

# MODELING OF A DISTILLATION COLUMN USING BOND GRAPHS

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## ABSTRACT

Modeling and simulating distillation columns are not new enterprises. The models used for distillation columns vary from the simple to the quite complex, depending on the nature of assumptions. 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 such a complex system. 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 using a specific model used by Steven Gallun. Results 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. INTRODUCTION

Modeling a distillation column is as simple or as complex as the assumptions made to create the model. Distillation models can be (and mostly are) very simple affairs that account for the mass and enthalpy balances using assumptions of constant pressures and flows and of simple thermodynamics of the components to be separated. Simple models are usually good for predicting steady-state behavior; most models forego the option of dynamic simulation. Fuller, more complete models of distillation have the advantages of accuracy and allowing dynamic simulation to test different control strategies, for instance. The disadvantage of these models is their size and complexity, requiring many specifications of the exact structure of the column and of the components used. In the last decade, models of distillation columns have dropped many of the simplifying assumptions, but problems still exist (Holland and Liapis 1983; Gani *et al.* 1986).

Problems are of two kinds, structural and theoretical. Distillation models are often rife with algebraic loops (an

index of nilpotency greater than zero, or zero-order causal paths). For instance, distillation models rarely (if ever) account for hydraulic inertia; only resistances are considered. The typical solutions are either to greatly simplify the model or use simulation techniques allowing such loops. Gear's algorithm allows for non-zero nilpotencies (Gear and Petzold 1984; van Dijk and Breedveld 1991). Of course, algebraic loops can be symptoms of deeper problems within the model. Some of the algebraic loops concern inadequacies in thermodynamic chemical theory. A major assumption in the formulation of thermal state equations and phase changing equations is the assumption of equilibrium between liquid and vapor on each stage: the pressures, temperatures and chemical potentials of the liquid and vapor are always identical. In distillation, the whole basis of the device is a continuous mass exchange between the liquid and vapor phases, yet the equations used do not predict this flow, the equations only predict the mass exchanged after a dynamic equilibrium is reached and steady-state flow is achieved.

Bond graphs have the advantage of clearly laying out the structure of a distillation column. Problems with the structure of a particular model are exposed. Because the structure changes with assumptions, and also as thermodynamic theory advances (hopefully), the inherent object-oriented nature of bond graphs allows for the easy change, expansion, or contraction of the model. Bond graphs thus become a convenient and useful tool in understanding the fundamentals of distillation.

## 2. DISTILLATION

The distillation column is a device to separate components of a mixture using the thermodynamic properties of the components. Heat is added to the bottom (QR) and removed at the top (QC) of the column. The column itself is adiabatic. Essentially, the components with the lower boiling-points will tend towards the top of the column as vapor and the components with the higher boiling-points will gravitate towards the bottom as liquid. The initial mixture is fed to the middle of the column (f), distillate is removed from the top (d), and bottoms (b) are removed from the base. Vapor and liquid make contact as the hot vapor rising from below ( $V_{j+1}$ ) flows through holes in stage trays containing the cooler liquid flowing from above ( $L_{j-1}$ ). The contact engenders heat and mass exchanges conducive to the separation goal of a distillation column. The entropy and molar flow between the

liquid and vapor phases is a complex affair. Convection, conduction, and heat of vaporization are taking place as the fluids are flowing through a stage, exchanging heat and mass. Figure 1 shows a small typical trayed column.

### 2.1 Traditional Models

The major aspects of a traditional model are energy balance, mass balance, vapor-liquid equilibrium, and hydraulics. Extensive thermodynamic data exist on many of the components that can be found in a distillation column (Perry and Chilton 1973). Most commonly, the data describe intensive enthalpy as a function of temperature. Entropy and chemical potential have no place in these calculations. By making the assumption of negligible vapor holdup in enthalpy and mass, a differential equation is generated expressing the change in the holdup of the liquid's enthalpy and mass on the  $j$ th stage and  $i$ th component as a function of incoming and outgoing flows of fluid; see Table 1. The vapor intensive enthalpy ( $h_{ji}^V$ ) is calculated using a polynomial function of temperature. Temperature is calculated using a polynomial function of liquid intensive enthalpy. Notice that this configuration does not require an explicit knowledge of the flow between the phases nor the heat of vaporizations.

$\frac{d(n_{ji}^L)}{dt} = (f_{ji} + L_{j-1} x_{j-1i} - L_j x_{ji}) + (v_{j+1i} - v_{ji})$
$\frac{dH_j^L}{dt} = F_j h_j^f + \frac{L_{j-1} H_{j-1}^L}{n_{j-1}^L} - \frac{L_j H_j^L}{n_j^L} + \sum_{vi} v_{j+1i} h_{j+1i}^V - \sum_{vi} v_{ji} h_{ji}^V$

Table 1. Mass and energy balance equations.

The vapor-liquid equilibrium equations, in essence, specify the mass flow between the phases. Although chemical potential is a convenient and theoretically potent concept, actual calculations of phase transfer are not made and chemical potential is never used. As seen in the mass balance equations, the vapor molar fractions ( $y_{ji}$ ) are required instead of the mass flow. Fugacity is used to estimate the molar fractions of each components. (Fugacity is essentially partial pressure with the deviation from ideal gas and mixture added in.) The equations used to calculate fugacity depend on the set of components and the required accuracy. By using Antoine's law, the vapor molar fractions become a function of liquid molar fractions, pressure and temperature. If activity and fugacity coefficients must be used, the vapor molar fractions also become functions of themselves. This is a non-linear algebraic loop.

The assumption of equilibrium is relaxed by using efficiencies. Essentially, it is recognized that the molar phase flow is being driven by differences in the fugacity of liquid and vapor. Efficiency is a resistance between the phases allowing for the differences. It does not effect the fundamental problems with phase flow.

### 2.2 Power Models

The major aspects of the distillation model are hydraulic power, thermal power, and chemical power. The hydraulic model equations must specify how liquid flows over a tray, over a weir, and through a downcomer to the next tray as well as vapor flow through the tray and fluid. There is also liquid flow outside the column through pumps and valves that may need to be included. Possible models vary from constants to partial differential continuity equations. The variants between begin with using just the Francis' weir formula for liquid flow. More complexity is added by using Bernoulli's equation for liquid downcomer flow and vapor plate flow. This is the extent of most models, though this paper advocates including inertial elements to model truly dynamic hydraulic flow as has been presented in the literature (Beaman and Breedveld 1988). A full model of compressible dynamic hydraulic flow would provide even more rigor, though with a high price of complexity. Empirical equations for the amount of foam formed, for instance, are inevitable to compensate for not including partial differential equations (Békássy-Molnár and Mustafa 1991).

The thermal model equations must specify entropy flow from the reboiler, into the condenser, and between the phases. The reboiler and condenser use conduction to

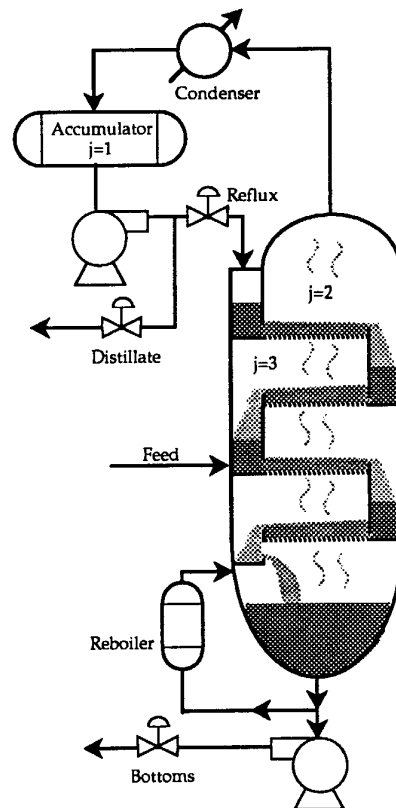


Figure 1. A simple distillation column.

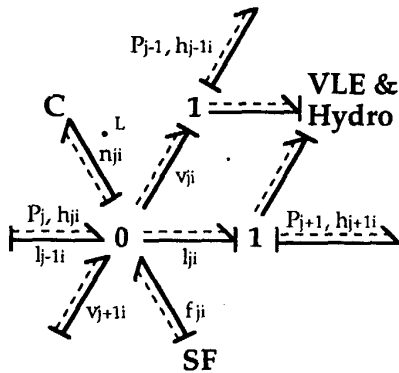


Figure 2. Stage bond graph with mass and energy balance.

transfer heat from hot and cold water to the mixture within the column. This is quite straightforward to model. Less straightforward is the entropy flow on the tray. Although conduction surely takes place, the major flow of entropy is in convection between the stages and between the phases. Heat of vaporization is the entropy flow necessary to excite a change of phase.

The chemical model equations must specify the mass balance and mass flow between the phases, just as the vapor-liquid equations. The stagnant-film model, used to derive certain efficiencies, theorizes flow to be driven by a difference in partial pressures, or in more advanced terms, by a difference in fugacities. The film between phases acts as a resistance to the flow (Holland 1981). The chemical power into this resistance, as well as the hydraulic power from such a dramatic density change, are related to the heat of vaporization. Unfortunately, the exact relationship is not known.

### 3. BOND GRAPH OF THE COLUMN

Bond graphs will be used to define the form of the equations used to describe a distillation column, if not the actual equations. Many good publications exist on distillation columns (Holland 1981; Deshpande 1985; Luyben 1973). However, none of these give the same perspective as bond graphs (Brooks 1992). The precise details of thermodynamic formulae are important here, but they are much too numerous and varying to actually list. The mass and energy balance equations of the traditional model can best be

expressed in bond graphs using the convection bonds of Brown (Brown 1991), see Figure 2. The convection bond perfectly expresses the traditional model of a distillation stage. The nature of the vapor-liquid equilibrium (VLE) equations and hydraulic equations depends on the exact model used. The VLE equations do not translate to bond graphs; they are linked to temperature, pressure, and molar fractions. In some models (Gallun 1979), the vapor flow is actually found using the VLE equations, creating one more algebraic loop. Breaking the convection bond model into normal bond graphs would require knowledge of entropy and chemical potential, revealing the incompatibility of normal bond graphs with the traditional model.

Figure 3 shows a bond graph of a hydraulic model of the two fluid flows. The Fw and DC elements are energy storage elements corresponding to the Francis' weir formula and the downcomer. The elements about the 1-nodes are expressions of Bernoulli's equation with inertial elements of the liquid and vapor flow; this is what is potentially contained with the Hydro-element of Figure 2. The 0-node represents the hydraulic power exchange on the stage between liquid and vapor; this is left out of traditional models. Note the HOV-element: the change of phase at this point is related to the mass flow between the phases and the heat of vaporization.

The exact nature of the chemical model is known only sketchily. Figure 4 shows the form of the chemical model. In the traditional model the chemical potentials are assumed equal, eliminating the central 1-node. The vapor mass is assumed negligible, eliminating the vapor's compliance node. Beyond the 1-node, the flow of mass is not being driven by chemical potential, but by hydraulic power, represented by the R-elements. The HOV-element determines the mass flow, but the exact relationship is not known.

The thermal model of convection is better known (Cellier 1991), as seen in Figure 5. The convection RS-elements are linked to the volume flow of the fluids. The central HOV-element combines heat of vaporization and convection due to mass flow. The heat of vaporization is entropy flow into the vapor occurring either at the temperature of the liquid (a vaporizing mass) or the temperature of the vapor (a condensing mass). The convection entropy flow is in the

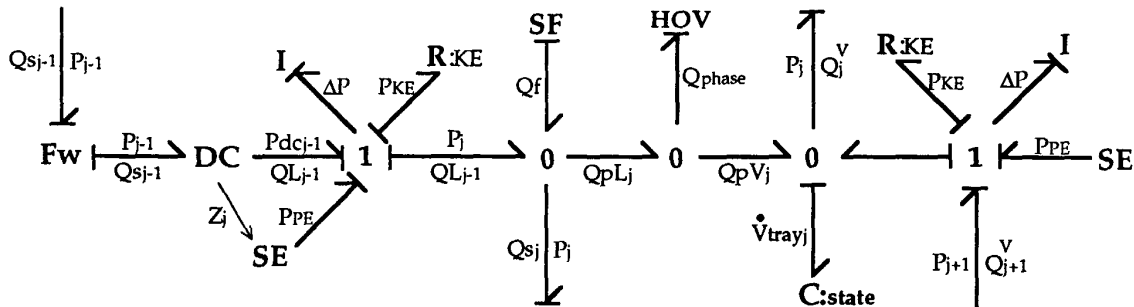


Figure 3. Hydraulic model of a distillation stage.

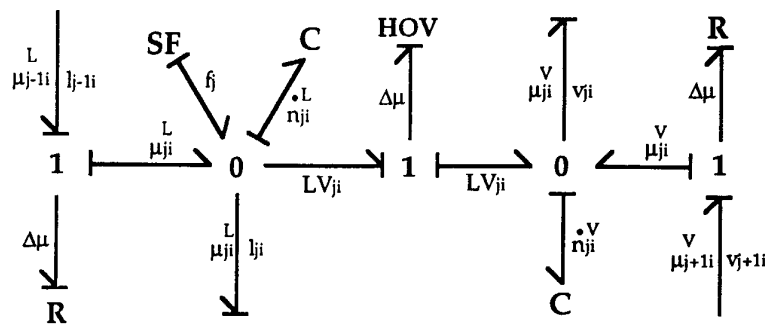


Figure 4. Chemical model of a distillation stage.

direction of the mass flow; the mass flow is either way, depending on the chemical potential difference.

Connecting together the three bond graphs creates a model of a distillation stage. Figure 6 shows the complete bond graph of a distillation column. Hierarchical bonds are required to show the entire model on one page. The elements, especially DCTray, are highly dependent on the particular model, although the power exchanged between the elements is the same. Each of the models above generalizes the stage to allow a feed on each stage. The same type of generalizations could be used to allow other complex configurations, such as sidestreams from each stage, heat conduction to or from each stage, or chemical reactions (Amrhein 1990).

#### 4. SIMULATION RESULTS

Any real distillation column model requires a large amount of thermodynamic data and parameters. A specific example of such a model is adapted from one presented by Gallun (Gallun 1979). The Gallun model is a 50 stage, 4 component column using precise models for fugacity. The model was changed and simplified in a number of ways; hydraulic inertial elements were included as well as hydraulic equations for vapor flow (as opposed to vapor flow equations based on vapor-liquid equilibrium), the number of

stages was reduced from 50 to 9, the ideal equation of state was used instead of the virial equation of state, and the vapor-liquid equations were simplified to use only Antoine's equation. The form of this simple model is expressed best by the convection-bond graph of Figure 2. The essence of a distillation column was the intended goal, not the exact duplication of existing models. In this form, the simple model contains 135 differential equations, 697 equations total, and no algebraic loops. The simple model was developed using DYMOLA (Cellier 1991; Elmqvist 1978), programmed in ACSL, and simulated using Gear's method with various experiments. Gallun's experiment is to change the set point of the 35th stage temperature, T35.

Of course, with a smaller column, the results of such a change should be different—faster and smoother. The simulation results bear this out. Figure 7 shows distillate flow of the two models. Figure 8 shows the temperature distribution of the simple model. The temperature of the 35th stage is controlled by the heat flow rising through convection from the base of the column. Heat flow into the base of the column is controlled by the steam flow in the reboiler tubes. Changing the set point of T35 up 6 degrees tests the control system of this column; does T35 move to its new set point without unduly oscillating T50 (only 2 stages away in the simple model) or T1, which has its own set point? The control system is PI control on all of the valves.

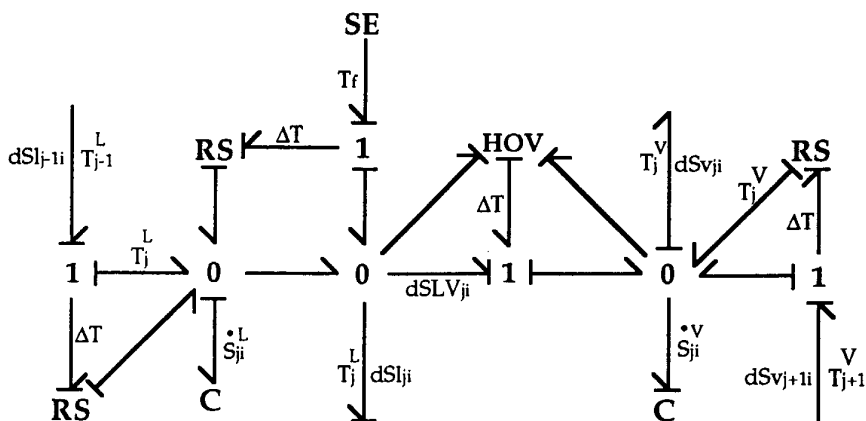


Figure 5. Thermal model of a distillation stage.

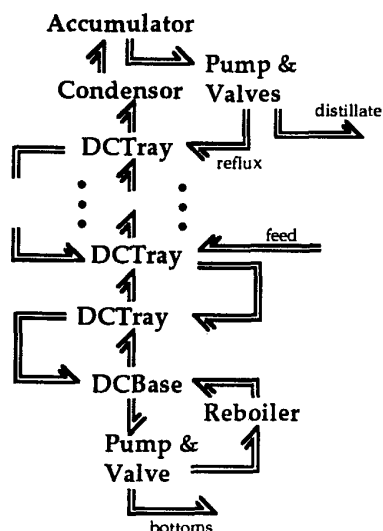


Figure 6. Hierarchical bond graph of column

## 5. CONCLUSION

A distillation column is a common device to be modeled. Yet such models are not free of problems. The unshelled nut within these problems is what exactly happens between two fluids, one liquid and one gaseous, each of varying temperature and flow that are known to be exchanging large quantities of mass and energy. We have not come across an adequate model of the situation. The equations used to express phase transfer are inadequate. There are extensive and precise models of equilibria between phases which include models (or at least calculation procedures) for

fugacities. Distillation models of the past have done well at ignoring this problem by focusing on those equations that are known. The hitch is that the precise models for fugacity can be used without algebraic loops only if the phase flow can be derived.

Using bond graphs as a paradigm for the workings of a distillation column, the problem is obvious. The structure of the bond graph model demands resolution. Convection bonds can successfully model distillation, but only at the expense of foregoing the exact nature of the power flows. Creating a truly dynamic, rigorous bond graph model of a distillation column requires more fundamental research; however, bond graphs do point the way towards the nature of the requisite research.

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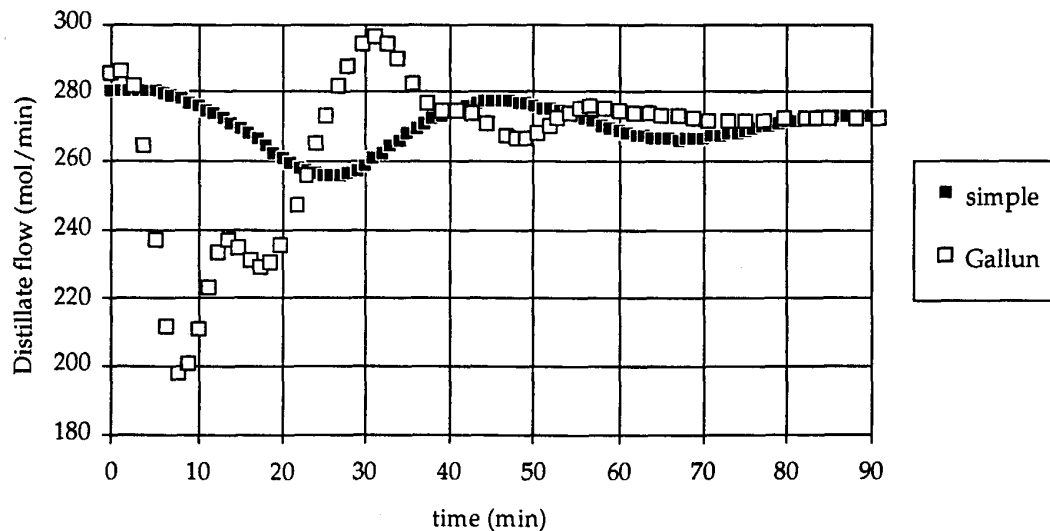


Figure 7. Comparison of Gallun and simple model simulations.

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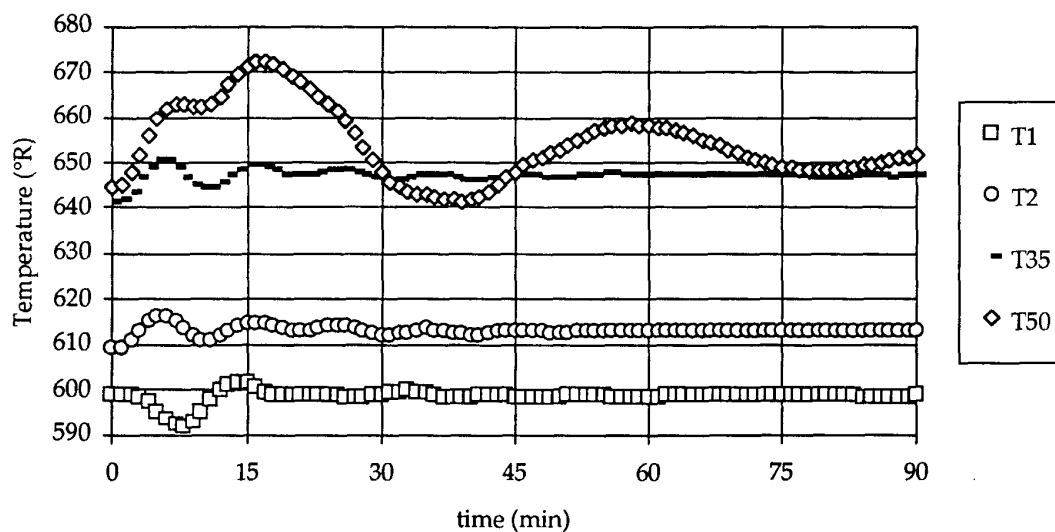


Figure 8. The temperature dynamics of the simple distillation model.