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VOC Reduction by Dynamic Condenser Design

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ABSTRACT

Organic solvents used in pharmaceutical manufacturing operations are volatile; thus, the vapor in equilibrium with the solvents contains species known as Volatile Organic Compounds (VOCs). The release of VOCs to the atmosphere is hazardous to the public health and is regulated by the EPA. Surface condensation is the preferred method for the reduction of VOCs in an emissions stream.\(^5\)

A mathematical model has been developed to simulate the operation of a surface condenser. It is based on the principle of diffusion-controlled condensation, which states that condensation will occur if the concentration gradient between the bulk gas and the gas-condensate interface promotes diffusion of the condensable species toward the interface and the vapor is saturated at the wall temperature. The model has been designed for a shell-and-tube condenser, where it is assumed that the condensate is removed from the condenser as it is formed, leaving only a thin film of liquid on outside walls of the coolant tubes. The thickness of this film is constant and its temperature is assumed to be equal to the wall temperature. The model uses finite volume discretization across the length of the condenser to form a system of equations (mass balances, energy balances, and diffusion equations) which must be solved simultaneously. These computations are performed using MATLAB. The algorithm outputs the temperature, concentration, and flow profiles along the length of the condenser for steady state operation. Output from the dynamic model traces the temperature change of a specified volume element with time, as well as the changes in flowrate of condensate, concentration in the bulk gas, and concentration near the wall.

Limitations on the validity of the diffusion-controlled condensation model were discovered. The model was updated to include the situation where the temperature of the bulk gas reaches the wall temperature and condensation occurs in the bulk phase without diffusion to the wall (i.e. heat transfer controlled condensation). The heat transfer limitation was imposed to ensure a physically valid solution; however, the change in fluid dynamics resulting from condensation in the bulk phase was not considered. Thus, the model should be used only in situations where diffusion-controlled condensation occurs.

The effect of uncertainty in system parameters has been analyzed, thus indicating which factors must be considered when designing a condenser to treat an inlet stream.
according to EPA regulations. A dynamic controller has been implemented in order to improve the efficiency and minimize the cost of the process. The controller minimizes the error between the outlet gas temperature and the desired set point by adjusting a system variable such as the coolant flowrate.
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INTRODUCTION

Motivation

Typical pharmaceutical processes involve the use of organic solvents, both within the reaction and separation steps and the cleaning of vessels after a reaction has occurred (see Figure 1). These organic solvents often have low vapor pressures, giving rise to volatile organic compounds (VOCs) in equilibrium with the liquid solvent. The emission of VOCs into the atmosphere is hazardous to the public health. In the presence of ultraviolet light, VOCs react with nitrogen oxides in the atmosphere to form tropospheric ozone, the primary component of smog. In the Clean Air Act Amendments of 1990, the Environmental Protection Agency (EPA) established regulations for VOC emissions. Individual states have developed their own procedures in order to comply with the EPA regulations. These state implementation plans can be found on the EPA’s website.

Figure 1: Flow Diagram for Typical Pharmaceutical Process

Many different methods exist for reducing the VOC concentration in a vapor stream. Although procedures such as combustion, adsorption, and absorption (scrubbing) are available, they possess inherent disadvantages which make surface condensation the preferred approach. Complete combustion of VOCs results in the formation of carbon dioxide and water. However, the efficiency and rate of combustion are dependent on the
residence time, temperature, and turbulence of the stream. For variable flowrates, the process becomes difficult to control and may result in incomplete combustion and the release of undesirable products into the atmosphere. Adsorption onto a catalyst bed is another technique used for removing VOCs from a vapor stream. However, when a bed becomes saturated, it must be regenerated before being returned to service. Regeneration involves desorbing the adsorbed gases, usually by heating or applying a vacuum, and results in an air stream which contains the original VOCs. In absorption, or scrubbing, components from the vapor stream are dissolved in a liquid solvent. This procedure is sensitive to the solubility of the VOC in the selected solvent and must be followed by a process to recover the VOC from the solvent.\(^5\) Condensation can be achieved by either lowering the system temperature or increasing the pressure. Components with lower vapor pressures will condense first, thus allowing for the separation of mixtures. In surface condensation, there is no contact between the vapor stream and the coolant. The VOCs condense on the outside walls of the coolant tubes and, since they have not been contaminated by the coolant, solvents can be recovered from the condensate and recycled.\(^6\)

The EPA has recognized the desirability of using surface condensers to reduce VOC emissions. Based on the vapor pressure of the VOC in the inlet stream, the EPA has specified acceptable temperatures for the gas leaving a condenser. Other types of air pollution equipment are merely governed by a required percent reduction in VOC emissions.\(^7\) Regulations for VOC emissions by pharmaceutical manufacturing facilities in Chicago, Illinois can be found in Appendix I.

The regulation of VOC emissions must be considered from an economic as well as environmental standpoint. Although VOC reduction is a necessary operation, it is a costly addition to a manufacturing process. In addition to the capital cost of the equipment, companies are also faced with operating costs such as materials, utilities, and labor. The cost of reducing VOC emissions must be weighed against the cost of generating VOC emissions. In an emissions treaty scheme, companies must purchase permits which allow them to emit a specific amount of VOCs during a set period of time. In the Chicago area, an allotment trading unit (ATU) represents 200 pounds of VOC emissions during the seasonal allotment period, which extends from May 1 to September
The allotment period is followed by a reconciliation period (October 1 to December 31) in which companies compile emissions data and submit an annual emissions report to the EPA. Companies must possess a sufficient amount of ATUs by the end of the reconciliation period to cover their actual emissions from the preceding season.\textsuperscript{8} The economic incentive to reduce both VOC emissions and operating costs leads to a design optimization problem. By implementing a dynamic control system, parameters such as the coolant flowrate can be adjusted as the inlet conditions change. Thus, the desired separation can be obtained at a minimum operating cost.

**Approach**

In order to optimize the design of a condenser, a thorough understanding of its operation is required. For this purpose, a mathematical model based on diffusion-controlled condensation was developed and was solved using MATLAB. Based on user-specified initial conditions and physical properties, the program computes the required heat and mass transfer variables and simulates the operation of the condenser by solving the system of mass and energy balances. The performance of the model was evaluated through trials using various initial conditions and modifications were made as necessary. The model is used as a basis for developing a dynamic control system for the operation of a condenser. The control system will reduce the cost associated with VOC emissions by allowing the process to continuously operate at the optimal balance between reduced operating cost and increased performance. The model has also been used to analyze the impact of uncertainty on the operation of the condenser.

**Outline**

The remainder of this paper is organized as follows. Typical operations in which VOCs are generated are described in the process description, followed by an explanation of how a surface condenser can be used to reduce the concentration of a VOC in a vapor stream. Next, the procedure for calculating the amount of VOC generated in an operation is outlined. The theory behind the operation of a condenser (including mass and energy balances and diffusion-controlled condensation) is presented before explaining the details of the mathematical model which has been developed. The dynamic control system for
the condenser is described and the procedure for evaluating the effect of uncertainty is given. Information on VOC emission regulations is contained in Appendix I, while Appendix II shows the method for calculating VOC emissions. The derivation of the diffusion equation is given in Appendix III. The correlations used for estimating system parameters are detailed in Appendix IV. Appendix V contains program code, and the results of the uncertainty evaluation are shown in Appendix VI.

**METHODOLOGY**

**Process Description**

As shown in Figure 1, organic solvent vapors are generated at various stages throughout the manufacture of a pharmaceutical product. This project focuses on the VOCs formed in the reactor and their treatment in the condenser located immediately after the reactor.

The use of organic solvents in the reaction itself, the subsequent separation steps, and the cleaning process used to prepare the vessel for future operations results in the formation of VOCs. After these operations, the tank is purged with nitrogen in order to displace the air present in the vessel. At temperatures low enough to condense the VOCs, moisture in the air would freeze inside the condenser and result in decreased performance.\(^2\) The presence of an inert such as nitrogen also prevents the vapor from becoming flammable.\(^9\)

The case studies used to evaluate the condenser model focused on the operation of charging a vessel with ethanol, followed by a nitrogen sweep. A diagram of the procedure is shown in Figure 2. After the charge and sweep operations, the used solvent is discharged from the reactor as a liquid. The vapor stream consists of the solvent vapors (VOCs) and nitrogen. The vapor stream is passed through a condenser, with its flow to the condenser being controlled by a valve. A shell-and-tube condenser is used for the separation. The vapor passes through the outer shell while the coolant flows through tubes contained within the interior of the shell. The condensate forms on the outer wall of the tubes. Both the condensate and the vapor containing nitrogen and uncondensed VOC exit from the shell of the condenser. A cryogenic coolant is used to efficiently achieve the low temperatures required for condensation of the VOCs.
VOC Emission Calculations

In order to determine the applicability of EPA regulations to a given operation, the VOC emissions must be calculated. EPA Publication 290580: “Control of Volatile Organic Emissions from Manufacture of Synthesized Pharmaceutical Products” outlines the methods for calculating emissions from the following operations:

- Charging
- Evacuation (Depressurizing)
- Nitrogen or Air Sweep
- Heating
- Gas Evolution
- Vacuum Distillation
- Drying

Calculations involving the charging of a vessel with ethanol followed by a nitrogen sweep can be found in Appendix II.

Another method for determining the VOC concentration in a process stream is to perform a computer simulation of the process. The program Batch Design Kit (BDK) was used to simulate the charge and sweep operations and the results were compared to those calculated according to the EPA documentation.
**Condenser Theory**

Figure 3 shows a two-dimensional view of a typical shell and tube condenser. The vapor stream flows through the outer shell while the coolant passes through the inner tube. (Multiple coolant tubes are usually used to improve efficiency.) The condensate is removed at various points along the length of the condenser. By using a finite volume discretization along the length of the condenser (see Figure 4), the applicable mass and energy balances form a system of differential and algebraic equations. The condenser model uses MATLAB to solve this system of equations and obtain flow, temperature, and concentration profiles along the length of the condenser.

![Figure 3: Diagram of Co-current Condenser](image)

**Figure 3: Diagram of Co-current Condenser** 11 Gas stream flows through outer shell of condenser while coolant passes through inner tube. Components from gas stream condense on outer surface of coolant tubes. Condensate is removed from the shell as it forms.

![Figure 4: Example of Finite Volume Discretization of a Condenser](image)

**Figure 4: Example of Finite Volume Discretization of a Condenser** 11 Flow of coolant, gas, and condensate streams entering and exiting each element is considered. Energy transfer between wall and coolant and wall and gas is also considered for each volume element.
The underlying assumption of the model is that condensation is diffusion controlled. When the concentration of VOC in the vapor stream is greater than the concentration of VOC near the tube wall (due to the vapor pressure of the VOC in equilibrium with the condensate), diffusion of the VOC from the bulk gas to the gas-condensate interface will occur. When the VOC molecules reach the gas-condensate interface, the temperature of the condensate is sufficiently low for condensation of the vapor to occur. It is assumed that the condensate is removed from the condenser as it is formed, leaving only a thin film of liquid on the tube wall. The thickness of this film is constant and its temperature is equal to the wall temperature.

Figure 5 shows the temperature and concentration profiles within a finite volume element of the condenser. The temperature and concentration of the bulk gas are constant. Within the gas boundary layer, the temperature and concentration of the gas change gradually until the conditions at the gas-condensate interface (as specified by vapor-liquid equilibrium) are reached. The condensate film consists solely of the condensable component of the gas, and its temperature is equal to the wall temperature. The coolant temperature changes from the wall temperature to that of the bulk phase throughout the coolant boundary layer.

Figure 5: Temperature and Concentration Profiles in a Finite Volume Element In the gas boundary layer, the gas temperature decreases from that of the bulk phase to that of the wall and condensate film. The concentrations of condensable and noncondensable species in the gas (designated as partial pressures) also change as prescribed by vapor-liquid equilibrium between the gas phase and the condensate. The temperature change of the coolant occurs in the coolant boundary layer rather than the bulk phase. The temperature and concentration gradients occur perpendicular to the direction of fluid flow through the element.
In order to obtain the system of equations describing the condenser, energy and mass balances must be performed on each finite volume element.\(^{11}\)

**Energy Balances**

Equation (1a) shows the energy balance for the gas phase: the change in energy of the gas phase is equal to the change in enthalpy between the inlet and outlet gas streams minus the enthalpy of the condensate and the energy transferred to the wall. Equations (1b), (1c), and (1d) manipulate equation (1a) to obtain a simplified form.

\[
C_{pg} \frac{d(N^n_g \cdot T^n_g)}{dt} = F^n_{g} \cdot C_{pg} \cdot T^{n-1}_g - F^n_{\text{condensate}} \cdot C_{pg} \cdot T^n_w - \dot{Q}^{n}_{w-g}
\]  
\[(1a)\]

\[
C_{pg} \left( N^n_g \frac{d(N^n_g)}{dt} + T^n_g \frac{d(T^n_g)}{dt} \right) = F^n_{g} \cdot C_{pg} \cdot T^{n-1}_g - F^n_{\text{condensate}} \cdot C_{pg} \cdot T^n_w - \dot{Q}^{n}_{w-g}
\]  
\[(1b)\]

\[
C_{pg} \left( N^n_g \frac{d(T^n_g)}{dt} + T^n_g (F^n_{g} \cdot C_{pg} \cdot T^{n-1}_g - F^n_{\text{condensate}} \cdot C_{pg} \cdot T^n_w) \right) = F^n_{g} \cdot C_{pg} \cdot T^{n-1}_g - F^n_{\text{condensate}} \cdot C_{pg} \cdot T^n_w - \dot{Q}^{n}_{w-g}
\]  
\[(1c)\]

\[
N^n_g \cdot C_{pg} \frac{dT^n_g}{dt} = F^n_{g} \cdot C_{pg} \cdot (T^{n-1}_g - T^n_g) + F^n_{\text{condensate}} \cdot C_{pg} \cdot (T^n_w - T^n_w) - \dot{Q}^{n}_{w-g}
\]  
\[(1d)\]

Equation (2) shows that the energy transferred to the wall from the gas phase is equal to the energy obtained from the cooling and condensation of the gas plus the heat convection from the gas phase to the gas-wall interface.

\[
\dot{Q}^{n}_{w-g} = \dot{Q}^{n}_g + F^{n}_{\text{condensate}} \left( C_{pg} \cdot (T^{n}_g - T^n_w) + \Delta H^\gamma_T(T^n_w) \right)
\]  
\[(2)\]

Equation (3) calculates the heat convection from the gas to the gas-wall interface.

\[
\dot{Q}^{n}_g = \alpha_g \cdot (T^n_g - T^n_w)
\]  
\[(3)\]

Equation (4) shows the energy balance for the coolant: the change in energy of the coolant is equal to the change in enthalpy between the inlet and outlet coolant streams plus the energy gained from the wall.

\[
N^{n}_{cool} \cdot C^{n}_{cool} \frac{dT^{n}_{cool}}{dt} = \dot{N}^{n}_{cool} \cdot C^{n}_{cool} \cdot (T^{n-1}_{cool} - T^{n}_{cool}) + \dot{Q}^{n}_{w-cool}
\]  
\[(4)\]

Equation (5) shows that the energy received by the coolant from the wall is equal to the heat convection from the wall-coolant interface to the coolant.
\[
\dot{Q}_{w-\text{cool}}^n = \alpha_{\text{cool}} \cdot (T_w^n - T_{\text{cool}}^n) \tag{5}
\]

Equation (6) shows the energy balance for the wall: the change in energy of the wall is equal to the energy it absorbs from the gas minus the energy it releases to the coolant.

\[
N_{\text{wall}} \cdot C_{\text{wall}} \frac{dT_w^n}{dt} = \dot{Q}_{w-g}^n - \dot{Q}_{w-\text{cool}}^n \tag{6}
\]

Mass Balances

Equation (7) shows the mass balance for the gas phase: the change in the gas flowrate is equal to the change in the gas flowrate between the inlet and outlet minus the flow of condensate.

\[
\frac{dN_g^n}{dt} = F_{g}^{n-1} - F_{g}^n - F_{\text{condensate}}^n \tag{7}
\]

Equation (8) shows the mass balance for the flow of the condensable component in the gas phase: the flow of condensable leaving a volume is equal to the flow of condensable entering the volume minus the amount condensed.

\[
F_{\text{Condensable}}^n = F_{\text{condensate}}^{n-1} - F_{\text{Condensate}}^n \tag{8}
\]

Equations (9) and (10), the ideal gas law, show the relation between temperature and the number of moles of gas in a control volume.

\[
N_g^n = V \cdot \rho_g^n \tag{9}
\]

\[
\rho_g^n = \frac{P}{R \cdot T_g^n} \tag{10}
\]

Equation (11) calculates the mole fraction of the condensable in the gas phase.

\[
y_g^n = \frac{F_{\text{Condensable}}^n}{F_g^n} \tag{11}
\]

Equation (12) calculates the mole fraction of the condensable at the gas-condensate interface, assuming that vapor-liquid equilibrium exists.

\[
y_s^n = \frac{P_s^n (T_w^n)}{P} \tag{12}
\]
Diffusion Equations

The diffusion controlled model is based on the assumption that if the concentration gradient of the condensable between the bulk gas and the gas-condensate interface favors diffusion of the condensable species toward the interface, condensation will occur if the vapor is saturated at the interface temperature.

Equation (13) considers the case where the concentration of condensable at the interface is greater than the concentration in the bulk gas, thus diffusion to the interface and the subsequent condensation will not occur.

\[
\text{if } y_f^n \geq y_g^n \Rightarrow F_{\text{condensate}}^n = 0
\]  

(13)

Equation (14) imposes the limitations of thermodynamics. In the condenser, the temperature of the gas cannot decrease below the temperature of the wall and the coolant. Thus, if the decrease in temperature of the gas as a result of condensation is sufficient to bring the gas temperature to the wall temperature, no further cooling of the gas can occur. At this point, the energy transferred between the gas and the coolant must only be the result of condensation, not cooling, of the gas. The amount of condensate that forms is dependent on the amount of heat that can be transferred to the coolant.

\[
\text{else if } T_g^n \leq T_w^n \Rightarrow T_g^n = T_w^n, F_{\text{condensate}}^n = \frac{\dot{Q}_{w-g}^n}{(\Delta H_f^k(T_w^n))}
\]

(14)

Equation (15) describes the situation where both the concentration and temperature gradients allow for diffusion of the condensable species to the gas-condensate interface and condensation of the species at the interface. The flowrate of condensate is a function of the diffusion coefficient, concentration difference, contact area, and boundary layer thickness. The derivation of Equation (15) from Fick’s Law is shown in Appendix III.

\[
\text{else } F_{\text{condensate}}^n = \frac{A D_{ab} C}{\delta} \ln \left( \frac{1 - y_f^n}{1 - y_g^n} \right)
\]

(15)
Condenser Model

A program has been developed in MATLAB to simulate the operation of a condenser. The user specifies the physical geometry of the condenser as well as the initial temperatures and flowrates. Properties of the species, such as molecular weight, molecular volume, density, viscosity, and Antoine equation coefficients, must also be specified. The program uses this data to calculate the relevant heat capacities, heat transfer coefficients, and diffusion coefficients for the system. MATLAB solvers are used to obtain a solution to the heat and mass transfer equations, thus simulating the operation of the condenser.

System Variable Calculations

While values for certain system properties can be found in literature, variables such as heat capacities of mixtures, heat transfer coefficients, and diffusion coefficients must be estimated for the given system. Many correlations regarding the calculation of these variables can be found in literature. The correlations used in this model are detailed in Appendix IV.

As an initial estimate, the values were calculated at the inlet gas conditions. Since these parameters are dependent on the gas temperature and flowrates of condensable and noncondensable species, it was necessary to analyze the impact of updating their values according to the position of the volume element. As the gas temperature and flowrate of condensable species decrease along the length of the condenser, the heat capacity of the gas mixture, heat transfer coefficient of the gas, and diffusion coefficient decrease. The heat transfer coefficients of the condensate film and coolant remain approximately constant. The calculation involves the addition of three equations to the coupled system. Equations must be written for the variables found explicitly in the heat and mass transfer equations: the heat capacity of the gas mixture, the diffusion coefficient, and alpha for the gas phase.
**Steady State Model**

In the steady state model, the MATLAB function \textit{fsolve} is used to solve the system of equations obtained from the mass and energy balances. For the steady state system, there is no accumulation of mass or energy within a volume element. Thus, the \( \frac{dN}{dt} \) and \( \frac{dT}{dt} \) terms must be equal to zero. Starting with the initial conditions specified by the user, the MATLAB function \textit{fsolve} performs iterative calculations to solve the system of equations. The solution of the system is found when the residuals are equal to zero.

The program plots the temperature, concentration, and flow profiles along the length of the condenser. To emphasize the heat transfer limitation imposed by Equation (14), the heat flows associated with the cooling of the gas, condensation, and heating of the coolant are calculated and plotted. Sample plots are shown in Figure 6. The program performs a numerical integration to determine the total amount of condensate and uses mass balances to calculate the error associated with the flowrate calculations for the condensable and noncondensable species. Code for the program can be found in Appendix V. The operating conditions for the simulations shown in the following figures are given in Table 1.

**Table 1: Operating Conditions for Condenser Simulations**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet Gas Temperature (K)</td>
<td>350</td>
</tr>
<tr>
<td>Inlet Coolant Temperature (K)</td>
<td>230</td>
</tr>
<tr>
<td>Initial Wall Temperature (K)</td>
<td>250</td>
</tr>
<tr>
<td>Operating Pressure (atm)</td>
<td>1</td>
</tr>
<tr>
<td>Condenser Length (m)</td>
<td>3</td>
</tr>
<tr>
<td>Shell Inner Diameter (m)</td>
<td>0.9079</td>
</tr>
<tr>
<td>Tube Outer Diameter (m)</td>
<td>0.0200</td>
</tr>
<tr>
<td>Number of Tubes</td>
<td>40</td>
</tr>
<tr>
<td>Coolant Flowrate (kg/s)</td>
<td>15</td>
</tr>
<tr>
<td>Inlet Gas Flowrate (mol/s)</td>
<td>75</td>
</tr>
</tbody>
</table>
Figure 6a: Temperature, Concentration, and Flow Profiles for Steady State Operation

Figure 6b: Heat Flow Profiles for Steady State Operation
**Dynamic Model**

A model has been developed in order to understand the behavior of a condenser under dynamic operation. The program introduces a change (such as temperature, flowrate, or composition of a stream) into the system over a specified time range and models the response. The solver *ode15s* is used to obtain a solution to the mass and energy balances both in position and time, where the initial conditions are obtained from the steady state solution. The program outputs the temperature, concentration, flow, and heat flow profiles for the steady state as shown in Figures 6a and 6b. Additional plots, shown in Figures 7a and 7b, trace the temperature change of a specified volume element with time, as well as changes in flowrate of condensate, concentration in the bulk gas, and concentration near the wall. In the case shown, an increase in the flowrate of the condensable species occurs quadratically between times $t = 3s$ and $t = 5s$.
7b: Temperature, Error, and Concentration Profiles for Dynamic Operation where inlet flowrate of condensable species undergoes quadratic increase between times t=3s and t=5s.

Uncertainty Evaluation

Several sources of uncertainty are associated with the use of a computer model to simulate the operation of a condenser. Operating conditions such as temperatures and flowrates can vary throughout a process or may not be known accurately due to errors in their measurement. Parameters calculated in the model, such as heat transfer and diffusion coefficients, also possess a degree of uncertainty associated with the specific correlation used and its applicability to the given system. When designing a condenser, sources of uncertainty must be considered to ensure that the operation of the condenser will conform to the set specifications.

The effect of uncertainty on the performance of the condenser was evaluated by selecting five uncertain variables and performing simulations at different treatment levels of these variables. Inlet gas temperature, inlet coolant temperature, and inlet flowrate of condensable species were selected to represent uncertainty in operating conditions. Uncertainty in estimated variables was considered by varying the heat transfer coefficient.
of the gas and the diffusion coefficient. Using the steady state model, three cases were considered:

- Independent variation of one variable; C_{pgas}, h_{gas}, D_{ab} constant
- Independent variation of one variable; C_{pgas}, h_{gas}, D_{ab} change with position
- Simultaneous variation of two variables; C_{pgas}, h_{gas}, D_{ab} change with position

**Control System**

A controller was implemented in order to improve the efficiency and reduce the operating cost of the condenser. A diagram of the control system is given in Figure 8. Without the control system, the process would have to operate continuously at the conditions that prevented a constraint violation in the worst case scenario. Using the control system, a specified variable is adjusted in order to influence the system toward a given set point. An error term is calculated as the difference between the outlet gas temperature and the set point T_{sp} (desired outlet gas temperature). In this case, the error is minimized by adjusting the coolant flowrate. The coolant flowrate can be increased as necessary to decrease the outlet gas temperature. However, if the outlet gas temperature is initially below the set point temperature, the coolant flowrate can be decreased, resulting in a lower cost.

![Figure 8: Control System Diagram](image)

**Figure 8: Control System Diagram**  
T = temperature; m = mass flowrate; n = molar flowrate; TT = temperature transmitter; constraint = outlet gas temperature
In a PI controller, the control action is determined by considering a term proportional to the error and an integral value. As seen in Equation (16), the error term is calculated as the difference between the outlet gas temperature and the set point temperature.

\[ e = Tg(n + 1) - Tsp \]  

(16)

The control action, a change in the mass flowrate of coolant, is determined by Equation (17), where \( kc \) and \( T_I \) are constants. Further study of dynamic control methods will involve optimizing the values of \( kc \) and \( T_I \). (Note: Program code defines \( Ti = 1/T_I \).)

\[ Gc = kc \cdot (e + \frac{1}{T_I} \int e \, dt) \]  

(17)

The units for the above variables are as follows: \( e \) [\( = \) K]; \( Gc \) [\( = \) kg/s]; \( kc \) [\( = \) (kg/s)\( \times \) (1/K)]; \( T_I \) [\( = \) s].

In Figures 9a-e, the set point temperature is 268.2K, five degrees below the maximum allowable outlet gas temperature of 273.2K. Since the outlet gas temperature is initially below the set point temperature, the coolant flowrate can be decreased until the outlet gas temperature equals the set point value.

Figure 9a is used as a reference point where both \( kc \) and \( Ti \) are set at zero; thus, no control action is carried out. Figure 9b shows that including only the proportional term results in a constant error after the system equilibrates. As seen in Figure 9c, including both the proportional and integral terms causes the error to approach zero. A comparison of Figures 9c-e reveals that gradual changes to the system (i.e. small \( kc \)) result in smooth transitions, while more dramatic changes (i.e. large \( kc \)) cause oscillations about the set point. Accordingly, an adequate safety margin must be considered when determining the set point in order to avoid overshooting the maximum allowed temperature.
Figure 9a: Control Method, Reference - $k_C = 0$; $T_i = 0$; $T_{sp} = 268.2 K$

Figure 9b: Control Method, Proportional Term - $k_C = 0.1$; $T_i = 0$; $T_{sp} = 268.2 K$
**Figure 9c:** Control Method, Proportional (low) and Integral Terms - $k_c = 0.1; T_i = 1.5; T_{sp} = 268.2K$

**Figure 9d:** Control Method, Proportional (mid) and Integral Terms - $k_c = 0.3; T_i = 1.5; T_{sp} = 268.2K$
In Figure 9f, the set point temperature has been reduced to 263.2K, ten degrees below the maximum allowable outlet gas temperature. Increasing the coolant flowrate alone cannot cause the gas temperature to decrease to the set point before the flowrate becomes unreasonably high.
The control model can also be used to simulate the system’s response to changes in operating conditions. Figures 9g and 9h show the situation where the system is allowed to equilibrate to the set point before a change in inlet coolant temperature is introduced. In Figure 9g, the coolant temperature is decreased; thus, the coolant flowrate is lowered in order to return the outlet gas temperature to the set point value. In Figure 9h, the coolant temperature is increased; accordingly, the coolant flowrate must be increased.

**Figure 9g: Control Method, Decrease in Inlet Coolant Temperature** - \( k_c = 0.1; \ T_i = 1.5; \ T_sp = 268.2\text{K}; \) 2% decrease in inlet coolant temperature occurs at \( t = 120s \)
RESULTS AND DISCUSSION

Steady State Uncertainty Evaluation

In order to determine the impact of uncertainty on condenser performance, five uncertain variables were selected (inlet gas temperature, inlet coolant temperature, inlet flowrate of condensable species, heat transfer coefficient of gas, and diffusion coefficient) and trials were performed using combinations of different levels of these variables. The treatment levels used for each variable are shown in Table A6.1. Using the steady state model, three cases were considered:

- Independent variation of one variable; $C_{p_{\text{gas}}}$, $h_{\text{gas}}$, $D_{ab}$ constant
- Independent variation of one variable; $C_{p_{\text{gas}}}$, $h_{\text{gas}}$, $D_{ab}$ change with position
- Simultaneous variation of two variables; $C_{p_{\text{gas}}}$, $h_{\text{gas}}$, $D_{ab}$ change with position
Table 2: Treatment Levels of Uncertain Variables

<table>
<thead>
<tr>
<th>Variable</th>
<th>Nominal</th>
<th>Action</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
<th>10</th>
<th>11</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tg(1)</td>
<td>350</td>
<td>add</td>
<td>-5</td>
<td>-4</td>
<td>-3</td>
<td>-2</td>
<td>-1</td>
<td>0</td>
<td>1</td>
<td>2</td>
<td>3</td>
<td>4</td>
<td>5</td>
</tr>
<tr>
<td>Tcool(1)</td>
<td>230</td>
<td>add</td>
<td>-2</td>
<td>-1.6</td>
<td>-1.2</td>
<td>-0.8</td>
<td>-0.4</td>
<td>0</td>
<td>0.4</td>
<td>0.8</td>
<td>1.2</td>
<td>1.6</td>
<td>2</td>
</tr>
<tr>
<td>Fconb(1)</td>
<td>15</td>
<td>add</td>
<td>-1</td>
<td>-0.8</td>
<td>-0.6</td>
<td>-0.4</td>
<td>-0.2</td>
<td>0</td>
<td>0.2</td>
<td>0.4</td>
<td>0.6</td>
<td>0.8</td>
<td>1</td>
</tr>
<tr>
<td>hgas</td>
<td>calculate</td>
<td>multiply by</td>
<td>0.8</td>
<td>0.84</td>
<td>0.88</td>
<td>0.92</td>
<td>0.96</td>
<td>1</td>
<td>1.04</td>
<td>1.08</td>
<td>1.12</td>
<td>1.16</td>
<td>1.2</td>
</tr>
<tr>
<td>Dab</td>
<td>calculate</td>
<td>multiply by</td>
<td>0.8</td>
<td>0.84</td>
<td>0.88</td>
<td>0.92</td>
<td>0.96</td>
<td>1</td>
<td>1.04</td>
<td>1.08</td>
<td>1.12</td>
<td>1.16</td>
<td>1.2</td>
</tr>
</tbody>
</table>

Numerical data from the simulations is found in Appendix VI.

Independent Variation of One Variable (Cpgas, hgas, Dab change with position)

In the following simulations, the maximum allowable outlet gas temperature at the nominal condition is 273.2K. Table 3 and Figure 10 show that the outlet gas temperature increases with increasing inlet gas temperature. Varying the inlet gas temperature five degrees above and below the nominal value did not result in a constraint violation.

Table 3: Outlet Gas Temperature vs. Inlet Gas Temperature

<table>
<thead>
<tr>
<th>Tg_in (K)</th>
<th>Delta Tg_in (K)</th>
<th>% Change</th>
<th>Tg_out (K)</th>
<th>Delta Tg_out (K)</th>
<th>% Change</th>
</tr>
</thead>
<tbody>
<tr>
<td>345</td>
<td>-5</td>
<td>-1.42</td>
<td>262.26</td>
<td>-4.39</td>
<td>-1.66</td>
</tr>
<tr>
<td>346</td>
<td>-4</td>
<td>-1.14</td>
<td>263.14</td>
<td>-3.51</td>
<td>-1.32</td>
</tr>
<tr>
<td>347</td>
<td>-3</td>
<td>-0.86</td>
<td>264.01</td>
<td>-2.64</td>
<td>-0.99</td>
</tr>
<tr>
<td>348</td>
<td>-2</td>
<td>-0.57</td>
<td>264.89</td>
<td>-1.76</td>
<td>-0.66</td>
</tr>
<tr>
<td>349</td>
<td>-1</td>
<td>-0.29</td>
<td>265.77</td>
<td>-0.88</td>
<td>-0.33</td>
</tr>
<tr>
<td>350</td>
<td>0</td>
<td>0.00</td>
<td>266.65</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>351</td>
<td>1</td>
<td>0.29</td>
<td>267.54</td>
<td>0.89</td>
<td>0.33</td>
</tr>
<tr>
<td>352</td>
<td>2</td>
<td>0.57</td>
<td>268.42</td>
<td>1.77</td>
<td>0.66</td>
</tr>
<tr>
<td>353</td>
<td>3</td>
<td>0.86</td>
<td>269.30</td>
<td>2.65</td>
<td>0.99</td>
</tr>
<tr>
<td>354</td>
<td>4</td>
<td>1.14</td>
<td>270.19</td>
<td>3.54</td>
<td>1.33</td>
</tr>
<tr>
<td>355</td>
<td>5</td>
<td>1.43</td>
<td>271.07</td>
<td>4.42</td>
<td>1.66</td>
</tr>
</tbody>
</table>

Figure 10: Outlet Gas Temperature vs. Inlet Gas Temperature

Table 4 and Figure 11 show that the outlet gas temperature also increases with increasing coolant temperature; however, the inlet coolant temperature has a smaller effect on the outlet gas temperature than the inlet gas temperature. For a range of inlet coolant temperatures two degrees above and below the nominal value, the condenser performed within the given constraints.
Table 4: Outlet Gas Temperature vs. Inlet Coolant Temperature

<table>
<thead>
<tr>
<th>Tcool_in (K)</th>
<th>Delta Tcool_in (K)</th>
<th>% Change</th>
<th>Tg_out (K)</th>
<th>Delta Tg_out (K)</th>
<th>% Change</th>
</tr>
</thead>
<tbody>
<tr>
<td>228.0</td>
<td>-2.3</td>
<td>-0.87</td>
<td>266.38</td>
<td>-0.27</td>
<td>-0.10</td>
</tr>
<tr>
<td>228.4</td>
<td>-1.6</td>
<td>-0.70</td>
<td>266.43</td>
<td>-0.22</td>
<td>-0.08</td>
</tr>
<tr>
<td>228.8</td>
<td>-1.2</td>
<td>-0.52</td>
<td>266.49</td>
<td>-0.16</td>
<td>-0.05</td>
</tr>
<tr>
<td>229.2</td>
<td>-0.8</td>
<td>-0.35</td>
<td>266.54</td>
<td>-0.11</td>
<td>-0.04</td>
</tr>
<tr>
<td>229.6</td>
<td>-0.4</td>
<td>-0.17</td>
<td>266.60</td>
<td>-0.06</td>
<td>-0.02</td>
</tr>
<tr>
<td>230.0</td>
<td>0.0</td>
<td>0.00</td>
<td>266.65</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>230.4</td>
<td>0.4</td>
<td>0.17</td>
<td>266.71</td>
<td>0.06</td>
<td>0.02</td>
</tr>
<tr>
<td>230.8</td>
<td>0.8</td>
<td>0.35</td>
<td>266.77</td>
<td>0.12</td>
<td>0.05</td>
</tr>
<tr>
<td>231.2</td>
<td>1.2</td>
<td>0.52</td>
<td>266.83</td>
<td>0.18</td>
<td>0.07</td>
</tr>
<tr>
<td>231.6</td>
<td>1.6</td>
<td>0.70</td>
<td>266.89</td>
<td>0.23</td>
<td>0.09</td>
</tr>
<tr>
<td>232.0</td>
<td>2.0</td>
<td>0.87</td>
<td>266.94</td>
<td>0.29</td>
<td>0.11</td>
</tr>
</tbody>
</table>

Figure 11: Outlet Gas Temperature vs. Inlet Coolant Temperature

Table 5 and Figure 12 show that the outlet gas temperature increases with decreasing inlet condensable flowrate. For a range of inlet condensable flowrates one mol/s above and below the nominal value, the condenser performed within the operating constraints.

Table 5: Outlet Gas Temperature vs. Inlet Condensable Flowrate

<table>
<thead>
<tr>
<th>Fconb_in (mol/s)</th>
<th>Delta Fconb_in (mol/s)</th>
<th>% Change</th>
<th>Tg_out (K)</th>
<th>Delta Tg_out (K)</th>
<th>% Change</th>
</tr>
</thead>
<tbody>
<tr>
<td>14.0</td>
<td>-1.0</td>
<td>-6.67</td>
<td>271.38</td>
<td>4.73</td>
<td>1.77</td>
</tr>
<tr>
<td>14.2</td>
<td>-0.8</td>
<td>-5.33</td>
<td>270.44</td>
<td>3.76</td>
<td>1.42</td>
</tr>
<tr>
<td>14.4</td>
<td>-0.6</td>
<td>-4.00</td>
<td>269.50</td>
<td>2.85</td>
<td>1.07</td>
</tr>
<tr>
<td>14.6</td>
<td>-0.4</td>
<td>-2.67</td>
<td>268.55</td>
<td>1.90</td>
<td>0.71</td>
</tr>
<tr>
<td>14.8</td>
<td>-0.2</td>
<td>-1.33</td>
<td>267.60</td>
<td>0.95</td>
<td>0.36</td>
</tr>
<tr>
<td>15.0</td>
<td>0.0</td>
<td>0.00</td>
<td>266.65</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>15.2</td>
<td>0.2</td>
<td>1.33</td>
<td>265.70</td>
<td>-0.95</td>
<td>-0.36</td>
</tr>
<tr>
<td>15.4</td>
<td>0.4</td>
<td>2.67</td>
<td>264.75</td>
<td>-1.90</td>
<td>-0.71</td>
</tr>
<tr>
<td>15.6</td>
<td>0.6</td>
<td>4.00</td>
<td>263.79</td>
<td>-2.94</td>
<td>-1.07</td>
</tr>
<tr>
<td>15.8</td>
<td>0.8</td>
<td>5.33</td>
<td>262.84</td>
<td>-3.81</td>
<td>-1.43</td>
</tr>
<tr>
<td>16.0</td>
<td>1.0</td>
<td>6.67</td>
<td>261.87</td>
<td>-4.78</td>
<td>-1.79</td>
</tr>
</tbody>
</table>

Figure 12: Outlet Gas Temperature vs. Inlet Condensable Flowrate

Table 6 and Figure 13 show that the outlet gas temperature increases with a decrease in the heat transfer coefficient of the gas. For low values of the heat transfer coefficient (i.e. the correlation used actually overestimates the coefficient), the temperature constraint is violated.
Table 6: Outlet Gas Temperature vs. Heat Transfer Coefficient of Gas

<table>
<thead>
<tr>
<th>Hgas (kJ/(s<em>m^2</em>K))</th>
<th>Delta Hgas (kJ/(s<em>m^2</em>K))</th>
<th>% Change</th>
<th>Tg_out (K)</th>
<th>Delta Tg_out (K)</th>
<th>% Change</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1061</td>
<td>-0.0265</td>
<td>-19.98</td>
<td>279.26</td>
<td>12.61</td>
<td>4.73</td>
</tr>
<tr>
<td>0.1114</td>
<td>-0.0212</td>
<td>-15.99</td>
<td>276.63</td>
<td>9.98</td>
<td>3.74</td>
</tr>
<tr>
<td>0.1167</td>
<td>-0.0159</td>
<td>-11.99</td>
<td>274.06</td>
<td>7.41</td>
<td>2.76</td>
</tr>
<tr>
<td>0.1220</td>
<td>-0.0106</td>
<td>-7.99</td>
<td>271.54</td>
<td>4.89</td>
<td>1.83</td>
</tr>
<tr>
<td>0.1273</td>
<td>-0.0053</td>
<td>-4.00</td>
<td>269.07</td>
<td>2.42</td>
<td>0.91</td>
</tr>
<tr>
<td>0.1326</td>
<td>0.0000</td>
<td>0.00</td>
<td>266.65</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>0.1379</td>
<td>0.0053</td>
<td>4.00</td>
<td>264.29</td>
<td>-2.36</td>
<td>-0.89</td>
</tr>
<tr>
<td>0.1432</td>
<td>0.0106</td>
<td>8.00</td>
<td>261.97</td>
<td>-4.68</td>
<td>-1.76</td>
</tr>
<tr>
<td>0.1486</td>
<td>0.0159</td>
<td>12.07</td>
<td>259.70</td>
<td>-6.95</td>
<td>-2.72</td>
</tr>
<tr>
<td>0.1539</td>
<td>0.0213</td>
<td>16.06</td>
<td>257.48</td>
<td>-9.17</td>
<td>-3.44</td>
</tr>
<tr>
<td>0.1592</td>
<td>0.0266</td>
<td>20.06</td>
<td>255.29</td>
<td>-11.02</td>
<td>-4.20</td>
</tr>
</tbody>
</table>

Outlet Gas Temperature vs. Heat Transfer Coefficient of Gas

Outlet Gas Temperature vs. Heat Transfer Coefficient of Gas (Initial Value)
y = -450.94x + 326.71
R² = 0.9991

Figure 13: Outlet Gas Temperature vs. Heat Transfer Coefficient of Gas

Table 7 and Figure 14 show that the outlet gas temperature increases with a decrease in the diffusion coefficient. For low values of the diffusion coefficient (i.e. the correlation used actually overestimates the diffusion coefficient), the temperature constraint is violated.

Table 7: Outlet Gas Temperature vs. Diffusion Coefficient

<table>
<thead>
<tr>
<th>Dab (mol/(s<em>m^2</em>atm))</th>
<th>Delta Dab (mol/(s<em>m^2</em>atm))</th>
<th>% Change</th>
<th>Tg_out (K)</th>
<th>Delta Tg_out (K)</th>
<th>% Change</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.1948</td>
<td>-0.7987</td>
<td>-20.00</td>
<td>278.66</td>
<td>12.01</td>
<td>4.59</td>
</tr>
<tr>
<td>3.3545</td>
<td>-0.6390</td>
<td>-16.00</td>
<td>276.18</td>
<td>9.53</td>
<td>3.57</td>
</tr>
<tr>
<td>3.5143</td>
<td>-0.4792</td>
<td>-12.00</td>
<td>273.74</td>
<td>7.09</td>
<td>2.66</td>
</tr>
<tr>
<td>3.6740</td>
<td>-0.3195</td>
<td>-8.00</td>
<td>271.34</td>
<td>4.69</td>
<td>1.76</td>
</tr>
<tr>
<td>3.8338</td>
<td>-0.1597</td>
<td>-4.00</td>
<td>268.95</td>
<td>2.33</td>
<td>0.89</td>
</tr>
<tr>
<td>3.9935</td>
<td>0.0000</td>
<td>0.00</td>
<td>266.56</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>4.1532</td>
<td>0.1597</td>
<td>4.00</td>
<td>264.17</td>
<td>-2.36</td>
<td>-0.88</td>
</tr>
<tr>
<td>4.3130</td>
<td>0.3195</td>
<td>8.00</td>
<td>262.13</td>
<td>-4.62</td>
<td>-1.70</td>
</tr>
<tr>
<td>4.4727</td>
<td>0.4792</td>
<td>12.00</td>
<td>259.95</td>
<td>-6.72</td>
<td>-2.52</td>
</tr>
<tr>
<td>4.6325</td>
<td>0.6390</td>
<td>16.00</td>
<td>257.54</td>
<td>-8.88</td>
<td>-3.35</td>
</tr>
<tr>
<td>4.7922</td>
<td>0.7987</td>
<td>20.00</td>
<td>255.13</td>
<td>-11.02</td>
<td>-4.13</td>
</tr>
</tbody>
</table>

Outlet Gas Temperature vs. Diffusion Coefficient (Initial Value)
y = -14.415x + 324.42
R² = 0.9994

Figure 14: Outlet Gas Temperature vs. Diffusion Coefficient

Figures 15 through 18 show the relationship between parameters. As seen in Figure 15, the diffusion coefficient is strongly dependent on the heat transfer coefficient of the gas. Weaker relationships exist between the diffusion coefficient and inlet gas temperature, heat transfer coefficient of the gas and inlet condensable flowrate, and diffusion coefficient and inlet condensable flowrate.
The same relationships between the uncertain parameters and outlet gas temperature as seen when the heat capacity of the gas mixture, heat transfer coefficient of the gas, and diffusion coefficient are assumed to be constant throughout the condenser as when they are updated with position. However, the numerical results are slightly different. When the variables are recalculated, the outlet gas temperature increases slightly, and the percent change from the nominal case is slightly less for the same change in the uncertain parameter.

**Simultaneous Variation of Two Variables (Cpgas, hgas, Dab change with position)**

After studying the effect of uncertainty in one parameter, the effect of varying two parameters simultaneously was examined. Since the aim of the uncertainty evaluation was to determine when a constraint violation would occur, each parameter was varied from the nominal value in the direction that would result in an increase in the outlet gas temperature. For the different treatment combinations, level zero is the situation where
both parameters are at the nominal value. Level five is the worst case scenario where both parameters are at their maximum deviation from the nominal value.

Table 8 and Figure 19 show that increasing the inlet gas and coolant temperatures simultaneously does not result in a constraint violation.

### Table 8: Outlet Gas Temperature vs. Inlet Gas Temperature and Inlet Coolant Temperature

<table>
<thead>
<tr>
<th>Level</th>
<th>T_{g_{in}} (K)</th>
<th>Delta T_{g_{in}} (K)</th>
<th>% Change</th>
<th>T_{cool_{in}} (K)</th>
<th>Delta T_{cool_{in}} (K)</th>
<th>% Change</th>
<th>T_{g_{out}} (K)</th>
<th>Delta T_{g_{out}} (K)</th>
<th>% Change</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>350</td>
<td>0</td>
<td>0.00</td>
<td>230.0</td>
<td>0.00</td>
<td>0.00</td>
<td>266.65</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>1</td>
<td>351</td>
<td>1</td>
<td>0.29</td>
<td>230.4</td>
<td>0.4</td>
<td>0.17</td>
<td>267.59</td>
<td>0.94</td>
<td>0.35</td>
</tr>
<tr>
<td>2</td>
<td>352</td>
<td>2</td>
<td>0.57</td>
<td>230.8</td>
<td>0.8</td>
<td>0.35</td>
<td>268.53</td>
<td>1.88</td>
<td>0.71</td>
</tr>
<tr>
<td>3</td>
<td>353</td>
<td>3</td>
<td>0.86</td>
<td>231.2</td>
<td>1.2</td>
<td>0.52</td>
<td>269.47</td>
<td>2.62</td>
<td>1.06</td>
</tr>
<tr>
<td>4</td>
<td>354</td>
<td>4</td>
<td>1.14</td>
<td>231.6</td>
<td>1.6</td>
<td>0.70</td>
<td>270.42</td>
<td>3.77</td>
<td>1.41</td>
</tr>
<tr>
<td>5</td>
<td>355</td>
<td>5</td>
<td>1.43</td>
<td>232.0</td>
<td>2.0</td>
<td>0.87</td>
<td>271.36</td>
<td>4.71</td>
<td>1.77</td>
</tr>
</tbody>
</table>

### Figure 19: Outlet Gas Temperature vs. Variation in Inlet Gas and Coolant Temperatures

\[ y = 0.9423x + 266.65 \]

\[ R^2 = 1 \]
Table 9 and Figure 20 show that increasing the inlet gas temperature and decreasing the inlet condensable flowrate simultaneously results in a constraint violation although performing either of these actions alone does not.

Table 9: Outlet Gas Temperature vs. Inlet Gas Temperature and Inlet Condensable Flowrate

<table>
<thead>
<tr>
<th>Level</th>
<th>Tg_in (K)</th>
<th>Delta Tg_in (K)</th>
<th>% Change</th>
<th>Fcomb_in (mol/s)</th>
<th>Delta Fcomb_in (mol/s)</th>
<th>% Change</th>
<th>Tg_out (K)</th>
<th>Delta Tg_out (K)</th>
<th>% Change</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>350</td>
<td>0</td>
<td>0.00</td>
<td>15.0</td>
<td>0.00</td>
<td>0.00</td>
<td>266.65</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>1</td>
<td>351</td>
<td>1</td>
<td>0.29</td>
<td>14.8</td>
<td>-0.2</td>
<td>-1.33</td>
<td>268.49</td>
<td>1.84</td>
<td>0.69</td>
</tr>
<tr>
<td>2</td>
<td>352</td>
<td>2</td>
<td>0.57</td>
<td>14.6</td>
<td>-0.4</td>
<td>-2.67</td>
<td>270.32</td>
<td>3.67</td>
<td>1.38</td>
</tr>
<tr>
<td>3</td>
<td>353</td>
<td>3</td>
<td>0.86</td>
<td>14.4</td>
<td>-0.6</td>
<td>-4.00</td>
<td>272.15</td>
<td>5.50</td>
<td>2.06</td>
</tr>
<tr>
<td>4</td>
<td>354</td>
<td>4</td>
<td>1.14</td>
<td>14.2</td>
<td>-0.8</td>
<td>-5.33</td>
<td>273.97</td>
<td>7.32</td>
<td>2.75</td>
</tr>
<tr>
<td>5</td>
<td>355</td>
<td>5</td>
<td>1.43</td>
<td>14.0</td>
<td>-1.0</td>
<td>-6.67</td>
<td>275.80</td>
<td>9.15</td>
<td>3.43</td>
</tr>
</tbody>
</table>

Outlet Gas Temperature vs. Variation in Inlet Gas Temperature and Inlet Condensable Flowrate

$$y = 1.8291x + 266.66$$

$$R^2 = 1$$

Figure 20: Outlet Gas Temperature vs. Variation in Inlet Gas Temperature and Inlet Condensable Flowrate
Table 10 and Figure 21 show that increasing the inlet coolant temperature and decreasing the inlet condensable flowrate simultaneously does not result in a constraint violation.

Table 10: Outlet Gas Temperature vs. Inlet Coolant Temperature and Inlet Condensable Flowrate

<table>
<thead>
<tr>
<th>Level</th>
<th>Tcool_in (K)</th>
<th>Delta Tcool_in (K)</th>
<th>% Change</th>
<th>Fcomb_in (mol/s)</th>
<th>Delta Fcomb_in (mol/s)</th>
<th>% Change</th>
<th>Tg_out (K)</th>
<th>Delta Tg_out (K)</th>
<th>% Change</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>230.0</td>
<td>0.0</td>
<td>0.00</td>
<td>15.0</td>
<td>0.0</td>
<td>0.00</td>
<td>266.65</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>1</td>
<td>230.4</td>
<td>0.4</td>
<td>0.17</td>
<td>14.8</td>
<td>-0.2</td>
<td>-1.33</td>
<td>267.66</td>
<td>1.01</td>
<td>0.38</td>
</tr>
<tr>
<td>2</td>
<td>230.8</td>
<td>0.8</td>
<td>0.35</td>
<td>14.6</td>
<td>-0.4</td>
<td>-2.67</td>
<td>268.67</td>
<td>2.02</td>
<td>0.76</td>
</tr>
<tr>
<td>3</td>
<td>231.2</td>
<td>1.2</td>
<td>0.52</td>
<td>14.4</td>
<td>-0.6</td>
<td>-4.00</td>
<td>269.67</td>
<td>3.02</td>
<td>1.13</td>
</tr>
<tr>
<td>4</td>
<td>231.6</td>
<td>1.6</td>
<td>0.70</td>
<td>14.2</td>
<td>-0.8</td>
<td>-5.33</td>
<td>270.67</td>
<td>4.02</td>
<td>1.51</td>
</tr>
<tr>
<td>5</td>
<td>232.0</td>
<td>2.0</td>
<td>0.87</td>
<td>14.0</td>
<td>-1.0</td>
<td>-6.67</td>
<td>271.67</td>
<td>5.02</td>
<td>1.88</td>
</tr>
</tbody>
</table>

Outlet Gas Temperature vs. Variation in Inlet Coolant Temperature and Inlet Condensable Flowrate

\[ y = 1.0037x + 266.66 \]

\[ R^2 = 1 \]

Figure 21: Outlet Gas Temperature vs. Variation in Inlet Coolant Temperature and Inlet Condensable Flowrate
Design Applications

A condenser model has been developed for application in processes for reducing VOC emissions. The model can be used to aid in the design of a condenser to treat a VOC stream, as well as control and optimization of the process.

The initial focus must be to conform to the operating constraints (maximum allowed outlet gas temperature) determined by EPA regulations. In the initial design stages, the steady state model can be used to determine whether a particular set of operating conditions and condenser geometry will adhere to or violate the constraints and adjustments can be made accordingly. The model can also be used to analyze the effect of uncertainty in system parameters. Uncertainty is present both in the operating conditions and the estimated parameters. The design must account for these uncertainties to ensure that they do not result in constraint violations. Due to the complex relationships between parameters, independent variation of one parameter at a time is not sufficient to analyze the impact of uncertainty in that particular variable. In the previously shown case, increasing the inlet gas temperature alone does not result in a constraint violation, nor does decreasing the inlet flowrate of the condensable species. However, a constraint violation does occur when these two parameters are varied simultaneously.

It must be recognized that the condenser does not always operate at steady state, particularly during startup or when a change is introduced into the system. Thus, a dynamic model was developed to simulate condenser operation under unsteady state conditions. This model can be used to determine the system’s response to conditions that change with time.

A control system has been implemented in order to prevent constraint violations. A control variable can be adjusted in order to influence the system toward steady state operation about a set point. As shown in Figure 9e, the control sequence can result in oscillations about the set point; thus, an adequate safety margin must be considered when determining the set point so that the oscillations themselves do not result in constraint violations.

Another feature of the control system is its role in process and cost optimization. The controller influences the system toward the set point, whether its initial state exceeded the set point or was in an acceptable operating range. Operating expenses can
be minimized by moving from the ‘acceptable’ range toward the limiting condition (the set point).

Model Robustness

The implementation of system variable calculations and outcome of case simulations resulted in the development of an improved model which can more accurately represent the behavior of a fluid as it passes through a condenser. When the calculations were inserted and the simulations begun, the heat transfer limitation described in Equation (14) had not yet been included in the model. Trials involving low concentrations of the condensable species in the inlet gas ran as expected; however, trials using higher concentrations yielded physically questionable results. Figures 22 and 23 show the difference in program output obtained by varying the mole fraction of the condensable species in the inlet gas for the operating conditions described in Table 1.

**Figure 22a: Temperature, Concentration, and Flow Profiles for 20% Inlet VOC Concentration without Heat Transfer Limitation**

**Figure 22b: Temperature, Concentration, and Flow Profiles for 40% Inlet VOC Concentration without Heat Transfer Limitation**

**Figure 23a: Heat Flow Profiles for 20% Inlet VOC Concentration without Heat Transfer Limitation**

**Figure 23b: Heat Flow Profiles for 40% Inlet VOC Concentration without Heat Transfer Limitation**
As seen in Figure 22b, trials using high inlet concentrations of the condensable species resulted in the gas temperature decreasing below the temperatures of both the wall and the coolant. However, the laws of thermodynamics restrict the temperature changes that can actually occur in a condenser. The temperature of the gas stream cannot fall below the wall temperature. The initial approach to this problem was to ensure that all of the calculations in the model were dimensionally correct and that there were no discrepancies between the derived equations and those entered into the program. After making these corrections and obtaining similar results, the model itself was scrutinized.

A conclusion was drawn that, in order to obtain a solution to the given system of equations, MATLAB was creating a physically invalid representation of the system. As written, the equations stated that condensation would occur when the concentration gradient favored diffusion of the condensable species toward the tube wall. Figure 23b shows that the system reaches a point where the amount of heat available from the coolant is less than the heat required to condense the amount of gas specified by the diffusion model (Equation (15)). Since the model forced condensation to occur in this situation, MATLAB was forced to compensate for the energy difference when computing the solution. As seen through the combination of Equations (2), (3), and (6) for the steady state system, the energy transferred from the wall to the coolant is equal to the heat convection from the bulk gas to the gas-wall interface plus the energy released through the condensation of the gas. Thus, the heat convection term was altered in order to obtain a solution. For the energy balance to be consistent, the heat convection term must be negative, forcing the temperature of the gas to be lower than the temperature of the wall. Since there was no restriction on the temperature of the gas, it was allowed to decrease below the coolant temperature as well.

The solution to this problem involved placing a temperature restriction on the model. When the gas temperature is greater than the wall temperature, the original diffusion controlled model holds. However, if the decrease in the temperature of the gas as a result of condensation is sufficient to make the gas temperature equal the wall temperature, no further cooling of the gas may occur. A heat transfer limitation is imposed, stating that when the gas temperature equals the wall temperature, the energy transfer between the gas and the coolant is a result of condensation only. This theory
holds since the gas is saturated at the wall temperature. The amount of condensate is then equal to the amount of heat that can be transferred to the coolant divided by the amount of heat required to condense the species (Equation (14)).

Figures 24 and 25 show the result of repeating the trials shown in Figures 22 and 23 with the addition of the heat transfer limitation.

In practice, a condenser designed based on this model should operate solely in the diffusion controlled region of the model. While the theory behind the heat transfer limitation is valid, it was imposed as a means to prevent the gas temperature from falling below the wall and coolant temperatures. The current model is based on diffusion controlled condensation where the condensate forms on the outside of the tube wall. In the region where the heat transfer limitation applies, the bulk gas is saturated and condensation will occur in the bulk gas, not only at the gas-wall interface. Corrections to account for changes in fluid dynamics resulting from condensation in the bulk gas have not been included in this model.
CONCLUSIONS

A mathematical model has been developed which can predict the behavior of a condenser under both steady state and unsteady state operation. This model is valid for situations in which condensation is diffusion controlled and the inlet gas stream is a mixture containing a condensable species and a noncondensable species. A dynamic control system has been implemented in order to respond to changes and return the system to steady state operation about a given set point.

The model may be used to analyze the effect of system parameters on condenser performance, either to determine the impact of making a conscious change or to evaluate the effect of uncertainty in the parameters. Coupled with cost data, this information may be used to optimize the design of a condenser. With increasingly strict regulations on VOC emissions being developed, companies are facing increased costs. The use of a computerized mathematical model will allow them to strike the desired balance between minimizing cost and improving performance when designing dynamic condensers to treat VOC emission streams.

FUTURE WORK

- Run simulations and uncertainty trials for systems with different species and condenser geometries.
- Introduce system variable calculations into model for treatment of inlet streams containing more than one condensable species.
- Create database of relevant properties for common VOCs.
- Gather information regarding cryogenic cooling systems and cost data for the construction and operation of a condenser.
- Compare simulation results with experimental data to judge accuracy and determine magnitude of error in parameter estimations (Cpgas, hgas, Dab).
- Optimize design under uncertainty.
ACKNOWLEDGEMENTS

- Faculty, graduate students, and post-doctoral researchers within the Chemical Engineering Department at the University of Illinois at Chicago, particularly Professor Andreas Linnerger and Andrés Malcolm.
- The National Science Foundation.
REFERENCES


3 United Stated Environmental Protection Agency. Website. www.epa.gov.


APPENDIX I: Regulations for VOC Emissions by Pharmaceutical Manufacturing Facilities in Chicago, Illinois

Pharmaceutical manufacturing operations are subject to the following regulations if their VOC emissions total more than 6.8 kg/day (15 lbs/day) or 2,268 kg/year (2.5 tons/year). The use of surface condensers to reduce VOC emissions must comply with the specifications shown in Table A1.1. If another type of air pollution control equipment is used, it must produce at least a 90 percent reduction in VOC emissions.

Table A1.1: Operating Specifications for Surface Condensers

<table>
<thead>
<tr>
<th>VOC Vapor Pressure (kPa) at 293.4K (70°F) greater than</th>
<th>Maximum Allowable Outlet Gas Temperature (K)</th>
<th>Maximum Allowable Outlet Gas Temperature (°F)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.45</td>
<td>298.2</td>
<td>77</td>
</tr>
<tr>
<td>7</td>
<td>283.2</td>
<td>50</td>
</tr>
<tr>
<td>10</td>
<td>273.2</td>
<td>32</td>
</tr>
<tr>
<td>20</td>
<td>258.2</td>
<td>5</td>
</tr>
<tr>
<td>40</td>
<td>248.2</td>
<td>-13</td>
</tr>
</tbody>
</table>
APPENDIX II: Calculation of VOC Emissions

Charging
The following procedure is used to calculate the emissions resulting from the charging of a liquid VOC into a vessel. Several assumptions have been made:
- Ideal Gas Law applies
- Volume of displaced gas equals volume of liquid charged into vessel
- Displaced air is saturated with VOC at exit temperature

1. Calculate rate of air displacement in ft³/hr.

\[
V_r = L_r \times (0.134 \text{ ft}^3/\text{gal}) \times (60 \text{ min}/\text{hr})
\]

Where: \( L_r \) = liquid pumping rate in gallons/minute

\[ V_r = (25 \text{ gal/min}) \times (0.134 \text{ ft}^3/\text{gal}) \times (60 \text{ min}/\text{hr}) = 201 \text{ ft}^3/\text{hr} \]

2. Determine the mole fraction \( x_i \) of each VOC in liquid mixture.

\[
x_i = \frac{\text{moles of } i \text{ in liquid mix}}{\text{total moles of liquid mix}}
\]

\[ x_i = 1 \]

3. Calculate the vapor pressure of the pure VOC using Antoine’s equation.

\[
\log_{10} P_i = a - \frac{b}{(c + T_i)}
\]

\[ P_i = 10^{a - \frac{b}{(c + T_i)}} \]

Where:
- \( P_i \) = vapor pressure of the VOC in mmHg
- \( T_i \) = air temperature in °C
- \( a, b, c \) = Antoine’s equation constants

\[ P_i = 10^{(8.1122 - 1592.864/(226.184 + 21.1))} = 46.86 \text{ mmHg} \]

4. Calculate the rate of VOC emission, \( S_e \), in lbs/hr for each VOC.

\[
S_e = \frac{P_i \times x_i \times V_r \times MW_i}{(R \times T)}
\]

Where:
- \( R = 999 \text{ (mmHg*ft}^3)/(\text{lbmol*K}) \)
- \( T \) = temperature in K
- \( MW_i \) = molecular weight of VOC in lbs/lbmol

\[ S_e = \frac{(46.86 \text{ mmHg} \times 1 \times 201 \text{ ft}^3/\text{hr} \times 46.07 \text{ lb/lbmol})}{(999 \text{ (mmHg*ft}^3)/(\text{lbmol*K}) \times 293.4 \text{ K})} = 1.48 \text{ lbs/hr} \]
Nitrogen Sweep

The following procedure is used to calculate the emissions resulting when nitrogen is used to sweep a vessel. Several assumptions have been made:

- Ideal Gas law applies
- Nitrogen leaving vessel is saturated with VOC at exit temperature

1. Calculate the rate of nitrogen sweep in standard ft³/hr.

\[ V_R = N_s \times (60 \text{ min/hr}) \]

Where: \( N_s \) = rate of nitrogen sweep in scfm

\[ V_R = 1 \text{ scfm} \times (60 \text{ min/hr}) = 60 \text{ ft}^3/\text{hr} \]

2. Calculate the mole fraction, \( x_i \), of each VOC in the liquid mixture.

\[ x_i = \frac{\text{moles of } i \text{ in liquid mix}}{\text{total moles of liquid mix}} \]  

\[ x_i = 1 \]

3. Calculate the vapor pressure, \( P_i \), of each VOC at the exit temperature.

\[ \log_{10} P_i = a - b / (c + T_e) \]  

\[ P_i = 10^{a - b / (c + T_e)} \]  

\[ P_i = 10^{(8.1122 - 1592.864 / (226.184 + 21.1))} = 46.86 \text{ mmHg} \]

4. Calculate the rate of total gas displaced from the vessel, \( V_{R2} \), in ft³/hr.

\[ V_{R2} = V_R \times (760) / (760 - \sum (P_i \times x_i)) \]

Where: \( P_{N2} = 760 = \) vapor pressure of nitrogen sweep in mmHg

\[ V_{R2} = 60 \text{ ft}^3/\text{hr} \times (760) / (760 - \sum (46.86 \text{ mmHg} \times 1)) = 63.94 \text{ ft}^3/\text{hr} \]

5. Calculate the rate of VOC emission, \( S_e \), in lbs/hr for each VOC.

\[ S_e = (P_i \times x_i \times V_{R2} \times MW_i) / (R \times T) \]

\[ S_e = (46.86 \text{ mmHg} \times 1 \times 63.94 \text{ ft}^3/\text{hr} \times 46.07 \text{ lb/mol}) / (999(\text{mmHg} \times \text{ft}^3) / (\text{lbmol} \times \text{K}) \times 293.4 \text{ K}) = 0.47 \text{ lbs/hr} \]
APPENDIX III: Derivation of Diffusion Equation from Fick’s Law

Fick’s Law:

\[ N_A = -C * D_{ab} * \Delta y_A + y_A (N_A + N_B) \]  

(A3.1)

where: \( N_i \) = molar flux of species i  
\( C \) = total concentration  
\( D_{ab} \) = diffusion coefficient  
\( y_i \) = mole fraction of species i  
\( A \) = condensable species  
\( B \) = noncondensable species

Assume: \( N_B = 0 \)  

(A3.2)

Thus: \( N_A = -(C * D_{ab} * \Delta y_A) / (1 - y_A) \)  

(A3.3)

\[ \Delta y_A = \frac{dy_A}{dx} \]  

(A3.4)

\[ N_A = -(C * D_{ab}) / (1 - y_A) * \left( \frac{dy_A}{dx} \right) \]  

(A3.5)

\[ \frac{N_A}{(C * D_{ab})} = -1 / (1 - y_A) * \left( \frac{dy_A}{dx} \right) = \text{constant} \]  

(A3.6)

\[ \int_0^\delta \frac{N_A}{(C * D_{ab})} dx = -\int_{y_G}^{y_i} 1 / (1 - y_A) dy_A \]  

(A3.7)

\[ N_A * \delta / (C * D_{ab}) = \ln \left( \frac{1 - y_i}{1 - y_G} \right) \]  

(A3.8)

Where: \( y_i \) = mole fraction of condensable at gas-condensate interface (\( x = \delta \))  
\( y_G \) = mole fraction of condensable in bulk gas (\( x = 0 \))

\[ N_A = \frac{F_A}{A} \]  

(A3.9)

Where: \( F_A \) = molar flowrate of condensable species  
\( A \) = area

\[ F_A = \frac{C * D_{ab} * A}{\delta} * \ln \left( \frac{1 - y_i}{1 - y_G} \right) \]  

(A3.10)
APPENDIX IV: System Variable Calculations and Correlations

Heat Capacity of Gas Mixture

Estimate Cp of each component.\(^\text{13}\)

\[
Cp = a + b \times T + c \times T^2 + d \times T^3
\]  \hspace{1cm} \text{(A5.1)}

or

\[
Cp = a + b \times T + c \times T^{-2}
\]  \hspace{1cm} \text{(A5.2)}

Cp \([\text{kJ/(mol*K)}]\); T \([\text{°C}]\); a,b,c are species-dependent parameters

Calculate Cp of mixture as a weighted average.

\[
C_{pgas} = \sum (y_i \times Cp_i)
\]  \hspace{1cm} \text{(A5.3)}

Diffusion Coefficient\(^\text{14}\)

\[
D_{ab} = h \times (c \times \mu / k)^{2/3} / (c \times p_{gf} \times M_m \times (\mu / (\rho \times k_d))^{2/3})
\]  \hspace{1cm} \text{(A5.4)}

Dab = diffusion coefficient; lbmol/(hr*ft\(^2\)*atm)

h = heat transfer coefficient; Btu/(hr*ft\(^2\)*°F)

c = specific heat of cold fluid; Btu/(lb*°F)

\(\mu\) = viscosity; lb/(ft*hr)

k = thermal conductivity; Btu/(hr*ft*°F)

\(\rho_{gf}\) = log mean pressure difference of the inert gas between \(p_a\) and \(p_a^\prime\); atm

\(p_a\) = partial pressure of the inert gas in the gas body; atm

\(p_a^\prime\) = partial pressure of the inert gas at the condensate film; atm

\(M_m\) = mean molecular weight of vapor mixture; lb/lbmol

\(\rho\) = density; lb/ft\(^3\)

\(k_d\) = diffusivity; ft\(^2\)/hr

\[
k_d = 0.0166 \times T^{2/3} \times (1 / M_A + 1 / M_B)^{1/2} / (p_t \times (v_A^{1/3} + v_B^{1/3})^2)
\]  \hspace{1cm} \text{(A5.5)}

T = temperature of gas mixture; K

\(M_A\) = molecular weight of diffusing species

\(M_B\) = molecular weight of inert species

\(p_t\) = total pressure; atm

\(v_A\) = molar volume of diffusing gas

\(v_B\) = molar volume of inert species

Heat Transfer Coefficients

Condensate Film\(^\text{15}\)

\[
h = 0.73 \times (k / D) \times ((D^3 \times \rho^2 \times g \times \lambda) / (k \times \mu \times \Delta t))^{1/4}
\]  \hspace{1cm} \text{(A5.6)}

\[
h_N = h \times N^{-1/4}
\]  \hspace{1cm} \text{(A5.7)}

h = heat transfer coefficient for 1 tube; kJ/(s*m\(^2\)*K)

\(h_N\) = heat transfer coefficient for N tubes; kJ/(s*m\(^2\)*K)

\(N\) = \((2/3)\times\)number of tubes across diameter of cylindrical tube bundle

k = thermal heat conductivity; kJ/(s*m*K)
D = tube diameter; m
ρ = density; kg/m³
g = gravitational constant; m/s²
λ = latent heat; kJ/kg
μ = viscosity; kg/(m*s) or centipoise*10
Δt = temperature difference between saturated vapor and surface; K

Gas

Valid for 2,000 ≤ Re ≤ 1,000,000

\[ h = 0.36*(k/De)^{0.55}*(c*μ/k)^{1/3}*(μ/μ_w)^{0.14} \]  
\[ Re = De*Gs/μ \]  
\[ Gs = W/a_s \]  
\[ a_s = (ID*C*B)/(P_T*144) \]

square pitch:  
\[ de = \frac{4*(P_T^2-\pi*d_o^2/4)}{\pi*d_o} \]

triangular pitch:  
\[ de = \frac{4*(0.5*P_T*0.86*P_T-0.5*\pi*d_o^2/4)}{0.5*\pi*d_o} \]

h = heat transfer coefficient; Btu/(hr*ft²*°F)
k = thermal conductivity; Btu/(hr*ft*°F)
De = equivalent diameter, ft
Re = Reynolds number
c = specific heat of cold fluid; Btu/(lb*°F)
μ = viscosity at bulk gas temperature; lb/(ft*hr)
μ_w = viscosity at gas-wall interface temperature; lb/(ft*hr)
Gs = mass flux of gas; lb/(hr*ft²)
W = mass flowrate of gas; lb/hr
a_s = shell-side crossflow area; ft²
ID = inner diameter of shell; inches
C' = clearance between tubes; inches
B = baffle spacing; inches
P_T = pitch; inches
de = equivalent diameter; inches
d_o = outer diameter of tube; inches
APPENDIX V: Condenser Model - MATLAB Program Code

Dynamic Model

Main Program: SimCondenser_Eval_Final.m

function SimCondenser(Kc,Ti,Tsp,nt,THotin,TColdin);

% Uncertainty Trial Factors
uf1 = 0; % Tg(1) - addition
uf2 = 0; % Tcool(1) - addition
uf3 = 0; % Fconb(1) - addition
uf4 = 1; % hgas - multiplication
uf5 = 1; % Dab - multiplication

% Condenser Geometry
L = 3; % total length in meters
n = 30; % number of volumes to integrate length over
dti = 0.019; % inner tube diameter in meters
wt = 0.001; % wall thickness in meters
dto = dti + wt; % outer tube diameter in meters
clr = 0.02; % clearance between coolant tubes in meters
pitch = clr + nto; % pitch in meters
nt = 40; % number of tubes
B = L; % baffle spacing in meters
pt = 1; % square pitch: pt = 1, triangular pitch: pt = 2

% approximate shell diameter based on number of tubes and layout
if pt == 1
    number = 1; % number of tubes interior to square
    Area = pitch^2; % area of square in m^2
else
    number = 0.75; % number of tubes interior to triangle
    Area = 3*(1/2)*pitch^2; % area of triangle
end
eleme1 = nt/number;
eleme2 = int32(element1);
eleme3 = real(element2);
elements = element3 + 1; % number of square/triangle elements for number of tubes
Area_req = elements*Area; % total area of required square/triangle elements in m^2
ds = (4*R*A)*Area_req
nt1 = ds/pitch; % approximate number of tubes at center of shell
dz = L/nt; % length increment
A = 3.14159*dto*nt*dz; % contact surface area of element in m^2
Atot = 3.14159*dto*nt*L; % total contact surface area of condenser in m^2
Vt = 3.14159*dti^2/4*nt*dz; % volume inside tube per element
VW = 3.14159*dz*nt*(dito^2-dti^2)/4; % volume of wall per element
Vs = 3.14159*dz*(ds^2-nt*dto^2)/4; % volume between shell and tube per element

% Operating Conditions
Fcool = 15; % mass flowrate of coolant in kg/s
P = 1; % total pressure in atm

% Constants
R = 8.314; % ideal gas constant in (m^3*Pa)/(mol*K)
g = 9.81; % gravitational constant in m/s^2
% Boundary Conditions
Tg(1) = 350 + uf1; % initial gas temperature in K
Tcool(1) = 230 + uf2; % initial coolant temperature in K
Twall(1) = 250; % initial wall temperature in K
Fgas(1) = 75; % initial molar flowrate of gas in mol/s
Fconb(1) = 15 + uf3; % initial molar flowrate of condensables in gas in mol/s
Fcon(1) = 0; % initial molar flowrate of condensate in mol/s
Ngas(1) = (Vs*P*101325)/(R*Tg(1)); % initial moles of gas
Fnc = Fgas(1)-Fconb(1); % molar flowrate of noncondensables in gas in mol/s

% Initial Values
for i = 1:n
y0(i) = Ngas(1);
y0(i+n) = Tg(1)/1.05;
y0(i+2*n) = Tcool(1);
y0(i+3*n) = Twall(1);
y0(i+4*n) = Fgas(1);
y0(i+5*n) = Fcon(1);
y0(i+6*n) = Fconb(1);
end

% Properties
% reference: appendices of Kern: "Process Heat Transfer"
Dcool = 1000; % density of coolant in kg/m^3
Dwall = 7830; % density of wall in kg/m^3
Dcond = 789; % density of condensate film in kg/m^3
Ccool = 4.184; % Cp of coolant in kJ/(kg*K)
Cwall = 0.4; % Cp of wall in kJ/(kg*K)
Cpc = 0.1031; % Cp of condensate in kJ/(mol*K) (Felder and Rousseau 636)
Visc_gas = 0.018*2.42; % gas viscosity at temperature of bulk gas lb/(ft*hr)
Visc_gas_wt = 0.015*2.42; % gas viscosity at wall temperature lb/(ft*hr)
Visc_cond = 2.5*10; % viscosity of condensate film in centipoise * 10 = kg/(m*s)
Visc_coool = 3.5*2.42; % coolant viscosity at temperature of bulk medium in lb/(ft*hr)
Visc_cool_wt = 2.5*2.42; % coolant viscosity at wall temperature in lb/(ft*hr)
M1 = 28; % molecular weight of noncondensable (nitrogen) g/mol or lb/lbmol
M2 = 46.07; % molecular weight of condensable (ethanol) g/mol or lb/lbmol
v1 = 2 * 15.6; % molecular volume of noncondensable (nitrogen) (Kern 344)
v2 = 2 * 14.8 + 6 * 3.7 + 7.4; % molecular volume of condensable (ethanol) (Kern 344)
Hv = 38.58; % heat of vaporization of condensable in kJ/mol (Felder and Rousseau 630)
kg = 0.01; % thermal conductivity of gas in Btu/(hr*ft*degreesF)
kf = 0.1/(9.486*10^-4)/1000/3600*3.28*1.8; % thermal conductivity of film in kJ/(s*m*K)
kc = 0.3; % thermal conductivity of coolant in Btu/(hr*ft*degreesF)

% Antoine Equation Coefficients for Condensable (ethanol)
Aa = 8.11220;
Ba = 1592.864;
Ca = 226.184;

% Calculations
Mc = Dcool*Vt; % mass of coolant in an element in kg
Nwall = Dwall*Vw; % mass of wall in a volume in kg
Cvel = Fcool/Dcool/(nt*3.14159*dti^2/4); % velocity of coolant stream in m/s
Tsat = Ba/(Aa-log10(Fconb(1)/Fgas(1)*P*760)-Ca+273); % saturation temperature of vapor
% Unit Conversions
pt = pitch*3.2808*12; % pitch in inches
do = dto*3.2808*12; % outer diameter in inches
di = dti*3.2808*12; % outer diameter in inches
crc = clr*3.2808*12; % clearance in inches
b = B*3.2808*12; % baffle spacing in inches

% Calculate Maximum Allowable Outlet Gas Temperature

Pconb = Fconb(1)/Fgas(1)*101.325; % inlet vapor pressure of condensable, kPa
z = Tg(1)/293.4; % correction factor to operating temperature
if Pconb >= 40*z
    Tg_max = 248.2 % maximum allowable outlet gas temperature in K
elseif ((Pconb < 40*z)&(Pconb >= 20*z))
    Tg_max = 258.2
elseif ((Pconb < 20*z)&(Pconb >= 10*z))
    Tg_max = 273.2
elseif ((Pconb < 10*z)&(Pconb >= 7*z))
    Tg_max = 283.2
elseif ((Pconb < 7*z)&(Pconb >= 3.45*z))
    Tg_max = 298.2
else
    fprintf('Outlet gas temperature not regulated. Specify maximum value.')
    Tg_max = 298.2
end

% Calculate Heat Capacity of Gas Mixture
% reference: Felder and Rousseau: "Elementary Principles of Chemical Processes" Table B.2
T(1) = Tg(1) - 273; % T = initial temperature of gas in degrees Celsius

% component 1 = nitrogen (noncondensable)
% Cp nitrogen = a + b*T + c*T^2 + d*T^3 where T is in degrees C
a1 = 29 * 10^-3;
b1 = 0.2199 * 10^-5;
c1 = 0.5723 * 10^-8;
d1 = -2.871 * 10^-12;
if T(1)>0 % correlation valid for T > 0 degrees C
    Cp1(1) = a1 + b1*T(1) + c1*T(1)^2 + d1*T(1)^3; % Cp of noncondensable in kJ/(mol*K)
else
    Cp1(1) = a1;
end
Cp_1(1) = Cp1(1)*1000*9.486*10^-4/1.8/M1*1000/2.2; % Cp of noncondensable in Btu/(lb*degF)

% component 2 = ethanol (condensable)
% Cp ethanol = a + b*T + c*T^2 + d*T^3 where T is in degrees C
a2 = 61.34 * 10^-3;
b2 = 15.72 * 10^-5;
c2 = -8.749 * 10^-8;
d2 = 19.83 * 10^-12;
if T(1)>0 % correlation valid for T > 0 degrees C
    Cp2(1) = a2 + b2*T(1) + c2*T(1)^2 + d2*T(1)^3; % Cp of condensable in kJ/(mol*K)
else
    Cp2(1) = a2;
Cp_2(1) = Cp2(1)*1000*9.486*10^-4/1.8/M2*1000/2.2; % Cp of condensable in Btu/(lb*degF)

% calculate Cpgas as a weighted average of the component Cps
Cpgas(1) = (Fnc/Fgas(1)) * Cp1(1) + (Fconb(1)/Fgas(1)) * Cp2(1); % kJ/(mol*K)
Cp_gas(1) = (Fnc*M1*Cp_1(1)+Fconb(1)*M2*Cp_2(1))/(Fnc*M1+Fconb(1)*M2); % Btu/(lb*degF)

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% Calculate Heat Transfer Coefficient for Gas

if pt == 1
    de = 4*(pt^2-3.14159*do^2/4)/3.14159/do; % equivalent diameter in inches
else
    de = 4*(0.5*pt*0.86*pt-0.5*3.14159*do^2/4)/(0.5*3.14159/do);
end
De = de/12; % equivalent diameter in feet
Ag = di*clrc*b/pt/144; % flow area of gas in ft^2
Wg(1) = (Fnc*M1+Fconb(1)*M2)/1000*2.2*3600; % mass flow rate of gas in lb/hr
Ga(1) = Wg(1)/Ag; % mass flux of gas in lb/(hr*ft^2)
Reg(1) = De*Ga(1)/Visc_gas; % Reynolds number for gas
hg(1) = uf4*0.36 * Reg(1)^0.55 * (Cp_gas(1)*Visc_gas/kg)^(1/3)*(Visc_gas/Visc_gas_wt)^0.14*kg/De;

hgas(1) = hg(1)/(9.486*10^-4)/1000/3600*(3.28^2)*1.8; % heat transfer coefficient for gas in kJ/(s*m^2*K)

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% Calculate Heat Transfer Coefficient for Condensate Film
% reference: Perry's Chemical Engineer's Handbook p. 5-20, 11-11

deltaT = Tsat-Twall(1); % temp difference between sat'd vapor and surface in K
h1film = heat transfer coefficient for film with 1 tube in kJ/(s*m^2*K)
h1film = 0.73*kf/dto*((dto^3*Dcond^2*g*Hv)/(kf*Visc_cond*deltaT*M2/1000))^(1/4);
nt2 = 2/3*nt1; % 2/3 of max number of tubes across diameter
nt3 = int32(nt2); % truncate to integer value
N = real(nt3); % convert to real number
hfilm = h1film*N^(-1/4); % correction for multiple tubes, kJ/(s*m^2*K)

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% Calculate Heat Transfer Coefficient for Coolant
% reference: Kern: "Process Heat Transfer" p. 103-105

Ac = 3.14159*dti^2/4*3.2808^2; % flow area of coolant in ft^2
Wc = Fcool/nt*3600*2.2; % mass flow rate of coolant per tube in lb/hr
Gc = Wc/Ac; % mass flux of coolant per tube in lb/(hr*ft^2)
Rec = dti*Gc/Visc_cool; % Reynolds number for coolant
c = Ccool*1000*(9.486*10^-4)/2.2/1.8; % specific heat of cold fluid in Btu/(lb*degreesF)

hc = heat transfer coefficient for coolant in Btu/(hr*ft^2*degreesF)
% note: eqs. valid for organic liquids, aqueous solutions, and gases, but not for water
if Rec > 2100
    hc = 0.027 * Rec^0.8 * (c*Visc_cool/kc)\(1/3)\(Visc_cool/Visc_cool\_wt\)\(0.14\*kc/dti;
else
    hc = 1.86*(Rec\(c*Visc_cool\_dti/kt/L)\(1/3)\(Visc_cool/Visc_cool\_wt\)\(0.14\*kc/dti;
end
hcoolant = hc/(9.486*10^-4)/1000/3600*(3.28^2)*1.8; % heat transfer coefficient for coolant in kJ/(s*m^2*K)
% correct to outer diameter of tube rather than inner diameter
hcool = hcoolant*dti/dto; % heat transfer coefficient for coolant in kJ/(s*m^2*K)
% Calculate General Heat Transfer Coefficients

alcool = hcool*A; % alpha for cooling fluid
alg(1) = 1/(1/hgas(1)+1/hfilm)*A; % alpha for gas and film
U(1) = 1/(1/hgas(1) + 1/hfilm + 1/hcool); % overall heat transfer coefficient kJ/(s*m^2*K)

% Calculate Diffusion Coefficient
% reference: Kern: "Process Heat Transfer" p. 343-344

% calculate diffusivity using Gilliland correlation
kd(1) = 0.0166 * (Tg(1))^(3/2)/ P / (v1^(1/3) + v2^(1/3))^2 * (1/M1 + 1/M2)^(1/2); % ft^2/hr
KD(1) = kd(1)/3600/3.28^2; % diffusivity in m^2/s

% calculate diffusion coefficient
pg1(1) = (Fnc/Fgas(1))*P; % partial pressure of the inert gas in the gas body, atm
pg2(1) = P-(10^(Aa-Ba/(Twall(1)-273+Ca)))/760; % partial pressure of the inert gas at the condensate film, atm
pgf(1) = (pg2(1)-pg1(1))/log(pg2(1)/pg1(1)); % log mean pressure difference of the inert gas between pg1 and pg2, atm
Mm(1) = ((Fnc/Fgas(1))*M1 + (Fconb(1)/Fgas(1))*M2); % mean molecular weight of the vapor mixture, lb/lbmol
Dgas(1) = P*Mm(1)/0.7302/(1.8*Tg(1)); % density of gas in lb/ft^3
Kg(1) = hg(1)*((Cp_gas(1)*Visc_gas/kg)^(2/3))/(Cp_gas(1)*pgf(1)*Mm(1)*(Visc_gas/Dgas(1)/kd)^(2/3)); % diffusion coefficient in lbmol/(hr*ft^2*atm)

% Set Initial Values of Heat Capacities, Heat Transfer Coefficients, and Diffusion Coefficient
for i=1:n
    % Heat Capacity
    cpg(i) = T(1);
    cpg(i+n) = Cp1(1);
    cpg(i+2*n) = Cp_1(1);
    cpg(i+3*n) = Cp2(1);
    y0(i+7*n) = Cpgas(1);
    cpg(i+5*n) = Cp_gas(1);
    % Heat Transfer Coefficient
    htc(i) = Wg(1);
    htc(i+n) = Ga(1);
    htc(i+2*n) = Reg(1);
    htc(i+3*n) = hg(1);
    htc(i+4*n) = hgas(1);
    y0(i+8*n) = alg(1);
    htc(i+5*n) = U(1);
    % Diffusion Coefficient
difc(i) = kd(1);
    difc(i+n) = KD(1);
    difc(i+2*n) = pg1(1);
    difc(i+3*n) = pg2(1);
    difc(i+4*n) = pgf(1);
    difc(i+5*n) = Mm(1);
    difc(i+6*n) = Dgas(1);
    difc(i+7*n) = Kg(1);
    y0(i+9*n) = Dab(1);
end
% Steady State Solution

options0 = optimset('Display','iter','MaxFunEvals',1e5);
[yss,eval,exitflag] =
fsolve(@(CondenserSS_Eval4,y0,options0,Tg,Tcool,Twall,Fgas,Fcon,Fconb,Fcool,A,alcool,Vs,P,R,Mc,Ccool,Cwall,Cpc,Nwall,Alcool,Hv,ngas,dz,cpg,htc,difc,Visc_gas,Visc_gas_wt,De,Ag,kf,g,Visc_cond,N,M1,M2,dto,Dcond,v1, v2,hcool,a1,b1,c1,d1,a2,b2,c2,d2,L,Tsat,hfilm,hgas,U,Cpgas,Dab,uf4,uf5);
yss;

% Plot Results
PlotSS_Eval(yss,n,Alcool,Ca,P,dz,Tg,Tcool,Twall,Fgas,Fcon,Fconb,Fcool,A,alcool,Hv,Cpc);

% Extract Variables from Steady State Solution
for i=1:n
    Ngas(i+1) = real(yss(i));
    Tg(i+1) = real(yss(i+n));
    Tcool(i+1) = real(yss(i+2*n));
    Twall(i+1) = real(yss(i+3*n));
    Fgas(i+1) = real(yss(i+4*n));
    Fcon(i+1) = real(yss(i+5*n));
    Fconb(i+1) = real(yss(i+6*n));
    ygas(i+1) = Fconb(i+1)/Fgas(i+1);
    Cpgas(i+1) = yss(i+7*n);
    alg(i+1) = yss(i+8*n);
    Dab(i+1) = yss(i+9*n);
end

% Error Calculations
Input=(Fgas(1));
TotalCond=trapz(Fcon);
FgasO=Fgas(n+1);
FconbO=Fconb(n+1);
Accumulated=Vs*P*101325/(R*Tg(n+1)^2)*(Tg(1)-Tg(n+1));
Output=TotalCond+FgasO+Accumulated;
FconbO=Fconb(1);
CAbsErr=Fconb(1)-TotalCond-FconbO;
CondbleError=(abs(CAbsErr))/(Fconb(1))*100;
NonCondError=Fnc-(FgasO*(1-ygas(n+1)));

% % Print results to file
% fid = fopen('Uncertainty_Evaluation_Change3.txt', 'a');
% fprintf(fid, 'Tg_in Tcool_in Fconb_in hgas Dab Tg_out Tcool_out Fconb_out Accum Error_C Error_NC uf1 uf2 uf3 uf4 uf5 exitflag 
', 'a');
% fprintf(fid, '%.1f %.1f %.1f %.4f %.4f %.2f %.2f %.2f %.3g %.3g %0f% %.1f%.1f%.2f%.2f%.3g \n', Tg(1), Tcool(1), Fconb(1), hgas(1), Dab(1), Tg(n+1), Tcool(n+1), Fconb(n+1), Accumulated, CondbleError, NonCondError, uf1, uf2, uf3, uf4, uf5, exitflag);
% fclose(fid);

% Dynamic Solution

tend = 30;
Mstep = tend/100;
tspan = [0:tend]; % time horizon integrated
nalg = 6; % number of algebraic eq
ndiff = 4; % number of differential equations

M = zeros((nalg+ndiff)*n,(nalg+ndiff)*n); % mass matrix for DAE

for j=1:(ndiff)*n
    M(j,j) = 1;
end

options = odeset('Mass',M,'Refine',5,'MaxStep',Mstep);
[t,y] = ode15s(@CondenserDyn_Eval_update,tspan,yss,options,Tg,Tcool,Twall,Fgas,Fcon,Fconb,Fnc,Fcool,A,alcool,Vs,P,R,
    Mc,Ccool,Cwall,Cp,Nwall,Aa,Ba,Ca,Hv,Ngas,n,cpg,htc,difc,Visc_gas,Visc_gas_wt,De,Ag,kg,kf,g,Visc_cond,N,M1,
    M2,dto,Dcond,v1,v2,hcool,a1,b1,c1,d1,a2,b2,c2,d2,L,Tsat,hfilm,uf4,uf5);

% Plot Results
a = n; % length to be displayed in time
PlotDynCond3(t,y,n,Aa,Ba,Ca,P,a,R,Vs);
PlotDynError(t,y,n,Aa,Ba,Ca,P,a,R,Vs);

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

Steady State Solution: CondenserSS_Eval4.m

function [out] = CondenserSS_Eval(y,Tg,Tcool,Twall,Fgas,Fcon,Fconb,Fnc,Fcool,A,alcool,Vs,P,R,Mc,Ccool,Cwall,Cp,Nwall,Aa,Ba,
    Ca,Hv,n,dz,cpg,htc,difc,Visc_gas,Visc_gas_wt,De,Ag,kg,kf,g,Visc_cond,N,M1,M2,dto,Dcond,v1,v2,hcool,a1,b1,c1,d1,
    a2,b2,c2,d2,L,Tsat,hfilm,hgas,U,Cpgas,Dab,uf4,uf5)

    % Variables Declaration
    for i=1:n
        Ngas(i+1) = real(y(i));
        Tg(i+1) = real(y(i+n));
        Tcool(i+1) = real(y(i+2*n));
        Twall(i+1) = real(y(i+3*n));
        Fgas(i+1) = real(y(i+4*n));
        Fcon(i+1) = real(y(i+5*n));
        Fconb(i+1) = real(y(i+6*n));
        Cpgas(i+1) = real(y(i+7*n));
        alg(i+1) = real(y(i+8*n));
        Dab(i+1) = real(y(i+9*n));
    end

    for i=1:n
        % Heat Capacity Values
        T(i+1) = cpg(i);
        Cp1(i+1) = cpg(i+n);
        Cp_1(i+1) = cpg(i+2*n);
        Cp2(i+1) = cpg(i+3*n);
        Cp_2(i+1) = cpg(i+4*n);
        Cp_gas(i+1) = cpg(i+5*n);

        % Heat Transfer Coefficient Values
        Wg(i+1) = htc(i);
        Ga(i+1) = htc(i+n);
        Reg(i+1) = htc(i+2*n);
        hgt(i+1) = htc(i+3*n);
        hgas(i+1) = htc(i+4*n);
        U(i+1) = htc(i+5*n);

        % Diffusion Coefficient Values
        kdi(i+1) = difc(i);
        KD(i+1) = difc(i+n);
\[
\begin{align*}
pg_{1}(i+1) &= \text{difc}(i+2*n); \\
pg_{2}(i+1) &= \text{difc}(i+3*n); \\
pg_{f}(i+1) &= \text{difc}(i+4*n); \\
M_{m}(i+1) &= \text{difc}(i+5*n); \\
D_{\text{gas}}(i+1) &= \text{difc}(i+6*n); \\
K_{g}(i+1) &= \text{difc}(i+7*n);
\end{align*}
\]

end

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

% System of Equations Declaration

% Differential Equations
for i=1:n

% Mass Balance For Gas
out(i)=F_{\text{gas}}(i)-F_{\text{gas}}(i+1)-F_{\text{con}}(i+1);

% Gas energy Balance
out(i+n)=(F_{\text{gas}}(i)*C_{\text{pgas}}(i+1)*(T_{g}(i)-T_{g}(i+1))-alg(i+1)*(T_{g}(i+1)-T_{\text{wall}}(i+1))-F_{\text{con}}(i+1)*H_{v})/(N_{\text{gas}}(i+1)*C_{\text{pgas}}(i+1));

% Coolant energy Balance
out(i+2*n)=(F_{\text{cool}}*C_{\text{cool}}*(T_{\text{cool}}(i)-T_{\text{cool}}(i+1))+alcool*(T_{\text{wall}}(i+1)-T_{\text{cool}}(i+1)))/(M_{c}*C_{\text{cool}});

% Wall energy Balance
out(i+3*n)=(alg(i+1)*(T_{g}(i+1)-T_{\text{wall}}(i+1))+F_{\text{con}}(i+1)*(H_{v}+C_{pc}(T_{g}(i+1)-T_{\text{wall}}(i+1)))-alcool*(T_{\text{wall}}(i+1)-T_{\text{cool}}(i+1)))/(N_{\text{wall}}*C_{\text{wall}});
end

% Algebraic Equations
for i=1:n

ywall(i+1)=10^{(A_{a} - B_{a}/(T_{\text{wall}}(i+1)-273+C_{a}))}/760/P;
ygas(i+1)=F_{\text{con}}b(i+1)/F_{\text{gas}}(i+1);

% Diffusion Equation
if (ygas(1+i)-ywall(i+1)) <= 1e-6
out(i+4*n)=F_{\text{con}}(i+1)-0;
elseif (T_{g}(i+1)-T_{\text{wall}}(i+1)) <= 1e-3
if T_{g}(i+1)-T_{\text{wall}}(i+1) < 0
T_{g}(i+1) = T_{\text{wall}}(i+1);
end
out(i+4*n)=F_{\text{con}}(i+1)-alcool*(T_{\text{wall}}(i+1)-T_{\text{cool}}(i+1))/H_{v};
else
out(i+4*n)=F_{\text{con}}(i+1)-A*D_{ab}(i+1)*P*log((1-ywall(1+i))/(1-ygas(i+1)));
end

% Mass Balance For Condensable in Gas phase
out(i+5*n)=F_{\text{con}}b(i)-F_{\text{con}}b(i+1)-F_{\text{con}}(i+1);

% Finite Volume Moles Change Due to Temperature using IG EoS
out(i+6*n)=N_{\text{gas}}(i+1)-Vs*P/(R*T_{g}(i+1));
end

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

% Update Heat Capacity, Heat Transfer Coefficients, and Diffusion Coefficient
for i=1:n

% Heat Capacity
T_{i+1} = T_{g}(i+1) - 273; % T = initial temperature of gas in degrees Celsius
% component 1 = nitrogen (noncondensable)
if T_{i+1}>0
\[ \text{Cp}_1(i+1) = a_1 + b_1 \cdot T(i+1) + c_1 \cdot T(i+1)^2 + d_1 \cdot T(i+1)^3; \] % Cp of noncondensable in kJ/(mol*K)

else
\[ \text{Cp}_1(i+1) = a_1; \]
end

\[ \text{Cp}_1(i+1) = \text{Cp}_1(i+1) \cdot 1000 \cdot 9.486 \cdot 10^{-4} / 1.8 / M_1 \cdot 1000 / 2.2; \] % Cp of noncondensable in Btu/(lb*degF)

\% component 2 = ethanol (condensable)

if T(i+1)>0
\[ \text{Cp}_2(i+1) = a_2 + b_2 \cdot T(i+1) + c_2 \cdot T(i+1)^2 + d_2 \cdot T(i+1)^3; \] % Cp of condensable in kJ/(mol*K)

else
\[ \text{Cp}_2(i+1) = a_2; \]
end

\[ \text{Cp}_2(i+1) = \text{Cp}_2(i+1) \cdot 1000 \cdot 9.486 \cdot 10^{-4} / 1.8 / M_2 \cdot 1000 / 2.2; \] % Cp of condensable in Btu/(lb*degF)

% calculate Cpgas as a weighted average of the component Cps
\[ \text{out}(i+7*n) = \left( \frac{\text{Fnc}}{\text{Fgas}(i+1)} \right) \cdot \text{Cp}_1(i+1) + \left( \frac{\text{Fconb}(i+1)}{\text{Fgas}(i+1)} \right) \cdot \text{Cp}_2(i+1) - \text{Cpgas}(i+1); \] % kJ/(mol*K)

\[ \text{Cp}_{\text{gas}}(i+1) = \left( \frac{\text{Fnc} \cdot M_1 \cdot \text{Cp}_1(i+1) + \text{Fconb}(i+1) \cdot M_2 \cdot \text{Cp}_2(i+1)}{\text{Fnc} \cdot M_1 + \text{Fconb}(i+1) \cdot M_2} \right); \] % Btu/(lb*degF)

% Heat Transfer Coefficient of Gas
\[ \text{Wg}(i+1) = \left( \frac{\text{Fnc} \cdot M_1 + \text{Fconb}(i+1) \cdot M_2}{1000 \cdot 2.2 \cdot 3600} \right); \] % mass flow rate of gas in lb/hr
\[ \text{Ga}(i+1) = \text{Wg}(i+1) / \text{Ag}; \] % mass flux of gas in lb/(hr*ft^2)

\[ \text{Reg}(i+1) = \text{De} \cdot \text{Ga}(i+1) / \text{Visc}_{\text{gas}}; \] % Reynolds number for gas

\[ \text{hgf}(i+1) = 0.36 \cdot \text{Reg}(i+1)^{0.55} \cdot \left( \frac{(\text{Cp}_{\text{gas}}(i+1) \cdot \text{Visc}_{\text{gas}} / \text{kg})^{1/3} \cdot (\text{Visc}_{\text{gas}} / \text{Visc}_{\text{gas}} \cdot \text{wt})^{0.14} \cdot \text{kg} / \text{De}}{\text{Btu} / (\text{hr} / \text{ft}^2 \cdot \text{degreesF})} \right); \]

\[ \text{hgas}(i+1) = \text{hgf}(i+1) \cdot (9.486 \cdot 10^{-4}) / 1000 / 3600 / (3.28^2) \cdot 1.8; \] % heat transfer coefficient for gas in kJ/(s*m^2*K)

% General Heat Transfer Coefficients
\[ \text{out}(i+8*n) = \frac{1}{1 / \text{hgas}(i+1) + 1 / \text{hfilm}} \cdot \text{A} - \text{alg}(i+1); \] % alpha for gas and film
\[ \text{U}(i+1) = 1 / (1 / \text{hgas}(i+1) + 1 / \text{hfilm} + 1 / \text{hcool}); \] % overall heat transfer coefficient kJ/(s*m^2*K)

% Diffusion Coefficient
\[ \text{kd}(i+1) = 0.0166 \cdot (\text{Tg}(i+1) / 3.2)^2 / P / (v1^1(1.3) + v2^2(1.3))^2 \cdot (1 / M_1 + 1 / M_2)^{(1/2)}; \] % diffusivity in ft^2/hr
\[ \text{Kd}(i+1) = \text{kd}(i+1) / 3600 / 3.28^2; \] % diffusivity in m^2/s

\[ \text{pg1}(i+1) = \left( \frac{\text{Fnc} \cdot \text{Fgas}(i+1)}{P} \right) \cdot \text{P} / (\text{Aa-Ba} / \text{Twall}(i+1) + 273 + \text{Ca}) / 760; \] % partial pressure of the inert gas in the gas body, atm

\[ \text{pg2}(i+1) = \left( \frac{\text{Fnc} \cdot \text{Fconb}(i+1) / \text{Fgas}(i+1)}{M_1} \right) / \log(\text{pg2}(i+1) / \text{pg1}(i+1)); \] % log mean pressure difference of the inert gas between pg1 and pg2, atm

\[ \text{Mm}(i+1) = ((\text{Fnc} / \text{Fgas}(i+1)) \cdot M_1 + (\text{Fconb}(i+1) / \text{Fgas}(i+1)) \cdot M_2); \] % mean molecular weight of the vapor mixture, lb/lbmol

\[ \text{Dgas}(i+1) = \text{P} \cdot \text{Mm}(i+1) / 0.7302 / (1.8 \cdot \text{Tg}(i+1)); \] % density of gas in lb/ft^3

\[ \% \text{Kg} = \text{diffusion coefficient in lbmol} / (\text{hr} \cdot \text{ft}^2 \cdot \text{atm}); \]

\[ \text{Kg}(i+1) = \left( \frac{\text{hgf}(i+1) \cdot (\text{Cp}_{\text{gas}}(i+1) \cdot \text{Visc}_{\text{gas}} / \text{kg})^{1/3} \cdot (\text{Visc}_{\text{gas}} / \text{Dgas}(i+1) / \text{kd}(i+1))^{2/3}}{\text{pgf}(i+1)^2} \right) / \text{pgf}(i+1) / \text{pg1}(i+1); \]

\[ \text{out}(i+9*n) = \text{uf5} \cdot \text{Kg}(i+1) \cdot(3.2808^2 / 3600 / 453.593 - \text{Dab}(i+1)); \] % diffusion coefficient in mol/(s*m^2*atm)

end

Steady State Plot: PlotSS_Eval.m

function [ ]=PlotSS_Eval(yss,n,Aa,Ba,Ca,P,dz,Tg,Tcool,Twall,Fgas,Fcon,Fconb,Fcool,alg,alcool,Hv,Cpc);

%Variables Declaration
for i=1:n
\[ \text{Tg}(i) = \text{real}(\text{yss}(i+n)); \]
\[ \text{Tcool}(i) = \text{real}(\text{yss}(i+2*n)); \]
\[ \text{Twall}(i) = \text{real}(\text{yss}(i+3*n)); \]
\[ \text{Fgas}(i) = \text{real}(\text{yss}(i+4*n)); \]
Fcon(i)=real(yss(i+5*n));
Fconb(i)=real(yss(i+6*n));
end

for i=1:n
ygas(i)=Fconb(i)/Fgas(i);
ywall(i)=10^(Aa - Ba/(Twall(i)-273+Ca))/760/P;
end

le=1:n;
lee=0+dz*le;
figure(1);
subplot(4,1,1),plot(lee,Tcool,'--', lee,Tg,'.:r',lee,Twall,'g')
title('Steady State Condenser');
legend('coolant', 'gas', 'wall');
% xlabel('Length');
ylabel('Temp (K)')

subplot(4,1,2),plot(lee,ygas,'.:r',lee,ywall,'g')
% title('Fg out vs L');
legend('gas', 'wall');
% xlabel('Time');
ylabel('VOC Conc. (mol fr.)')

subplot(4,1,3),plot(lee,Fconb,'g')
% title('Control vs time');
% xlabel('Length');
ylabel('Fconb (mol/s)')

subplot(4,1,4),plot(lee,Fcon,'b')
% title('Control vs time');
% xlabel('Length (m)');
ylabel('Fcon (mol/s)')

figure(2);
qgas=alg*(Tg-Twall);
qcond=Fcon.*(Hv+Cpc*(Tg-Twall));
qdisp=alcool*(Twall-Tcool);
diff=qdisp-qgas;

subplot(3,1,1),plot(lee,qgas)
title('Steady State Condenser');
% xlabel('Length');
ylabel('Qgas (kJ/s)')

subplot(3,1,2),plot(lee,qcond,lee,diff,'r.')
% title('Fg out vs L');
% xlabel('Time');
ylabel('Qcond (kJ/s)')

subplot(3,1,3),plot(lee,qdisp)
% title('Control vs time');
% xlabel('Length (m)');
ylabel('Qdisp (kJ/s)')

Dynamic Solution: CondenserDyn_Eval_update.m

function [out] = 
CondenserDyn_Eval_update(t,y,Tg,Tcool,Twall,Fgas,Fcon,Fconb,Fnc,Fcool,A,alcool,Vs,P,R,Mc,Ccool,Cwall,Cpc,Nw
all,Aa,Ba,Ca,Hv,Ngas,n,cpg,htc,difc,Visc_gas,Visc_gas_wt,De,Ag,kf,g,Visc_cond,N,M1,M2,dto,Dcond,v1,v2,hcoo
l,a1,b1,c1,d1,a2,b2,c2,d2,L,Tsat,hfilm,uf4,uf5)

% Variables Declaration
for i=1:n
    Ngas(i+1) = real(y(i));
    Tg(i+1) = real(y(i+n));
    Tcool(i+1) = real(y(i+2*n));
    Twall(i+1) = real(y(i+3*n));
    Fgas(i+1) = real(y(i+4*n));
    Fcon(i+1) = real(y(i+5*n));
    Fconb(i+1) = real(y(i+6*n));
    Cpgas(i+1) = real(y(i+7*n));
    alg(i+1) = real(y(i+8*n));
    Dab(i+1) = real(y(i+9*n));
end

for i=1:n
    % Heat Capacity Values
    T(i+1) = cpg(i);
    Cp1(i+1) = cpg(i+n);
    Cp_1(i+1) = cpg(i+2*n);
    Cp_2(i+1) = cpg(i+3*n);
    Cp_gas(i+1) = cpg(i+5*n);
    % Heat Transfer Coefficient Values
    Wg(i+1) = htc(i);
    Ga(i+1) = htc(i+n);
    Reg(i+1) = htc(i+2*n);
    hg(i+1) = htc(i+3*n);
    hgas(i+1) = htc(i+4*n);
    U(i+1) = htc(i+5*n);
    % Diffusion Coefficient Values
    kd(i+1) = difc(i);
    KD(i+1) = difc(i+n);
    pg1(i+1) = difc(i+2*n);
    pg2(i+1) = difc(i+3*n);
    pgf(i+1) = difc(i+4*n);
    Mm(i+1) = difc(i+5*n);
    Dgas(i+1) = difc(i+6*n);
    Kg(i+1) = difc(i+7*n);
end

% Simulation Changes
Fconb0=Fconb(1);
if (t >= 3) & (t < 5)
    Fconb(1)=Fconb0+1*(t-3)^2;
elseif t >= 5
    Fconb(1)=Fconb0+1*(5-3)^2;
end

% System of Equations Declaration

% Differential Equations
for i=1:n
% Mass Balance For Gas
out(i)=Vs*P*(R*(Tg(i+1))^2)*(Fgas(i)*Cpgas(i+1)*(Tg(i)-Tg(i+1))-alg(i+1)*(Tg(i+1)-Twall(i+1))-Fcon(i+1)*Hv)/(Ngas(i+1)*Cpgas(i+1));

% Gas energy Balance
out(i+n)=(Fgas(i)*Cpgas(i+1)*(Tg(i)-Tg(i+1))-alg(i+1)*(Tg(i+1)-Twall(i+1))-Fcon(i+1)*Hv)/(Ngas(i+1)*Cpgas(i+1));

% Coolant energy Balance
out(i+2*n)=(Fcool*Ccool*(Tcool(i)-Tcool(i+1))+alcool*(Twall(i+1)-Tcool(i+1)))/(Mc*Ccool);

% Wall energy Balance
out(i+3*n)=(alg(i+1)*(Tg(i+1)-Twall(i+1))+Fcon(i+1)*(Hv+Cpc*(Tg(i+1)-Twall(i+1)))-alcool*(Twall(i+1)-Tcool(i+1)))/(Nwall*Cwall);

end

% Algebraic Equations
for i=1:n
    ywall(i+1)=10^(Aa - Ba/(Twall(i+1)-273+Ca))/760/P;
    ygas(i+1)=Fconb(i+1)/Fgas(i+1);
    % Diffusion Equation
    if (ygas(i+1)-ywall(i+1)) <= 1e-6
        out(i+4*n)=Fcon(i+1)-0;
    elseif (Tg(i+1)-Twall(i+1)) <= 1e-3
        if Tg(i+1)-Twall(i+1) < 0
            Tg(i+1) = Twall(i+1);
        end
        out(i+4*n)=Fcon(i+1)-alcool*(Twall(i+1)-Tcool(i+1))/Hv;
    else
        out(i+4*n)=Fcon(i+1)-A*Dab(i+1)*P*log((1-ywall(1+i))/(1-ygas(i+1)));
        % ygas(i+1) = Fconb(i+1)/Fgas(i+1);
    end
end

% Mass Balance For Condensable in Gas phase
out(i+5*n)=Fconb(i)-Fconb(i+1)-Fcon(i+1);

% Finite Volume Moles Change Due to Temperature using IG EoS
out(i+6*n)=Fgas(i)-Fgas(i+1)-Fcon(i+1)+Vs*P*(R*(Tg(i+1))^2)*(Fgas(i)*Cpgas(i+1)*(Tg(i)-Tg(i+1))-alg(i+1)*(Tg(i+1)-Twall(i+1))-Fcon(i+1)*Hv)/(Ngas(i+1)*Cpgas(i+1));

end

% Update Heat Capacity, Heat Transfer Coefficients, and Diffusion Coefficient
for i=1:n
    % Heat Capacity
    T(i+1) = Tg(i+1) - 273; % T = initial temperature of gas in degrees Celsius
    % component 1 = nitrogen (noncondensable)
    if T(i+1)>0
        Cp1(i+1) = a1 + b1*T(i+1) + c1*T(i+1)^2 + d1*T(i+1)^3; % Cp of noncondensable in kJ/(mol*K)
    else
        Cp1(i+1) = a1;
        end
    Cp_1(i+1) = Cp1(i+1)*1000*9.486*10^-4/1.8/M1*1000/2.2; % Cp of noncondensable in Btu/(lb*degF)
    % component 2 = ethanol (condensable)
    if T(i+1)>0
        Cp2(i+1) = a2 + b2*T(i+1) + c2*T(i+1)^2 + d2*T(i+1)^3; % Cp of condensable in kJ/(mol*K)
    else
        Cp2(i+1) = a2;
    end
    Cp_2(i+1) = Cp2(i+1)*1000*9.486*10^-4/1.8/M2*1000/2.2; % Cp of condensable in Btu/(lb*degF)
    % calculate Cpgas as a weighted average of the component Cps
out(i+7*n) = (Fnc/Fgas(i+1)) * Cp1(i+1) + (Fconb(i+1)/Fgas(i+1)) * Cp2(i+1) - Cpgas(i+1); % kJ/(mol*K)
Cp_gas(i+1) = (Fnc*M1*Cp_1(i+1)+Fconb(i+1)*M2*Cp_2(i+1))/(Fnc*M1+Fconb(i+1)*M2); % Btu/(lb*degF)

% Heat Transfer Coefficient of Gas
Wg(i+1) = (Fnc*M1+Fconb(i+1)*M2)/1000*2.2*3600; % mass flow rate of gas in lb/hr
Ga(i+1) = Wg(i+1)/Ag; % mass flux of gas in lb/(hr*ft^2)
Reg(i+1) = De*Ga(i+1)/Visc_gas; % Reynolds number for gas
hgas(i+1) = hg(i+1)(9.486*10^-4)/1000/3600*(3.28^2)*1.8; % heat transfer coefficient for gas in kJ/(s*m^2*K)

% General Heat Transfer Coefficients
out(i+8*n) = 1/(1/hgas(i+1)+1/hfilm)*A - alg(i+1); % alpha for gas and film
U(i+1) = 1/(1/hgas(i+1) + 1/hfilm + 1/hcool); % overall heat transfer coefficient kJ/(s*m^2*K)

% Diffusion Coefficient
kd(i+1) = 0.0166 * (Tg(i+1))^(3/2)/ P / (v1^(1/3) + v2^(1/3))^2 * (1/M1 + 1/M2)^(1/2); % diffusivity in ft^2/hr
KD(i+1) = kd(i+1)/3600/3.28^2; % diffusivity in m^2/s
pg1(i+1) = (Fnc/Fgas(i+1))*P; % partial pressure of the inert gas in the gas body, atm
pg2(i+1) = P*10^((Aa-Ba/(Twall(i+1)-273+Ca))/760); % partial pressure of the inert gas at the condensate film, atm
pgf(i+1) = (pg2(i+1)-pg1(i+1))/log(pg2(i+1)/pg1(i+1)); % log mean pressure difference of the inert gas between pg1 and pg2, atm

Mm(i+1) = ((Fnc/Fgas(i+1))*M1 + (Fconb(i+1)/Fgas(i+1))*M2); % mean molecular weight of the vapor mixture, lb/lbmol
Dgas(i+1) = P*Mm(i+1)/0.7302/(1.8*Tg(i+1)); % density of gas in lb/ft^3
Kg(i+1) = hg(i+1)*((Cp_gas(i+1)*Visc_gas/kg)^(2/3))/(Cp_gas(i+1)*pgf(i+1)*Mm(i+1)*(Visc_gas/Dgas(i+1)/kd(i+1))^(2/3)); % diffusion coefficient in mol/(s*m^2*atm)

Dynamic Plot 1: PlotDynCond3.m

function []=PlotDynCond(t,y,n,Aa,Ba,Ca,P,a,R,Vs)
tfin = size(y);
for i=1:tfin
Ngas(i)=(y(i,a));
Tg(i)=(y(i,n+a));
Tcool(i)=(y(i,2*n+a));
Twall(i)=(y(i,3*n+a));
Fgas(i)=(y(i,4*n+a));
Fcon(i)=(y(i,5*n+a));
Fconb(i)=(y(i,6*n+a));
ygas(i)=Fconb(i)/Fgas(i);
ywall(i)=10^(Aa - Ba/(Twall(i)-273+Ca))/760/P;
diff(i)=Ngas(i)-Vs*P/(R*Tg(i));
end

figure(3);
subplot(2,3,4),plot(t,Fcon)
xlabel('Time (s)');
ylabel('Fcond (mol/s)');
Dynamic Plot 2: PlotDynError.m

function []=PlotDynCond(t,y,n,Aa,Ba,Ca,P,a,R,Vs)

    tfin = size(y);
    for i=1:tfin
        Ngas(i)=(y(i,a));
        Tg(i)=(y(i,n+a));
        Tcool(i)=(y(i,2*n+a));
        Twall(i)=(y(i,3*n+a));
        Fgas(i)=(y(i,4*n+a));
        Fcon(i)=(y(i,5*n+a));
        Fconb(i)=(y(i,6*n+a));
        ygas(i)=Fconb(i)/Fgas(i);
        ywall(i)=10^(Aa - Ba/(Twall(i)-273+Ca))/760/P;
        diff(i)=Ngas(i)-Vs*P/(R*Tg(i));
    end

    figure(4);
    subplot(2,3,4),plot(t,diff)
    xlabel('Time (s)');
    ylabel('NgasError (mol)');

    subplot(2,3,5),plot(t,ygas,'r')
    xlabel('Time (s)');
    ylabel('Ygas');

    subplot(2,3,6),plot(t,ywall,'g')
    xlabel('Time (s)');
    ylabel('Ywall');

    subplot(2,1,1),plot(t,Tg,':r',t,Tcool,'--b',t,Twall,'g')
    title('Temporary reponse of element a');
    xlabel('Time (s)');
    ylabel('Temp (K)');
    legend('Gas', 'Coolant', 'Wall');
function SimCondenser(Kc,Ti,Tsp,nt,THotin,TColdin);

% Condenser Geometry
L = 3; % total length in meters
n = 30; % number of volumes to integrate length over - must be even number
di = 0.019; % inner tube diameter in meters
wt = 0.001; % wall thickness in meters
do = di + wt; % outer tube diameter in meters
clr = 0.02; % clearance between coolant tubes in meters
pitch = clr + do; % pitch in meters
nt = 40; % number of tubes
B = L; % baffle spacing in meters
pt = 1; % square pitch: pt = 1, triangular pitch: pt = 2

% approximate shell diameter based on number of tubes and layout
if pt == 1
    number = 1; % number of tubes interior to square
    Area = pitch^2; % area of square in m^2
else
    number = 0.75; % number of tubes interior to triangle
    Area = 3*(1/2)*pitch^2; % area of triangle
end
element1 = nt/number;
element2 = int32(element1);
element3 = real(element2);
elements = element3 + 1; % number of square/triangle elements for number of tubes
Area_req = elements*Area; % total area of required square/triangle elements in m^2
ds = (4*3.14159*Area_req)^(1/2); % minimum required shell diameter in meters
nt1 = ds/pitch; % approximate number of tubes at center of shell
dz = L/n; % length increment
A = 3.14159*do^2*nt*dz; % contact surface area of element in m^2
A_tot = 3.14159*do^2*nt*L; % total contact surface area of condenser in m^2
V_t = 3.14159*di^2/4*nt*dz; % volume inside tube per element
V_w = 3.14159*do^2/4*(do^2-di^2)/4; % volume of wall per element
V_s = 3.14159*dz*(ds^2-nt*do^2)/4; % volume between shell and tube per element

% Operating Conditions
F_cool(1) = 15; % mass flowrate of coolant in kg/s
P = 1; % total pressure in atm

% Constants
R = 8.314; % ideal gas constant in (m^3*Pa)/(mol*K)
g = 9.81; % gravitational constant in m/s^2

% Boundary Conditions
T_g(1) = 350; % initial gas temperature in K
T_cool(1) = 230; % initial coolant temperature in K
T_wall(1) = 250; % initial wall temperature in K
F_gas(1) = 75; % initial molar flowrate of gas in mol/s
F_conb(1) = 15; % initial molar flowrate of condensables in gas in mol/s
F_con(1) = 0; % initial molar flowrate of condensate in mol/s
N_gas(1) = (Vs*P*101325)/(R*T_g(1)); % initial moles of gas
\[
F_{nc} = F_{gas(1)} - F_{conb(1)}; \text{ \% molar flowrate of noncondensables in gas in mol/s}
\]

% Initial Values
for i = 1:n
y0(i) = Ngas(1);
y0(i+n) = Tg(1)/1.05;
y0(i+2*n) = Tcool(1);
y0(i+3*n) = Twall(1);
y0(i+4*n) = Fgas(1);
y0(i+5*n) = Fcon(1);
y0(i+6*n) = Fconb(1);
end

% Properties
% reference: appendices of Kern: "Process Heat Transfer"
Dcool = 1000; \% density of coolant in kg/m^3
Dwall = 7830; \% density of wall in kg/m^3
Dcond = 789; \% density of condensate film in kg/m^3
Ccool = 4.184; \% Cp of coolant in kJ/(kg*K)
Cwall = 0.4; \% Cp of wall in kJ/(kg*K)
Cpc = 0.1031; \% Cp of condensate in kJ/(mol*K) (Felder and Rousseau 636)
Visc_gas = 0.018*2.42; \% gas viscosity at temperature of bulk gas lb/(ft*ft/hr)
Visc_gas_wt = 0.015*2.42; \% gas viscosity at wall temperature lb/(ft*ft/hr)
Visc_cond = 2.5*10; \% viscosity of condensate film in centipoise * 10 = kg/(m*s)
Visc_cool = 3.5*2.42; \% coolant viscosity at temperature of bulk medium in lb/(ft*ft/hr)
Visc_cool_wt = 2.5*2.42; \% coolant viscosity at wall temperature in lb/(ft*ft/hr)
M1 = 28; \% molecular weight of noncondensable (nitrogen) g/mol or lb/lbmol
M2 = 46.07; \% molecular weight of condensable (ethanol) g/mol or lb/lbmol
v1 = 2 * 15.6; \% molecular volume of noncondensable (nitrogen) (Kern 344)
v2 = 2 * 14.8 + 6 * 3.7 + 7.4; \% molecular volume of condensable (ethanol) (Kern 344)
Hv = 38.58; \% heat of vaporization of condensable in kJ/mol (Felder and Rousseau 630)
kg = 0.01; \% thermal conductivity of gas in Btu/(hr*ft*degreesF)
kf = 0.1/(9.486*10^-4)*1000/3600*3.28*1.8; \% thermal conductivity of film in kJ/(s*m*K)
kc = 0.3; \% thermal conductivity of coolant in Btu/(hr*ft*degreesF)

% Antoine Equation Coefficients for Condensable (ethanol)
Aa = 8.11220;
Ba = 1592.864;
Ca = 226.184;

% Calculations
Mc = Dcool*Vt; \% mass of coolant in an element in kg
Nwall = Dwall*Vw; \% mass of wall in a volume in kg
Cvel = Fcool(1)/Dcool/(nt*3.14159*dti^2/4); \% velocity of coolant stream in m/s
Tsat = Ba/(Aa*log10(Fconb(1)/Fgas(1)*P*760))-Ca+273; \% saturation temperature of vapor

% Unit Conversions
pt = pitch*3.2808*12; \% pitch in inches
do = dto*3.2808*12; \% outer diameter in inches
di = dti*3.2808*12; \% inner diameter in inches
cclr = clr*3.2808*12; \% clearance in inches
b = B*3.2808*12; \% baffle spacing in inches

% Calculate Maximum Allowable Outlet Gas Temperature
Pconb = Fconb(1)/Fgas(1)*P*101.325; % inlet vapor pressure of condensable, kPa

z = Tg(1)/293.4; % correction factor to operating temperature

if Pconb >= 40*z
    Tg_max = 248.2; % maximum allowable outlet gas temperature in K
elseif ((Pconb < 40*z)&(Pconb >= 20*z))
    Tg_max = 258.2;
elseif ((Pconb < 20*z)&(Pconb >= 10*z))
    Tg_max = 273.2;
elseif ((Pconb < 10*z)&(Pconb >= 7*z))
    Tg_max = 283.2;
elseif ((Pconb < 7*z)&(Pconb >= 3.45*z))
    Tg_max = 298.2;
else
    % fprintf('Outlet gas temperature not regulated. Specify maximum
    % value.')
    Tg_max = 298.2;
end

% Calculate Heat Capacity of Gas Mixture
% reference: Felder and Rousseau: "Elementary Principles of Chemical Processes" Table B.2

T = Tg(1) - 273; % T = initial temperature of gas in degrees Celsius

% component 1 = nitrogen (noncondensable)
% Cp nitrogen = a + b*T + c*T^2 + d*T^3 where T is in degrees C
a1 = 29 * 10^-3;
b1 = 0.2199 * 10^-5;
c1 = 0.5723 * 10^-8;
d1 = -2.871 * 10^-12;
if T>0 % correlation valid for T > 0 degrees C
    Cp1 = a1 + b1*T + c1*T^2 + d1*T^3; % Cp of noncondensable in kJ/(mol*K)
else
    Cp1 = a1;
end
Cp_1 = Cp1*1000*9.486*10^-4/1.8/M1*1000/2.2; % Cp of noncondensable in Btu/(lb*degF)

% component 2 = ethanol (condensable)
% Cp ethanol = a + b*T + c*T^2 + d*T^3 where T is in degrees C
a2 = 61.34 * 10^-3;
b2 = 15.72 * 10^-5;
c2 = -8.749 * 10^-8;
d2 = 19.83 * 10^-12;
if T>0
    Cp2 = a2 + b2*T + c2*T^2 + d2*T^3; % Cp of condensable in kJ/(mol*K)
else
    Cp2 = a2;
end
Cp_2 = Cp2*1000*9.486*10^-4/1.8/M2*1000/2.2; % Cp of condensable in Btu/(lb*degF)

% calculate Cpgas as a weighted average of the component Cps
Cpgas = (Fnc/Fgas(1)) * Cp_1 + (Fconb(1)/Fgas(1)) * Cp_2; % kJ/(mol*K)
Pgas = (Fnc*M1*Cp_1+Fconb(1)*M2*Cp_2)/(Fnc*M1+Fconb(1)*M2); % Btu/(lb*degF)

% Calculate Heat Transfer Coefficient for Gas
if \( pt \) == 1
\[
de = 4 \times \left( pt^2 - 3.14159 \times do^2 \right) / 3.14159 / do; \quad \text{% equivalent diameter in inches}
\]
else
\[
de = 4 \times \left( 0.5 \times pt^2 - 0.5 \times 3.14159 \times do^2 \right) / 0.5 \times 3.14159 / do; \quad \text{end}
\]
\[
De = de / 12; \quad \text{% equivalent diameter in feet}
\]
\[
Ag = di \times clrc \times b / pt / 144; \quad \text{flow area of gas in ft}^2
\]
\[
Wg = (Fnc \times M1 + Fconb(1) \times M2) / 1000 \times 2.2 \times 3600; \quad \text{mass flow rate of gas in lb/hr}
\]
Ga = Wg / Ag; \quad \text{mass flux of gas in lb/(hr*ft^2)}
\]
\[
Reg = De \times Ga / Visc_gas; \quad \text{Reynolds number for gas}
\]
\[
hg = \text{heat transfer coefficient for gas in Btu/(hr*ft^2*degreesF)} \quad \text{for 2000 < Reg < 1,000,000}
\]
\[
hg = 0.36 \times \text{Reg}^{0.55} \times (Cp_gas \times Visc_gas / kg)^{(1/3)} \times (Visc_gas / Visc_gas_wt)^{0.14} \times kg / De;
\]
\[
hgas = hg / (9.486 \times 10^{-4} / 1000 / 3600) / 3.28^2 / 1.8; \quad \text{heat transfer coefficient for gas in kJ/(s*m^2*K)}
\]
\[
\]
% Calculate Heat Transfer Coefficient for Condensate Film
% reference: Perry's Chemical Engineer's Handbook p. 5-20, 11-11
\]
\[
delta T = T_sat - T_wall(1); \quad \text{temp difference between sat'd vapor and surface in K}
\]
\[
h1film = \text{heat transfer coefficient for film with 1 tube in kJ/(s*m^2*K)}
\]
\[
h1film = 0.73 \times k_f / dt_t \times (d_t_t^3 \times \text{Dcond}^2 \times g \times H_v) / (k_f \times Visc_cond \times \delta T \times M_2 / 1000) / (1/4);
\]
\[
nt_2 = 2/3 \times nt_1; \quad \text{% 2/3 of max number of tubes across diameter}
\]
\[
nit_3 = \text{int3(nt2)}; \quad \text{% truncate to integer value}
\]
\[
N = \text{real(nt3)}; \quad \text{% convert to real number}
\]
\[
hfilm = h1film \times N^{-1/4}; \quad \text{correction for multiple tubes, kJ/(s*m^2*K)}
\]
\[
\]
% Calculate Heat Transfer Coefficient for Coolant
% reference: Kern: "Process Heat Transfer" p. 103-105
\]
\[
Ac = 3.14159 \times dt_i^2 / 4 \times 3.2808^2; \quad \text{flow area of coolant in ft}^2
\]
\[
Wc = F_cool(1) / nt \times 3600 \times 2.2; \quad \text{mass flow rate of coolant per tube in lb/hr}
\]
\[
Gc = Wc / Ac; \quad \text{mass flux of coolant per tube in lb/(hr*ft^2)}
\]
\[
Rec = dt_i \times Gc / Visc_cool; \quad \text{Reynolds number for coolant}
\]
\[
c = C_cool \times 1000 \times (9.486 \times 10^{-4}) / 2.2 / 1.8; \quad \text{specific heat of cold fluid in Btu/(lb*degreesF)}
\]
\[
hc = \text{heat transfer coefficient for coolant in Btu/(hr*ft^2*degreesF)}
\]
\[
% note: eqs. valid for organic liquids, aqueous solutions, and gases, but not for water
\]
\[
% if Rec > 2100
hc = 0.027 \times \text{Rec}^{0.8} \times (c \times Visc_cool / kc) / (1/3) / (Visc_cool / Visc_cool_wt) \times 0.14 / kc / dt_i;
\]
\[
% else
hc = 1.86 / (Rec \times c \times Visc_cool / dt_i / L) / (1/3) / (Visc_cool / Visc_cool_wt) \times 0.14 / kc / dt_i;
\]
\[
% end
hcoolant = hc / (9.486 \times 10^{-4} / 1000 / 3600 / 3.28^2 / 1.8); \quad \text{heat transfer coefficient for coolant in kJ/(s*m^2*K)}
\]
\[
% correct to outer diameter of tube rather than inner diameter
hcool = hcoolant * dt_i / dt_o; \quad \text{heat transfer coefficient for coolant in kJ/(s*m^2*K)}
\]
\[
\]
% Calculate General Heat Transfer Coefficients
alcool = hcool * A; \quad \text{% alpha for cooling fluid}
\]
\[
alg = 1 / (1 / hg + 1 / hfilm) * A; \quad \text{% alpha for gas and film}
\]
\[
U = 1 / (1 / hg + 1 / hfilm + 1 / hcool); \quad \text{% overall heat transfer coefficient kJ/(s*m^2*K)}
\]
\[
\]
% Calculate Diffusion Coefficient
% reference: Kern: "Process Heat Transfer" p. 343-344

% calculate diffusivity using Gilliland correlation
kd = 0.0166 * (Tg(1))^(3/2) / P / (v1(1/3) + v2(1/3))^2 * (1/M1 + 1/M2)^2; % ft^2/hr
KD = kd/3600/3.28^2; % diffusivity in m^2/s

% calculate diffusion coefficient
pg1 = (Fnc/Fgas(1))*P; % partial pressure of the inert gas in the gas body, atm
pg2 = P-(10^(Aa-Ba/(Twall(1)-273+Ca)))/760; % partial pressure of the inert gas at the condensate film, atm
pgf = (pg1-pg2)/log(pg2/pg1); % log mean pressure difference of the inert gas between pg1 and pg2, atm
Mm = ((Fnc/Fgas(1))*M1 + (Fconb(1)/Fgas(1))*M2); % mean molecular weight of the vapor mixture, lb/lbmol
Dgas = P*Mm/0.7302/(1.8*Tg(1)); % density of gas in lb/ft^3
% Kg = diffusion coefficient in lbmol/(hr*ft^2*atm)
Kg = hg*((Cp_gas*Visc_gas/kg)^(2/3))/(Cp_gas*pgf*Mm*(Visc_gas/Dgas(1)/kd)^(2/3));
Dab = Kg*(3.2808^2)/3600*453.593; % diffusion coefficient in mol/(s*m^2*atm)

% Steady State Solution
options0 = optimset('Display','iter','MaxFunEvals',1e5);
[yss,fval,exitflag] = fsolve(@CondenserSS8b,y0,options0,Tg,Tcool,Twall,Fgas,Fcon,Fconb,Fnc,Fcool,A,alcool,Vs,P,R,Mc,Ccool,Cwall,Cpc,Nwall,Al,Alcool,Hv,Cpc);
yss;
yss(7*n+1) = 0; % set integral value Io = 0

% Plot Results
PlotSST3b(yss,n,Aa,Ba,Ca,P,dz,Tg,Tcool,Twall,Fgas,Fcon,Fconb,alg,alcool,Hv,Cpc);

% Extract Variables from Steady State Solution
for i=1:n
    Ngas(i+1) = real(yss(i));
    Tg(i+1) = real(yss(i+n));
    Tcool(i+1) = real(yss(i+2*n));
    Twall(i+1) = real(yss(i+3*n));
    Fgas(i+1) = real(yss(i+4*n));
    Fcon(i+1) = real(yss(i+5*n));
    Fconb(i+1) = real(yss(i+6*n));
ygas(i+1) = Fconb(i+1)/Fgas(i+1);
end

% Error Calculations
Input=(Fgas(1));
TotalCond=trapz(Fcon);
FgasO=Fgas(n+1);
FcondbO=Fconb(n+1);%
Accumulated=Vs*101325/(R*Tg(n+1)^2)*(Tg(1)-Tg(n+1));
Output=TotalCond+FgasO+Accumulated;
Fconblein=Fconb(1);
CondbleError=(abs(CAbsErr))/(Fconblein)
NonCondError=Fnc-(FgasO*(1-ygas(n+1)));

% Dynamic Solution
kc = .1;
Ti = 1.5;
Tsp = Tg_max-5; % temperature set point in K
tend = 240;
Mstep = tend/100;
tspan = [0:tend]; % time horizon integrated

nalg = 3; % number of algebraic eq
ndiff = 4; % number of differential equations

M = zeros((nalg+ndiff)*n:(nalg+ndiff)*n); % mass matrix for DAE

for j=1:(ndiff)*n
    M(j,j) = 1;
end

M((ndiff+nalg)*n + 1, (ndiff+nalg)*n + 1) = 1; % control

options = odeset('Mass',M,'Refine',5,'MaxStep',Mstep);

[t,y] = ode15s(@CondenserDyn8b,tspan,yss,options,Tg,Tcool,Twall,Fgas,Fcon,Fconb,Fnc,Fcool,A,alcool,Vs,P,R,Mc,Ccool,Cwall,Cpc,Nwall,Aa,Ba,Ca,Hv,Ngas,n,alg,Cpgas,Dab,Tsp,kc,Ti);

% Plot Results
a = n; % length to be displayed in time
PlotDynCond3(t,y,n,Aa,Ba,Ca,P,a,R,Vs);
PlotDynError(t,y,n,Aa,Ba,Ca,P,a,R,Vs);
PlotDynCondControl(t,y,n,Aa,Ba,Ca,P,a,R,Vs,Tsp,kc,Ti,Fcool);

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
Steady State Solution: CondenserSS8b.m

function [out] = CondenserSS8b(y,Tg,Tcool,Twall,Fgas,Fcon,Fconb,Fnc,Fcool,A,alcool,Vs,P,R,Mc,Ccool,Cwall,Cpc,Nwall,Aa,Ba,Ca,Hv,n,alg,Cpgas,Dab)

% Variables Declaration
for i=1:n
    Ngas(i+1) = real(y(i));
    Tg(i+1) = real(y(i+n));
    Tcool(i+1) = real(y(i+2*n));
    Twall(i+1) = real(y(i+3*n));
    Fgas(i+1) = real(y(i+4*n));
    Fcon(i+1) = real(y(i+5*n));
    Fconb(i+1) = real(y(i+6*n));
end

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% System of Equations Declaration

% Differential Equations
for i=1:n
    % Mass Balance For Gas
    out(i)=Fgas(i)-Fgas(i+1)-Fcon(i+1);

    % Gas energy Balance
    out(i+n)=(Fgas(i)*Cpgas*(Tg(i)-Tg(i+1))-alg*(Tg(i+1)-Twall(i+1))-Fcon(i+1)*Hv)/(Ngas(i+1)*Cpgas);

    % Coolant energy Balance
    out(i+2*n)=(Fcool(1)*Ccool*(Tcool(i)-Tcool(i+1))+alcool*(Twall(i+1)-Tcool(i+1)))/(Mc*Ccool);

    % Wall energy Balance
out(i+3*n)=(alg*(Tg(i+1)-Twall(i+1))+Fcon(i+1)*(Hv+Cpc*(Tg(i+1)-Twall(i+1)))-alcool*(Twall(i+1)-Tcool(i+1)))/(Nwall*Cwall);
end

% Algebraic Equations
for i=1:n
    ywall(i+1)=10^(Aa - Ba/(Twall(i+1)-273+Ca))/760/P;
ygas(i+1)=Fconb(i+1)/Fgas(i+1);
% Diffusion Equation
if (ygas(i+1)-ywall(i+1)) <= 1e-6
    out(i+4*n)=Fcon(i+1)-0;
elseif (Tg(i+1)-Twall(i+1)) <= 1e-3
    if Tg(i+1)-Twall(i+1) < 0
        Tg(i+1) = Twall(i+1);
    end
    out(i+4*n)=Fcon(i+1)-alcool*(Twall(i+1)-Tcool(i+1))/Hv;
else
    out(i+4*n)=Fcon(i+1)-A*Dab*P*log((1-ywall(i+1))/(1-ygas(i+1)));
end
% Mass Balance For Condensable in Gas phase
out(i+4*n)=Fconb(i)-Fconb(i+1)-Fcon(i+1);
% Finite Volume Moles Change Due to Temperature using IG EoS
out(i+6*n)=Ngas(i+1)-Vs*P/(R*Tg(i+1));
end

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
out=out';
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

Steady State Plot: PlotSS3b.m

function []=PlotSS3b(yss,n,Aa,Ba,Ca,P,dz,Tg,Tcool,Twall,Fgas,Fcon,Fconb,alg,alcool,Hv,Cpc);

%Variables Declaration
for i=1:n
    Tg(i)=real(yss(i+n));
    Tcool(i)=real(yss(i+2*n));
    Twall(i)=real(yss(i+3*n));
    Fgas(i)=real(yss(i+4*n));
    Fcon(i)=real(yss(i+5*n));
    Fconb(i)=real(yss(i+6*n));
end

for i=1:n
    ygas(i)=Fconb(i)/Fgas(i);
    ywall(i)=10^(Aa - Ba/(Twall(i)-273+Ca))/760/P;
end
le=1:n;
lee=0+dz*le;
figure(1);
subplot(4,1,1),plot(lee,Tcool,'--',lee,Tg,'.:r',lee,Twall,'g')
title('Steady State Condenser');
legend('coolant', 'gas', 'wall');
% xlabel('Length');
ylabel('Temp (K)')
subplot(4,1,2),plot(lee,ygas,'.:r',lee,ywall,'g')
% title('Fg out vs L');
legend('gas', 'wall');
% xlabel('Time');
ylabel('VOC Conc. (mol fr.)')

subplot(4,1,3),plot(lee,Fconb,'g')
% title('Control vs time');
% xlabel('Length (m)');
ylabel('Fconb (mol/s)')

subplot(4,1,4),plot(lee,Fcon,'b')
% title('Control vs time');
% xlabel('Length (m)');
ylabel('Fcon (mol/s)')

figure(2);
qgas=alg*(Tg-Twall);
qcond=Fcon.*(Hv+Cpc*(Tg-Twall));
diff=qdisp-qgas;

subplot(3,1,1),plot(lee,qgas)
% title('Steady State Condenser');
% xlabel('Length');
ylabel('Qgas (kJ/s)')

subplot(3,1,2),plot(lee,qcond,lee,diff,'r.')
% title('Fg out vs L');
% xlabel('Time');
ylabel('Qcond (kJ/s)')

subplot(3,1,3),plot(lee,qdisp)
% title('Control vs time');
% xlabel('Length (m)');
ylabel('Qdisp (kJ/s)')

**Dynamic Solution: CondenserDyn8b.m**

function [out] = CondenserDyn8b(t,y,Tg,Tcool,Twall,Fgas,Fcon,Fconb,Fnc,Fcool,A,alcool,Vs,P,R,Mc,Ccool,Cwall,Cpc,Nwall,Aa,Ba,Ca,Hv,Ngas,n,alg,Cpgas,Dab,Tsp,kc,Ti)

% Variables Declaration
for i=1:n
   Ngas(i+1) = real(y(i));
   Tg(i+1) = real(y(i+n));
   Tcool(i+1) = real(y(i+2*n));
   Twall(i+1) = real(y(i+3*n));
   Fgas(i+1) = real(y(i+4*n));
   Fcon(i+1) = real(y(i+5*n));
   Fconb(i+1) = real(y(i+6*n));
end

I = real(y(7*n+1));
% Simulation Changes
Tcool0 = Tcool(1);
if t >= 120
    Tcool(1) = 0.98*Tcool0;
end

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

% System of Equations Declaration
% Differential Equations
for i=1:n

% Mass Balance For Gas
out(i)=-Vs*P/(R*(Tg(i+1))^2)*(Fgas(i)*Cpgas*(Tg(i)-Tg(i+1))-alg*(Tg(i+1)-Twall(i+1))-
Fcon(i+1)*Hv)/(Ngas(i+1)*Cpgas);

% Gas energy Balance
out(i+n)=(Fgas(i)*Cpgas*(Tg(i)-Tg(i+1))-alg*(Tg(i+1)-Twall(i+1))-Fcon(i+1)*Hv)/(Ngas(i+1)*Cpgas);

% Coolant energy Balance
du = kc*(Tg(n+1)-Tsp+I);
if (Fcool(1)+du) <= 1e-3
    out(i+2*n)=(1e-3*Ccool*(Tcool(i)-Tcool(i+1))+alcool*(Twall(i+1)-Tcool(i+1)))/(Mc*Ccool);
else
    out(i+2*n)=((Fcool(1)+du)*Ccool*(Tcool(i)-Tcool(i+1))+alcool*(Twall(i+1)-Tcool(i+1)))/(Mc*Ccool);
end

% Wall energy Balance
out(i+3*n)=(alg*(Tg(i+1)-Twall(i+1))+Fcon(i+1)*(Hv+Cpc*(Tg(i+1)-Twall(i+1)))-alcool*(Twall(i+1)-Tcool(i+1)))/(Nwall*Cwall);
end

% Algebraic Equations
for i=1:n

ywall(i+1)=10^(Aa - Ba/(Twall(i+1)-273+Ca))/760/P;
ygas(i+1)=Fconb(i+1)/Fgas(i+1);

% Diffusion Equation
if (ygas(i+1)-ywall(i+1)) <= 1e-6
    out(i+4*n)=Fcon(i+1)-0;
elseif (Tg(i+1)-Twall(i+1)) <= 1e-3
    if Tg(i+1)-Twall(i+1) < 0
        Tg(i+1) = Twall(i+1);
    end
    out(i+4*n)=Fcon(i+1)-alcool*(Twall(i+1)-Tcool(i+1))/Hv;
else
    out(i+4*n)=Fcon(i+1)-A*Dab*P*log((1-ywall(1+i))/(1-ygas(i+1)));
end

% Mass Balance For Condensable in Gas phase
out(i+5*n)=Fconb(i)-Fconb(i+1)-Fcon(i+1);

% Finite Volume Moles Change Due to Temperature using IG EoS
out(i+6*n)=Fgas(i)-Fgas(i+1)-Fcon(i+1)+Vs*P/(R*(Tg(i+1))^2)*(Fgas(i)*Cpgas*(Tg(i)-Tg(i+1))-alg*(Tg(i+1)-Twall(i+1))-Fcon(i+1)*Hv)/(Ngas(i+1)*Cpgas);
end

% Control
out(7*n+1) = (Tg(n+1)-Tsp)*Ti; % dl/dt = e*Ti
Dynamic Plot 1: PlotDynCond3.m (See Dynamic Model Code)

Dynamic Plot 2: PlotDynError.m (See Dynamic Model Code)

Dynamic Controller Plot: PlotDynCondControl.m

function []=PlotDynCondControl(t,y,n,Aa,Ba,Ca,P,a,R,Vs,Tsp,kc,Ti,Fcool)

tfin = size(y);

for i=1:tfin
Ngas(i)=(y(i,a));
Tg(i)=(y(i,n+a));
Tcool(i)=(y(i,2*n+a));
Twall(i)=(y(i,3*n+a));
Fgas(i)=(y(i,4*n+a));
Fcon(i)=(y(i,5*n+a));
Fconb(i)=(y(i,6*n+a));
error(i) = Tg(i)-Tsp;
I(i) = y(i,7*n+1);
du(i) = kc*(error(i)+I(i));
Fcool_control(i) = Fcool(1)+du(i);
end

figure(5);

subplot(2,2,1),plot(t,Tg,'.:r',t,Tcool,'--b',t,Twall,'g')
title('Temporary response of element a')
xlabel('Time (s)');
ylabel('Temp (K)');
legend('Gas', 'Coolant', 'Wall');

subplot(2,2,2),plot(t,Tg,'r')
xlabel('Time (s)');
ylabel('Gas Temp (K)');

subplot(2,2,3),plot(t,error,'r')
xlabel('Time (s)');
ylabel('Error (K)');

subplot(2,2,4),plot(t,Fcool_control,'b')
xlabel('Time (s)');
ylabel('Coolant Flowrate (kg/s)');
APPENDIX VI: Steady State Uncertainty Evaluation

Independent Variation of One Variable (Cpgas, hgas, Dab constant)

Data resulting from the independent variation of one variable in the steady state model is shown in Table A6.1.

Table A6.1: Simulation Data for SS Uncertainty Evaluation: Independent Variation of One Variable (Cpgas, hgas, Dab constant with position)

<table>
<thead>
<tr>
<th>Tg_in</th>
<th>Tcool_in</th>
<th>Fconb_in</th>
<th>hgas</th>
<th>Dab</th>
<th>Tg_out</th>
<th>Tcool_out</th>
<th>Fconb_out</th>
<th>Accum</th>
<th>Error_C</th>
<th>Error_NC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nominal</td>
<td>350</td>
<td>230</td>
<td>15</td>
<td>0.1326</td>
<td>3.9935</td>
<td>266.37</td>
<td>234.23</td>
<td>9.56</td>
<td>0.912</td>
<td>0.491</td>
</tr>
<tr>
<td>Change</td>
<td>349</td>
<td>230</td>
<td>15</td>
<td>0.1326</td>
<td>3.9897</td>
<td>265.46</td>
<td>234.22</td>
<td>9.56</td>
<td>0.917</td>
<td>0.490</td>
</tr>
<tr>
<td>351</td>
<td>230</td>
<td>15</td>
<td>0.1327</td>
<td>3.9973</td>
<td>267.27</td>
<td>234.23</td>
<td>9.55</td>
<td>0.907</td>
<td>0.491</td>
<td></td>
</tr>
<tr>
<td>352</td>
<td>230</td>
<td>15</td>
<td>0.1327</td>
<td>4.0011</td>
<td>268.17</td>
<td>234.26</td>
<td>9.55</td>
<td>0.902</td>
<td>0.491</td>
<td></td>
</tr>
<tr>
<td>353</td>
<td>230</td>
<td>15</td>
<td>0.1327</td>
<td>4.0049</td>
<td>269.08</td>
<td>234.28</td>
<td>9.54</td>
<td>0.897</td>
<td>0.491</td>
<td></td>
</tr>
<tr>
<td>354</td>
<td>230</td>
<td>15</td>
<td>0.1328</td>
<td>4.0087</td>
<td>269.98</td>
<td>234.30</td>
<td>9.54</td>
<td>0.892</td>
<td>0.492</td>
<td></td>
</tr>
<tr>
<td>355</td>
<td>230</td>
<td>15</td>
<td>0.1328</td>
<td>4.0124</td>
<td>270.89</td>
<td>234.32</td>
<td>9.54</td>
<td>0.887</td>
<td>0.492</td>
<td></td>
</tr>
<tr>
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Matlab files: SimCondenser_Eval_07_20_04.m, CondenserSS_Eval.m, PlotSS_Eval.m
Independent Variation of One Variable (Cpgas, hgas, Dab change with position)

Data resulting from the independent variation of one variable in the steady state model is shown in Table A6.2.

Table A6.2: Simulation Data for SS Uncertainty Evaluation: Independent Variation of One Variable (Cpgas, hgas, Dab change with position)

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Matlab files: SimCondenser_Eval4_07_23_04_loop.m, CondenserSS_Eval4.m, PlotSS_Eval.m

Cpgas, hgas, Dab change with position
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<td>236.61</td>
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<td>0.884</td>
<td>0.430</td>
<td>-7.1E-15</td>
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<td>1.6</td>
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</table>

Data from the simultaneous variation of two variables in the steady state model is shown in Table A6.3.