

HEAT AND MASS TRANSFER MODELS FOR THE UNIVERSITY OF TENNESSEE AT
CHATTANOOGA DISTILLATION COLUMN

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ABSTRACT

The distillation column in the University of Tennessee at Chattanooga is a Pyrex glass unit with 12 separation stages, overhead receiver and a reboiler as shown on figure 8. In this thesis, mathematical models that relate to heat and mass transfer during a binary distillation of methanol-water mixture are developed and simulated through analytical and numerical methods [1]. Collections of these models were generated from theoretical correlations which yielded algebraic and differential equations that were solvable simultaneously. [2].

Thermal transfer due to temperature gradient caused heat flux through conduction, convection, and radiation respectively [3]. These heat transfer equations facilitated approximations of the reboiler surface temperature during heating and cooling processes.

Mass transfer was considered during the binary distillation process; where dynamic and steady state mass transfer models were derived from methanol component's mole balance. An average relative volatility of 4.0 for the methanol water mixture promoted reparability and mass transfer during the experimental and modeling processes. [3].

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LIST OF SYMBOLS

π , pi value (3.412).

e , Emissivity of the boiler's material.

σ , Radiation coefficient Stefan-Boltzmann constant.

C , Rayleigh dimensionless number correlation constant.

n , Rayleigh dimensionless number correlation constant.

β , Coefficient of thermal expansion for air.

R_a , Rayleigh dimensionless number.

G_r , Grashof dimensionless number.

N_{uc} , Nusselt dimensionless number for the reboiler's cylindrical part.

N_{uh} , Nusselt dimensionless number for the reboiler's hemispherical part.

x_i , Mole fractions of i^{th} component in liquid phase.

y_i , Mole fractions of i^{th} component in vapor phase.

p , Partial pressure.

P^* , Vapor pressure.

α , Relative volatility.

\dot{x} , state derivative dx/dt

∇T , 3 dimensional thermal diffusivity

CHAPTER 1

INTRODUCTION

1.1 Background

A wide application of mixture separation has made distillation to be a major process operation amongst petroleum, food, drugs and hosts of chemicals manufacturing industries, and thus, prompting an over 40% of the overall energy consumption in North America alone [4]. While energy transfer occurs across the walls of the distillers, mass transfer is due to separation process of the pure components from the mixture.

1.2 Modeling description

The extent of heat transfers during distillation could be tracked through the thermodynamic relations of Fourier, Newton, and Stefan-Boltzmann laws. Mass transfer models on the other hand are started with consideration of Raoult's and Dalton's laws of ideal vapor-liquid equilibrium (VLE) relationship. VLE brings forth the definition of methanol's vapor phase concentration (y_m), as a function of relative volatility (α) and methanol's liquid phase concentration (x_m) as shown by equation1 [5]:

$$y_m = \frac{\alpha x_m}{1 + (\alpha - 1)x_m} \quad (1)$$

1.3 Heat transfer experiment

Heat transfer data was gathered during heating and cooling experiments. A Power of 200, 300, and 400 watts was supplied each time to the column's reboiler shown on figure 1 until a steady temperature on the inner surface was reached. Cooling experiment was performed for the reboiler while containing pure water at an initial temperature of 98 °C. It was allowed to attain ambient temperature by setting the power supply to zero watts, while monitoring the temperature data. A model for this case was built through an assumption that a negligible heat was transferred through radiation. In so doing, the rate of change of reboiler's heat content was only equated to heat transfer by natural convection.



Figure 1 Distillation column reboiler

1.4 Mass transfer experiment

Mass transfer experiments were conducted when the reboiler containing pure water was initially heated up to boiling point of about 100°C for all the stages. Then, a feed of 10%

methanol concentration and a quality (qF) of 1.2 was feed continuously through the feed stage at a rate of 1.4 moles per min. Feed composition was prepared with quantities shown on table 2. The feed quality defined its sub-cooled phase characteristic at 20 °C and was computed as on table 5 using equation 2.

$$qF = 1 + c_p \frac{(T_b - T_a)}{\lambda} \quad (2)$$

As shown on equation 2, specific heat capacity of mixture (C_p), feed stage temperature (T_b), ambient temperature (T_a), and latent heat of vaporization (λ) were determined from the experimental correlations.

The experimental distillate product from the overhead stage had a constant flow rate of 0.26 moles per min and the reflux was set to a constant rate of 80%. From these identities for the feed, distillate, and reflux, other distillation parameters like liquid and vapor flow rates in rectifying and stripping stages were determined by material balance. Both steady and dynamic mass transfer models which were developed as differential equations mole balances were all dependent on equation 1. The schematic block diagrams shown on figure 2 below indicate important streams within the column from where the balances were performed.

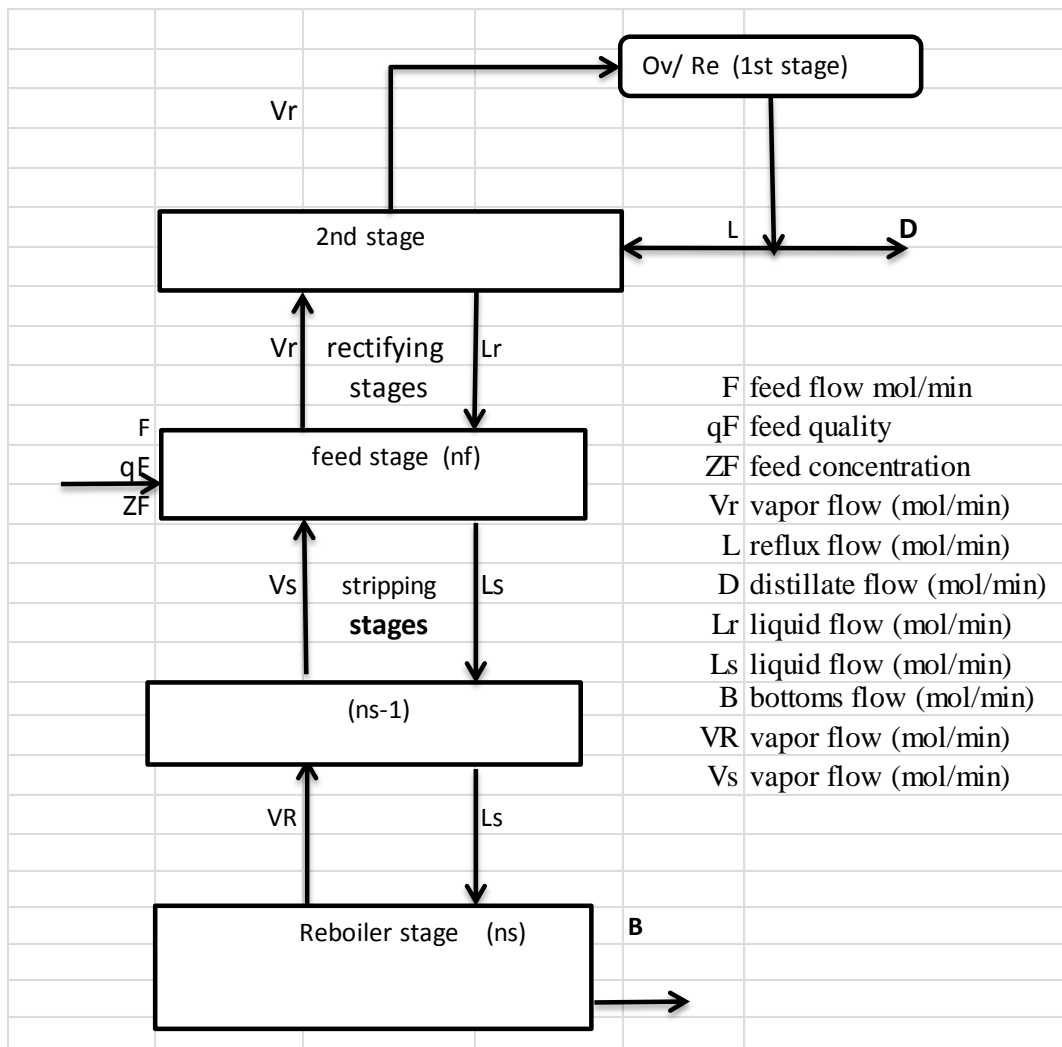


Figure 2 Material balance block diagram

Figure 2 indicates the feed position where feed flow rate (F), feed quality (qF), and feed composition (ZF) are introduced. The exit of distillate product (D) and Bottoms (B) are shown at the top and bottom of the figure respectively. As stated earlier, the components mole balance was performed at each stages of the column; and was achieved from the product of mass flow rate and its mole fraction [15].

1.5 Significance of the study

The experimental heat and mass transfer data, together with the necessary theoretical correlations were simulated into the generated models with the goal of approximating the reboiler's outer surface temperature and the methanol composition at every stage. Comparisons of the results obtained from the experiment and the models simulations would provide deductions for the differences on correlations adapted from real experiments.

CHAPTER 2

LITERATURE REVIEW

2.1 Heat transfer mechanisms

2.1.1 Conduction

In this thesis, the reboiler is simplified into a hollow cylindrical shell with one end closed by a hemispherical geometry while the other is considered to be thermally insulated. By citing the Fourier law of conduction with an assumption that heat flux is occurring only in the radial direction at steady state, a model for the reboiler's heat transfer is generated through separation of variables and integration [6]. Equation 3 and 4 represent the magnitude of reboiler's heat transfer by conduction through its cylindrical and hemispherical parts; with k , L , T_i , T_s , r_1 , and r_2 , representing thermal conductivity, length, inner surface temperature, outer surface temperature, inner radius, outer radius and the length of the reboiler respectively.

$$Q = 2\pi kL(T_i - T_s)/\ln\left(\frac{r_2}{r_1}\right) \quad (3)$$

$$Q = k2\pi(T_i - T_s)/\left(\frac{1}{r_1} - \frac{1}{r_2}\right) \quad (4)$$

Since the boundary conditions are similar, the notable difference between the above equations is the integration related to the surface area for cylinder ($2\pi rL$) and that of a hemisphere ($2\pi r^2$) [11]. However, total heat flux across the reboiler's wall is the sum from the two models.

2.1.2 Natural convection

Magnitude of heat transferred through natural convection was determined through Newton's law of cooling as displayed by equation 5 [7].

$$Q = hA(T_s - T_a) \quad (5)$$

The heat transfer coefficient (h) is obtained through correlations from Nusselt's (Nu) dimensionless numbers which incorporate the Grashof's (Gr), Raleigh (Ra), and Prandtl numbers. These correlations account for the buoyancy-driven thermal convection as influenced by gravitational field. The correlations also put into considerations the geometry characteristic length and diameter [8]. Equation 6 and 7 are the Nusselt's number (N_{uc}) for the cylindrical and hemispherical part (N_{uh}) for the reboiler respectively.

$$N_{uc} = \frac{hD}{k_a} = c \left[\frac{g\beta(T_s - T_a)D^3\rho^2}{\mu^2} \left(\frac{c_p u}{k_a} \right) \right]^n = c[GrPr]^n \quad (6)$$

$$N_{uh} = \frac{hD}{k_a} = 2 + c \left[\frac{g\beta(T_s - T_a)D^3\rho^2}{\mu^2} \left(\frac{c_p u}{k_a} \right) \right]^n = c[GrPr]^n \quad (7)$$

The correlation values (c) are given as 0.53 for cylindrical part and 0.45 for hemispherical part, while n is ¼ for both forms of the reboiler geometry [9]. Coefficient of volumetric thermal expansion (β) is approximated by the reciprocal of the average of the reboiler surface temperature (T_s) and ambient temperature (T_a). Surface temperature was to be determined from the heating experiment as indicated earlier, while the ambient temperature was taken to be 298 K. The other properties these correlations are as tabulated on table 1. [14]:

Table 1 Theoretical correlation constants

Conductivity of air (k_a)	0.03 W/m.K
Specific heat capacity of air (C_{pa})	1009J/kg.K
Viscosity of air (μ)	$1.95 \cdot 10^{-5}$ Kg/s.m
Gravitational acceleration (g)	9.81m/s^2
Density of air (ρ)	1.0 Kg/m^3

2.1.3 Radiation

The contribution of radiation to the heat transfer at the reboiler surface is approximated by use of Stephan-Boltzmann's law, where,

$$Q = Ae\sigma(T_s^4 - T_a^4) \quad (8)$$

Once the surface temperature (T_s) was experimentally determined, the radiated heat becomes a function of surface emissivity (e). This is because the reboiler's surface area (A) and Stephan-Boltzmann constant (σ) and ambient temperature (T_a) had constant values. With a surface emissivity value of 0.9 for the Pyrex glass, the magnitude of the radiated energy can be determined with the Stefan-Boltzmann constant value of $5.67\text{E-}8\text{W/m}^2\cdot\text{K}^4$ [9].

2.2 Steady state heat transfer

2.2.1 Theoretical correlation model

The goal of the steady state heat transfer models was to generate energy balance analysis model which would facilitate approximation of the reboiler's surface temperature once the inner surface is experimentally determined. This model was achieved by performing an energy balance that equated the magnitude of heat transfer through conduction to the sum of heat transfer through convection and radiation as represented by equation 9.

$$Q = \frac{2\pi kL(T_i - T_s)}{\ln\left(\frac{r_2}{r_1}\right)} + \frac{2\pi i kL(T_i - T_s)}{\frac{1}{r_1} - \frac{1}{r_2}} = (h_c A_c + h_h A_h)(T_s - T_a) + Ae\sigma(T_s^4 - T_a^4) \quad (9)$$

Since reboiler dimensions with its temperature boundary conditions have already been defined on the previous generated equations, equation 9 would be functional once the heat transfer coefficient for the cylindrical geometry (h_c) and heat transfer coefficient for the cylindrical shape (h_h) are determined, together with their respective surface areas A_c and A_h .

2.2.2 Finite element model

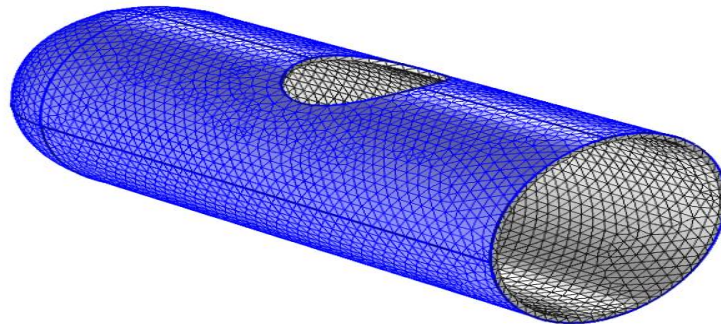
For the finite element analysis method, a heat transfer model shown by equation 10 within Comsol software is used.

$$Q = -n \cdot A(-k\nabla T) = h \cdot A(T_a - T_s) + e\sigma A(T_a^4 - T_s^4) \quad (10)$$

∇T represents a 3 dimensional vector representation of thermal conductivity [11]. The surface emissivity (e) and Stefan-Boltzmann constant (σ) of a radiating surface are as defined on section 2.1.3.

The activity of designing reboiler geometry of figure 3 was done by Comsol's Computer Aided Design (CAD) capability, which specifies its dimensions, thermal properties, and mesh-grids (n). These were necessary for the computations of model results.

Figure 3 Comsol's Reboiler design



The parameters required by the model are specified on table 1 and defined as global variables in the comsol's command window [10]. The model evaluates numerically the value for the surface temperature and heat transfer by conduction, convection and radiation.

2.3 Unsteady state natural convection heat transfer

During cooling process, the reboiler power supply was turned off while monitoring the reboiler temperature data over time. By observing the nature of the temperature decline curve, an exponential distribution model for the cooling situation was built through the assumption that heat transfer occurred only through natural convection. In doing so, rate of change of heat content for the reboiler and water was equated to heat transfer by free convection as in equation

11. Separation of variables and integration yielded equation 12 which would approximate the reboiler wall temperature in real time.

$$(\hat{h}_c A_c + \hat{h}_h A_h)(T_a - T_s) = -(m_g C_{pg} + m_w C_{pw}) \frac{dT_s}{dt} \quad (11)$$

$$T_{st} = (T_{so} - T_a) \exp\left(\frac{(\hat{h}_c A_c + \hat{h}_h A_h)t}{m_g C_p + m_w C_{pw}}\right) + T_a \quad (12)$$

The mass of the pyrex-glass (m_g) and water (m_w) were determined from their respective density and volume. While their specific heat capacities (C_{pg} , and C_{pw}) were obtained from theoretical data. Other variable in equations 11 and 12 were as defined earlier on the preceding sections. Equation 12 was simulated using dimensions that matched the reboiler geometry shown on figure 3 on section 2.2.2. A similar work on cooling analysis for the column's reboiler had been done to determine the overall heat transfer coefficient (U) using equation 13, but its geometry was not considered [12]:

$$T_{st} = [T_a - T_{so}](1 - \exp\left(-\frac{UA t}{m C_p}\right)) + T_{so} \quad (13)$$

2.4 Mass transfer

2.4.1 Vapor liquid equilibrium

Modeling of mass transfer during distillation process started with the vapor-liquid equilibrium relationship as defined by the Raoult's and Dalton's laws for an ideal situation. Raoult's law has methanol partial pressure (p_m) at a fixed temperature equals to the product of its vapor pressure (P^*) and mole fraction in the liquid phase (x_m) [8]. A similar case occurs to water component as shown by equation 14.

$$p_m = P_m^* x_m \quad \text{and} \quad p_w = P_w^*(x_w) \quad (14)$$

For the Dalton's law, the vapor phase has its components partial pressure (p) as the product of the mole fraction in the vapor (y) and total pressure (P) of the system shown in equation 15 for both methanol and water [9].

$$P_m = Py_m \text{ and } p_w = Py_w \quad (15)$$

Using equations 14 and 15, relative volatility for methanol-water mixture (α_{mw}) is derived as the ratio of their vapor pressures when pure as shown by equation 16 [8].

$$\alpha_{mw} = \frac{P_m^*}{P_w^*} = \frac{\frac{y_m}{x_m}}{\frac{y_w}{x_w}} = \frac{y_m x_w}{y_w x_m} \quad (16)$$

Simplification of equation 16 models the equilibrium mole fraction for the lighter component (methanol) in the vapor phase (y_m) as a function of relative volatility (α_{mw}) and the mole fraction of methanol in liquid phase (x_m) as in equation 17.

$$y_m = \frac{\alpha x_m}{1 + (\alpha - 1)x_m} \quad (17)$$

2.4.2 Dynamic and Steady state models:

Dynamic models are rate-based differential equations that can be solved simultaneously and numerically, while steady state models are obtained when the rate of change in the dynamic state is constant or non-changing [12]. All the mass transfer models are dependent on equation 17. While developing these models for the University of Tennessee at Chattanooga's column, a consideration of the mass transfer models as developed by Bequette's distillation process modeling was made [1]. The models developed for each stage of the column are outlined in the proceeding sub-sections.

2.4.2.1 Overhead receiver

Starting with the columns overhead receiver's mole balance, the rate of accumulation of the lighter component is given by the difference of the inlet and outlet flow rates as shown in equation 18 and 19 for dynamic and steady state respectively. These model equations incorporate the relative volatility expression and are solved by numerically through ode45 method, and Newton- based algebraic technique [1].

$$m_d \frac{dx_i}{dt} = [V_R(y_2 - x_1)] \quad (18)$$

$$f_1 = (y_2 - x_1) = 0 \quad (19)$$

Where the molar hold up for the overhead receiver (m_d) is assumed to be 1 mole and the vapor flow rate at the rectifying stage (V_R) is determined by experimental mole balances across the rectifying stage. The symbols y_2 and x_1 represents the molar composition for the vapor and liquid phase across the overhead stage which is represented as stage 1 in the model [15].

2.4.2.2 Rectifying and stripping stages

The rectifying and stripping stages are represented by a collection of finite number (i^{th}) of stages with mole fraction of lighter component expressed as x_i . Just like at the overhead, a mass balance is also performed between the incoming and the outgoing components streams in molar quantities as given by equation 20 and 21. Their respective steady state models are shown by equation 22 and 23 respectively.

$$m_{st} \frac{dx_i}{dt} = (L_R x_{i-1} + V_R y_{i+1} - L_R x_i - V_R y_i) \quad (20)$$

$$f_{ir} = (L_R x_{i-1} + V_R y_{i-1} - L_R x_i - V_R y_i) = 0 \quad (21)$$

$$m_{st} \frac{dx_i}{dt} = (L_S x_{i-1} + V_S y_{i+1} - L_S x_i - V_S y_i) \quad (22)$$

$$f_{is} = (L_S x_{i-1} + V_S y_{i+1} - L_S x_i - V_S y_i) = 0 \quad (23)$$

Symbols used in this equations represents stage molar hold up (m_{st}), reflux flow rate (L_R), methanol vapor phase (y_i), and liquid phase composition (x_i) in the i th stage. Also included are the vapor flow rates V_R and V_S in both rectifying and stripping stages respectively.

2.4.2.3 Feed stage

For the feed stage, component balance equation includes feed flow rate (F) and its quality (qF). The liquid flow rate leaving the stage (L_{nf}) is therefore given as;

$$L_{nf} = L_r + FqF \quad (24)$$

Where, L_r is the reflux flow rate from the rectifying stage and FqF is the product of feed flow rate (F) and feed quality (qF). The vapor flow rate leaving the stage is expressed as $V_S + F(1-qF)$, and its final form of dynamic and steady state concentration of liquid phase component (x_{nf}) across the feed stage is expressed as equation 25 and 26 respectively [1].

$$m_{st} \frac{dx_{nf}}{dt} = [L_R x_{nf-1} + V_S y_{nf+1} + Fz_F - L_S x_{nf} - V_R y_{nf}] \quad (25)$$

$$f_{nf} = [L_R x_{nf-1} + V_S y_{nf+1} + Fz_F - L_S x_{nf} - V_R y_{nf}] = 0 \quad (26)$$

With the product of feed (F) and its composition (Z_F) being an input into the feed.

2.4.2.4 Bottoms stage

At the bottom stage, a mole balance is performed between the liquid entering the reboiler, vapor leaving out and the bottom being drawn. The differential expression for the final models yielded the form of equations 27 and 28.

$$m_b \frac{dx_{nS}}{dt} = (L_S x_{nS-1} - Bx_{nS} - V_S y_{nS}) \quad (27)$$

$$f_{ns} = (L_S x_{nS-1} - B x_{nS} - V_S y_{nS}) = 0 \quad (28)$$

Where B represents the bottoms molar flow rate in moles per minute, and m_b the molar hold up at the bottoms in moles. A complete derivation for these algebraic and differential equations are as outlined at section 5.0 of the model gallery.

CHAPTER 3

METHODOLOGIES

Matlab programs created for simulating heat transfer models are and mass shown on programs 10.1.1 and 10.1.2 for heating and cooling process respectively. Programs 10.2.1 through 10.2.2 are for steady state and dynamic mass transfer modeling. The comsol multiphysics program utilized the parameters on table 3 to simulate its in-built finite element model [10].

3.1 Model simulations

Simulation for heat transfer model of equation 9 during steady state heating involved altering the values for the approximated surface temperature (T_s) until the heat transfer by conduction across the reboiler wall was equivalent to the sum of heat transfer by convection and radiation. Program 10.1.1 has a provision for input command that calls for a change of the surface temperature. On the other hand, the cooling model has a command that provides for adjustment of heat transfer coefficient conversion factor for both cylindrical and hemispherical geometry. This adjustment is iterated until an approximation that provided the best fit curve for the cooling experimental data was achieved.

Collection of the mass transfer models simulation variables defined in the theory section and adapted from experiment and theoretical correlation constants are tabulated on table 6. These parameters were defined as DIST_PAR variables in the programs 10.2.1 and 10.2.2. The

DIST_PAR was set up as a global vector file in the matlab software editor [1]. In order to simulate the mass transfer programs, a script program 10.2.3 was set up to run them sequentially in order for the dynamic model to utilize the steady state results as the initial methanol concentration [14].

CHAPTER 4

RESULTS

4.1 Heat transfer

The steady state temperatures attained during a steady power supply to the reboiler are as shown in figure 4.

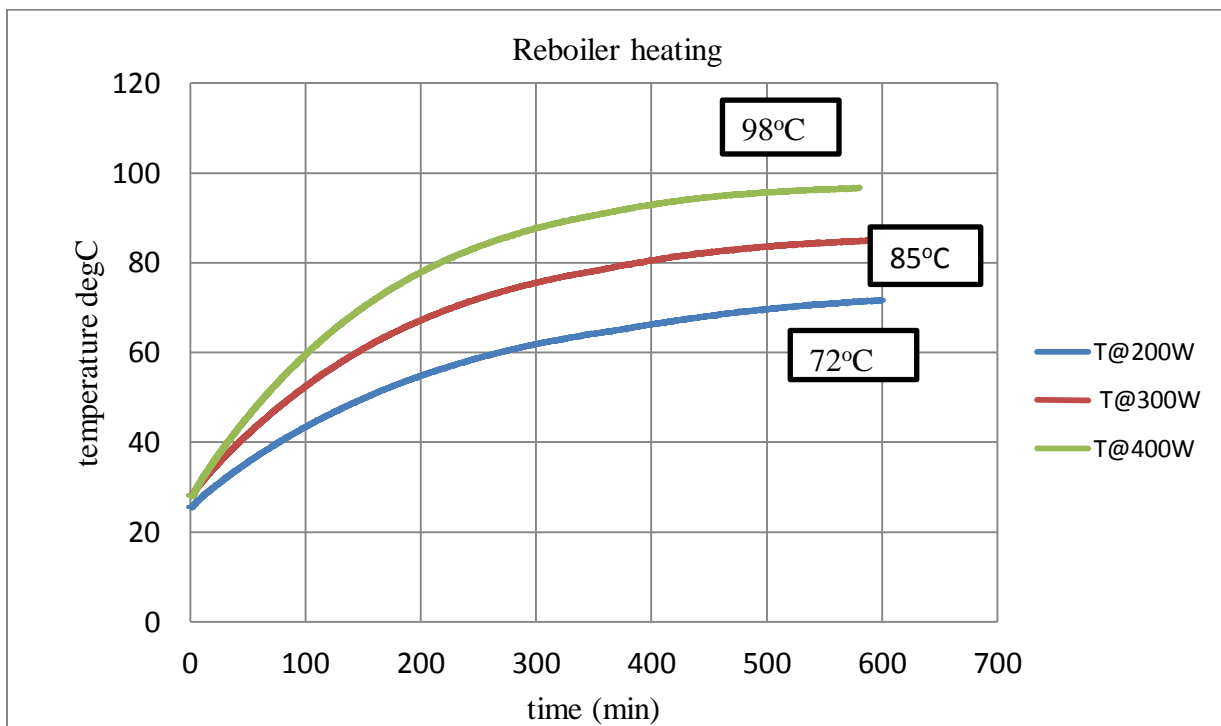


Figure 4 Steady state reboiler heating experiment

By supplying some fixed amount of energy to the reboiler, a steady state was eventually attained where inner surface temperature of the reboiler does not change with time. Such is the steady state condition achieved through the heating experiment.

By slotting the steady state conditions of power and temperature on equations 9 and 10, results for surface temperature (T_s) were obtained as shown on table 2.

Table 2 Reboiler outer surface temperature (T_s)

Theoretical model's outer surface temperature (T_s) °C	Finite element model's outer surface temperature (T_s) °C
91	92
80	81
69	69

These values above for the reboiler surface temperature were obtained through matlab programs 1 and 2 simulations. A similar data for the comsol simulation is also shown on figure 8.

For natural convection cooling, the results for the reboiler temperature profile for experiment and the model are displayed on figure 5.

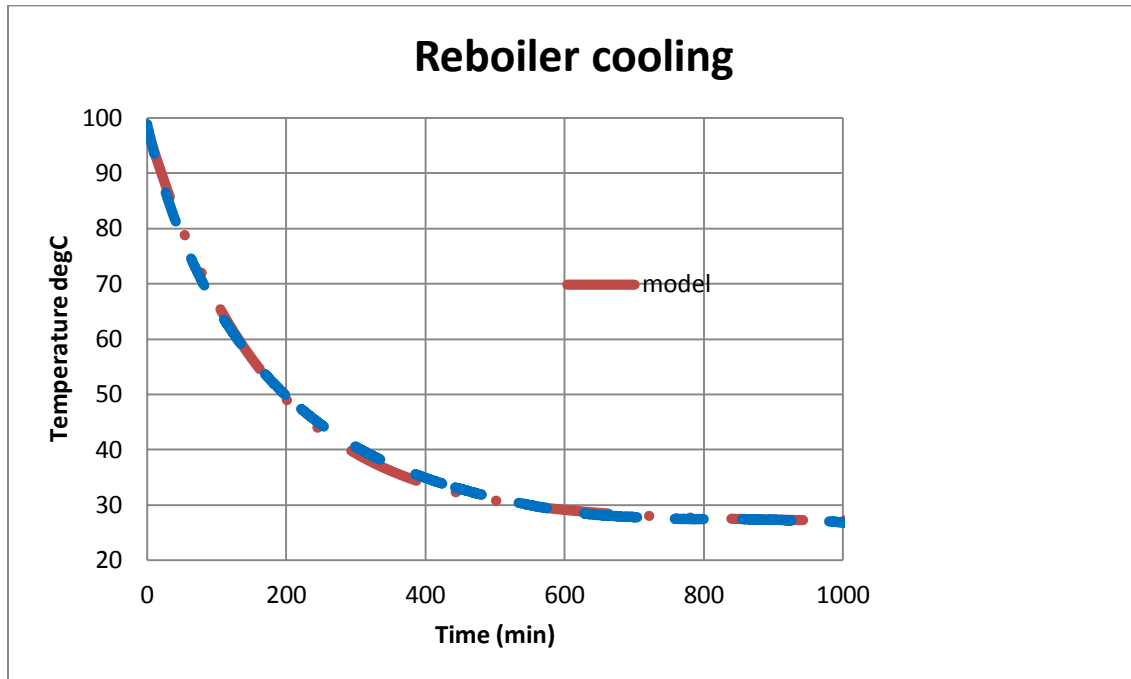


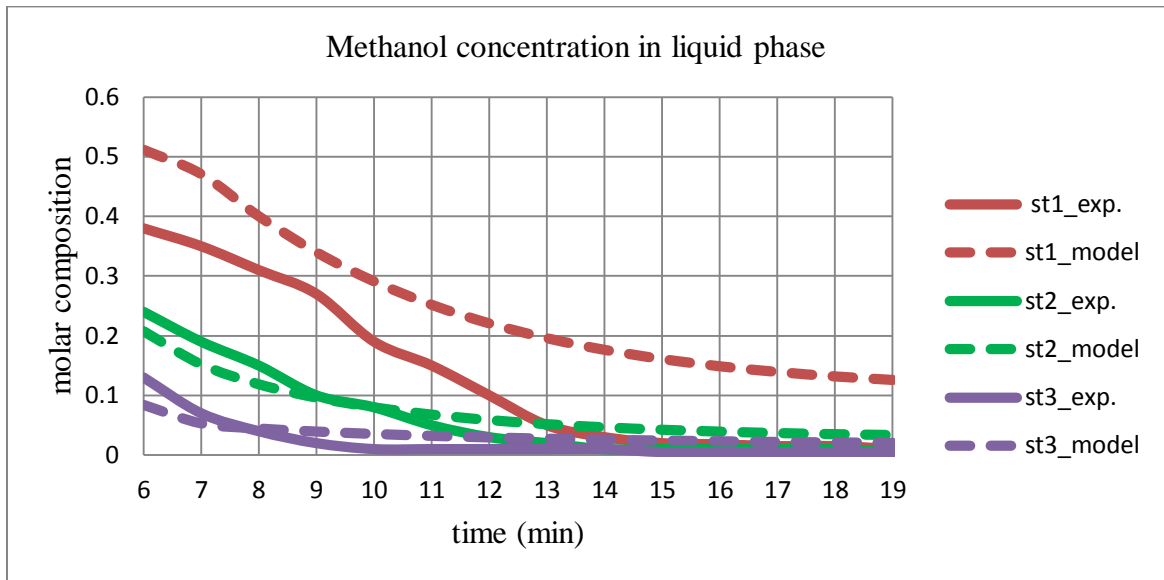
Figure 5 Reboiler cooling temperature profile

The experimental data was best fitted with a heat transfer coefficient value of 14.4 W/m².K for the cylindrical part and 12.9 W/m².K for the hemispherical part. These values of coefficients were higher by a factor of 2.5 from those approximated by theoretical correlations. Achievement for the best fit curve occurred by the simulation of program 10.1.2 with various conversion factor for the heat transfer coefficients.

4.2 Mass transfer

Figure 6 indicates methanol concentration from the experimental and simulated model results for the 3 top stages of separation:

Figure 6 Methanol stage compositions



Each pair of curves bearing similar color represents a particular stage; with the experimental shown by the solid curve and the model by the broken one. Only the first three top stages of separation had a considerable methanol composition for both the experiment and the model, and thus these three were more significant to compare with each other

CHAPTER 5

DISCUSSION AND CONCLUSION

5.1 Heat transfer

By heating the reboiler with a constant power supply, a steady temperature occurred when the reboiler and its content's internal energy equaled the energy supplied. The steady temperature attained was proportional to the power supplied as evidenced by figure 4. These experimental data were necessary in this study for the approximation of surface temperature and heat transfer coefficients through energy analysis.

For the cooling experiment, equating the rate of heat change to heat transfer by natural convection for the reboiler's content did not model the experiment. But, a factor of 2.5 for the respective heat transfer coefficients was sort for the model to fit for the experimental data. This factor indicates the deviation of the model that was generated by theoretical correlations from the real experimental situation. The factor also accounted for the assumption made while designing the reboiler geometry shown on chapter 2.

5.2 Mass transfer

The general decreasing trend of methanol concentration for both the model and the experimental results in figure 6 indicate reduction of methanol content from the mixture due to mass transfer. However, methanol stage concentration has disparities between the model and the experimental results. These differences are attributed by tray efficiencies, heat transfers and

temperature considerations. While the ideal model assumes 100% tray efficiency, the experimental column trays are about 50 %. Also, the ideal model does not account for the temperatures and heat transfers while the experimental depended entirely on input of heat and temperatures.

CHAPTER 6
MODEL GALLERY

6.1 Heat transfer models

1) Conduction:

a) Cylindrical part:

$$Q = -kA \frac{dT}{dr} = -k2\pi rL \frac{dT}{dr}$$

$$Q \int_{r_1}^{r_2} \frac{1}{r} dr = -k\pi 2L \int_{T_1}^{T_2} dT$$

$$Q_c = \frac{2\pi kL(T_1 - T_2)}{\ln\left(\frac{r_2}{r_1}\right)}$$

b) Hemispherical part:

$$Q = -kA \frac{\Delta T}{\Delta r} = -k2\pi r^2 \frac{\Delta T}{\Delta r}$$

$$Q \int_{r_1}^{r_2} \frac{1}{r^2} dr = -k2\pi \int_{T_1}^{T_2} dT$$

$$Q_h = \frac{k2\pi(T_i - T_s)}{\frac{1}{r_1} - \frac{1}{r_2}}$$

Natural convection (Newton's law of cooling)

$$Q = hA(T_s - T_\infty)$$

Dimensionless correlations:

$$N_{uc} = \frac{hD}{k_a} = c \left[\frac{g\beta(T_s - T_\infty)D^3\rho^2}{\mu^2} \left(\frac{c_p u}{k_a} \right) \right]^n \quad \text{Nusselt's number for cylindrical part.}$$

$$N_{uh} = \frac{hD}{k_a} = 2 + c \left[\frac{g\beta(T_s - T_\infty)D^3\rho^2}{\mu^2} \left(\frac{c_p u}{k_a} \right) \right]^n \quad \text{Nusselt's number for spherical part.}$$

$$G_r = \frac{g\beta(T_s - T_\infty)D^3\rho^2}{\mu^2} \quad \text{Grashof's modulus.}$$

$$\nu^2 = \frac{u^2}{\rho^2} \quad \text{Kinematic viscosity.}$$

$$P_r = \frac{c_p u}{k_a} \quad \text{Prandtl number.}$$

$$R_a = G_r P_r \quad \text{Rayleigh's number.}$$

3) Radiation:

$$Q = e\sigma A(T_s^4 - T_a^4)$$

3) Reboiler's Surface temperature model:

$$\frac{2\pi kL(T_i - T_s)}{\ln\left(\frac{r_2}{r_1}\right)} + \frac{2\pi kL(T_i - T_s)}{\frac{1}{r_1} - \frac{1}{r_2}} = hA(T_s - T_a) + Ae\sigma(T_s^4 - T_a^4)$$

4) Finite element models:

$$Q = -n \cdot A(k\nabla T) = h \cdot A(T_a - T_s) + e\sigma A(T_a^4 - T_s^4)$$

6) Cooling process model:

$$(h_c A_c + h_h A_h)(T_a - T_s) = -(m_g C_{pg} + m_w C_{pw}) \frac{dT_s}{dt}$$

$$-\frac{h_c A_c + h_h A_h}{m_g C_{pg} + m_w C_{pw}} \int_0^t dt = \int_{T_{s0}}^{T_{st}} \frac{dT_s}{T_a - T_s}$$

$$-\frac{h_c A_c + h_h A_h}{m_g C_p + m_w C_{pw}} t = \ln(T_{st} - T_a) - \ln(T_{s0} - T_a) = \ln\left(\frac{T_{st} - T_a}{T_{s0} - T_a}\right)$$

$$T_{st} = (T_{so} - T_a) \exp\left(\frac{h_c A_c + h_h A_h}{m_g c_p + m_w c_{pw}}\right) + T_a$$

6.2 Mass transfer models

1) Raoult's and Dalton's law

$$p_m = P_m x_m \quad \text{and} \quad p_w = P_w x_w$$

$$P_m = P y_m \quad \text{and} \quad p_w = P y_w$$

$$\frac{P_m x_m}{P_w x_w} = \frac{y_m}{y_w} \quad \text{thus,} \quad \frac{P_m}{P_w} = \frac{y_m x_w}{y_w x_m}$$

2) Relative volatility

$$\alpha_{mw} = \frac{P_m}{P_w} = \frac{K_m}{K_w} = \frac{\frac{y_m}{x_m}}{\frac{y_w}{x_w}} = \frac{y_m x_w}{y_w x_m} = \frac{y_m(1 - x_m)}{x_m(1 - y_m)}$$

K value = vapor liquid distribution ratio at vapor-liquid equilibrium interphase.

$$\alpha_{mw} x_m (1 - y_m) = y_m (1 - x_m)$$

$$y_m = \frac{\alpha_{mw} x_m}{1 - x_m + \alpha_{mw} x_m}$$

$$y_m = \frac{\alpha x_m}{1 + (\alpha - 1)x_m}$$

2) Overhead receiver:

Overall material balance:

$$L_D + D = V_2 = V_R$$

Component material balance:

$$\frac{M_d dx_1}{dt} = V_R y_2 - (L + D)x_1$$

$$\frac{dx_1}{dt} = \frac{1}{M_d} V_R (y_2 - x_1)$$

$$f_1 = (y_2 - x_1)$$

3) Rectifying stages:

Liquid stream molar flow rate:

$$L_R = L$$

Vapor stream molar flow rate:

$$V_R = V_S + F(1 - q_F)$$

Component balance:

$$\frac{M_t dx_i}{dt} = L_{i-1} x_{i-1} + V_{i+1} y_{i+1} - L_i x_i - V_i y_i$$

$$\frac{dx_i}{dt} = \frac{1}{M_t} (L_R x_{i-1} + V_R y_{i-1} - L_R x_i - V_R y_i)$$

$$f_{ir} = (L_R x_{i-1} + V_R y_{i-1} - L_R x_i - V_R y_i)$$

4) Feed stage:

Feed quality (qF)

$$qF = 1 + C_p * \frac{T_b - T_a}{\lambda}$$

Vapor molar flow rate into the feed stage

$$V_{nf} = V_{nf+1} + F(1 - q_F) = V_S + F(1 - q_F)$$

Liquid molar flow rate out of the feed stage:

$$L_{nf} = L_{nf-1} + Fq_F = L_R + Fq_F$$

Methanol molar balance:

$$\frac{M_t dx_{nf}}{dt} = [L_{nf} x_{nf-1} + V_{nf} y_{nf+1} + Fz_F - L_{nf} x_{nf} - V_{nf} y_{nf}]$$

$$\frac{dx_{nf}}{dt} = \frac{1}{M_t} [L_R x_{nf-1} + V_S y_{nf+1} + F Z_F - L_S x_{nf} - V_R y_{nf}]$$

$$f_{nf} = [L_R x_{nf-1} + V_S y_{nf+1} + F Z_F - L_S x_{nf} - V_R y_{nf}]$$

5) Stripping stage:

Liquid molar flow rate leaving the stage: $L_S = L_R + F_{qF}$

Vapor molar flow rate into the stage:

$$V_S = V_r$$

Component mole balance:

$$\frac{M_t dx_i}{dt} = (L_S x_{i-1} + V_S y_{i+1} - L_S x_i - V_S y_i)$$

$$\frac{dx_i}{dt} = \frac{1}{M_t} (L_S x_{i-1} + V_S y_{i+1} - L_S x_i - V_S y_i)$$

$$f_{is} = (L_S x_{i-1} + V_S y_{i+1} - L_S x_i - V_S y_i)$$

6) Bottom stage:

Material balance:

$$B = L_{ns-1} - V_r$$

Component balance:

$$\frac{dx_{ns}}{dt} = \frac{1}{M_b} (L_S x_{ns-1} - B x_{ns} - V_S y_{ns})$$

$$f_{ns} = (L_S x_{ns-1} - B x_{ns} - V_S y_{ns})$$

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APPENDIX A
LIST OF FIGURES

Figure 7 Distillation column

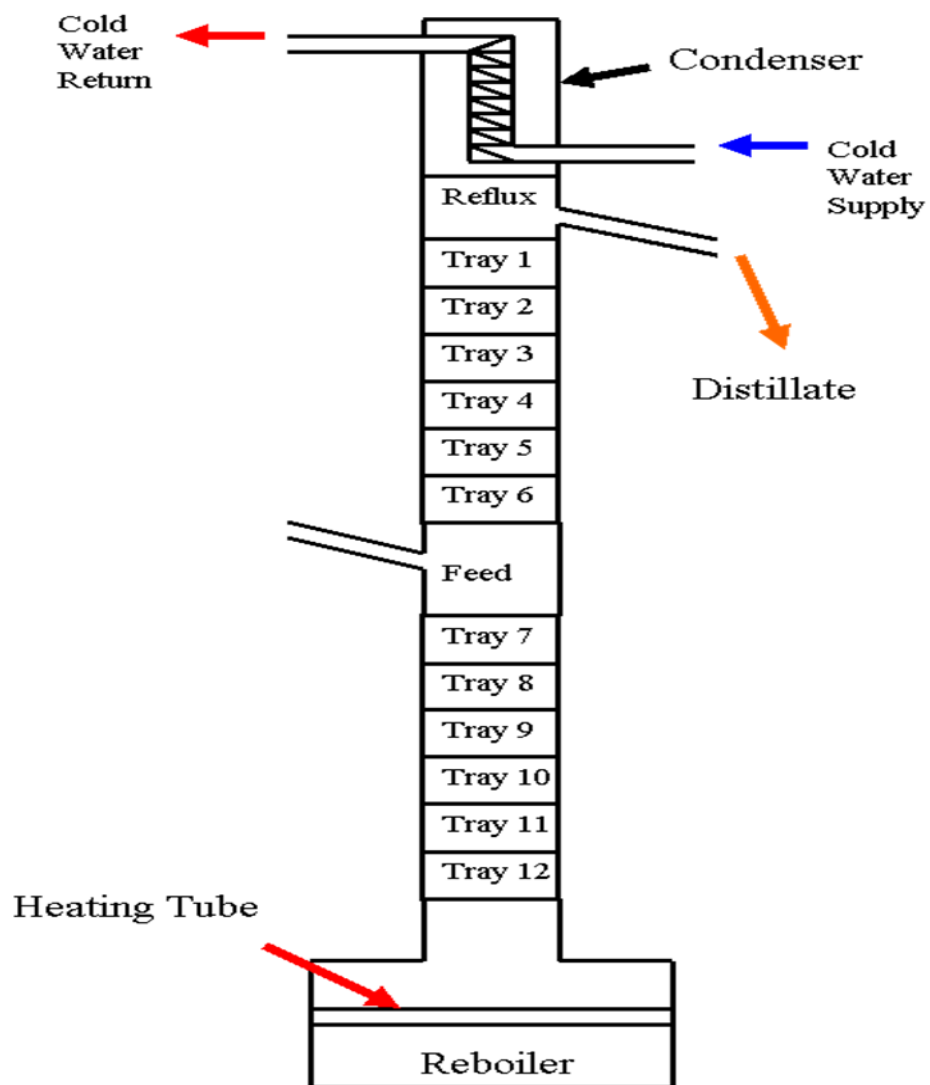
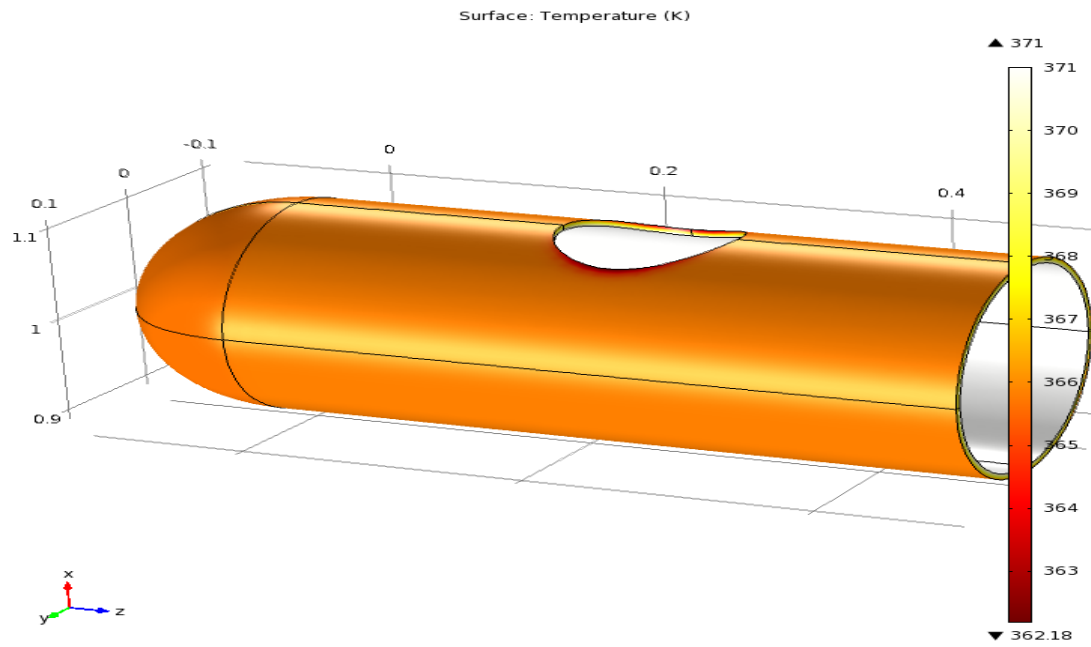


Figure 8 Comsol's design simulation results



APPENDIX B
LIST OF TABLES

Table 2 Comsol's heat transfer parameters

Parameter	Value	Parameter	Value
L	0.55m	P1	-400W
T ₁	371 K	P ₂	-300W
T ₂	358 K	P ₃	-200W
T ₃	345	P _{atm}	101300pa
D	0.21 m	e _s	0.9
d _{air}	1 kg/m ³	k _{air}	0.03 W/m.K
C _{pair}	1000 J/kg/K	T _a	293K

Table 4 feed composition

Mixture components	Volume in gallons	Mass in grams	Mole	Mole %
Methanol	0.75	2271	71	10
Water	3	11335	631	90

Table 5 feed quality calculation

Specific heat C_p (cal/g)	Heat of vaporization λ (cal/g)	Feed stage temperature (T_b) ($^{\circ}C$)	Feed temperature (T_a) ($^{\circ}C$)	Quality (q)
0.95	277.64	76	20	1.2

Table 6 Distillation Parameters (DIST_PAR)

Alpha (α)	ns	nf	Ff	Zf	qF	reflux	VR	M_d	M_b
4	6	3	1.4	0.1	1.2	1.04	1.58	1	5
M_{st}	stepr	tstepr	stepvs	tstepvs	stepzf	tstepzf	stepFf	tstepFf	
0.5	0	0	-0.2	6	0	0	-1.1	6	

APPENDIX C
MATLAB'S SIMULATION PROGRAMS

HEAT TRANSFER

Reboiler heating:

```
% The objective of this program is to compute:
% (1) Heat transfer through conduction, convection, and radiation mechanisms.
% (2) Outer surface temperature of the reboiler.

% REBOILER GEOMETRY.

s0=0.022; % spout outer diameter [m].
si=0.016; % spout inner diameter [m].
T=(s0-si); % reboiler Thickness [m].
L=0.55; % horizontal length [m].
D=0.21; % Reboiler's outer diameter [m].
r2=D/2; % outer radius [m].
r1=r2-T; % inner radius [m]

% input variables.

Ti=input('Enter inner surface temperature T_i '); % reboiler surface temperature, [K].
Ts=input('Guess the outer surface temperature T_s '); % reboiler surface temperature,[K].
Ta=input('Enter ambient temperature T_a '); % air ambient temperature,(K).

% PROPERTIES OF PYREX GLASS:

kg=1.0;% thermal conductivity of pyrex glass[W/m.K].
e=0.9; % surface emissivity of pyrex glass.

% PROPERTIES OF AIR @ [ 300K-350K].
```

```

ka=0.03; % thermal conductivity of air [W/m.K].

Cpa=1000; % heat capacity of air [J/kg.K].

da=1.0; % density of air [kg/m3]

u=1.95E-5; % viscosity of air [Kg/s.m].

v=u/d_a; % kinematic viscosity; [m3/s].

B=2/(Ts+Ta); % coefficient of thermal expansion[k-1]

%CORRELATIONS OF DIMENSIONLESS NUMBERS:

Sb=5.70E-8; %Stephan Boltzman constant, [W/m2.K4].

Pr=Cpa*u/ka; %Prandtl Number

g=9.81; % gravitational acceleration, [m/s2].

Gr=(g*B*(Ts-Ta)*D3)/v2;%Grashof's modulus

Ra=Gr*Pr; % Rayleigh number

Cc=0.53; % Correlation constant for Rayleigh Number

Ch=0.45; % Correlation constant for hemispherical part

n=1/4; % Correlation constant for Rayleigh Number

%COMPUTATIONS OF HEAT TRANSFER MODEL:

Ac=2*pi*r2*L; % area of the cylindrical part.

Ah=2*pi*r2; % area of hemispherical.

A=Ac+Ah; % total area of reboiler.

% HEAT TRANSFER COEFFICIENTS

hc =k_a/D*Cc*(Ra)n; % cylindrical part,[W/m2-K].

hh =k_a/D*(2+Ch*(Ra)n); % spherical part,[W/m2-K].

% HEAT TRANSFER MAGNITUDES:

```

```

Qcond=k*2*pi*L/log(r2/r1)*(Ti-Ts)+k*2*pi*L*(Ti-Ts)/(1/r1-1/r2); % conduction
Qconv=hc*Ac*(Ts-Ta) + hh*Ah*(Ts-Ta); % natural convection
Qrad=A*e*Sb*(Ts^4-Ta^4); % radiation
Qconvrad=Qconv+Qrad; % heat transfer due to convection and radiation
fprintf('Heat transfer through conduction           %8.0fW  \n', Qcond);
fprintf('Heat transfer through convection           %8.0fW  \n', Qconv);
fprintf('Heat transfer through radiation              %8.0fW  \n', Qrad)

```

Reboiler cooling

```
% The objective of this program is to approximate.
% (1) Heat transfer coefficient by free convection.
% (2) The outer surface temperature of the cooling reboiler.
% REBOILER PROPERTIES:
r2=0.105; % outer radius[m]
D=2*r2; % outer diameter[m]
r1=0.099; % inner radius[m]
L=0.55; % length of the reboiler
Cpr=750; % specific heat capacity of pyrex glass [J/kg.K]
k=1.0; % thermal conductivity of pyrex glass [W/m.K].
e=0.9; % surface emissivity of pyrex glass.
dg=2200; % density of pyrex glass kg/m3
% CONSTANTS
g=9.81; % gravitational acceleration, [m/s2].
S_b=5.7E-8; % Stefan Boltzmann constant[W/m2.K4]
Cpw=4184; % specific heat capacity of water [J/kg.K]
Cpa=1006; % heat capacity of air [J/kg.K].
k_a=0.03; % thermal conductivity of air [W/m.K].
dw=1000; % density of water [KG.M3]
da=1.0; % density of air [kg/m3]
u=1.95E-5; % viscosity of air [Kg/s.m].
```


$v=u/\alpha$; % kinematic viscosity; [m²/s].

%TEMPERATURES AND TIME FOR THE MODEL SIMULATION

$T_a=27$; % the final steady state reboiler temperature/ ambient temperature [degC];

$T_y=T_a+273$; % [temperature in K]

$T_{w0}=98$; % reboiler initial surface [degC].

$T_w=T_{w0}+273$; % reboiler initial surface [K].

$\Delta T=T_{w0}-T_a$; % pre-exponential factor for temperature difference;

$t_{span}=0:10:1200$; % time span for the cooling process [min];

$B=2/(T_w+T_y)$; % coefficient of thermal expansion [k⁻¹]

%DIMENSIONLESS CORRELATIONS:

$SB=5.70E-8$; % Stephan Boltzmann constant [W/m².K⁴].

$Pr=C_{pa} \cdot u/\alpha$; % Prandtl Number

$Gr=(g \cdot B \cdot (T_w - T_y) \cdot D^3)/v^2$; % Grashof's modulus

$Ra=Gr \cdot Pr$; % Raleigh number

$C_c=0.53, C_s=0.45, n=1/4$; % Raleigh number correlations

$Nuc=C_c \cdot Ra^n$; % Nusselt's correlation for cylindrical part

$Nus=2+C_s \cdot Ra^n$; % Nusselt's correlation number of spherical part

% VOLUME AND AREA AND MASS

$V_w=0.014$; % volume of water in the Reboiler [m³].

$A_c=2 \cdot \pi \cdot r^2 \cdot L$; % surface area of the cylindrical part [m²]

$V_c=\pi \cdot (r^2 - r_1^2) \cdot L$; % volume of the cylindrical part [m³]

$A_h=2 \cdot \pi \cdot r^2$; % surface area of the hemispherical part [m²]

$V_h=2/3 \cdot \pi \cdot (r^3 - r_1^3)$; % volume of the hemisphere [m³]

```

Vt=Vc+Vh;%total volume of Reboiler [m3]

mw=dw*Vw; % mass of water in the reboiler [Kg].

mr=dg*vt; % mass of the reboiler [Kg].

% HEAT TRANSFER CORRELATION APPROXIATIONS:

cf=input('enter HEAT TRANSFER factor'); % conversion factor for heat transfer coefficient.

hc=cf*k_a/D*Nuc;% heat transfer coefficient for the cylindrical part, [W/m2-K]

hh=cf*k_a/D*Nuh;% heat transfer coefficient due to hemispherical part,[W/m2-K].

% MODEL SIMULATION

[T,t]=meshgrid(del_T,tspan); % mapping of g and t into 2D matrices;

HA=(hc*Ac+As*hs); % sum of product of heat transfer coefficient and respective areas

s=1/(mr*Cpr+mw*Cpw); % pre-exponential value.

T_wt=T.*exp(-t*hA*s*60)+Ta; % temperature decay model;

% NATURAL CONVECTION HEAT TRANSFER

Qc=hc*Ac*(Tw-Ty), Qs=hs*As*(Tw-Ty), Qconv=Qc+Qs; % convection, conduction, radiation.

% PLOTTING

plot(tspan,T_wt), axis([0,1200,0,100]); % axes scaling set up.

title('Reboiler cooling trend'),xlabel('Time (min)'), ylabel('Temperature DegC'),grid on;

```

MASS TRANSFER

Steady state

```
% This program models the steady state stage composition of an ideal binary
% distillation column using matlab's f-solver algebraic method.

% Program overview:

% All the flow rates are molar quantities.

% Stages are numbered from the top to bottom.

% Stage 1 is the overhead receiver, nf is feed while the reboiler (ns) is the last stage.

% The column parameters are specified as global variables within DIST-PAR .

function f = dist_ss(s) % A differential function that numerically evaluates
                        % the new state derivatives.

global DIST_PAR; % vector of distillation column parameters in the global variables.

% A loop that checks availability of the global variables.

if length(DIST_PAR) < 8;

    disp('not enough parameters given in dist_par')

    disp(' ')

    disp('check to see that global dist_par has been defined')

    return

end

% Specification of distillation variables as declared in the global variables:

alpha=DIST_PAR(1); % relative volatility.

ns=DIST_PAR(2); % total number of stages.
```

```

nf=DIST_PAR(3); % number of feed stage.

F=DIST_PAR(4); % initial feed flow rate [mol/min].

zF=DIST_PAR(5); % initial feed composition [mol fraction].

qF=DIST_PAR(6); % feed quality.

L=DIST_PAR(7); % initial reflux molar flowrate [mol/min].

VR=DIST_PAR(8); % initial reboiler vapor flowrate [mol/min].

% flowrates [mol/min]

% rectifying section;

Lr=L; % liquid flow rate.

% Stripping section

Ls=L+F*qF; % liquid flow rate.

% Stripping section

Vs=VR; % vapor flow rate.

% Rectifying section.

Vr=Vs+F*(1-qF); % vapor flow rate.

% Distillate stage.

D=Vr-L; % distillate product flow rate.

% Bottom stage.

B=Ls-Vs; % bottoms product flow rate.

% errors detection.

if D < 0; % detection of distillate composition.

disp('error in specifications, distillate flow<0')

return

```

```

end

if B<0; % detection of error on bottoms flowrate.

    disp('error in specifications, stripping section ')

    disp(' ')

    disp('liquid flow rate is negative')

    return

end

% AT STEADY STATE FUNCTION VECTOR IS ZERO:

f=zeros(ns,1); % xdot is the state derivatives equals zero at steady state.

% calculation of the VLE compositions using relative volatility:

for i=1:ns;

    y(i)=(alpha*s(i))/(1.+(alpha-1.)*s(i)); % vapor compositions at equilibrium curve

end

% LIGHT COMPONENT MATERIAL BALANCE:

% overhead receiver stage:

f(1)=(Vr*y(2)-(D+L)*s(1));

% rectifying stages:

for i=2:nf-1

    f(i)=Lr*s(i-1)+Vr*y(i+1)-Lr*s(i)-Vr*y(i);

end

% feed stage:

f(nf)=Lr*s(nf-1)+Vs*y(nf+1)-Ls*s(nf)-Vr*y(nf)+ F*zF;

% stripping stages:

```

```
for i=nf+1:ns-1;
    f(i)=Ls*s(i-1)+Vs*y(i+1)-Ls*s(i)-Vs*y(i);
end

% reboiler stage:
f(ns)=Ls*s(ns-1)-B*s(ns)-Vs*y(ns);
```

Dynamic state

```
% This program models dynamic state of methanol stage composition
% Mixture using the ODE45 numerical method.

% Program overview:

% All the flow rates are molar quantities.

% Stages are numbered from the top to bottom.

% Stage 1 is the overhead receiver, nf is feed while reboiler (ns) last stage.

% The column parameters are specified as global variables.
% within the DIST-PAR.

function xdot = dist_dyn(t,x) % A differential function that numerically evaluates
% the new state derivatives.

global DIST_PAR; % vector of distillation column parameters in the global variables.

% A loop that checks availability of the global variables.

if length(DIST_PAR) < 11;

    disp('not enough parameters given in DIST_PAR')

    disp(' ')

    disp('check to see that global DIST_PAR has been defined')

return

end

% Specification of distillation variables as declared in the global variables:

alpha =DIST_PAR(1); % relative volatility

ns=DIST_PAR(2); % total number of stages

nf=DIST_PAR(3); % feed stage
```

```

F=DIST_PAR(4); % initial feed flow rate
zF=DIST_PAR(5); % initial feed composition
qF=DIST_PAR(6); % feed quality
L=DIST_PAR(7); % initial reflux molar flow rate
VR=DIST_PAR(8); % initial reboiler vapor flow rate
md=DIST_PAR(9); % overhead receiver molar hold up
mb=DIST_PAR(10);% reboiler molar hold-up
mst=DIST_PAR(11);% stage molar hold-up
if length (DIST_PAR)==19;
    stepL=DIST_PAR(12);% magnitude step in reflux
    tstepL=DIST_PAR(13);%time of reflux step change
    stepVR=DIST_PAR(14);% magnitude step in vapor flowrate
    tstepVR=DIST_PAR(15);%time of vapor step change
    stepzF=DIST_PAR(16);% magnitude of feed composition change
    tstepzF=DIST_PAR(17);%time of feed composition change
    stepF=DIST_PAR(18);%magnitude of feed flow change
    tstepF=DIST_PAR(19);%time of feed flow change
else
    stepL=0;tstepL=0;stepVR=0;tstepVR=0;stepzF=0;tstepzF=0;stepF=0;tstepF=0;
end
% checking for the process disturbances
% reflux
if t<tstepL;

```



```

    reflow=L;% reflux flow equals the initial reflux flow rate
else
    reflow=L+stepL; % sum of initial reflux & its magnitude step
end

% vapor from the reboiler
if t<tstepVR;
    vapflow=VR; % reboiler vapor flow equals initial vapor flow rate
else
    vapflow=VR+stepVR; % sum of initial reboiler vapor flow & its step change
end

% feed composition
if t<tstepzF;
    fcom=zF; % feed composition equals initial feed composition
else
    fcom=zF+stepzF;% sum of initial feed flow & feed composition change
end

% feed
if t<tstepF;
    fflow=F; % feed flow rate equals initial feed flow.
else
    fflow=F+stepF; % sum of initial feed flow & magnitude of feed flow change.
end

% FLOWRATES:

```

```

% % rectifying section;

Lr=reflow;% liquid flow rate

% stripping section

Ls=reflow+fflow*qF;% liquid flow rate

% stripping section

Vs=vapflow; % vapor flow rate (3.2)

%rectifying section

Vr=Vs+fflow*(1-qF); % vapor flow rate.(3.2+1.0=3.3)

% distillate stage

D=Vr-reflow; % distillate product flow rate: (3.3-2.7=0.6)

% bottom stage

B=Ls-Vs;% bottoms product flow rate:(3.8-3.2=0.6)

% ERRORS DETECTION.

if D < 0; % detection of distillate composition

    disp('error in specifications, distillate flow<0')

    return

end

if B<0; % detection of error on bottoms flowrate

    disp('error in specifications, stripping section ')

    disp(' ')

    disp('liquid flow rate is negative')

    return

end

```

```

% AT STEADY STATE RATE OF CHANGE WITH TIME:
xdot=zeros(ns,1); % xdot is the state derivatives equals zero at steady state
% calculation of the VLE compositions using relative volatility:
for i=1:ns;
    y(i)=(alpha*x(i))/(1.+(alpha-1)*x(i)); % vapor compositions at equilibrium curve
end
% light component material balance:
% overhead receiver stage:
xdot(1)=(1/md)*(Vr*y(2)-(D+reflow)*x(1));
% rectifying stages:
for i=2:nf-1
    xdot(i)=(1/mst)*(Lr*x(i-1)+Vr*y(i+1)-Lr*x(i)-Vr*y(i));
end
% feed stage:
xdot(nf)=(1/mst)*(Lr*x(nf-1)+Vs*y(nf+1)-Ls*x(nf)-Vr*y(nf)+ fflow*fcom);
% stripping stages:
for i=nf+1:ns-1;
    xdot(i)=(1/mst)*(Ls*x(i-1)+Vs*y(i+1)-Ls*x(i)-Vs*y(i));
end
% reboiler stage:
xdot(ns)=(1/mb)*Ls*x(ns-1)-B*x(ns)-Vs*y(ns);

```

Script program

```
% This script file runs both steady state and dynamic models

ns=input('enter number of stages '); % total number of stages.

% steady state stage composition solver.

s=fsolve('dist_ss',s0); % solution for the steady state model

    % dynamic differential models using the steady state initialization.

tspan=(6:20); % Interval for the integration.

x0=s; % dynamic model uses the steady state concentrations as the initial value

[t,x]=ode45('dist_dyn',tspan,x0); % solving the dynamic model

    % plotting response curves.

plot(t,x); % methanol stages composition against time.

xlabel('Time (min)'); % labeling axis.

ylabel('Molar composition'); % labeling axis

title('Methanol transient stage composition') % graph's a title.

axis([6,20,0,0.6]); % axes scaling set up.

grid on; % grids on the graph's axes.
```

VITA

Simon Irungu was born in Central Kenya to the parent of Rosemary and Anthony who were peasants. After a selection into United States free diversity immigration Visa program, he moved to America in April 2004. He worked at Maytag Steel factory at Cleveland Tennessee before enrolling for Pre- engineering classes at Cleveland Community College on the spring of 2005. Simon transferred his credits to the University of Tennessee at Knoxville on April 2006 and graduated in December 2009 with a bachelor degree in Chemical Engineering concentration.

On the Fall of 2010, he moved to the university of Tennessee at Chattanooga for his Masters on the same Engineering major and completed the course requirement on August of 2012. Simon has laid up plans to pursue a PhD in chemical engineering in the near future.