...
0.0,0.099,0.1,0.19,0.2,0.29,0.3,0.39,0.4,0.49,...
0.5,0.59,0.6,0.69,0.7,0.79,0.8,0.89,0.9,1.0,...

```

0.0, 0.0, 0.6759999E2, -0.6691973E3, 0.6691969E4, ...
 0.0, 0.0, 0.6759999E2, -0.6691973E3, 0.6691969E4, ...
 0.1, 0.676E1, 0.1345197E3, -0.1167920E4, 0.8667223E4, ...
 0.1, 0.676E1, 0.1345197E3, -0.1167920E4, 0.8667223E4, ...
 0.2, 0.5810001E2, 0.9598074E3, -7506973E4, 0.8598887E5, ...
 0.2, 0.5810001E2, 0.9598074E3, -7506973E4, 0.8598887E5, ...
 0.3, 0.165E3, .2038081E4, -0.768066E4, 0.8299831E5, ...
 0.3, 0.165E3, .2038081E4, -0.768066E4, 0.8299831E5, ...
 0.4, 0.375E3, 0.2991901E4, -0.6826715E4, 0.4807690E5, ...
 0.4, 0.375E3, 0.2991901E4, -0.6826715E4, 0.4807690E5, ...
 0.5, 0.654E3, 0.3068865E4, -0.5726895E4, 0.6382414E4, ...
 0.5, 0.654E3, 0.3068865E4, -0.5726895E4, 0.6382414E4, ...
 0.6, 0.91E3, 0.2114958E4, -0.2852868E5, 0.2237909E6, ...
 0.6, 0.91E3, 0.2114958E4, -0.2852868E5, 0.2237909E6, ...
 0.7, 0.106E4, 0.3122954E4, 0.1411841E5, -0.9347956E5, ...
 0.7, 0.106E4, 0.3122954E4, 0.1411841E5, -0.9347956E5, ...
 0.8, 0.142E4, 0.3142248E4, -0.2419347E5, 0.1177098E6, ...
 0.8, 0.142E4, 0.3142248E4, -0.2419347E5, 0.1177098E6, ...
 0.9, 0.161E4, 0.1834851E4, -0.6969128E3, 0.3484387E4, ...
 0.9, 0.161E4, 0.1834851E4, -0.6969128E3, 0.3484387E4 /

TABLE CV2CO, 2, 5, 20/...

1,2,3,4,5, ...
 0.0, 0.099, 0.1, 0.19, 0.2, 0.29, 0.3, 0.39, 0.4, 0.49, ...
 0.5, 0.59, 0.6, 0.69, 0.7, 0.79, 0.8, 0.89, 0.9, 1.0, ...
 0.0, 0.0, 0.6759999E2, -0.6691973E3, 0.6691969E4, ...
 0.0, 0.0, 0.6759999E2, -0.6691973E3, 0.6691969E4, ...
 0.1, 0.676E1, 0.1345197E3, -0.1167920E4, 0.8667223E4, ...
 0.1, 0.676E1, 0.1345197E3, -0.1167920E4, 0.8667223E4, ...
 0.2, 0.172E2, 0.1609525E3, -0.5040024E3, 0.5344770E4, ...
 0.2, 0.172E2, 0.1609525E3, -0.5040024E3, 0.5344770E4, ...
 0.3, 0.3360001E2, 0.2204954E3, -0.1038741E4, 0.8337859E4, ...
 0.3, 0.3360001E2, 0.2204954E3, -0.1038741E4, 0.8337859E4, ...
 0.4, 0.5360001E2, 0.2628831E3, -0.9942312E3, 0.8153996E4, ...
 0.4, 0.5360001E2, 0.2628831E3, -0.9942312E3, 0.8153996E4, ...
 0.5, 0.7810001E2, 0.3086567E3, -0.1381982E4, 0.1085412E5, ...
 0.5, 0.7810001E2, 0.3086567E3, -0.1381982E4, 0.1085412E5, ...
 0.6, 0.106E3, 0.3578840E3, -0.1145935E4, 0.8670914E4, ...
 0.6, 0.106E3, 0.3578840E3, -0.1145935E4, 0.8670914E4, ...
 0.7, 0.139E3, 0.3888247E3, -0.1526535E4, 0.1038285E5, ...
 0.7, 0.139E3, 0.3888247E3, -0.1526535E4, 0.1038285E5, ...
 0.8, 0.173E3, 0.3950034E3, -0.6824436E3, 0.2324071E4, ...
 0.8, 0.173E3, 0.3950034E3, -0.6824436E3, 0.2324071E4, ...
 0.9, 0.208E3, 0.3282368E3, -0.1564725E4, 0.7823613E4, ...
 0.9, 0.208E3, 0.3282368E3, -0.1564725E4, 0.7823613E4 /

TABLE CV3CO, 2, 5, 20/...

1,2,3,4,5, ...
 0.0, 0.099, 0.1, 0.19, 0.2, 0.29, 0.3, 0.39, 0.4, 0.49, ...
 0.5, 0.59, 0.6, 0.69, 0.7, 0.79, 0.8, 0.89, 0.9, 1.0, ...
 0.0, 0.0, 0.6689999E2, -0.17743E3, 0.1742997E4, ...
 0.0, 0.0, 0.6689999E2, -0.17743E3, 0.1742997E4, ...
 0.1, 0.669E1, 0.8432991E2, -0.8532524E3, 0.5009532E4, ...
 0.1, 0.669E1, 0.8432991E2, -0.8532524E3, 0.5009532E4, ...
 0.2, 0.116E2, 0.6396542E2, -0.3343521E3, 0.3846974E4, ...
 0.2, 0.116E2, 0.6396542E2, -0.3343521E3, 0.3846974E4, ...
 0.3, 0.185E2, 0.1125043E3, -0.6310693E3, 0.6060258E4, ...
 0.3, 0.185E2, 0.1125043E3, -0.6310693E3, 0.6060258E4, ...
 0.4, 0.295E2, 0.1680985E3, -0.9577654E3, 0.9167789E4, ...
 0.4, 0.295E2, 0.1680985E3, -0.9577654E3, 0.9167789E4, ...
 0.5, 0.4589999E2, 0.2515793E3, -0.132549E4, 0.1269696E5, ...
 0.5, 0.4589999E2, 0.2515793E3, -0.132549E4, 0.1269696E5, ...
 0.6, 0.705E2, 0.3673904E3, -0.1754303E4, 0.1630397E5, ...

0.6, 0.705E2, 0.3673904E3, -0.1754303E4, 0.1630397E5, ...
 0.7, 0.106E3, 0.5056489E3, -0.2605563E4, 0.2349071E5, ...
 0.7, 0.106E3, 0.5056489E3, -0.2605563E4, 0.2349071E5, ...
 0.8, 0.154E3, 0.6892578E3, -0.2990246E4, 0.2697664E5, ...
 0.8, 0.154E3, 0.6892578E3, -0.2990246E4, 0.2697664E5, ...
 0.9, 0.22E3, 0.9005083E3, -0.1210117E4, 0.6050512E4, ...
 0.9, 0.22E3, 0.9005083E3, -0.1210117E4, 0.6050512E4/

TABLE CV5CO, 2, 5, 20/...

1,2,3,4,5, ...
 0.0,0.099,0.1,0.19,0.2,0.29,0.3,0.39,0.4,0.49, ...
 0.5,0.59,0.6,0.69,0.7,0.79,0.8,0.89,0.9,1.0, ...
 0.0, 0.0, 0.463E3, -0.3610995E4, 0.3610991E5, ...
 0.0, 0.0, 0.463E3, -0.3610995E4, 0.3610991E5, ...
 0.1, 0.463E2, 0.8240989E3, -0.5206883E4, 0.3035894E5, ...
 0.1, 0.463E2, 0.8240989E3, -0.5206883E4, 0.3035894E5, ...
 0.2, 0.107E3, 0.6934902E3, -0.1574331E4, 0.1039425E5, ...
 0.2, 0.107E3, 0.6934902E3, -0.1574331E4, 0.1039425E5, ...
 0.3, 0.171E3, 0.6904519E3, -0.2672921E4, 0.1468400E5, ...
 0.3, 0.171E3, 0.6904519E3, -0.2672921E4, 0.1468400E5, ...
 0.4, 0.228E3, 0.5963877E3, -0.2192055E4, 0.1328175E5, ...
 0.4, 0.228E3, 0.5963877E3, -0.2192055E4, 0.1328175E5, ...
 0.5, 0.279E3, 0.5564294E3, -0.1604116E4, 0.8398187E4, ...
 0.5, 0.279E3, 0.5564294E3, -0.1604116E4, 0.8398187E4, ...
 0.6, 0.327E3, 0.4875520E3, -0.1870622E4, 0.9950992E4, ...
 0.6, 0.327E3, 0.4875520E3, -0.1870622E4, 0.9950992E4, ...
 0.7, 0.367E3, 0.4119575E3, -0.4696677E3, -0.1499096E4, ...
 0.7, 0.367E3, 0.4119575E3, -0.4696677E3, -0.1499096E4, ...
 0.8, 0.402E3, 0.2730510E3, -0.1572119E4, 0.6416082E4, ...
 0.8, 0.402E3, 0.2730510E3, -0.1572119E4, 0.6416082E4, ...
 0.9, 0.42E3, 0.1511098E3, -0.4221873E3, 0.2110922E4, ...
 0.9, 0.42E3, 0.1511098E3, -0.4221873E3, 0.2110922E4/

TABLE CSCO, 2, 5, 20/...

1,2,3,4,5, ...
 0.0,0.099,0.1,0.19,0.2,0.29,0.3,0.39,0.4,0.49, ...
 0.5,0.59,0.6,0.69,0.7,0.79,0.8,0.89,0.9,1.0, ...
 0.0, 0.0, 0.112E3, -0.280999E3, 0.2809984, ...
 0.0, 0.0, 0.112E3, -0.280999E3, 0.2809984, ...
 0.1, 0.193E2, 0.9875446E2, -0.6029138E3, 0.6653684E4, ...
 0.1, 0.193E2, 0.9875446E2, -0.6029138E3, 0.6653684E4, ...
 0.2, 0.193E2, 0.9875446E2, -0.6029138E3, 0.6653684E4, ...
 0.2, 0.193E2, 0.9875446E2, -0.6029138E3, 0.6653684E4, ...
 0.3, 0.298E2, 0.1777826E3, -0.8587102E3, 0.8508832E4, ...
 0.3, 0.298E2, 0.1777826E3, -0.8587102E3, 0.8508832E4, ...
 0.4, 0.475E2, 0.2613057E3, -0.1764654E4, 0.1651596E5, ...
 0.4, 0.475E2, 0.2613057E3, -0.1764654E4, 0.1651596E5, ...
 0.5, 0.725E2, 0.4038538E3, -0.2260444E4, 0.2271903E5, ...
 0.5, 0.725E2, 0.4038538E3, -0.2260444E4, 0.2271903E5, ...
 0.6, 0.133E3, 0.6333362E3, -0.2353483E4, 0.2220118E5, ...
 0.6, 0.133E3, 0.6333362E3, -0.2353483E4, 0.2220118E5, ...
 0.7, 0.175E3, 0.8286753E3, -0.2622047E4, 0.1935291E5, ...
 0.7, 0.175E3, 0.8286753E3, -0.2622047E4, 0.1935291E5, ...
 0.8, 0.251E3, 0.8848535E3, -0.6906321E3, -0.4579047E4, ...
 0.8, 0.251E3, 0.8848535E3, -0.6906321E3, -0.4579047E4, ...
 0.9, 0.328E3, 0.6093555E3, -0.4187094E4, 0.2093548E5, ...
 0.9, 0.328E3, 0.6093555E3, -0.4187094E4, 0.2093548E5/

"-----Physical constants "

TABLE PCC, 2, 4, 4/...

1,2,3,4, 1,2,3,4, ...
 78.5, 59.6, 70.0, 127.8, ...
 59.6, 46.6, 54.0, 93.5, ...
 70.0, 54.0, 63.0, 111.9, ...

127.8, 93.5, 111.9, 218.3/
 TABLE TCC, 2, 4, 4/...
 1,2,3,4, 1,2,3,4,...
 513.2, 510.9, 514.1, 576.4,...
 510.9, 508.7, 512.3, 573.9,...
 514.1, 512.3, 516.0, 578.0,...
 576.4, 573.9, 578.0, 647.4/
 TABLE TC, 1, 4/...
 1,2,3,4,...
 513.2, 508.7, 516.0, 647.4/
 TABLE PC, 1, 4/...
 1,2,3,4,...
 78.5, 46.6, 63.0, 218.3/
 TABLE VC, 1, 4/...
 1,2,3,4,...
 118.0, 213.5, 161.3, 55.2/
 TABLE WW, 1, 4/...
 1,2,3,4,...
 0.557, 0.309, 0.637, 0.344/
 TABLE WWH, 1, 4/...
 1,2,3,4,...
 0.105, 0.187, 0.152, 0.010/
 TABLE MU, 1, 4/...
 1,2,3,4,...
 1.66, 2.88, 1.69, 1.83/
 TABLE ETTA, 2, 4, 4/...
 1,2,3,4, 1,2,3,4,...
 1.21, 0.605, 1.155, 0.605,...
 0.605, 0.0, 0.55, 0.0,...
 1.155, 0.55, 1.1, 0.55,...
 0.605, 0.0, 0.55, 0.0/
 TABLE MUR, 2, 4, 4/...
 1,2,3,4, 1,2,3,4,...
 4.408, 4.693, 4.308, 4.761,...
 4.693, 5.006, 4.607, 5.008,...
 4.308, 4.607, 4.213, 4.640,...
 4.761, 5.008, 4.640, 5.161/
 TABLE WH, 2, 4, 4/...
 1,2,3,4, 1,2,3,4,...
 0.105, 0.146, 0.1285, 0.0575,...
 0.146, 0.187, 0.1695, 0.0985,...
 0.1285, 0.1695, 0.152, 0.081,...
 0.0575, 0.0985, 0.081, 0.01/
 TABLE MOL, 1, 4/...
 1,2,3,4,...
 32.04, 58.08, 46.07, 18.016/
 "-----Column constants and forcing functions "
 TABLE AH, 1, 4/...
 1,3,4,50,...
 18,18,13,13/
 TABLE CD, 1, 4/...
 1, 3, 4, 50,...
 0.75, 0.75, 0.72, 0.72/
 TABLE F, 2, 10, 4/...
 1,2,3,4,5,6,20,21,22,50,...
 1,2,3,4,...
 0., 0., 0., 0., 65.25, 0., 0., .0, 0., 0., ...
 0., 0., 0., 0., 25.5, 0., 0., .0, 0., 0., ...
 0., 0., 0., 0., 10.0, 0., 0., .0, 0., 0., ...
 0., 0., 0., 0., 208.5, 0., 0., .0, 0., 0./
 TABLE Hf, 1, 10/...

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1,2,3,4,5,6,20,21,22,50,...
0.0, 0.0, 0.0, 0.0, 868000., 0.0, ...
0.0, 0.0, 0.0, 0.0/
"-----RECeiver liquid height to volume function"
TABLE RECVOL, 1, 27/...
    0.0,2.12692,5.99764,10.9848,16.8604,23.4904,42.8183,...
    65.4004,90.6624,118.2,178.918,245.674,317.069,391.969,...
    469.392,548.452,628.319,708.185,787.245,864.668,939.568,...
    1010.96,1077.72,1138.44,1191.24,1233.15,1256.64,...
    0.0,0.1,0.2,0.3,0.4,0.5,0.75,1.0,1.25,1.5,2.0,2.5,3.0,...
    3.5,4.0,4.5,5.0,5.5,6.0,6.5,7.0,7.5,8.0,8.5,9.0,9.5,10.0/

TABLE LF, 2, 2,4/...
    1,50,      1,2,3,4, ...
    10.,10.,   10., 10.,   10.,10.,   10.,10./

"-----Gas Constant in atm*ft**3/lBmol*K, cm**3*mmHg/gmol*K,"
"      ft**3*mmHg/lBmol*R, cal/gmol*K, lb*ft**3/ft**2*lBmol*R"
TABLE RR, 1, 5/...
    1,2,3,4,5,...
    1.314, 62361.0, 555.0, 1.987, 1545.0/

"    Twi changed from 545."

INITIAL
Constant...
pii=3.14159 , Twi=530. , Pw1=60 , Pw3=35 , PD=40 ,...
PB=30 , TSH=960.0 , PSH=255.0 , HSH=1262.8 , TSAT=862.7 ,...
AA=141.372 , AD=17.6715 , AN=141.372 , AT=176.714 ,...
AUD=0.908375 , DH=0.1875,  DTT=15.0 , HW=1.0 , HWSP=1.25 ,...
LW=130.806 , LWSP=149.0 , TT=0.09375 , Apc=16022.16 ,...
Aw=13940.0 , Ccw=1.0 , Cmc=0.12 , DR=10.0 , LR=16.0 ,...
Pw2Pw3=9.0 , Qcwo=8653.0 , Ucw=17160.0 , Umc=45000.0 ,...
Upmo=213.0 , Uwmo=1250.0 , Sv2IR=105.8752 , ZC=5.0 ,...
ALPHA=0.2 , RHO2VR=0.002549852, As=3844.168 ,...
Apmr=3361.826 , Cmr=0.12 , Us=1000.0 , Umr=11000.0,...
Upmr=300.0 , Vr=68.83 , ZB=10.0 , ...
TAUM=0.20 , P1P2R=27.09, REF1 = 0.947775644, REF2 = 9.0,...
sumv1 = 1.0, g = 115523.24, Cx = .58, REF3=2.69413,...
LH = 0.011208333, Cvc = .65
"gravitational acceleration, g, in ft/min**2"

"-----Energy models-----"
MACRO engder(dBmj, dB11, dB12, dB13, dB14, dB22, dB23, dB24, ...
    dB33, dB34, dB44,Yj1, Yj2, Yj3, Yj4,Tj, TKj)

    MACRO Redefine df311, df312, df313, df314, df322, df323, df324,
...
    df333, df334, df344, df411, df412, df413, df414, ...
    df422, df423, df424, df433, df434, df444, ...
    df511, df512, df513, df514, df522, df523, df524, ...
    df533, df534, df544, df611, df612, df613, df614, ...
    df622, df623, df624, df633, df634, df644

"    The variables here are partial derivitives with respect to Tj"

    dBmj = (Yj1*Yj1*dB11 + Yj1*Yj2*dB12 ...
    + Yj1*Yj3*dB13 + Yj1*Yj4*dB14 ...
    + Yj2*Yj1*dB12 + Yj2*Yj2*dB22 ...
    + Yj2*Yj3*dB23 + Yj2*Yj4*dB24 ...
    + Yj3*Yj1*dB13 + Yj3*Yj2*dB23 ...

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+ Yj3*Yj3*dB33 + Yj3*Yj4*dB34 ...
+ Yj4*Yj1*dB14 + Yj4*Yj2*dB24 ...
+ Yj4*Yj3*dB34 + Yj4*Yj4*dB44)
dB11 = RR(1.0)*TCC(1.0,1.0)/PCC(1.0,1.0)*(df311 + WH(1.0,1.0)...
*df411 + df511 + ETTA(1.0,1.0)*df611)
dB12 = RR(1.0)*TCC(1.0,2.0)/PCC(1.0,2.0)*(df312 + WH(1.0,2.0)...
*df412 + df512 + ETTA(1.0,2.0)*df612)
dB13 = RR(1.0)*TCC(1.0,3.0)/PCC(1.0,3.0)*(df313 + WH(1.0,3.0)...
*df413 + df513 + ETTA(1.0,3.0)*df613)
dB14 = RR(1.0)*TCC(1.0,4.0)/PCC(1.0,4.0)*(df314 + WH(1.0,4.0)...
*df414 + df514 + ETTA(1.0,4.0)*df614)
dB22 = RR(1.0)*TCC(2.0,2.0)/PCC(2.0,2.0)*(df322 + WH(2.0,2.0)...
*df422 + df522 + ETTA(2.0,2.0)*df622)
dB23 = RR(1.0)*TCC(2.0,3.0)/PCC(2.0,3.0)*(df323 + WH(2.0,3.0)...
*df423 + df523 + ETTA(2.0,3.0)*df623)
dB24 = RR(1.0)*TCC(2.0,4.0)/PCC(2.0,4.0)*(df324 + WH(2.0,4.0)...
*df424 + df524 + ETTA(2.0,4.0)*df624)
dB33 = RR(1.0)*TCC(3.0,3.0)/PCC(3.0,3.0)*(df333 + WH(3.0,3.0)...
*df433 + df533 + ETTA(3.0,3.0)*df633)
dB34 = RR(1.0)*TCC(3.0,4.0)/PCC(3.0,4.0)*(df334 + WH(3.0,4.0)...
*df434 + df534 + ETTA(3.0,4.0)*df634)
dB44 = RR(1.0)*TCC(4.0,4.0)/PCC(4.0,4.0)*(df344 + WH(4.0,4.0)...
*df444 + df544 + ETTA(4.0,4.0)*df644)
df311 = -0.330*TCC(1.0,1.0)/TKj**2 +
0.1385*TCC(1.0,1.0)**2/TKj**3 ...
+ 0.0121*TCC(1.0,1.0)**3/TKj**4
df312 = -0.330*TCC(1.0,2.0)/TKj**2 +
0.1385*TCC(1.0,2.0)**2/TKj**3 ...
+ 0.0121*TCC(1.0,2.0)**3/TKj**4
df313 = -0.330*TCC(1.0,1.0)/TKj**2 +
0.1385*TCC(1.0,3.0)**2/TKj**3 ...
+ 0.0121*TCC(1.0,3.0)**3/TKj**4
df314 = -0.330*TCC(1.0,4.0)/TKj**2 +
0.1385*TCC(1.0,4.0)**2/TKj**3 ...
+ 0.0121*TCC(1.0,4.0)**3/TKj**4
df322 = -0.330*TCC(2.0,2.0)/TKj**2 +
0.1385*TCC(2.0,2.0)**2/TKj**3 ...
+ 0.0121*TCC(2.0,2.0)**3/TKj**4
df323 = -0.330*TCC(2.0,3.0)/TKj**2 +
0.1385*TCC(2.0,3.0)**2/TKj**3 ...
+ 0.0121*TCC(2.0,3.0)**3/TKj**4
df324 = -0.330*TCC(2.0,4.0)/TKj**2 +
0.1385*TCC(2.0,4.0)**2/TKj**3 ...
+ 0.0121*TCC(2.0,4.0)**3/TKj**4
df333 = -0.330*TCC(3.0,3.0)/TKj**2 +
0.1385*TCC(3.0,3.0)**2/TKj**3 ...
+ 0.0121*TCC(3.0,3.0)**3/TKj**4
df334 = -0.330*TCC(3.0,4.0)/TKj**2 +
0.1385*TCC(3.0,4.0)**2/TKj**3 ...
+ 0.0121*TCC(3.0,4.0)**3/TKj**4
df344 = -0.330*TCC(4.0,4.0)/TKj**2 +
0.1385*TCC(4.0,4.0)**2/TKj**3 ...
+ 0.0121*TCC(4.0,4.0)**3/TKj**4
df411 = - 0.4600*TCC(1.0,1.0)/TKj**2 ...
+ 0.5000*TCC(1.0,1.0)/TKj**3 ...
+ 0.0970*TCC(1.0,1.0)**3/TKj**4 ...
+ 0.0073*TCC(1.0,1.0)**8/TKj**9
df412 = - 0.4600*TCC(1.0,2.0)/TKj**2 ...
+ 0.5000*TCC(1.0,2.0)/TKj**3 ...
+ 0.0970*TCC(1.0,2.0)**3/TKj**4 ...
+ 0.0073*TCC(1.0,2.0)**8/TKj**9

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df413 = - 0.4600*TCC(1.0,3.0)/TKj**2 ...
      + 0.5000*TCC(1.0,3.0)/TKj**3 ...
      + 0.0970*TCC(1.0,3.0)**3/TKj**4 ...
      + 0.0073*TCC(1.0,3.0)**8/TKj**9
df414 = - 0.4600*TCC(1.0,4.0)/TKj**2 ...
      + 0.5000*TCC(1.0,4.0)/TKj**3 ...
      + 0.0970*TCC(1.0,4.0)**3/TKj**4 ...
      + 0.0073*TCC(1.0,4.0)**8/TKj**9
df422 = - 0.4600*TCC(2.0,2.0)/TKj**2 ...
      + 0.5000*TCC(2.0,2.0)/TKj**3 ...
      + 0.0970*TCC(2.0,2.0)**3/TKj**4 ...
      + 0.0073*TCC(2.0,2.0)**8/TKj**9
df423 = - 0.4600*TCC(2.0,3.0)/TKj**2 ...
      + 0.5000*TCC(2.0,3.0)/TKj**3 ...
      + 0.0970*TCC(2.0,3.0)**3/TKj**4 ...
      + 0.0073*TCC(2.0,3.0)**8/TKj**9
df424 = - 0.4600*TCC(2.0,4.0)/TKj**2 ...
      + 0.5000*TCC(2.0,4.0)/TKj**3 ...
      + 0.0970*TCC(2.0,4.0)**3/TKj**4 ...
      + 0.0073*TCC(2.0,4.0)**8/TKj**9
df433 = - 0.4600*TCC(3.0,3.0)/TKj**2 ...
      + 0.5000*TCC(3.0,3.0)/TKj**3 ...
      + 0.0970*TCC(3.0,3.0)**3/TKj**4 ...
      + 0.0073*TCC(3.0,3.0)**8/TKj**9
df434 = - 0.4600*TCC(3.0,4.0)/TKj**2 ...
      + 0.5000*TCC(3.0,4.0)/TKj**3 ...
      + 0.0970*TCC(3.0,4.0)**3/TKj**4 ...
      + 0.0073*TCC(3.0,4.0)**8/TKj**9
df444 = - 0.4600*TCC(4.0,4.0)/TKj**2 ...
      + 0.5000*TCC(4.0,4.0)/TKj**3 ...
      + 0.0970*TCC(4.0,4.0)**3/TKj**4 ...
      + 0.0073*TCC(4.0,4.0)**8/TKj**9
df511 = (5.769770 - 6.181427*MUR(1.0,1.0)) ...
      + 2.283270*MUR(1.0,1.0)**2 ...
      - 0.2649074*MUR(1.0,1.0)**3) *TCC(1.0,1.0)/TKj**2
df512 = (5.769770 - 6.181427*MUR(1.0,2.0)) ...
      + 2.283270*MUR(1.0,2.0)**2 ...
      - 0.2649074*MUR(1.0,2.0)**3) *TCC(1.0,2.0)/TKj**2
df513 = (5.769770 - 6.181427*MUR(1.0,3.0)) ...
      + 2.283270*MUR(1.0,3.0)**2 ...
      - 0.2649074*MUR(1.0,3.0)**3) *TCC(1.0,3.0)/TKj**2
df514 = (5.769770 - 6.181427*MUR(1.0,4.0)) ...
      + 2.283270*MUR(1.0,4.0)**2 ...
      - 0.2649074*MUR(1.0,4.0)**3) *TCC(1.0,4.0)/TKj**2
df522 = (5.769770 - 6.181427*MUR(2.0,2.0)) ...
      + 2.283270*MUR(2.0,2.0)**2 ...
      - 0.2649074*MUR(2.0,2.0)**3) *TCC(2.0,2.0)/TKj**2
df523 = (5.769770 - 6.181427*MUR(2.0,3.0)) ...
      + 2.283270*MUR(2.0,3.0)**2 ...
      - 0.2649074*MUR(2.0,3.0)**3) *TCC(2.0,3.0)/TKj**2
df524 = (5.769770 - 6.181427*MUR(2.0,4.0)) ...
      + 2.283270*MUR(2.0,4.0)**2 ...
      - 0.2649074*MUR(2.0,4.0)**3) *TCC(2.0,4.0)/TKj**2
df533 = (5.769770 - 6.181427*MUR(3.0,3.0)) ...
      + 2.283270*MUR(3.0,3.0)**2 ...
      - 0.2649074*MUR(3.0,3.0)**3) *TCC(3.0,3.0)/TKj**2
df534 = (5.769770 - 6.181427*MUR(3.0,4.0)) ...
      + 2.283270*MUR(3.0,4.0)**2 ...
      - 0.2649074*MUR(3.0,4.0)**3) *TCC(3.0,4.0)/TKj**2
df544 = (5.769770 - 6.181427*MUR(4.0,4.0)) ...
      + 2.283270*MUR(4.0,4.0)**2 ...

```



```

- 0.2649074*MUR(4.0,4.0)**3) *TCC(4.0,4.0)/TKj**2
df611 = 101.49*EXP(-6.6*TKj/TCC(1.0,1.0))
df612 = 101.49*EXP(-6.6*TKj/TCC(1.0,2.0))
df613 = 101.49*EXP(-6.6*TKj/TCC(1.0,3.0))
df614 = 101.49*EXP(-6.6*TKj/TCC(1.0,4.0))
df622 = 101.49*EXP(-6.6*TKj/TCC(2.0,2.0))
df623 = 101.49*EXP(-6.6*TKj/TCC(2.0,3.0))
df624 = 101.49*EXP(-6.6*TKj/TCC(2.0,4.0))
df633 = 101.49*EXP(-6.6*TKj/TCC(3.0,3.0))
df634 = 101.49*EXP(-6.6*TKj/TCC(3.0,4.0))
df644 = 101.49*EXP(-6.6*TKj/TCC(4.0,4.0))
MACRO END

MACRO engb1(Tj, TKj, R, QC, Ej, Lj, sumuj, EVjp, ...
uj1, uj2, uj3, uj4, duj1,duj2,duj3,duj4, J)

MACRO Redefine Ejdot, jj, dTj, hLj1, hLj2,hLj3,hLj4

jj = J/1.0
Ejdot = Hf(jj) + EVjp - (1 + R)*Lj*Ej/(R * sumuj) - QC
Ej = INTEG(Ejdot, E0&J)

hLj1 = hLCO(1.0,1.0) + hLCO(2.0,1.0)*Tj + hLCO(3.0,1.0)*Tj**2
hLj2 = hLCO(1.0,2.0) + hLCO(2.0,2.0)*Tj + hLCO(3.0,2.0)*Tj**2
hLj3 = hLCO(1.0,3.0) + hLCO(2.0,3.0)*Tj + hLCO(3.0,3.0)*Tj**2
hLj4 = hLCO(1.0,4.0) + hLCO(2.0,4.0)*Tj + hLCO(3.0,4.0)*Tj**2

Tj = INTEG(dTj, T0&J)
TKj = 5.0*Tj/9.0
dTj = (Ejdot - hLj1*duj1 - hLj2*duj2 - hLj3*duj3 - hLj4*duj4)/ ...
      ((hLCO(2.0,1.0) + 2*hLCO(3.0,1.0)*Tj)*uj1 ...
      + (hLCO(2.0,2.0) + 2*hLCO(3.0,2.0)*Tj)*uj2 ...
      + (hLCO(2.0,3.0) + 2*hLCO(3.0,3.0)*Tj)*uj3 ...
      + (hLCO(2.0,4.0) + 2*hLCO(3.0,4.0)*Tj)*uj4)

MACRO END

MACRO engbj(Ej, Lj, Ljm, Ejm,uj1, uj2, uj3, uj4, ...
sumuj, ujm1,ujm2,ujm3,ujm4,sumujm, ...
duj1, duj2, duj3, duj4, Vj, EVj, EVjp, ...
Yj1,Yj2,Yj3,Yj4, Tj, TKj, Bmj, Pj, ZZj, J)

MACRO Redefine Ejdot,jj, dTj, OMEGAj, H01, H02,H03,H04, ...
dBmj, dB11, dB12, dB13, dB14, dB22, dB23, dB24, ...
dB33, dB34, dB44, hLj1,hLj2,hLj3,hLj4, ...
HVj1, HVj2, HVj3,HVj4

engder(dBmj, dB11, dB12, dB13, dB14, dB22, dB23, dB24, ...
dB33, dB34, dB44,Yj1, Yj2, Yj3, Yj4,Tj, TKj)

jj = J/1.0
Ejdot = Hf(jj) + Ljm*Ejm/sumujm - Lj*Ej/sumuj - ...
      EVj + EVjp
Ej = INTEG(Ejdot, E0&J)

hLj1 = hLCO(1.0,1.0) + hLCO(2.0,1.0)*Tj + hLCO(3.0,1.0)*Tj**2
hLj2 = hLCO(1.0,2.0) + hLCO(2.0,2.0)*Tj + hLCO(3.0,2.0)*Tj**2
hLj3 = hLCO(1.0,3.0) + hLCO(2.0,3.0)*Tj + hLCO(3.0,3.0)*Tj**2
hLj4 = hLCO(1.0,4.0) + hLCO(2.0,4.0)*Tj + hLCO(3.0,4.0)*Tj**2

EVj = Vj*Yj1*HVj1 + Vj*Yj2*HVj2 + Vj*Yj3*HVj3 + ...
      Vj*Yj4*HVj4

```

```

HVj1 = H01 + OMEGAj
HVj2 = H02 + OMEGAj
HVj3 = H03 + OMEGAj
HVj4 = H04 + OMEGAj

H01 = HVCO(1.0,1.0) + HVCO(2.0,1.0)*Tj + HVCO(3.0,1.0)*Tj**2 + ...
      HVCO(4.0,1.0)*Tj**3 + HVCO(5.0,1.0)*Tj**4
H02 = HVCO(1.0,2.0) + HVCO(2.0,2.0)*Tj + HVCO(3.0,2.0)*Tj**2 + ...
      HVCO(4.0,2.0)*Tj**3 + HVCO(5.0,2.0)*Tj**4
H03 = HVCO(1.0,3.0) + HVCO(2.0,3.0)*Tj + HVCO(3.0,3.0)*Tj**2 + ...
      HVCO(4.0,3.0)*Tj**3 + HVCO(5.0,3.0)*Tj**4
H04 = HVCO(1.0,4.0) + HVCO(2.0,4.0)*Tj + HVCO(3.0,4.0)*Tj**2 + ...
      HVCO(4.0,4.0)*Tj**3 + HVCO(5.0,4.0)*Tj**4

OMEGAj = (2 - 1/ZZj)*Pj/(2*ZZj - 1) * (TKj*dBmj - Bmj)

Tj = INTEG(dTj, T0&J)
TKj = 5.0*Tj/9.0
dTj = (Ejdot - hLj1*duj1 - hLj2*duj2 - hLj3*duj3 - hLj4*duj4)/ ...
      ((hLCO(2.0,1.0) + 2*hLCO(3.0,1.0)*Tj)*uj1 ...
      + (hLCO(2.0,2.0) + 2*hLCO(3.0,2.0)*Tj)*uj2 ...
      + (hLCO(2.0,3.0) + 2*hLCO(3.0,3.0)*Tj)*uj3 ...
      + (hLCO(2.0,4.0) + 2*hLCO(3.0,4.0)*Tj)*uj4)
MACRO END

MACRO engbN(Lj, Ljm, Ejm, QR,uj1, uj2, uj3, uj4, ...
sumuj,ujm1, ujm2, ujm3, ujm4, sumujm, ...
duj1, duj2, duj3, duj4, Vj, EVj, ...
Yj1,Yj2,Yj3,Yj4, Tj, TKj, Bmj, Pj, ZZj, J)

MACRO Redefine Ej, Ejdot, jj, dTj, H01,H02,H03,H04,...
      OMEGAj, dBmj,dB11,dB12,dB13,dB14,dB22,dB23,dB24, ...
      dB33, dB34, dB44, hLj1,hLj2,hLj3,hLj4, ...
      HVj1, HVj2, HVj3,HVj4

engder(dBmj, dB11, dB12, dB13, dB14, dB22, dB23, dB24, ...
      dB33, dB34,dB44,Yj1, Yj2, Yj3, Yj4,Tj, TKj)

jj = J/1.0
Ejdot = Hf(jj) + Ljm*Ejm/sumujm - Lj*Ej/sumuj - EVj + QR
Ej = INTEG(Ejdot, E0&J)

hLj1 = hLCO(1.0,1.0) + hLCO(2.0,1.0)*Tj + hLCO(3.0,1.0)*Tj**2
hLj2 = hLCO(1.0,2.0) + hLCO(2.0,2.0)*Tj + hLCO(3.0,2.0)*Tj**2
hLj3 = hLCO(1.0,3.0) + hLCO(2.0,3.0)*Tj + hLCO(3.0,3.0)*Tj**2
hLj4 = hLCO(1.0,4.0) + hLCO(2.0,4.0)*Tj + hLCO(3.0,4.0)*Tj**2

EVj = Vj*Yj1*HVj1 + Vj*Yj2*HVj2 + Vj*Yj3*HVj3 + ...
      Vj*Yj4*HVj4

HVj1 = H01 + OMEGAj
HVj2 = H02 + OMEGAj
HVj3 = H03 + OMEGAj
HVj4 = H04 + OMEGAj

H01 = HVCO(1.0,1.0) + HVCO(2.0,1.0)*Tj + HVCO(3.0,1.0)*Tj**2 + ...
      HVCO(4.0,1.0)*Tj**3 + HVCO(5.0,1.0)*Tj**4
H02 = HVCO(1.0,2.0) + HVCO(2.0,2.0)*Tj + HVCO(3.0,2.0)*Tj**2 + ...
      HVCO(4.0,2.0)*Tj**3 + HVCO(5.0,2.0)*Tj**4
H03 = HVCO(1.0,3.0) + HVCO(2.0,3.0)*Tj + HVCO(3.0,3.0)*Tj**2 + ...

```

```

      HVCO(4.0,3.0)*Tj**3 + HVCO(5.0,3.0)*Tj**4
H04 = HVCO(1.0,4.0) + HVCO(2.0,4.0)*Tj + HVCO(3.0,4.0)*Tj**2 + ...
      HVCO(4.0,4.0)*Tj**3 + HVCO(5.0,4.0)*Tj**4

OMEGAj = (2 - 1/ZZj)*Pj/(2*ZZj -1) * (TKj*dBmj - Bmj)

Tj = INTEG(dTj, T0&J)
TKj = 5.0*Tj/9.0
dTj = (Ejdot - hLj1*duj1 - hLj2*duj2 - hLj3*duj3 - hLj4*duj4)/ ...
      (hLCO(2.0,1.0) + 2*hLCO(3.0,1.0)*Tj)*uj1 ...
      + (hLCO(2.0,2.0) + 2*hLCO(3.0,2.0)*Tj)*uj2 ...
      + (hLCO(2.0,3.0) + 2*hLCO(3.0,3.0)*Tj)*uj3 ...
      + (hLCO(2.0,4.0) + 2*hLCO(3.0,4.0)*Tj)*uj4)
MACRO END

"-----Material-balance models-----"

MACRO matb1(uj1, uj2, uj3, uj4, sumuj,duj1, duj2, duj3, duj4, ...
  Yjp1, Yjp2, Yjp3, Yjp4, Vjp, Suvj, LVj1,LVj2,LVj3,LVj4,...
  Yj1,Yj2,Yj3,Yj4, R, Lj, J)

MACRO Redefine jj, uvj1, uvj2, uvj3, uvj4

jj = J/1.0

duj1 = f(jj,1.0) - (1 + R)*Lj*uj1/(R*sumu1) + Vjp*Yjp1 - LVj1
uj1 = INTEG(duj1, u10&J)
duj2 = f(jj,2.0) - (1 + R)*Lj*uj2/(R*sumu1) + Vjp*Yjp2 - LVj2
uj2 = INTEG(duj2, u20&J)
duj3 = f(jj,3.0) - (1 + R)*Lj*uj3/(R*sumu1) + Vjp*Yjp3 - LVj3
uj3 = INTEG(duj3, u30&J)
duj4 = f(jj,4.0) - (1 + R)*Lj*uj4/(R*sumu1) + Vjp*Yjp4 - LVj4
uj4 = INTEG(duj4, u40&J)
sumuj = uj1 + uj2 + uj3 + uj4

uvj1 = INTEG(LVj1, uv10&J)
uvj2 = INTEG(LVj2, uv20&J)
uvj3 = INTEG(LVj3, uv30&J)
uvj4 = INTEG(LVj4, uv40&J)
Suvj = uvj1 + uvj2 + uvj3 + uvj4

Yj1 = uvj1/Suvj
Yj2 = uvj2/Suvj
Yj3 = uvj3/Suvj
Yj4 = uvj4/Suvj

MACRO END

MACRO matbj(uj1, uj2, uj3, uj4, sumuj,ujm1,ujm2, ujm3, ujm4, ...
  sumujm,duj1, duj2, duj3, duj4, Yj1,Yj2,Yj3,Yj4, Vj, ...
  Yjp1,Yjp2,Yjp3,Yjp4, Vjp, Lj, Ljm, ...
  LVj1,LVj2,LVj3,LVj4, Suvj, J)

MACRO Redefine jj, duvj1,duvj2,duvj3,duvj4, ...
  uvj1,uvj2,uvj3,uvj4

jj = J/1.0

duj1 = f(jj,1.0) + Ljm*ujm1/sumujm - Lj*uj1/sumuj - LVj1
uj1 = INTEG(duj1, u10&J)
duj2 = f(jj,2.0) + Ljm*ujm2/sumujm - Lj*uj2/sumuj - LVj2

```

```

uj2 = INTEG(duj2, u20&J)
duj3 = f(jj,3.0) + Ljm*ujm3/sumujm - Lj*uj3/sumuj - LVj3
uj3 = INTEG(duj3, u30&J)
duj4 = f(jj,4.0) + Ljm*ujm4/sumujm - Lj*uj4/sumuj - LVj4
uj4 = INTEG(duj4, u40&J)
sumuj = uj1 + uj2 + uj3 + uj4

```

```

duvj1 = Vjp*Yjp1 - Vj*Yj1 + LVj1
uvj1 = INTEG(duvj1, uv10&J)
duvj2 = Vjp*Yjp2 - Vj*Yj2 + LVj2
uvj2 = INTEG(duvj2, uv20&J)
duvj3 = Vjp*Yjp3 - Vj*Yj3 + LVj3
uvj3 = INTEG(duvj3, uv30&J)
duvj4 = Vjp*Yjp4 - Vj*Yj4 + LVj4
uvj4 = INTEG(duvj4, uv40&J)
Suvj = uvj1 + uvj2 + uvj3 + uvj4

```

```

Yj1 = uvj1/Suvj
Yj2 = uvj2/Suvj
Yj3 = uvj3/Suvj
Yj4 = uvj4/Suvj

```

MACRO END

```

MACRO matbN(uj1, uj2, uj3, uj4, sumuj,ujm1,ujm2, ujm3, ujm4, ...
sumujm,duj1, duj2, duj3, duj4, Suvj, ...
Vj, Vjp, Lj, Ljm, ...
Yj1,Yj2,Yj3,Yj4, LVj1,LVj2,LVj3,LVj4, J)

```

MACRO Redefine jj, duvj1, duvj2, duvj3, duvj4

```

jj = J*1.0/1.0
duj1 = f(jj,1.0) + Ljm*ujm1/sumujm - Lj*uj1/sumuj - LVj1
uj1 = INTEG(duj1, u10&J)
duj2 = f(jj,2.0) + Ljm*ujm2/sumujm - Lj*uj2/sumuj - LVj2
uj2 = INTEG(duj2, u20&J)
duj3 = f(jj,3.0) + Ljm*ujm3/sumujm - Lj*uj3/sumuj - LVj3
uj3 = INTEG(duj3, u30&J)
duj4 = f(jj,4.0) + Ljm*ujm4/sumujm - Lj*uj4/sumuj - LVj4
uj4 = INTEG(duj4, u40&J)
sumuj = uj1 + uj2 + uj3 + uj4

```

```

duvj1 = - Vj*uvj1/Suvj + LVj1
uvj1 = INTEG(duvj1, uv10&J)
duvj2 = - Vj*uvj2/Suvj + LVj2
uvj2 = INTEG(duvj2, uv20&J)
duvj3 = - Vj*uvj3/Suvj + LVj3
uvj3 = INTEG(duvj3, uv30&J)
duvj4 = - Vj*uvj4/Suvj + LVj4
uvj4 = INTEG(duvj4, uv40&J)
Suvj = uvj1 + uvj2 + uvj3 + uvj4

```

```

Yj1 = uvj1/Suvj
Yj2 = uvj2/Suvj
Yj3 = uvj3/Suvj
Yj4 = uvj4/Suvj

```

MACRO END

"-----pressure models-----"

```

MACRO pres1(Pj, Pjp, Z1, RHMLj, sumuj, Vjp, Tj, ZZj, Suvj, ...
  RHMvj, J)

  MACRO Redefine VOLREC, dP

    Pj = RR(5.0)*Tj*RHMvj*ZZj
    RHMvj = Suvj/(1256.6 - VOLREC)
    VOLREC = sumuj/RHMLj
    Z1 = RECVOL(VOLREC)

    dP = Pjp - Pj
    Vjp = SIGN(1.0,dP)*SQRT(ABS(dP)/(RHMvj*REF3))

  MACRO END

MACRO presj(Pj, Pjp, Lj, Ljm, HCTRj, HCTRjp, QQsj, ...
  RHOvj, RHMvj, RHMLj, RHOLj, RHOvj, RHOvj, RHOvj, ...
  sumuj, Vj, Vjp, Suvj, Yj1,Yj2,Yj3,Yj4, Tj, Zj, ZZj, ...
  LVj1,LVj2,LVj3,LVj4, Jp, J)

  MACRO Redefine HOj, FOAMj, QLj, FVAj, UVAj, UHj, HLUdj, ...
    MOLV, HOLDj, jj, dPdc, Pdc, dVdc, ...
    Vdc, dhow, howj, PUD, Qs, dQs, Cdd, dsumuj, dQVjp, ...
    dvjp, dZj, Pke

    jj = J/1.0
    RHMvj = Suvj/(883.57 - sumuj/RHMLj)
    MOLV = Yj1*MOL(1.0) + Yj2*MOL(2.0) + Yj3*MOL(3.0) + ...
    Yj4*MOL(4.0)
    RHOvj = MOLV*RHMvj
    Pj = RR(5.0)*Tj*RHMvj*ZZj

    HCTRj = FOAMj*(howj + HW/12)
    FOAMj = 1 - 0.372192*FVAj**0.177709
    FVAj = UVAj*SQRT(RHOvj)
    UVAj = Vjp/(AN*RHMvj*60)

    " UHj = Vjp/(AH(jj)*RHMvj) "
    " --HOj-- POj = (UHj/CD(jj))**2 * RHOvj/(2*g) "
    Pke = RHOvj*(Vjp/(AH(jj)*Cvc*RHMvj))**2 / (2*g)
    dQVjp = Cvc**2*AH(jj)*(Pjp - Pj - HCTRj*RHOLj - Pke)/(RHOvj*LH)
    dvjp = dQVjp*RHMvj
    Vjp = INTEG(dVjp, V0&Jp)

    " -----downcomer hydrolic capacitance"
    " dPdc = RHOLj*dZj "
    " Pdc = INTEG(dPdc, (Zj*RHOLj)) "
    dVdc = dZj * AD
    dZj = (Qs - QLj)/AD
    Vdc = Zj * AD
    Zj = INTEG(dZj, Z0&J)
    " --note that flows are allowed to become negative"
    QLj = Cx*AUD*SIGN(1.0,PUD)*SQRT(2*g*ABS(PUD))
    PUD = (Pj - Pjp)/RHOLj - HCTRjp + Zj
    Lj = QLj*RHMLj

    " -----wier equations"
    dQs = Cdd*LW*dhow*SIGN(1.0,howj)*SQRT(2*g*ABS(howj))/12.0
    QQsj = INTEG(dQs, Qs0&J )
    Qs = FCNSW(howj, 0.0, 0.0, QQsj)
    Cdd = (1.368*(1.01 + .0063*(Qs*(12/LW)**2.5)))*1.5

```

```

dhow = (dsumuj/RHMLj - dVdc)/(AN*FOAMj)
dsumuj = f(jj,1.0) + f(jj,2.0) + f(jj,3.0) + f(jj,4.0) + ...
        Ljm - Lj - (LVj1 + LVj2 + LVj3 + LVj4)
howj = INTEG(dhow, how0&J )
MACRO END

"-----Liquid-Vapor equilibrium models-----"
MACRO eqlcom(LMBjik, ALPHji, ALPHjk, Bjik,Tj, TKj, i, k)

        MACRO Redefine TRRjik, f3jik, f4jik, f5jik, f6jik

LMBjik = ALPHjk/ALPHji * EXP(WLMB(i,k)/(RR(4.0)*TKj))

"        TRRjik is reduced temperature here, as confirmed by"
"        [Perry, '73] , [°Kelvin/°Kelvin]"
TRRjik = TKj/TCC(i,k)
Bjik = RR(1.0)*TCC(i,k)*(f3jik + WH(i,k)*f4jik + f5jik + ...
        ETTA(i,k)*f6jik)/PCC(i,k)
f3jik = 0.1445 - 0.330/TRRjik - 0.1385/(TRRjik**2) - ...
        0.0121/(TRRjik**3)
f4jik = 0.073 + 0.46/TRRjik - 0.5/(TRRjik**2) - 0.097/(TRRjik**3)
...
        - 0.0073/(TRRjik**8)
f5jik = -5.237220 + 5.665807*MUR(i,k) - 2.133816*MUR(i,k)**2 +
...
        0.2525373*MUR(i,k)**3 + (5.769770 - 6.181427*MUR(i,k) + ...
        2.283270*MUR(i,k)**2 - 0.2649074*MUR(i,k)**3)/TRRjik
f6jik = EXP(4.62 - 6.6*TRRjik)

MACRO END

MACRO eql(uj1, uj2, uj3, uj4, sumuj,Tj,TKj, ...
        Pj, Yj1, Yj2, Yj3, Yj4, RHMLj, RHOLj, ...
        ZZj, Bmj, RHMVj, ...
        LVj1,LVj2,LVj3,LVj4, J)

MACRO Redefine PSj1, PSj2, PSj3, PSj4, Kj1, Kj2, Kj3 ,Kj4, ...
        ALPHj1, ALPHj2, ALPHj3, ALPHj4, ...
        PHIVj1, PHIVj2, PHIVj3, PHIVj4, ...
        GAMj1, GAMj2, GAMj3, GAMj4, ...
        PHILj1, PHISj1, f1j1, f2j1, TRj1, ...
        PHILj2, PHISj2, f1j2, f2j2, TRj2, ...
        PHILj3, PHISj3, f1j3, f2j3, TRj3, ...
        PHILj4, PHISj4, f1j4, f2j4, TRj4, ...
        Bj11, Bj12, Bj13, Bj14, Bj21, Bj22, Bj23, Bj24, Bj31, ...
        Bj32, Bj33, Bj34, Bj41, Bj42, Bj43, Bj44, ...
        LMBj11, LMBj12, LMBj13, LMBj14, LMBj21, LMBj22, ...
        LMBj23, LMBj24, LMBj31, LMBj32, LMBj33, LMBj34, ...
        LMBj41, LMBj42, LMBj43, LMBj44, jj, ...
        FgRj1, FgRj2, FgRj3, FgRj4, ...
        FgLj1,FgLj2,FgLj3,FgLj4, FgVj1,FgVj2,FgVj3,FgVj4, ...
        Rf1,Rf2,Rf3,Rf4, GAMs1,GAMs2,GAMs3,GAMs4

        eqlcom(LMBj11, ALPHj1, ALPHj1, Bj11,Tj, TKj, 1.0, 1.0)
        eqlcom(LMBj12, ALPHj1, ALPHj2, Bj12,Tj, TKj, 1.0, 2.0)
        eqlcom(LMBj13, ALPHj1, ALPHj3, Bj13,Tj, TKj, 1.0, 3.0)
        eqlcom(LMBj14, ALPHj1, ALPHj4, Bj14,Tj, TKj, 1.0, 4.0)
        eqlcom(LMBj21, ALPHj2, ALPHj1, Bj21,Tj, TKj, 2.0, 1.0)
        eqlcom(LMBj22, ALPHj2, ALPHj2, Bj22,Tj, TKj, 2.0, 2.0)
        eqlcom(LMBj23, ALPHj2, ALPHj3, Bj23,Tj, TKj, 2.0, 3.0)

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eqlcom(LMBj24, ALPHj2, ALPHj4, Bj24,Tj, TKj, 2.0, 4.0)
eqlcom(LMBj31, ALPHj3, ALPHj1, Bj31,Tj, TKj, 3.0, 1.0)
eqlcom(LMBj32, ALPHj3, ALPHj2, Bj32,Tj, TKj, 3.0, 2.0)
eqlcom(LMBj33, ALPHj3, ALPHj3, Bj33,Tj, TKj, 3.0, 3.0)
eqlcom(LMBj34, ALPHj3, ALPHj4, Bj34,Tj, TKj, 3.0, 4.0)
eqlcom(LMBj41, ALPHj4, ALPHj1, Bj41,Tj, TKj, 4.0, 1.0)
eqlcom(LMBj42, ALPHj4, ALPHj2, Bj42,Tj, TKj, 4.0, 2.0)
eqlcom(LMBj43, ALPHj4, ALPHj3, Bj43,Tj, TKj, 4.0, 3.0)
eqlcom(LMBj44, ALPHj4, ALPHj4, Bj44,Tj, TKj, 4.0, 4.0)

jj = J/1.0

" ---liquid and vapor fugacity is calculated and then molar flow---"
" The Rf values are guesses at this point"

FgLj1 = GAMj1*uj1*PSj1*PHILj1/sumuj
FgVj1 = PHIVj1*Yj1*Pj
Rf1 = uvj1*Rf + 1.
LVj1 = (FgLj1 - FgVj1)/Rf1

FgLj2 = GAMj2*uj2*PSj2*PHILj2/sumuj
FgVj2 = PHIVj2*Yj2*Pj
Rf2 = uvj2*Rf + 1.
LVj2 = (FgLj2 - FgVj2)/Rf2

FgLj3 = GAMj3*uj3*PSj3*PHILj3/sumuj
FgVj3 = PHIVj3*Yj3*Pj
Rf3 = uvj3*Rf + 1.
LVj3 = (FgLj3 - FgVj3)/Rf3

FgLj4 = GAMj4*uj4*PSj4*PHILj4/sumuj
FgVj4 = PHIVj4*Yj4*Pj
FgRj4 = LVj4*Rf4
Rf4 = uvj4*Rf + 1.
LVj4 = (FgLj4 - FgVj4)/Rf4

"-----Liquid fugacity stuff-----"

PSj1 = 2.784605*10.** (ANT(1.0,1.0) - (ANT(2.0,1.0)/(ANT(3.0,1.0) +
...
(TKj - 273.15))))
PSj2 = 2.784605*10.** (ANT(1.0,2.0) - (ANT(2.0,2.0)/(ANT(3.0,2.0) +
...
(TKj - 273.15))))
PSj3 = 2.784605*10.** (ANT(1.0,3.0) - (ANT(2.0,3.0)/(ANT(3.0,3.0) +
...
(TKj - 273.15))))
PSj4 = 2.784605*10.** (ANT(1.0,4.0) - (ANT(2.0,4.0)/(ANT(3.0,4.0) +
...
(TKj - 273.15))))

GAMs1 = uj1*LMBj11 + uj1*LMBj12 + uj1*LMBj13 ...
+ uj1*LMBj14
GAMs2 = uj2*LMBj21 + uj2*LMBj22 + ...
uj2*LMBj23 + uj2*LMBj24
GAMs3 = uj3*LMBj31 + uj3*LMBj32 + ...
uj3*LMBj33 + uj3*LMBj34
GAMs4 = uj4*LMBj41 + uj4*LMBj42 + uj4*LMBj43 + ...
uj4*LMBj44
GAMj1 = EXP(1 - uj1*LMBj11/GAMs1 - uj2*LMBj21/GAMs2 - ...
uj3*LMBj31/GAMs3 - uj4*LMBj41/GAMs4) * ...

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sumuj/(uj1*LMBj11 + uj2*LMBj12 + ...
uj3*LMBj13 + uj4*LMBj14)
GAMj2 = EXP(1 - uj1*LMBj12/GAMs1 - uj2*LMBj22/GAMs2 - ...
uj3*LMBj32/GAMs3 - uj4*LMBj42/GAMs4) * ...
sumuj/(uj1*LMBj21 + uj2*LMBj22 + uj3*LMBj23 + ...
uj4*LMBj24)
GAMj3 = EXP(1 - uj1*LMBj13/GAMs1 - uj2*LMBj23/GAMs2 - ...
uj3*LMBj33/GAMs3 - uj4*LMBj43/GAMs4) * ...
sumuj/(uj1*LMBj31 + uj2*LMBj32 + ...
uj3*LMBj33 + uj4*LMBj34)
GAMj4 = EXP(1 - uj1*LMBj14/GAMs1 - uj2*LMBj24/GAMs2 - ...
uj3*LMBj34/GAMs3 - uj4*LMBj44/GAMs4) * ...
sumuj/(uj1*LMBj41 + uj2*LMBj42 + ...
uj3*LMBj43 + uj4*LMBj44)

PHISj1 = EXP(f1j1 + f2j1*WW(1.0))
PHISj2 = EXP(f1j2 + f2j2*WW(2.0))
PHISj3 = EXP(f1j3 + f2j3*WW(3.0))
PHISj4 = EXP(f1j4 + f2j4*WW(4.0))

"      Note that TRji is 9/5 of reduced temperature.      "
"      Otherwise, PHILji <<1.0 for all Tj, which is improbable"
"      Hence, the dimension of TRji is [°Rankine/°Kelvin]"
TRj1 = Tj/TC(1.0)
TRj2 = Tj/TC(2.0)
TRj3 = Tj/TC(3.0)
TRj4 = Tj/TC(4.0)

f1j1 = -3.5021358 + TRj1*( 5.6085595 + TRj1*(-3.076574 + ...
TRj1*0.57335015))
f2j1 = -3.7690418 + TRj1*( 4.3538729 + TRj1*( 0.3166137 + ...
TRj1*( ...
0.12666184 + TRj1*(-1.1662283 + TRj1*(-0.10665730 + TRj1*( ...
0.12147436 + TRj1*( 0.18927037 + TRj1*(0.14936906 + ...
TRj1*(0.024364816 + TRj1*(-0.068603516 + TRj1*(-0.015172164
...
+ TRj1*0.012089114)))))))))
f1j2 = -3.5021358 + TRj2*( 5.6085595 + TRj2*(-3.076574 + ...
TRj2*0.57335015))
f2j2 = -3.7690418 + TRj2*( 4.3538729 + TRj2*( 0.3166137 +
TRj2*(...
0.12666184 + TRj2*(-1.1662283 + TRj2*(-0.10665730 + TRj2*( ...
0.12147436 + TRj2*( 0.18927037 + TRj2*(0.14936906 + ...
TRj2*(0.024364816 + TRj2*(-0.068603516 + TRj2*(-0.015172164
...
+ TRj2*0.012089114)))))))))
f1j3 = -3.5021358 + TRj3*( 5.6085595 + TRj3*(-3.076574 + ...
TRj3*0.57335015))
f2j3 = -3.7690418 + TRj3*( 4.3538729 + TRj3*( 0.3166137 +
TRj3*(...
0.12666184 + TRj3*(-1.1662283 + TRj3*(-0.10665730 + TRj3*( ...
0.12147436 + TRj3*( 0.18927037 + TRj3*(0.14936906 + ...
TRj3*(0.024364816 + TRj3*(-0.068603516 + TRj3*(-0.015172164
...
+ TRj3*0.012089114)))))))))
f1j4 = -3.5021358 + TRj4*( 5.6085595 + TRj4*(-3.076574 + ...
TRj4*0.57335015))
f2j4 = -3.7690418 + TRj4*( 4.3538729 + TRj4*( 0.3166137 +
TRj4*(...
0.12666184 + TRj4*(-1.1662283 + TRj4*(-0.10665730 + TRj4*( ...
0.12147436 + TRj4*( 0.18927037 + TRj4*(0.14936906 + ...

```



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TRj4*(0.024364816 + TRj4*(-0.068603516 + TRj4*(-0.015172164
...
+ TRj4*0.012089114)))))))))
PHILj1 = PHISj1*EXP(ALPHj1*(- PSj1)/(2.784605*RR(2.0)*TKj))
PHILj2 = PHISj2*EXP(ALPHj2*(- PSj2)/(2.784605*RR(2.0)*TKj))
PHILj3 = PHISj3*EXP(ALPHj3*(- PSj3)/(2.784605*RR(2.0)*TKj))
PHILj4 = PHISj4*EXP(ALPHj4*(- PSj4)/(2.784605*RR(2.0)*TKj))

"-----Liquid densities-----"
ALPHj1 = MV(1.0,1.0) + MV(2.0,1.0)*Tj + MV(3.0,1.0)*Tj**2
ALPHj2 = MV(1.0,2.0) + MV(2.0,2.0)*Tj + MV(3.0,2.0)*Tj**2
ALPHj3 = MV(1.0,3.0) + MV(2.0,3.0)*Tj + MV(3.0,3.0)*Tj**2
ALPHj4 = MV(1.0,4.0) + MV(2.0,4.0)*Tj + MV(3.0,4.0)*Tj**2

RHMLj = 62.43*sumuj/(ALPHj1*uj1 +ALPHj2*uj2 + ...
ALPHj3*uj3 + ALPHj4*uj4)
RHOLj = 62.43*sumuj/(ALPHj1*uj1/MOL(1.0) + ...
ALPHj2*uj2/MOL(2.0) + ...
ALPHj3*uj3/MOL(3.0) + ...
ALPHj4*uj4/MOL(4.0))

"---Vapor fugacity stuff---"
PHIVj1 = EXP(2*(Yj1*Bj11 + Yj2*Bj12 + Yj3*Bj13 + Yj4*Bj14)* ...
RHMvj) / ZZj
PHIVj2 = EXP(2*(Yj1*Bj21+Yj2*Bj22 + Yj3*Bj23 + Yj4*Bj24)* ...
RHMvj) / ZZj
PHIVj3 = EXP(2*(Yj1*Bj31 + Yj2*Bj32 + Yj3*Bj33+Yj4*Bj34)* ...
RHMvj) / ZZj
PHIVj4 = EXP(2*(Yj1*Bj41 + Yj2*Bj42 + Yj3*Bj43+Yj4*Bj44)* ...
RHMvj) / ZZj

Bmj = (Yj1*(Yj1*Bj11 + Yj2*Bj12 + Yj3*Bj13 + Yj4*Bj14) + ...
Yj2*(Yj1*Bj21 + Yj2*Bj22 + Yj3*Bj23 + Yj4*Bj24) + ...
Yj3*(Yj1*Bj31 + Yj2*Bj32 + Yj3*Bj33 + Yj4*Bj34) + ...
Yj4*(Yj1*Bj41 + Yj2*Bj42 + Yj3*Bj43 + Yj4*Bj44))

ZZj = 1.0 + Bmj*RHMvj

MACRO END

"-----condenser and receiver model-----"

MACRO condsr(QC, L1, RHMLj, R, Pjp, Z1, Pj, q1, RHOL1, ...
T1,T2, Vjp,CV1, CV2, CV3)

MACRO Redefine Pd1, Ps1, q2, Qcw, Tmc, Two,...
Z, Y, X, PDD

Two = INTEG(((Qcw*Ccw*(Twi - Two)*8.34 + Uwmo/60 * Aw*(Tmc - ...
Two)*(Qcw/Qcwo)**1.8 )/(Ucw*Ccw)), Two0)
QC = (105.8752/(Vjp))**0.33 *(Upmo/60 * Apc*( ...
(1-ALPHA)*T2 + ALPHA*T1 - Tmc))
Tmc = INTEG(((QC - Uwmo/60 * (Qcw/Qcwo)**1.8 * Aw*(Tmc - Two)) ...
/(Umc*Cmc)), Tmc0)
Qcw = ((Pw1 - Pw3)*CV1**2/(0.25 + ...
REF2*CV1**2/Qcwo**1.8))**0.5157507757

"--recevier flow"
R = q1/q2

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L1 = q1*RHMLj/7.481

Pd1 = Pj + Ppmp + Ppe
Ppmp = (HEDCO(1,1) + HEDCO(2,1)*(q1 + q2) + ...
        HEDCO(3,1)*(q1 + q2)**2 + HEDCO(4,1)*(q1 + q2)**3)*RHOL1
Ppe = (Z1 + ZC)*RHOL1

"hydraulic inductance = rho*volume/area is guessed at in the following"
Pv1 = (q1/CV1)**2 / 144
q1 = INTEG((Pd1 + Pv1 - PD)/(RHOL1*100),q10)
Pv2 = (q2/CV2)**2 / 144
q2 = INTEG((Pd1 + Pv2 - Pjp)/(RHOL1*50),q20)

MACRO END

"-----reboiler model-----"

MACRO reboil(HCTRj, QR, P50, Z50, L50, QQsj, Ljm, ...
    Wsh, RHOVj, RHMVj, RHMLj, RHOL50, RHMLjm, ...
    sumuj, Suvj,Yj1, Yj2, Yj3, Yj4, T50, CS4, CV5, ZZj)

    MACRO Redefine Tsc, Tmr, Ps2, Pd2, q50, RHOSC, hLSC, HVSC, ...
        VOLBTW, MOLV, HP, dHVSC, FVAj, Csc, dRHOSC, ...
        dhowj, howj, Qs, dQs, Cdd

"-----pressure----"

    RHMVj = Suvj/(2297.290 - Z50*176.7146)
    MOLV = Yj1*MOL(1.0) + Yj2*MOL(2.0) + Yj3*MOL(3.0) + ...
        Yj4*MOL(4.0)
    RHOVj = MOLV*RHMVj
    VOLBTW = 100 + pii*Z50*DTT**2/4

    HCTRj = howj + 1.25/12
    dhowj = (Ljm/RHMLjm - Qs)/11.01
    howj = INTEG(dhowj, how050 )
    dQs = Cdd*149.0*dhowj*SIGN(1.0,howj)*SQRT(2*g*ABS(howj))/12.0
    QQsj = INTEG(dQs, Qs050 )
    Qs = FCNSW(howj, 0.0, 0.0, QQsj)
    Cdd = (1.368*(1.01 + .0063*(Qs*(12/LW)**2.5)))*1.5

    Z50 = 4/(pii*DTT**2)*(sumuj/RHMLj - 100)
    P50 = RR(5.0)*T50*RHMVj*ZZj

"-----reboiler enthalpy balance and pump pressures----"

    Tmr = INTEG((Us*As/60 * (Tsc - Tmr) - QR)/(Umr*Cmr), ...
        Tmr0)
    Tsc = INTEG(((Wsh*(HSH - hLSC) - Us*As/60 * (Tsc - Tmr)) ...
        /(Csc*Vr*RHOSC - hLSC*dRHOSC*Vr)), Tsc0)
    Csc = dHVSC + HVSC*dRHOSC/RHOSC
    QR = Upmr*Apmr/60 * (Tmr - T50)
    q50 = (0.0156369 + SQRT((0.0156369)**2 - 4*(-2.7865E-5 - ...
        144/(62.4*CV5**2)) * (70.3698 - HP)))/(2* ...
        (-2.7865E-5 - 144/(62.4*CV5**2)) )
    HP = PB*144/RHOL50 - Ps2
    L50 = q50*RHMLj/7.481
    Wsh = 2*PSH*CS4/(60*(1.0 + 0.00065*(TSH - TSAT)))
    RHOSC = 1.031951E-2 + 1.427797E1*Tsc/610 + 0.9414444* ...
        (Tsc/610)**2 ...
        + 2.048037*(Tsc/610)**3 + 5.956991*(Tsc/610)**4
    dRHOSC = ( RHOSCO(2.0) + 2*RHOSCO(3.0)*Tsc/610 + 3*RHOSCO(4.0) ...

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      *(Tsc/610)**2 + 4*RHOSCO(5.0)*(Tsc/610)**3 )/610
hLSC = -1.6029E2 + 8.06427E-2*Tsc + 7.361453E-5*Tsc**2 + ...
      1.501012E-6*Tsc**3 - 9.9964334E-10*Tsc**4
dHVSC = 8.039637E-1 + 2*1.931794E-3*Tsc - 3*3.938661E-6* ...
      Tsc**2 + 4*1.907853E-9 * Tsc**3
HVSC = 5.448738E2 + 8.039637E-1*Tsc + 1.931794E-3*Tsc**2 - ...
      3.938661E-6*Tsc**3 + 1.907853E-9*Tsc**4
Ps2 = P50/RHOL50 + Z50 + ZB
MACRO END

"-----Controllers model-----"

MACRO contrl(CV1, CV2, CV3, CS4, CV5, ...
  T35, TK35, Pj, ql, Z1, Z50, Wsh)

MACRO Redefine CI1, CI2, CI3, CI4, CI5, CI6, CO1, CO2, CO3, ...
  CO4, CO5, CO6, I1, I2, I3, I4, I5, I6, TM, ZETA1, ZETA2, ...
  ZETA3, ZETA4, ZETA5, dZETA1, dZETA2, dZETA3, dZETA5

CV1 = CV1CO(2.0,ZETA1) + CV1CO(3.0,ZETA1)*( ZETA1 ...
  - CV1CO(1.0,ZETA1)) + CV1CO(4.0,ZETA1)*( ZETA1 ...
  - CV1CO(1.0,ZETA1))**2 ...
  + CV1CO(5.0,ZETA1)*(ZETA1 - CV1CO(1.0,ZETA1))**3
CV2 = CV2CO(2.0,ZETA2) + CV2CO(3.0,ZETA2)*( ZETA2 ...
  - CV2CO(1.0,ZETA2)) + CV2CO(4.0,ZETA2)*( ZETA2 ...
  - CV2CO(1.0,ZETA2))**2 ...
  + CV2CO(5.0,ZETA2)*(ZETA2 - CV2CO(1.0,ZETA2))**3
CV3 = CV3CO(2.0,ZETA3) + CV3CO(3.0,ZETA3)*( ZETA3 ...
  - CV3CO(1.0,ZETA3)) + CV3CO(4.0,ZETA3)*( ZETA3 ...
  - CV3CO(1.0,ZETA3))**2 ...
  + CV3CO(5.0,ZETA3)*(ZETA3 - CV3CO(1.0,ZETA3))**3
CS4 = CSCO(2.0,ZETA4) + CSCO(3.0,ZETA4)*(ZETA4 ...
  - CSCO(1.0,ZETA4)) + CSCO(4.0,ZETA4)*(ZETA4 ...
  - CSCO(1.0,ZETA4))**2 + CSCO(5.0,ZETA4)*(ZETA4 ...
  - CSCO(1.0,ZETA4))**3
CV5 = CV5CO(2.0,ZETA5) + CV5CO(3.0,ZETA5)*(ZETA5 ...
  - CV5CO(1.0,ZETA5)) + CV5CO(4.0,ZETA5)*(ZETA5 ...
  - CV5CO(1.0,ZETA5))**2 + CV5CO(5.0,ZETA5)*(ZETA5 ...
  - CV5CO(1.0,ZETA5))**3

Pbob = Pj/2.784605

CI1 = 0.032*Pbob - 12.0
I1 = INTEG((CI1 - CISP1), I01)
CO1 = XKC(1.0)*(CI1 - CISP1 + I1/TAUI(1.0))
ZETA1 = INTEG(dZETA1, ZET01)
dZETA1 = (-0.25 + 0.0625*CO1 - ZETA1)/TAUV(1.0)

CI2 = (ql/200)**2 + 4.0
I2 = INTEG(CISP2 - CI2, I02)
CO2 = XKC(2.0)*(-CI2 + CISP2 + I2/TAUI(2.0))
ZETA2 = INTEG( dZETA2, ZET02)
dZETA2 = (-0.25 + 0.0625*CO2 - ZETA2)/TAUV(2.0)

CI3 = 4.0 + 1.6*Z1
I3 = INTEG(CI3 - CISP3, I03)
CO3 = XKC(3.0)*(CI3 - CISP3 + I3/TAUI(3.0))
ZETA3 = INTEG(dZETA3, ZET03)
dZETA3 = (-0.25 + 0.0625*CO3 - ZETA3)/TAUV(3.0)

CI5 = -20.0 + 4*Z50

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```

I5 = INTEG(CI5 - CISP5, I05)
CO5 = XKC(5.0)*(CI5 - CISP5 + I5/TAUI(5.0))
ZETA5 = INTEG(dZETA5, ZET05)
dZETA5 = (-0.25 + 0.0625*CO5 - ZETA5)/TAUV(5.0)

CI4 = 4 + 16*(Wsh/3000)**2
I4 = INTEG(CO6 - CI4, I04)
CO4 = XKC(4.0)*(CO6 - CI4 + I4/TAUI(4.0))
ZETA4 = INTEG((-0.25 + 0.0625*CO4 - ZETA4)/TAUV(4.0), ...
ZET04)
TM = INTEG((T35 - TM)/TAUM , TM0)
CI6 = 0.4*TM - 232.
CO6 = XKC(6.0)*(CISP6 - CI6 + I6/TAUI(6.0))
I6 = INTEG(CISP6 - CI6, I06)
MACRO END

"-----stage 1 model-----"
MACRO cond(Tj,Tjp, Vjp, uj1, uj2, uj3, uj4, sumuj,...
Yjp1,Yjp2,Yjp3,Yjp4, CV1, CV2, CV3, EVjp, ...
RHOLj, RHMLj, RHOVjp, RHMVjp, ...
Pj, Pjp, HCTRjp, Lj, Ej, q1, Zj)

MACRO Redefine R, QC, TKj, RHMLj, Yj1,Yj2,Yj3,Yj4, ...
duj1,duj2,duj3,duj4, Suvj, LVj1, LVj2, LVj3,LVj4, ...
ZZj, Bmj, RHMVj

engb1(Tj, TKj, R, QC, Ej, Lj, sumuj, EVjp,...
uj1, uj2, uj3, uj4, duj1,duj2,duj3,duj4, 1)
matb1(uj1, uj2, uj3, uj4, sumuj,duj1, duj2, duj3, duj4, ...
Yjp1, Yjp2, Yjp3, Yjp4, Vjp, Suvj,LVj1,LVj2,LVj3,LVj4, ...
Yj1,Yj2,Yj3,Yj4, R, Lj, 1)
eql(uj1, uj2, uj3, uj4, sumuj,Tj,TKj, ...
Pj, Yj1, Yj2, Yj3, Yj4, RHMLj, RHOLj, ...
ZZj, Bmj, RHMVj , ...
LVj1,LVj2,LVj3,LVj4, 1)
pres1(Pj, Pjp, Zj, RHMLj, sumuj, Vjp, Tj, ZZj, Suvj, ...
RHMVj, 1)
condsr(QC, Lj, RHMLj, R, Pjp, Zj, Pj, q1, RHOLj, ...
Tj,Tjp, Vjp,CV1, CV2, CV3)
MACRO END

"-----stage 2-49 model-----"
MACRO stage(uj1, uj2, uj3, uj4, sumuj,ujm1, ujm2, ujm3, ujm4, ...
sumujm, Tj,TKj, Vj,Vjp, Yjp1,Yjp2,Yjp3,Yjp4, ...
Yj1,Yj2,Yj3,Yj4, EVj, EVjp, Qsj, ...
RHOLj, RHOVj, RHMVj, RHMLj, RHOVjp, RHMVjp, ...
Zj, Pjp, HCTRjp,Pj, HCTRj,Ljm, Ejm,Lj, Ej, Jp, J)

MACRO Redefine duj1, duj2, duj3, duj4, ...
LVj1,LVj2,LVj3,LVj4, Bmj, ZZj, Suvj

eql(uj1, uj2, uj3, uj4, sumuj,Tj,TKj, ...
Pj, Yj1, Yj2, Yj3, Yj4, RHMLj, RHOLj, ...
ZZj, Bmj, RHMVj, ...
LVj1,LVj2,LVj3,LVj4, J)
matbj(uj1, uj2, uj3, uj4, sumuj,ujm1,ujm2, ujm3, ujm4, ...
sumujm,duj1, duj2, duj3, duj4, Yj1,Yj2,Yj3,Yj4, Vj, ...
Yjp1,Yjp2,Yjp3,Yjp4, Vjp, Lj, Ljm, ...
LVj1,LVj2,LVj3,LVj4, Suvj, J)
engbj(Ej, Lj, Ljm, Ejm,uj1, uj2, uj3, uj4, ...

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sumuj,ujm1, ujm2, ujm3, ujm4, sumujm, ...
duj1, duj2, duj3, duj4, Vj, EVj, EVjp, ...
Yj1,Yj2,Yj3,Yj4, Tj, TKj, Bmj, Pj, ZZj, J)
presj(Pj, Pjp, Lj, Ljm, HCTRj, HCTRjp, Qsj, ...
RHOVj, RHMVj, RHMLj, RHOLj, RHOVjp, RHMVjp, ...
sumuj, Vj, Vjp, Suvj, Yj1,Yj2,Yj3,Yj4, Tj, Zj,ZZj, ...
LVj1,LVj2,LVj3,LVj4, Jp,J)
MACRO END

"-----stage 50 model-----"
MACRO rebo(uj1, uj2, uj3, uj4, sumuj,ujm1, ujm2, ujm3, ujm4, ...
sumujm, Vj, Yj1, Yj2, Yj3, Yj4, ...
RHOLj, RHOVj, RHMVj, EVj, Pj, Qsj, ...
HCTRj,Ljm, Ejm,CS4, CV5, Zj, Wsh, Lj, Tj, J)

MACRO Redefine QR, RHMLj, TKj, FgLj1,FgLj2,FgLj3,FgLj4, ...
Suvj, Bmj, ZZj, LVj1,LVj2,LVj3,LVj4

engbn(Lj, Ljm, Ejm, QR,uj1, uj2, uj3, uj4, ...
sumuj,ujm1, ujm2, ujm3, ujm4, sumujm, ...
duj1, duj2, duj3, duj4, Vj, EVj, ...
Yj1,Yj2,Yj3,Yj4, Tj, TKj, Bmj, Pj, ZZj, J)
matbn(uj1, uj2, uj3, uj4, sumuj,ujm1,ujm2, ujm3, ujm4, ...
sumujm,duj1, duj2, duj3, duj4, Suvj, ...
Vj, Vjp, Lj, Ljm, ...
Yj1,Yj2,Yj3,Yj4, LVj1,LVj2,LVj3,LVj4, J)
eq1(uj1, uj2, uj3, uj4, sumuj,Tj,TKj, ...
Pj, Yj1, Yj2, Yj3, Yj4, RHMLj, RHOLj, ...
ZZj, Bmj, RHMVj, ...
LVj1,LVj2,LVj3,LVj4, J)
reboil(HCTRj, QR, Pj, Zj, Lj, Qsj, Ljm, ...
Wsh, RHOVj, RHMVj, RHMLj, RHOLj, RHMLj, ...
sumuj, Suvj,Yj1, Yj2, Yj3, Yj4, Tj, CS4, CV5, ZZj)
MACRO END

END $" of INITIAL"
"-----"
DYNAMIC
DERIVATIVE

cond(T1,T2, V2, u11, u12, u13, u14, sumu1,...
Y21,Y22,Y23,Y24, CV1, CV2, CV3, EV2, ...
RHOL1, RHML2, RHOV2, RHMV2, ...
P1, P2, HCTR2, L1, E1, q1, Z1)

stage(u21, u22, u23, u24, sumu2,u11, u12, u13, u14, ...
sumu1, T2,TK2, V2,V3, Y31,Y32,Y33,Y34, ...
Y21,Y22,Y23,Y24, EV2, EV3, Qs2, ...
RHOL2, RHOV2, RHMV2, RHML2, RHOV3, RHMV3, ...
Z2, P3, HCTR3,P2, HCTR2,L1, E1,L2, E2, 3,2)
stage(u31, u32, u33, u34, sumu3,u21, u22, u23, u24, ...
sumu2, T3,TK3, V3,V4, Y41,Y42,Y43,Y44, ...
Y31,Y32,Y33,Y34, EV3, EV4, Qs3, ...
RHOL3, RHOV3, RHMV3, RHML3, RHOV4, RHMV4, ...
Z3, P4, HCTR4,P3, HCTR3,L2, E2,L3, E3, 4,3)
stage(u41, u42, u43, u44, sumu4,u31, u32, u33, u34, ...
sumu3, T4,TK4, V4,V5, Y51,Y52,Y53,Y54, ...
Y41,Y42,Y43,Y44, EV4, EV5, Qs4,...
RHOL4, RHOV4, RHMV4, RHML4, RHOV5, RHMV5, ...
Z4, P5, HCTR5,P4, HCTR4,L3, E3,L4, E4, 5,4)
stage(u51, u52, u53, u54, sumu5,u41, u42, u43, u44, ...

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    sumu4, T5,TK5, V5,V21, Y211,Y212,Y213,Y214, ...
    Y51,Y52,Y53,Y54, EV5, EV21, Qs5,...
    RHOL5, RHOV5, RHMV5, RHML5, RHOV21, RHMV21, ...
    Z5, P21, HCTR21,P5, HCTR5,L4, E4,L5, E5, 21,5)
stage(u211, u212, u213, u214, sumu21,u51, u52, u53, u54, ...
    sumu5, T21,TK21, V21,V35, Y351,Y352,Y353,Y354, ...
    Y211,Y212,Y213,Y214, EV21, EV35, Qs21,...
    RHOL21, RHOV21, RHMV21, RHML21, RHOV35, RHMV35, ...
    Z21, P35, HCTR35,P21, HCTR21,L5, E5,L21, E21, 35,21)
stage(u351,u352,u353,u354, sumu35,u211,u212,u213,u214, ...
    sumu21, T35,TK35, V35,V49, Y491,Y492,Y493,Y494, ...
    Y351,Y352,Y353,Y354, EV35, EV49, Qs35,...
    RHOL35, RHOV35, RHMV35, RHML35, RHOV49, RHMV49, ...
    Z35, P49, HCTR49,P35, HCTR35,L21, E21,L35, E35, 49,35)
stage(u491,u492,u493,u494, sumu49,u351,u352,u353,u354, ...
    sumu35, T49,TK49, V49,V50, Y501,Y502,Y503,Y504, ...
    Y491,Y492,Y493,Y494, EV49, EV50, Qs49,...
    RHOL49, RHOV49, RHMV49, RHML49, RHOV50, RHMV50, ...
    Z49, P50, HCTR50,P49, HCTR49,L35, E35,L49, E49, 50,49)

rebo(u501,u502,u503,u504, sumu50, u491,u492,u493, u494, ...
    sumu49, V50, Y501, Y502, Y503, Y504, ...
    RHOL50, RHOV50, RHMV50, EV50, P50, Qs50, ...
    HCTR50,L49, E49,CS4, CV5, Z50, Wsh, L50, T50, 50)

contrl(CV1, CV2, CV3, CS4, CV5, ...
    T35, TK35, P1, q1, Z1, Z50, Wsh)

END $ "of DERIVATIVE"
    Termt(t .ge.tmx)
END $ "of DYNAMIC"
END $"of Program distcom.csl"

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