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Enhancement of heat transfer in an adsorbent bed

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**ENHANCEMENT OF HEAT TRANSFER
IN AN ADSORBENT BED**

A Thesis

Presented to

**The Faculty of the Department of
Chemical and Materials Engineering
San Jose State University**

**In Partial Fulfillment
Of the Requirements for the Degree
Masters of Science**

**By
Francesco Corral
August, 2001**

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ABSTRACT

ENHANCEMENT OF HEAT TRANSFER IN AN ADSORBENT BED

By Francesco Corral

The efficiency, as represented by the Coefficient of Performance (COP), of adsorption heat pumps must be increased in order for such devices to compete with the ubiquitous mechanical vapor compression heat pumps. To increase the COP, an adsorption heat pump design needs to improve heat transfer within the adsorption beds. Metal gauze was bonded to the heating medium to distribute heat throughout an adsorption bed and increase the COP.

The metal gauze minimized the COP dependency on the adsorbent thermal conductivity. An ideal pin size was 0.1 mm. The ideal volume ratio of pin fins to adsorbent material was 20%. Time variation simulations had quick rise to the maximum and then a steady decrease in COP. Finally, a comparative simulation indicated that activated carbon achieved a higher COP than Zeolite 13X. The metal gauze design allows exploration of adsorbents with low thermal conductivity, but high adsorptive capacity.

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LIST OF SYMBOLS

Symbol	Definition
A	Vapor specific volume, dimensionless
A_C	Heat exchanger/adsorbent contact area, (mm^2)
b	Tube wall thickness of HTF pipe, (m)
Bi	Biot number, dimensionless
Bi_c	Contact Biot number, dimensionless
C_a	Specific heat of adsorbent, (kJ/kg K)
C_{av}	Heat of vaporization, dimensionless
C_{fl}	Specific heat of heat transfer fluid, (kJ/kg K)
C_p	Vapor specific heat, dimensionless
C_{Pr}	Compression work, dimensionless
$C_{p,v}$	Specific heat of refrigerant vapor, ($\text{kJ/kg } ^\circ\text{C}$)
C_{if}	HTF pipe thermal capacitance, dimensionless
C_t	Specific heat of the HTF pipe, (kJ/kg K)
c	Condenser
COP_C	Coefficient of Performance for cooling
COP_H	Coefficient of Performance for heating
$d_{\max}$	Maximum distance from heat exchanger to any position within the adsorbent bed, (mm)
e	Evaporator

Fo	Fourier number, dimensionless
Ho	Time ratio, dimensionless
h	Heat transfer coefficient, ($\text{W}/\text{m}^2 \text{ K}$)
h_a	Contact heat transfer coefficient at tube/adsorbent interface, ($\text{W}/\text{m}^2 \text{ K}$)
h_η	Convective heat transfer coefficient at fluid/tube interface, ($\text{W}/\text{m}^2 \text{ K}$)
h_{av}^s	Specific enthalpy of refrigerant, (kJ/kg)
k	Thermal conductivity, ($\text{W}/\text{m K}$)
k_a	Thermal conductivity of adsorbent, ($\text{W}/\text{m K}$)
k_η	Thermal conductivity of heat transfer fluid, ($\text{W}/\text{m K}$)
kg_a	Mass of adsorbent, (kg)
kg_r	Mass of adsorbate, (kg)
K	Kelvin
L	Length of the adsorbent bed, (m)
N_l	Aspect ratio, dimensionless
NTU	Number of Transfer Units, dimensionless
P_c	Condenser pressure, (kPa)
Pe	Peclet number, dimensionless
Q	Heat transfer, (kJ)
Q_{cd}	Condenser heat transfer, (kJ)
Q_{ev}	Evaporator heat transfer, (kJ)
SCP	Specific cooling power, (W/kg)
r_a	Radius of adsorbent, (m)

r_t	Inside radius of the HTF pipe, (m)
T_h	Highest temperature, (K)
T_{hr}	Heater temperature, (K)
T_{cool}	Cooler temperature, (K)
T_{Lift}	Temperature difference between evaporator and condenser, (K), $T_{Lift} = T_{Ev} - T_{Cd}$
t^s_t	Time to saturation, (sec)
t_c	Cycle time, (s)
u_a	Adsorbent internal energy, (kJ/kg)
u_r	Refrigerant internal energy, (kJ/kg)
V_{ADS}	Volume of adsorbent, (mm ³)
V_{fl}	Heat transfer fluid velocity, (m/s)
v	Refrigerant velocity, (m/s)
ϵ	Void volume, dimensionless
κ	Permeability, (m ²)
θ	Dimensionless bed temperature
ϕ	Dimensionless fluid temperature
ρ	Density, (kg/m ³)
ρ_a	Density of adsorbent, (kg/m ³)
ρ_{fl}	Density of the heat transfer fluid, (kg/m ³)
ρ_r	Density of adsorbate, (kg/m ³)

ρ_t	Density of HTF pipe, (kg/m ³)
ρ_v^s	Density of saturated refrigerant, (kg/m ³)
$Re_{\sqrt{\kappa}}$	Reynolds number with permeability, dimensionless
η_{Carnot}	Carnot thermodynamic efficiency
Ωt	Tube resistance, dimensionless
μ	Dynamic Viscosity, (N s/m ²)
ω	Adsorption level, (kg _r /kg _a)

LIST OF ACRONYMS/ABBREVIATIONS

CFC	Chlorofluorocarbon
CFC-12	Dichlorodifluoromethane
COP	Coefficient of Performance
HCFC	Hydro-chlorofluorocarbon
HTF	Heat transfer fluid
HVAC	Heating Ventilating and Air Conditioning

Enhancement of Heat Transfer in an Adsorbent Bed

1. Introduction

1.1 Introduction to Heat Pumps

Heat pumps transfer heat from a cold temperature source to a warm temperature source. Depending upon the application, the heat pump is used to remove or add heat to a system. Heat pumps accomplish their tasks with the aid of a circulating fluid medium, called the working fluid or refrigerant. Figure 1 (Cengel and Boles, 1998) shows the flow path of the refrigerant for a standard vapor compression cycle.

Figure 1: Process flow for ideal vapor-compression refrigeration cycle, (Cengel and Boles, 1998)

Figure 2 is the corresponding temperature vs. entropy diagram for this process. The vapor compression refrigeration cycle consists of the following steps. A very low

Figure 2: Temperature (T) vs. Entropy (S) diagram for ideal vapor-compression refrigeration cycle (Cengel and Boles, 1998)

temperature and pressure refrigerant vapor enters a compressor (1). The compressor pressurizes and heats the refrigerant. Hot refrigerant vapor (2) then enters a condenser, where it cools and condenses, as heat is rejected. Heat from the condenser (Q_{cd}) warms the surrounding medium, either the outdoor environment or some indoor space. The liquid refrigerant (3) then passes through a Joule-Thomson expansion valve, which reduces the pressure and temperature. Cold refrigerant (4) flows through an evaporator, boiling as it absorbs heat (Q_{ev}) from a cool space. Finally, the refrigerant vapor re-enters the compressor, thus completing the thermodynamic cycle.

The COP is a measure of the heat pump efficiency. COP is defined as the ratio of net heat transferred at the lower temperature to the net work into the heat pump, W_{in} .

$$\text{COP} = \frac{Q}{W_{\text{in}}} \quad (1)$$

Displaced heat is either from the cooling process, Q_{ev} , or heating process, Q_{cd} , which characterizes the heat pump either as an air conditioner or as a heater. Net work is the energy supplied to the compressor for mechanical vapor compression or the energy supplied to the heating element for adsorption heat pumps.

1.2 Adsorption Heat Pumps

1.2.1 History of Adsorption Heat Pumps

Michael Faraday first demonstrated solid-vapor adsorption refrigeration in 1848 (Miles and Shelton 1991). Faraday noticed a pressure decrease as vapor was passed over an adsorbent material. Faraday also noticed an increase in pressure as heat was applied to the adsorbent. In 1929, Miller devised a refrigeration system based on Faraday's discovery (Miller 1929). Miller's refrigeration device marks the transition of theory and laboratory data into practical application. Beds of solid adsorbent are employed for the same purpose as mechanical compressors in vapor compression systems; to compress the refrigerant vapor. The power source for solid-vapor adsorption systems can be solar energy, natural gas, or electricity. Early designs required no electricity, an important feature in the days before national electrification. The last milestone (1970s) is the development of regeneration, which is the use of waste heat rejected from an adsorption bed during its cooling phase for partially heating another adsorption bed during its respective heating phase. Early, non-regenerative, single-bed, adsorption heat pumps

functioned at a 0.4 COP value (Shelton, et al. 1988). Regeneration techniques now allow these devices to operate at COP near 1.0. Discovery of the adsorption process and the first practical design mark the beginning of the adsorption heat pump and regeneration marks a major improvement in COP.

Dichlorodifluoromethane (CFC-12, the first freon) was developed in 1931 and allowed mechanical vapor compression (reversed Rankine cycle) to displace solid vapor adsorption cooling techniques. Before freons and national electrification, adsorption pumps served the heating and cooling market (Shelton, et al. 1988). Freons allowed mechanical vapor compression to operate at a higher efficiency than the adsorption heat pumps. Nearly fifty years passed before interest in the adsorption heat pumps was rekindled by concerns over the ozone depletion potential of CFC and HCFC refrigerants and the prospect of energy savings. These potential environmental and economic advantages will continue to drive research in adsorption heat pumps.

1.2.2 Process Description

Figure 3 illustrates the process flow for the heating of a cold adsorbent bed 1 in an adsorption refrigeration cycle. The system includes parallel bed adsorbers, which switch between adsorption and desorption operation. In the first phase of the two-part refrigeration cycle, adsorption bed #1 is cool (adsorption), while adsorption bed #2 is hot (desorption). Heat transfer fluid (HTF) from the fluid heater enters adsorption bed #1

through tubing, thereby heating the bed. Figure 4 displays the tubing coil (HTF pipe) running through an adsorption bed. HTF flows from adsorption bed #1 to the fluid cooler

Figure 3: Adsorption Heat Pump Flow Diagram (Heating Adsorbent Bed 1)

to reduce its temperature. The HTF then passes into bed #2, where it cools the adsorbent. Finally, the HTF returns to the boiler, which supplies make-up heat to complete the HTF thermal cycle.

Figure 4: Adsorbent Bed with HTF Coil

As the heated adsorbent (e.g. activated carbon) in bed #1 approaches the peak cycle temperature, the adsorbent begins to release trapped refrigerant vapor (e.g., ammonia) at an elevated pressure. Once the pressure exceeds the condenser pressure, the refrigerant flows from bed #1 into the condenser as a hot pressurized vapor. The condenser cools and condenses the refrigerant. The liquid refrigerant passes through the expansion (throttling) valve becoming a low pressure, very low temperature, and liquid-vapor mixture. This mixture then flows into the evaporator, where it absorbs heat from the

space being cooled and boils, emerging as a low-pressure vapor. Refrigerant finally enters bed #2 and adsorbs onto the adsorbent at low temperature and pressure. After adsorption bed #2 reaches the cycle time, the HTF pump reverses direction, beginning the second (reversed) phase of the cooling cycle in which the now hot bed #1 is cooled and the now cool bed #2 is heated. Figure 5 illustrates the system configuration for cooling of a warm bed #1. HTF now flows in the reverse direction, and bed #2 discharges refrigerant at the peak cycle temperature.

1.2.3 Economic Significance

Adsorption heat pumps provide an alternative to mechanical vapor compression devices for refrigeration and space heating applications. Common mechanical vapor compression requires electricity, an expensive energy source, to compress the refrigerant. Adsorption systems demand only a fraction of the electrical energy and rely upon plentiful, inexpensive, and clean burning natural gas or even solar energy to compress the refrigerant. Electricity costs \$3.22 per therm (1 therm = 100,000 Btu), which is about five times that of natural gas (assuming \$0.11 per kWh for electricity and \$0.63 per therm for gas). This large difference allows systems powered by natural gas to exhibit lower thermodynamic efficiencies yet still cost less to operate than conventional mechanical vapor compression devices. The following example illustrates the potential electrical savings for Los Angeles (LA), Riverside, and Orange County (OC).

Figure 5: Adsorption Heat Pump Flow Diagram (Cooling Adsorbent Bed 1)

Potential energy savings for an adsorption heat pump in LA, Riverside, and OC.

Given:

Population

L.A., Riverside, O.C. = 14.5 million

(Population Division U.S. Bureau of the Census 1999)

Houses (3 people per house)

Cooling Degree Days (DD_c) °F days: (Base 70 °F)

L.A., Riverside, O.C. = 460

(Western Region Climate Center Los Angeles 1999)

House Description

Floor plan: (25ft × 70ft) = 1750 ft²

Ceiling height = 8.5 ft

Wall Area: (50 + 140)ft × 8.5ft = 1615 ft²

Cooling Load per House

Ceiling U-Value = 0.026 BTU/hr °F ft²

Wall U-Value = 0.12 BTU/hr °F ft²

Floor U-Value = 0.05 BTU/hr °F ft²

Mechanical Heat Pump Efficiency = 3.5

Adsorption Heat Pump Efficiency = 2.0

Electricity Unit Cost = \$0.11 / kW hr

Natural Gas Unit Cost = \$0.63 / therm

Calculations:

Number of houses in L.A., Riverside, O.C.;

$$14.5e6 \div 3 = 4.8 \text{ million}$$

UA Value, UA = U - Value $\times$ Area

Ceiling UA

$$0.026 \frac{\text{BTU}}{\text{hr} \cdot ^\circ \text{F} \cdot \text{ft}} \times 1750 \text{ft} = 46 \text{ BTU/hr } ^\circ \text{F}$$

Wall UA

$$0.12 \frac{\text{BTU}}{\text{hr} \cdot ^\circ \text{F} \cdot \text{ft}} \times 1615 \text{ft} = 194 \text{ BTU/hr } ^\circ \text{F}$$

Floor UA

$$0.05 \frac{\text{BTU}}{\text{hr} \cdot ^\circ \text{F} \cdot \text{ft}} \times 1750 \text{ft} = 88 \text{ BTU/hr } ^\circ \text{F}$$

$$\text{Total UA}_{\text{total}} = 330 \text{ BTU/hr } ^\circ \text{F house}$$

Mechanical Heat Pump Cooling

$$\text{Load, } Q_{c, \text{yr}} = \frac{\text{UA}_{\text{total}} * \text{DD}_c * \text{houses}}{\text{efficiency}} \quad (2)$$

(ASHRAE, 1993)

$$\frac{330 \frac{\text{BTU}}{\text{hr} \cdot ^\circ \text{F} \cdot \text{house}} \times 460 ^\circ \text{F days} \times 4.8e6 \text{ houses} \times \frac{24 \text{ hr}}{\text{day}}}{3.5} = 5.0 e12 \text{ BTU}$$
$$= 1.5e9 \text{ kW hr}$$

Mechanical Heat Pump Cost

$$1.5e9 \text{ kW hr} \times \frac{\$0.11}{\text{kW hr}} = \$170 \text{ million}$$

Adsorption Heat Pump Cooling

$$\frac{330 \frac{\text{BTU}}{\text{hr} \cdot ^\circ \text{F} \cdot \text{house}} \times 460 ^\circ \text{F days} \times 4.8e6 \text{ houses} \times \frac{24 \text{ hr}}{\text{day}}}{2.0} = 8.7e12 \text{ BTU}$$
$$= 8.7e7 \text{ therm}$$

Adsorption Heat Pump Cost

$$8.7e7 \text{ therm} \times \frac{\$0.63}{\text{therm}} = \$55 \text{ million}$$

Adsorption vs. Mechanical Heat Pump Savings

$$\text{Savings; } \$170e6 - \$55e6 = \$115 \text{ million}$$

$$\text{Savings; } \frac{115e6}{170e6} \times 100\% = 68\%$$

Equation 3 is a representation of degree-days at a base of 70 °F.

$$DD_c = (1 \text{ day}) \sum_{\text{days}} \left(\frac{\text{Temp}_{\text{high}} + \text{Temp}_{\text{low}}}{2} \right) - 70^\circ \text{F} \quad (3)$$

There is one-degree day of cooling for each day that the average temperature is above 70 °F. Although the above example illustrated the economic benefit for the residential market, the industrial market would also see savings on electricity. Also of significance is the fact that space heating and cooling accounts for 20% of the electrical power consumed in the United States (DOE and ICF Consultants, 2001). Thus, a large-scale

shift to adsorption heat pumps could relieve some of the increasing strain on the nation's power electricity generation and distribution grid. New power plants are very expensive and do not provide adequate returns for investors. Utility companies would rather reduce the electrical requirement than build another power plant. Adsorption heat pumps have a great potential to impact the conservation of energy.

1.2.4 Environmental Advantage

Mechanical vapor compression systems utilizing chlorofluorocarbon (CFC) and hydrochlorofluorocarbon (HCFC) refrigerants (e.g., freon) dominate the heating and cooling market. CFC and HCFC refrigerants are purported to cause the loss of stratospheric ozone (EPA Global Warming Site, 2001). The new replacement hydrofluorocarbon (HFC) refrigerants do not deplete stratospheric ozone. However, HFCs are suspected of forming hydro-fluoric acid (HF) and formaldehyde in the upper atmosphere. Adsorption heat pumps can utilize environmentally benign refrigerants such as ammonia, methanol, butane, or even water and complies with the Montreal Protocol of 1988. The Montreal Protocol prescribed the phase out of CFC and HCFC refrigerants. Another environmental benefit is the adsorption heat pumps reliance on clean-burning natural gas. Fifty-four percent of the world's electrical energy comes from coal. Natural gas burns cleaner than coal and does not pollute the environment like coal. Adsorption heat pumps do not threaten the ozone layer or contribute to pollution via electrical generation.

1.2.5 Efficiency

Currently, commercially available adsorption heat pumps operate at a COP of 1.0, and are marginally less expensive to operate than mechanical vapor compression systems. Adsorption heat pumps with a cooling COP of 0.8 have the same operating costs as typical mechanical vapor compression systems (Shelton et al. 1988 and Shelton et al. 1990). However, adsorption heat pumps cost 30% more than mechanical vapor compression systems, and the energy savings payoff period is on the order of twenty years (Cacciola and Restuccia 1994). This time scale is too long for such devices to be economically competitive. One way to decrease the payoff period is to decrease the operating cost. An increase in COP would decrease the operating cost. Optimization of heat transfer within the adsorption beds can increase COP. It is quite feasible that COP could be raised to 1.5, perhaps even to 2.0. An improved COP of 1.5 will reduce the time to break even economically, making adsorption heat pumps strongly competitive. The following example illustrates the reduction in the payback period

Reduction in the payback period from increasing the COP from 1.0 to 2.0

for the LA, Riverside, and OC area.

Given:

Cost of Mechanical Heat Pump = \$650 / house

Cost of Adsorption Heat Pump:

$1.3 \times \$650$ = \$850 / house

Natural Gas Unit Cost = \$0.63 / therm

$$\text{Electricity Unit Cost} = \$0.11 / \text{kW hr}$$

Calculations:

Cost Difference between Adsorption and Mechanical Heat Pumps

$$\$850 - \$650 = \$200 / \text{house}$$

Cooling Load for an adsorption efficiency of 2.0

$$\frac{8.7 \times 10^{12} \text{ BTU/year}}{4.8 \times 10^6 \text{ houses}} = 1.8 \times 10^6 \text{ BTU / year house}$$

$$= 18 \text{ therms / year house}$$

Adsorption efficiency of 2.0 cost per house

$$\$0.63 \times 18 \text{ therms/year house} = \$11 / \text{year house}$$

Adsorption efficiency of 1.0 cost per house

$$\frac{\$11}{\text{year house}} \times \frac{2.0}{1.0} = \$22 / \text{year house}$$

Cooling Load for mechanical heat pump efficiency of 3.5

$$\frac{5.0 \times 10^{12} \text{ BTU/year}}{4.8 \times 10^6 \text{ houses}} = 1.0 \times 10^6 \text{ BTU / year house}$$

$$= 305 \text{ kW hr/ year house}$$

Mechanical heat pump efficiency of 3.5 cost per house

$$\frac{\$0.11}{\text{kW hr}} \times \frac{305 \text{ kW hr}}{\text{year house}} = \$34 / \text{year house}$$

Savings per Year with 2.0 Adsorption Heat Pump Efficiency

$$\$34 - \$11 = \$23 / \text{year house}$$

Savings per Year with 1.0 Adsorption Heat Pump Efficiency

$$\text{\$34} - \text{\$22} = \text{\$12 / year house}$$

Payback Calculation of 2.0 Adsorption Heat Pump Efficiency

$$\frac{\text{\$200}}{\text{house}} \times \frac{\text{year house}}{\text{\$23}} = \text{8.7 years}$$

Payback Calculation of 1.0 Adsorption Heat Pump Efficiency

$$\frac{\text{\$200}}{\text{house}} \times \frac{\text{year house}}{\text{\$12}} = \text{16.7 years}$$

COP improvement from 1.0 to 2.0 reduces the payback time from 16.7 years to 8.7 years.

1.3 Related Technology

The mechanical vapor compression cycle is the overwhelmingly prevalent heat pump technology in use today. Almost every residential and light commercial building uses mechanical vapor compression. Low initial costs keep mechanical vapor compression systems competitive against adsorption heat pumps. Efficiency of mechanical vapor compression will remain at the current COP of 3.5, because the compressor is already optimized. Adsorption heat pumps have not reached their peak efficiency. Improvement of the heat transfer would allow adsorption heat pumps to increase efficiency and decrease operating costs. Although the initial costs are favorable for mechanical vapor compression, the operational costs for adsorption heat pumps may be reduced.

Absorption heat pumps are another form of refrigeration technology. The refrigerant flow path for the absorption heat pump is similar to mechanical vapor compression. Refrigerant flows through a condenser, evaporator, and expansion valve. However, an absorber and generator are added to compress the refrigerant with a liquid absorbent. The absorber section absorbs refrigerant from the evaporator. A generator section delivers heat to the absorbent/refrigerant mixture to achieve a high pressure and separate the refrigerant from the absorbent. Typical refrigerant/absorbent combinations are ammonia/water and water/lithium bromide. Single effect designs achieved a COP 0.52 and double-effect designs achieved a COP of 0.88 (Sauer and Howell, 1983). The best COP of 1.2 was achieved by the Iron Fireman double-effect chiller design (Sauer and Howell, 1983).

2. Literature Search

2.1 Current Areas of Research and Development

A literature review was conducted for the thermal hindrances, mathematical modeling, variation of parameters, and adsorbate/adsorbent combinations. An account of the efficiency hindrances highlights the heat transfer problem. This section also includes a discussion about consolidated adsorbents. Differential equations that depict the adsorption heat pump were found in literature (Ellis and Wepfer, 1999). Information about the parameters provided insight on which parameters to manipulate for the best COP. Finally, the adsorbate/adsorbent literature highlighted suitable combinations for the refrigerant and adsorbent.

2.2 Thermal Hindrances

The controlling mechanism for COP is the heat transfer in the adsorption beds (Watanabe, et al., 1996; Pons, et al., 1996; and Zheng, et al., 1995). Heat transfer is greatly hindered in two areas of the adsorbent bed; heat transfer through the adsorbent and heat transfer from the heating medium to the adsorbent. Figure 6 is a representation of an adsorption bed.

Figure 6: Representation of Adsorption Bed (Ellis and Wepfer, 1999)

Conduction of heat through the adsorbent bed follows many paths; through a poor conductor (adsorbent material), from adsorbent particle to adsorbent particle across a contact resistance, from adsorbent material through adsorbed refrigerant, and through the refrigerant vapor in the voids. All these paths of heat conduction are very poor, which leads to poor heat transfer. Conduction from the HTF pipe to the adsorbent bed is across another contact resistance, which hinders heat transfer.

2.2.1 Consolidated Adsorbents

Consolidated adsorbents were reviewed to counter the heat transfer problem (Guilleminot, et al., 1996; Guilleminot, et al., 1998; Pons, et al, 1996; Poyelle, et al, 1999; and Poyelle, et al, 1996). Adsorbent material was compacted and a binder was added to produce consolidated adsorbent granules. An additive is used to combine individual adsorbent granules to produce bricks. The binder and compression of the adsorbent increased the thermal conductivity, however the amount of sorption decreased. Reduction of the adsorbent sorption capacity resulted in decreased COP. The adverse effects of reducing adsorbent sorption were illustrated in a permeability study (Ellis and Wepfer, 1999). Figure 7 demonstrates the decrease in COP as permeability decreases. A range of consolidation exists that is acceptable for reduced mass transfer. Consolidated adsorbents with permeability lower than $1\text{e-}10\text{ m}^2$ sacrificed too much of the sorption capacity, and as a result the COP decreased.

Figure 7: COP versus Permeability, replicated version (Ellis and Wepfer, 1999)

2.3 Mathematical Modeling

Mathematical modeling varied between researchers. Heat transfer was modeled in the axial plane only (Shelton, et al, 1988). Heat of adsorption was included in some models (Teng, et al, 1997). The contact resistance between the heating medium and the adsorbent material was accounted for in some models (Ben Amar, et al, 1996). This thesis is based upon a model that incorporated heat of adsorption, heat transfer in the radial direction, and heat transfer across a contact resistance from the heating medium to the adsorbent (Ellis and Wepfer, 1999). Modeling in the radial direction was required, because of the geometrical design, which will be explained in chapter three. Models without the heat of adsorption deviated from experimental results (Worm, et al, 1993). COP is also sensitive to the contact resistance (Ellis and Wepfer, 1999). Figure 8

illustrates the impact that contact resistance and adsorbent thermal conductivity has on COP.

Figure 8: Effect of contact resistance and adsorbent thermal conductivity on COP, replicated version (Ellis and Wepfer, 1999)

An 80% increase in heat transfer between the HTF pipe and the adsorbent bed improved the COP by 17%. The increase in the convective coefficient shifted the COP curve up. Thermal conductivity of the adsorption bed was varied from 0 to 10 W/m K to produce values of COP. The COP sharply rises up and levels off after 1 W/ m K. A great benefit in COP is realized for the initial improvement of the thermal conductivity. However, the increase of COP after 1 W/m K is minimal.

The following equations are the transient differential equation for the adsorbent bed (Ellis and Wepfer, 1999). Conservation of mass for the adsorbent bed is Equation 4.

$$\frac{\partial}{\partial t}(\epsilon \rho_r + (1 - \epsilon) \rho_a \omega) + \nabla \cdot (\rho_r v) = 0 \quad (4)$$

The first part of the time differential accounts for the refrigerant in the void volume (ϵ) and adsorbed on the adsorbent. Other variables are: refrigerant density is ρ_r , adsorbent density is ρ_a , refrigerant velocity is v , and adsorbed refrigerant per amount of adsorbent is ω . The second part of the differential equation is the del operator accounting for the refrigerant leaving and entering the adsorbent bed. Equation 5 describes Equation 4 in terms of average refrigerant properties and velocity in the axial direction.

$$\frac{\partial}{\partial t}(\epsilon \bar{\rho}_r + (1 - \epsilon) \rho_a \bar{\omega}) + \frac{\partial}{\partial z}(\bar{\rho}_r v_z) = 0 \quad (5)$$

Refrigerant mass in the void volume, adsorbed on the adsorbent, and in flux is now averaged. Pressure drop and velocity of the refrigerant were related by the Ergun approach in Equation 6 (Ellis and Wepfer, 1999).

$$\frac{\partial P}{\partial z} = -\frac{\mu \bar{v}_z}{\kappa} \left(1 + C_E \text{Re}_{\sqrt{\kappa}} \right) \quad (6)$$

Pressure drop along the axial axis is now related to the dynamic viscosity (μ), permeability (κ), average velocity ($\bar{v}_z$), and Reynolds number ($\text{Re}_{\sqrt{\kappa}}$). The 1 in equation 6 account for the viscous component of the friction. The constant C_E accounts for the turbulent flow from friction and was set at 0.55 (Ward, 1964). Equation 7 allows the Reynolds number to account for permeability.

$$\text{Re}_{\sqrt{\kappa}} = \frac{\rho |v| \sqrt{\kappa}}{\mu} \quad (7)$$

Equation 8 is the conservation of energy for the adsorbent.

$$\frac{\partial}{\partial t}(\epsilon \rho_r u_r + (1-\epsilon) \rho_a u_a + (1-\epsilon) \rho_a \omega u_r) + \frac{\partial(h_a \overline{\rho_r v_z})}{\partial z} - \nabla \cdot (k_a \nabla T_a) = 0 \quad (8)$$

The partial time derivative accounts for the energy change in the refrigerant vapor, adsorbent, and adsorbed refrigerant. Refrigerant and adsorbent internal energy is represented by u_r and u_a . The second differential represents the convection of energy in the refrigerant vapor. Heat conduction through the adsorbent is the last part of equation 8. Equation 8 then incorporates Equations 5-7 to give Equation 9.

$$\epsilon \rho_r c_{pv} \frac{\partial T_a}{\partial t} + (1-\epsilon) \rho_a c_a \frac{\partial T_a}{\partial t} + (1-\epsilon) \rho_a \omega \frac{\partial u_a}{\partial t} - (1-\epsilon) \rho_a h_{av} \frac{\partial \omega}{\partial t} - \epsilon \frac{\partial P}{\partial t} - k_a \nabla^2 T_a + c_{pv} \overline{\rho_r v_z} \frac{\partial T_a}{\partial z} = 0$$

Transient energy change in the refrigerant vapor is the first term. Transient energy change in the adsorbent is the second term. The internal energy for the refrigerant is the third term. Fourth term is the differential enthalpy of adsorption. Pressure drop is the fifth term. Heat conduction throughout the adsorption bed is the sixth term. Finally, the seventh term accounts for the convection transfer of energy. Equation 10 describes the adsorption equilibrium behavior.

$$\omega = \omega_o \exp \left(-DT^2 \left(\ln \left(\frac{P_s}{P} \right) \right)^2 \right) \quad (10)$$

The amount of adsorbed refrigerant is a modified form of the Dubinin-Raduschkovich equation (Ellis and Wepfer, 1999). The initial adsorption level, ω_o , and the Dubinin-Raduschkovich coefficient, D , are experimentally determined for each refrigerant/adsorbent combination. Equation 11 is the Refrigerant vapor pressure.

$$\ln P_s = B - \frac{m}{T} \quad (11)$$

Constant, B, coefficient in vapor pressure curve correlation (m), and temperature describe the refrigerant saturation pressure. Differential enthalpy of adsorption is represented by equation 12 (Ellis, 1996).

$$h_{av}(\omega) = \left[Rm + \frac{1.58R}{\sqrt{D}} \right] - \left[\frac{1.42R}{\sqrt{D}\omega_0} \right] \omega \quad (12)$$

Equation 12 is a linear expression that describes the enthalpy in terms of the gas constant (R), m, D, and ω_0 . Equation 13 describes the internal energy of the refrigerant in terms of the adsorbed phase enthalpy.

$$u_r \approx h_r \approx h_{ref} + C_{p,v} (T - T_{ref}) - \Delta \bar{h}_{av} \quad (13)$$

The relation described in equation 13 was accomplished by assuming that the specific volume of the adsorbed phase is small. Equation 14 is the incorporation of equation 12 into 13.

$$u_a \equiv h_a = h_{refv} + c_{pv} (T - T_{ref}) - \left[Rm + \frac{1.58R}{\sqrt{D}} \right] + \frac{1}{2} \left[\frac{1.42R}{\sqrt{D}\omega_0} \right] \omega \quad (14)$$

Equation 9 is the main form of the conservation of energy, and equations 10, 11, and 14 are the sub equations.

2.4 Variation of Parameters

Design parameters were reviewed to increase COP. Cycle time displayed a parabolic response with a maximum for COP (Zheng, et al, 1995). An increase in Biot number displayed an increase in COP (Fuller, et al, 1994). A thorough review of the dimensionless variables was performed to study COP (Zheng, et al, 1995). Bed-

switching frequency (ω), number of transfer units (NTU), adsorbent Biot number (Bi_d), contact Biot number (Bi_c), inert alpha number (α_{w-d}), and fluid alpha number (α_{w-f}) were the varied parameters. Low values for the bed-switching frequency correspond to a long time between alternating the heating and cooling of the adsorption beds. NTU is related to the size of the heating medium for the adsorbent bed. High thermal conductivity through the adsorbent material produces low sorbent Biot numbers. Also, a high contact heat transfer coefficient between the adsorbent and HTF pipe produces low values for the contact Biot number. The inert alpha number is the ratio of the energy change of the inert mass to the energy change of the adsorbent mass. Typically, a good design directs most of the energy into the adsorbent material, which produces low values for the inert alpha number. The heat capacity ratio of the heat transfer fluid and the adsorbent material is the fluid alpha number. Appendix B contains the mathematical relations of the dimensionless parameters.

2.4.1 Switching Frequency

The switching frequency displayed an ideal maximum for COP. Figure 9 is COP as a function of switching frequency and NTU. This result agrees with intuition about regeneration schemes. If the HTF flow is switched too fast, then refrigerant does not entirely desorb and adsorb onto the adsorbent. If the HTF flow is switched too slow, then excessive desorption and adsorption occurs and energy is wasted.

Figure 9: Effects of ω on COP at NTU = 10 to 50 (Zheng, et al, 1995)

2.4.2 NTU

NTU may be increased up to a practical point. As illustrated in Figure 9, the NTU performed ideally in the model down to a value of twenty. Low values of NTU were unfavorable, and very high values of NTU did not produce major improvements in the COP. This suggests that an increase in the heat exchanger size provided a benefit up to a practical point. Afterwards, any size increase in the heating medium produced marginal improvement.

2.4.3 Biot Number

The reduction of the adsorbent Biot number and contact Biot number improved the COP up to a certain point. Figure 10 displays the effects of the adsorbent Biot number.

Figure 10: Effects of ω on COP for $Bi_d = .25$ to 4 (Zheng, et al, 1995)

Figure 11 displays the effects of the contact Biot number.

Figure 11: Effects of ω on COP for $Bi_c = .001$ to 10 (Zheng, et al, 1995)

The adsorbent and contact Biot number reached a point where further reduction in the contact resistance produced marginal benefits in the COP.

2.4.4 Alpha Number

Reduction of the inert alpha number was minimally favorable for COP. Figure 12 displays the effects of the inert alpha number.

Figure 12: Effects of ω on COP for $\alpha_{w-d} = .25$ to 4 (Zheng, et al, 1995)

Figure 13 displays the effects of the fluid alpha number. Increase in the fluid alpha number displayed minimal improvement for the COP. An increase in the inert mass does impact COP, but not as much as the dimensionless Biot, NTU, and switching frequency parameters.

2.4.4 Spacing

COP also depends on the amount of adsorbent around the HTF pipe (Miles and Shelton 1991). There is a definite position that uses heat efficiently. If the tubes are too close together then the heat exchanger mass is over designed and the device has excess area. If

Figure 13: Effects of ω on COP for $\alpha_{f-d} = .25$ to 4 (Zheng, et al, 1995)

the spacing is too large, then the adsorbent does not receive all of the intended heat and the COP suffers. Figure 14 is COP as a function of tube spacing from 0.25 mm to 20 mm.

Figure 14: COP versus tube spacing

COP is very low for small spacing, quickly rises to maximum, and falls off. This variation of spacing helped optimize the heat exchanger design to 4 mm spacing.

2.5 Adsorbate/Adsorbent Combinations

A common scheme to improve efficiency is the use of different adsorbent/adsorbate combinations. Common adsorbent/adsorbate combinations are Zeolite/Water, Zeolite/Ammonia, Active Carbon/Methanol, Active Carbon/Ammonia, and Silica Gel/Water (Poyelle, et al, 1999; Saha, et al, 1997; Ito, et al, 1996; Watanabe, et al, 1996; and Tchernev and Clinch, 1989). Each combination holds merit with different applications and preferences.

2.5.1 Refrigerant

The adsorbate (commonly referred to as the refrigerant) should possess the following characteristics: high latent heat per unit volume, good thermal stability, environmentally friendly, and non-flammable (Cacciola, G. and Restuccia, 1994). Table 1 summarizes the thermal characteristics of some common refrigerants. Although water has a high specific heat, the boiling point is too high, which restricts the refrigerant to warm geographical locations. Water was identified as an ideal refrigerant (Cacciola, and Restuccia, 1994). Water would be problematic in areas where the climate approaches the freezing point temperature. Ammonia has an acceptable specific heat and the boiling point is suitable for low temperature zones.

Table 1: Thermophysical Properties of Common Refrigerants

Refrigerant	$\Delta H_f^{a,i}$ (kJ/kg)	Boiling Point ^{a,ii} (K)	Thermal Conductivity ⁱⁱⁱ (W/m K)	Density (kg/m ³)
Ammonia, NH ₃	1357	240	.0247 ^b	.6894 ^{b,iv}
Carbon Dioxide, CO ₂	231	195	.0166 ^b	1.7730 ^{b,iv}
Methane, CH ₄	510	112	.0342 ^c	.7167 ^{c,v}
Water, H ₂ O	2257	373	.0196 ^b	.0256 ^{b,iv}

a (Cengel and Boles, 1998)

b (Incropera and Dewitt, 1996)

c (Perry, et al, 1984)

i Heat of Vaporization at normal boiling point and 1 atm

ii Boiling Point at 1 atm

iii Temperature at 300 K

iv Density at 300 K and 1 atm

v Density at 273 K and 1 atm

2.5.2 Adsorbent

Suitable characteristics of the adsorbent include: high adsorption of refrigerant, wide concentration change for small temperature change, good thermal conductivity, and low cost (Cacciola, and Restuccia, 1994). Table 2 lists the thermodynamic and physical properties of some common adsorbents. Zeolite 13X has the best sorptive capacity, and

activated graphite has the worst sorptive capacity for water. However, activated graphite has the best thermal conductivity.

Table 2: Thermodynamic and Physical Properties of Common Adsorbents

Adsorbent	Specific Heat (kJ/kg K)	Thermal Conductivity (W/m K)	Density (kg/m ³)	Sorptive Capacity of H ₂ O kg/kg (dry)
Activated Carbon, C•H ₂ O	.837 ^b	.138 ^b	465 ^b	.12 ^c
Activated Graphite, C•H ₂ O	.709 ^{a, iii}	5.7 ^{a, iii}	2210 ^{a, iii}	7.75 x 10 ⁻⁴ c, ix
Alumina, Al ₂ O ₃ •H ₂ O	.960 ^{a, iv, v}	1.0 ^{a, iv, v}	2645 ^{a, iv, v}	.16 ^{d, viii}
Zeolite 13X, Na ₂ O•Al ₂ O ₃ •2.5 SiO ₂ •6H ₂ O	.837 ^{f, vii}	.14 ^{f, vii}	640 ^{f, vii}	.24 ^{d, viii}

a (Incropera and Dewitt, 1996)

b (Fuller, et al, 1994)

c (El-Nabaray, et al, 1997)

d (Breck, 1974)

e (Miura and Morimoto, 1991)

f (Miles and Shelton, 1991)

- i Temperature at 298 K and Pressure at 700 torr.
- ii Temperature at 308 K and Pressure at 700 torr.
- iii Temperature at 300 K.
- iv Temperature at 478 K.
- v Fire brick clay data is similar to Alumina.
- vi Silicon Dioxide (polycrystalline) is similar to silica gel.
- vii Temperature at 423 K.
- viii Temperature at 298 K and Pressure at 20 torr.
- ix Temperature at 298 K and Pressure at 8 torr.

2.5.3 Zeolite 13X

Zeolite 13X is a common synthetic zeolite used in the application and testing of adsorption heat pumps. Pore size, overall size, and structure are the unique physical properties of zeolites. Pore size allows zeolites to achieve adsorption selectivity. Although many different size molecules will adsorb to the outside surface of the zeolite, large molecules are denied access to the interior surface area. Molecules with a size greater than the pore diameter on the zeolite are restricted to the outside surface area. Zeolites have pore sizes that range from 3 to 10 angstroms (Catlow 1993). Zeolite 13X has a nominal pore size of 10 angstroms, which decreases the selectivity of this particular adsorbent (Adsorbents and Desiccants Corporation of America 2000).

Structure orientation is an interesting attribute associated with zeolites. Individual molecules of zeolite have body center cubic structure. However, zeolite molecules chain

together with other zeolite molecules to form some elaborate geometric structures. The synthetically derived zeolite 13X is labeled as a Faujasite (FAU) structure. Figure 15 is a FAU framework structure that consists of linked truncated octahedral (β -cages). This cage like structure is similar to sodalite (Breck, 1974). Geometric arrangement also determines the degree of hydration, density, structure stability, cation exchange properties, electrical conductivity, adsorption of gases, and catalytic properties (Breck, 1974).

Figure 15: FAU framework for zeolite (Breck, 1974)

Zeolite 13X is a synthetically altered form of zeolite type X. Zeolite refers to material like aluminosilicate, aluminophosphate, and germinates (Breck, 1974). Zeolite may be represented by TO_4 as the chemical compound (with T as Silicon, Aluminum, or Phosphorus ion) (Catlow, 1993). The tetrahedral corners are shared to form the elaborate zeolite structures. Complex geometry may be represented by the structural formula

$M_{x/n}[(AlO_2)_x(SiO_2)_y \cdot wH_2O]$ (M is the exchangeable cation, n is the cation valence, w is the number of water molecules, and the ratio y/x has values 1 to 5 (Breck, 1974). Zeolite type X is synthetically altered to increase the pore size and form zeolite 13X. Common cations for zeolites are from group I and II in the periodic table. However, Sodium remains the primary cation for zeolite 13X.

Zeolite 13X fulfills the adsorbent requirements for adsorption heat pumps. Selectivity is low, so a wide range of refrigerants may be used as the adsorbate. Synthetic zeolites have less variability in properties than natural zeolites. The properties of natural zeolites vary from region to region and lead to variability in tests. Low selectivity, wide spread usage, and low variability in properties made zeolite 13X a logical material for the adsorbent.

2.6 Summary of Current Research

Researchers engaged in a number of activities for the advancement of the adsorption heat pump. After the development of the regeneration, heat transfer in the adsorption bed remained a primary interest. Other areas of interest include parameter optimization, proper experimental set up, mathematical modeling, device fabrication, and adsorbate/adsorbent selection.

2.6.1 Tchernev, et al

Tchernev, et al produced articles that distinguish the benefits of regeneration

(Tchernev and Clinch, 1989 and Tchernev, et al, 1989). Regeneration elevated the COP of adsorption heat pumps. This new level of COP allows adsorption heat pumps to operate more efficiently than mechanical vapor compression.. Tchernev developed regeneration for adsorption heat pumps that are commercially available.

2.6.2 Cacciola, et al

Cacciola, et al provided a thorough review of adsorption heat pumps (Cacciola and Restuccia, 1994). This review explained the problem with heat transfer and the regeneration process. A theoretical limit was provided along with recommendations to achieve that limit. Later designs with finned heat exchangers were an attempt to improve heat transfer (Cacciola and Restuccia, 1995). Cacciola, et al provided insight and recommendations for all pertinent development areas of adsorption heat pumps.

2.6.3 Meunier, Guilleminot, et al

Meunier, Guilleminot, et al developed consolidated materials to improve thermal conductivity (Guilleminot, et al., 1996; Guilleminot, et al., 1998; and Poyelle, et al, 1996). Adsorbent materials are poor thermal conductors, which interfere with heat transfer during the regeneration process. Meunier, Guilleminot, et al compacted the Zeolite material and used a binder to improve thermal conductivity. However, the high thermal conductivity was achieved at the expense of mass transfer.

2.6.4 Miles, Shelton, et al

Miles, Shelton, et al pursued the development of mathematical models for adsorption heat pumps (Shelton, et al, 1988; Shelton, et al, 1990; and Miles, et al, 1991). This group realizes that an accurate model allows the exploration of parameters. Once all of the parameters are understood, a proper design can be pursued. Other researchers provided additional work in the area of mathematical modeling (Ben Amar, et al, 1996; Zheng, et al, 1995; Ellis and Wepfer, 1999; Worm, et al, 1993; and Hajji, et al, 1993).

2.6.5 Overall

Table 3 is a summary of some researchers findings of COP.

Table 3: COP_c Achievement (Lambert, 1999)

Researcher	COP _c	Comments	Reference
Cacciola & Restuccia	.75-.85	Predicted	Cacciola, and Restuccia, 1995
Ben Amar et al	1.07	Predicted	Ben Amar, et al, 1996
Pons et al	0.89	Experimental	Pons et al, 1996
Meunier et al	1.06	Experimental	Meunier et al, 1990
Miles et al	0.80	Experimental	Miles et al, 1993
Jones	1.0	Predicted	Green, 1991
Guilleminot et al	0.41-0.68	Experimental	Guilleminot, et al, 1998

3. Thesis Proposal

3.1 Hypothesis

Metal gauze should increase the contact area between the heat source and the adsorbent, and diffuse the heat throughout the adsorbent to increase the overall heat transfer of an adsorption heat pump.

3.2 Objective

This thesis developed a theoretical model that studied the enhancement to heat transfer by the incorporation of metal gauze into an adsorption heat pump. Metal gauze was bonded to the outer wall of the HTF pipe and allowed heat to diffuse throughout the adsorbent bed. The metal gauze addressed the two primary problems of heat transfer within an adsorption heat pump; heat transfer between the adsorption bed and HTF pipe and heat transfer throughout the adsorption bed. These two problems restrict the total benefit that could be realized with regeneration. Contact area between adsorbent and the HTF pipe was maximized while the distance between adsorbent and the path from the HTF pipe to the adsorbent was minimized.

3.3 Justification

Improvement of heat transfer depends in large part upon increasing the heat transfer between the HTF pipe and the adsorption bed. The HTF pipe transports heat from the hot adsorption bed to the cold adsorption bed and delivers additional heat from the boiler. Metal gauze increases the surface area of the heat source. Heat may

effectively diffuse throughout the adsorbent with the aid of metal gauze interspersed throughout the adsorbent. A pin fin network represents the metal gauze connected to the HTF pipe and extended from the surface. Metal gauze (pin fins) augments the contact area between the metal components of the HTF plumbing and the adsorbent.

3.4 Modeling Approach

3.4.1 Overview

Evaluation of the metal gauze design is broken down into three phases of model verification, optimization, and adsorbent material evaluation. Model verification is the baseline comparison between an activated carbon adsorption bed with and without metal gauze. This requires the development of a finite difference model to represent the adsorption bed. The baseline model represents a defined adsorption bed with no metal gauze. The comparative model has a pin fin network that represents the metal gauze. Optimization of pin size, amount of pin fins and cycle time in second phase allows the metal gauze design to achieve the best efficiency results. Then, the baseline model is compared with the comparative model. Finally the adsorbent material evaluation reviews zeolite 13X in the last phase. Figure 16 is a flow diagram that represents the sequence of this thesis.

3.4.2 Model Justification

Model justification begins development of a series of differential equations to define an adsorption heat pump (Ellis and Wepfer 1999). Three main sections comprise

Figure 16: Flow Diagram

the adsorption heat pump; HTF, HTF pipe wall, and the adsorbent as illustrated in the Figure 17. Transient differential equations describe each of these sections and produce refrigerant flow, refrigerant temperature, and HTF temperature data.

The heat transfer of the working fluid, HTF, will be described by equation 15.

$$\pi r_i^2 \rho_n C_n \frac{\partial T_n}{\partial t} - \pi r_i^2 k_n \frac{\partial}{\partial z} \left(\frac{\partial T_n}{\partial z} \right) + [\pm] \pi r_i^2 \rho_n C_n V_n \frac{\partial T_n}{\partial z} + 2\pi r_i h_n (T_n - T_t) = 0 \quad (15)$$

Figure 17: Cross Section View of Grid Network

Equation 15 incorporates the following assumptions.

- Constant mass flow rate of the HTF.
- Constant thermal conductivity, density, and specific heat for all materials, the average thermal conductivity for the maximum and minimum temperature will be used.
- Radial temperature gradient is negligible.
- Convective heat transfer from the HTF to the HTF pipe wall

Figure 18 illustrates the node for the HTF.

Equation 16 will describe heat transfer through the HTF pipe.

$$2\pi r_t b \rho_t C_t \frac{\partial T_t}{\partial t} - 2\pi r_t b k_t \frac{\partial}{\partial z} \left(\frac{\partial T_t}{\partial z} \right) - 2\pi r_t h_{\Pi} (T_{\Pi} - T_t) + 2\pi r_t h_a (T_t - T_a(r_{t,z})) = 0 \quad (16)$$

Figure 18: Cylindrical node representation of HTF

Equation 16 has the following assumptions.

- Cylindrical HTF pipe with adsorbent material inside and HTF outside.
- Adsorbent material is continuous with a contact resistance between the HTF pipe and adsorbent material.
- Constant thermal conductivity, density, and specific heat for all materials, the average thermal conductivity for the maximum and minimum temperature will be used.
- Radial temperature gradients are negligible.

Figure 19 illustrates the HTF pipe

Equation 9 will describe the heat transfer through the adsorbent bed.

$$\varepsilon \rho_r c_{pv} \frac{\partial T_a}{\partial t} + (1 - \varepsilon) \rho_a c_a \frac{\partial T_a}{\partial t} + (1 - \varepsilon) \rho_a \omega \frac{\partial u_a}{\partial t} - (1 - \varepsilon) \rho_a h_{av} \frac{\partial \omega}{\partial t} - \varepsilon \frac{\partial P}{\partial t} - k_a \nabla^2 T_a + c_{pu} \rho_r v_z \frac{\partial T_a}{\partial z} = 0 \quad (9)$$

Figure 19: Cylindrical node representation of HTF pipe

Equation 9 has the following assumptions.

- Adsorbed phase internal energy is equal to the adsorbed phase enthalpy.
- Adsorbent material is continuous.
- Refrigerant vapor is free to move throughout the void space.
- Fraction of bed not occupied is the void space.
- Adsorbent material, adsorbed refrigerant, and refrigerant vapor exist at the same temperature.
- Constant thermal conductivity, density, and specific heat for all materials, the average thermal conductivity for the maximum and minimum temperature will be used.
- Refrigerant vapor behaves as an ideal vapor.
- Adsorbate (adsorbed refrigerant) behaves as a liquid with a very small specific volume.
- Adsorbent phases are stationary.

- Local adsorption equilibrium.
- Mass, momentum, and energy are unsteady.
- Vapor flow is axial.
- Momentum can be neglected.
- Heat transfer in the axial and radial directions.
- Bulk convective and viscous terms in the momentum equation are small.
- Specific volume of the adsorbed phase is small.

These equations will be broken down by finite difference methods in the explicit form to represent a cylindrical array. The array is five nodes in the radial direction and seven hundred in the axial direction. In the radial direction, the inner node represents a solid cylindrical slice and the proceeding radial nodes resemble discs. The innermost node is adsorbent material and the next two nodes are adsorbent material. The fourth node is the HTF pipe and convective heat transfer occurs at both radial interfaces. One interface is the heat transfer from the HTF pipe to the adsorbent material. Another interface is the heat transfer from the HTF to the HTF pipe and the fifth node is the HTF. The stability criterion for the explicit method requires the coefficients of the calculated node from the previous time step to be greater than zero. This criterion will be accomplished by decreasing the interval time step to low values (i.e. 10 milliseconds). A C++ program solves the differential equations by following the flow chart in Figure 20.

Figure 20: Flow Diagram of C++ Program

Equations 9, 15, and 16 are cycled for cooling of hot bed and heating of cold bed.

Transient temperatures and flow are recorded. Transient data is necessary for the calculation of COP. Equation 17 will describe the evaporator.

$$\bar{q}_c = (h_g(P_c) - h_f(P_c)) \frac{1}{t_{1/2}} \int_0^{t_{1/2}} \dot{m} dt \quad (17)$$

This equation has the following assumptions.

- The average rate of heat transfer describes the amount of heat transfer for a refrigerant flow rate of zero (pressurization stage) to a maximum flow rate (desorption stage).
- No heat loss.
- Constant specific enthalpy.

Equation 18 will describe the fluid heater.

$$\bar{q}_{hr} = \frac{1}{t_{1/2}} \int_0^{t_{1/2}} \dot{m}_{fl} C_{fl} (T_{hr} - T_{fl,exit}(t)) dt \quad (18)$$

Equation 18 has the following assumptions.

- Constant specific heat, the average specific heat for the maximum and minimum temperature will be used.
- Constant flow rate of working fluid, HTF.
- Average rate of heat transfer describes the amount of heat transfer over a cycle with changing T_{fl} and T_{hr} .
- No heat loss.

Equations 17 and 18 will determine COP via Equation 19.

$$COP = \frac{\bar{q}_c}{\bar{q}_h} \quad (19)$$

A finite difference program will be developed to solve Equations 9, 15, and 16, and obtain the COP value with equation 19.

Validation of the model requires reproduction of the COP response to change in thermal conductivity. Ellis and Wepfer revealed that COP quickly rises from a low thermal conductivity value of 0.2 W/m K and then sharply rolls off to a slowly increasing COP value. Comparing the COP response to an existing system defined by Ellis and Wepfer validates the model produced in this thesis.

Boundary conditions exist for each differential equation that describes subsections within the adsorption heat pump. The initial condition for the temperature throughout the adsorption bed, HTF, and HTF pipe is described by the following.

$t = 0$, all z , all r , for the initial heating up of a cooled bed, all nodes in Figure 17.

$$T = T_{cool}, 280K \quad (20)$$

The next set of boundary conditions applies at time greater than zero. Equation 9 has the following conditions for the heating up of a cooled bed.

all z , $r = r_a$ (edges of adsorbent layer next to HTF pipe, see Figure 9):

$$h_a * (T_i - T_a) = q \quad (21)$$

all z , $r = 0$ (center of adsorbent bed):

$$\frac{dT}{dr} = 0 \quad (22)$$

Equation 16 (heat transfer through HTF) has the following conditions for the heating up of a cooled bed, see Figure 18.

$z = 0$, all r (beginning of HTF):

$$T = T_{\text{heat}}, 503\text{K} \quad (23)$$

all z , $r = r_o$ (outside radius of HTF):

$$\frac{dT}{dr} = 0 \quad (24)$$

all z , $r = r_{in}$ (inside radius of HTF):

$$h_r * (T_i - T_r) = q \quad (25)$$

Figure 21 illustrates one of cylindrical nodes for the adsorbent bed.

Figure 21: Cylindrical node representation of adsorbent

A list of physical properties is given in Table 4.

Table 4: Adsorption Heat Pump Parameters

Parameter	Value	Units	Reference
Convective heat transfer between HTF pipe and adsorbent	180	W/m ² K	Ellis and Wepfer 1999
Adsorbent density	450	kg/m ³	Ben Amar, et al. 1996
Adsorbent specific heat	920	J/kg K	Ben Amar, et al. 1996
Adsorbent thermal conductivity	0.2 to 10	W/m °C	Ellis and Wepfer 1999
Density of steel HTF pipe	7832	kg/m ³	Incropera and Dewitt 1996
Specific heat of steel HTF pipe	490.1	J/kg K	Incropera and Dewitt 1996
Adsorbent bed length	4.0	m	Ellis and Wepfer 1999
HTF pipe wall thickness	0.6	mm	Ellis and Wepfer 1999
Distance from edge of HTF to HTF pipe	3.0	mm	Ellis and Wepfer 1999
HTF pipe thermal conductivity	17.3	W/m °C	Back calculated from Ellis and Wepfer 1999
HTF density	914	kg/m ³	Ellis and Wepfer 1999
HTF specific heat	1930	J/kg °C	Ellis and Wepfer 1999
HTF thermal conductivity	0.115	W/m °C	Ellis and Wepfer 1999

Temperature of heater	503	K	Ellis and Wepfer 1999
Temperature of cooler	280	K	Ellis and Wepfer 1999
Temperature at refrigerant flow	314	K	Ellis and Wepfer 1999
Void Volume	0.27	-	Back calculated from Ellis and Wepfer 1999

Metal gauze (pin fins) will be added to the adsorbent bed to improve heat transfer from the HTF pipe to the adsorbent bed. The metal gauze will be modeled as a thin disc immersed between the adsorbent. An overall representation is alternating discs of adsorbent and pin fins. Figure 22 is the pin fins with the HTF pipe, HTF, and adsorbent.

Figure 22: Adsorption Bed Geometry

Equation 26 will describe heat transfer through the pin fin.

$$\pi r_p^2 \rho_p C_p \frac{\partial T_p}{\partial t} - \pi r_p^2 k_p \frac{\partial}{\partial z} \left(\frac{\partial T_p}{\partial z} \right) + 2\pi r_p h_o (T_p - T_a) = 0 \quad (26)$$

Equation 26 has the following assumptions:

- Pin fin has a cylindrical geometry that is surrounded by adsorbent material at the axial interfaces.
- A contact resistance between the pin fin and adsorbent material describes the heat transfer across this boundary.
- Thermal conductivity, density, and specific heat are constant for all materials, the average thermal conductivity for the maximum and minimum temperature will be used.

Equation 26 (heat transfer through the pin fin) has the following conditions for the heating up of a cooled bed.

All z , $r = r_a$:

$$k_{pf} * \frac{dT}{dr} = q \quad (27)$$

All z , $r = 0$ (center of adsorption bed):

$$\frac{dT}{dr} = 0 \quad (28)$$

$z = 0, z_a$, all r (edges of adsorbent layer next to pin fin, see Figure 22):

$$h_a * (T_a - T_{pf}) = q \quad (29)$$

$z = 0$ to z_{pf} , $r = r_{in-t}$ (HTF pipe surface next to pin fin, see Figure 22):

$$k_{pf} * \frac{dT}{dr} = q \quad (30)$$

As a result in limitations of available memory for a C++ program, the number of pin fins were set at 466, and the adsorbent bed thickness was reduced. Optimization of the Pin/Adsorbent volume ratio, pin fin size, and flow rate of at a 360 second cycle time was conducted for optimal COP results. This optimization was necessary before justifying the benefit of the metal gauze.

3.4.3 Optimization of Metal Gauze

Introduction of pin fins allows for optimization of key parameters; the size of the pin fin, the volume ratio of the pin fins to adsorbent, and the HTF flow at a 360-cycle time. Pin fin designs often require fine-tuning of the physical design to achieve optimum efficiency. The pin fin structure from the metal gauze will undergo the same kind of fine-tuning.

The size of the pin fin is geometric factor that will be varied. By keeping the adsorbent volume constant, the axial length of the pin fin will be varied. COP should respond as the size of the pin fin is optimized.

Varying the distance between the pins will optimize the volume of metal gauze in the adsorbent beds. The mass of the non-adsorbent material must be minimized (Miles and Shelton 1991), but still provide for adequate heat transfer. Thus, the optimal space between the pins fins must be determined that incurs the smallest possible non-absorbing mass penalty while simultaneously providing maximal thermal diffusivity. Model

simulations at different pin fin (gauze) spacing will be used to optimize the geometry of the gauze.

At a constant HTF flow, the frequency will be changed to observe the change in COP. Frequency is the length of time that the adsorption beds have to adsorb or desorb the refrigerant. By keeping the HTF flow constant and allowing the simulation to process a range of 350 to 385 seconds of process time, the COP will respond to a change in time.

3.4.4 Adsorbent Selection

The heart of the adsorption heat pump begins with the adsorbent material. Ellis and Wepfer used activated carbon AX21 to adsorb an ammonia refrigerant. Ellis and Wepfer indicated that the Dubinin-Radusch-Kovich coefficient was $1.2 \times 10^{-6} \text{ K}^{-2}$ and the initial adsorption level was $0.55 \text{ kg}_r/\text{kg}_a$. These parameters will be used throughout the model simulations except for the comparison simulation between activated carbon AX21 and zeolite 13X.

Zeolite 13X will be compared with activated carbon for the adsorbent material. This comparison will be evaluated for Ammonia as the refrigerant. This portion of the study illustrates the importance of adsorbent/refrigerant combinations. Physical parameters for zeolite 13X will be 640 kg/m^3 for the density, 837 J/kg K for the specific heat, 6.226×10^{-8} for the Dubinin-Radusch-kovich coefficient, and the initial adsorbent level will be $0.16 \text{ kg}_r/\text{kg}_a$.

4. Results

4.1 Model Validation

4.1.1 Model Results

The finite difference program is a suitable model for the depiction of COP. At a convective heat transfer coefficient of $180 \text{ W/m}^2\text{K}$, the new model in Figure 23 correlated with previous published results (Ellis and Wepfer 1999).

Figure 23: Thesis Model Validation

Low values of thermal conductivity resulted in low COP values (i.e. COP equal 0.03 at k_a equal to 0.14). COP rises rapidly from 0.03 to 0.68, when the thermal conductivity is varied from 0.14 to 0.8 W/m K . After the knee of the curve is obtained, the COP rolls off to a 1.08 value from a k_a value of 0.8 to 10.0 W/m K . This COP response is identical to published results (Ellis and Wepfer, 1999).

4.1.2 Model Comparison with Published Results

Differences exist between the thesis model and the published results by Ellis and Wepfer. Below a thermal conductivity value of 1.0 W/m K, the thesis model exhibits lower values for COP than the results from Ellis and Wepfer. Above 1.0 W/m K, the results from the thesis model is now inversed and COP is higher than the published results from Ellis and Wepfer. These differences could be a result from the geometrical arrangement of the adsorption bed. Ellis and Wepfer modeled the adsorption bed with the heating medium in the center of the bed. In this thesis, the heating medium was at the outer walls of the cylindrical adsorption bed.

4.1.3 Model Validation

Constant temperature, refrigerant flow, and thermal conductivity simulations validated the model without metal gauze. Constant HTF temperature at the initial bed kept the rest of the temperature nodes the same. By holding this boundary condition constant, the rest of the temperature nodes behaved as expected by not changing temperature. Refrigerant correctly flowed from the adsorption bed at the condenser operating pressure and portrayed an adsorption heat pump. Varied values for thermal conductivity produced the same COP response as illustrated by Ellis and Wepfer. All of the above simulations produced the expected results (see Figure 23) to validate the finite difference program.

4.2 Optimal Pin Size

Pin geometry is a parameter that requires optimization for the metal gauze design. The distribution of the metal gauze throughout the adsorbent bed corresponds to a pin fin network. Each pin acts as a source of heat for the neighboring adsorbent material. Adsorbent distance between the pin fins was held constant at 0.002m, while the pin fin size was varied. Figure 24 depicts the COP response to pin size.

Figure 24: COP Response to Pin Size

By varying the pin fin size from 5.0×10^{-5} meters to 1.0×10^{-4} , the COP increases from 1.16 to a maximum of 1.21. After the maximum, further increase in pin size results in counterproductive results for the addition of metal gauze. COP quickly falls to 0.33 for a pin fin size of 0.01 meters. As indicated in Figure 24, the COP response to a change in pin size is not very sensitive from 0.00005 to 0.005 meters. The pin size has to change by a factor of ten before the COP changes. An optimized pin fin size is 0.0001 meters.

4.3 Optimal Pin Volume

Another optimized parameter for the metal gauze design is the amount of pin fins. As the volume of the metal gauze was varied, a maximum COP of 1.11 was achieved at twenty percent (metal gauze/adsorbent*100%). Pin fin size was held constant at 0.0005 meters, while the adsorbent length between each pin fin was varied. Figure 25 depicts the COP varied from 0.07 to 0.33 pin volumes.

Figure 25: COP Response to Pin/Adsorbent Volume

The COP shows some sensitivity to changes in the volume ratio. As with other pin fin designs, the number of pin fins or in this case the volume of pin fins will have an optimum value to achieve the best COP.

4.4 Time Variation

Cycle time is an optimization parameter that is common with heat pumps. As with other adsorption heat pumps, switching frequency is optimized to achieve the best COP. Pin fin size was held constant at 0.0005m and the volume ratio was held constant at 20%. Figure 26 illustrates the importance of varying the time at a constant HTF flow of 0.01 m/s.

Figure 26: COP versus Time (Switching Frequency)

The beginning of the curve illustrates the importance of allowing enough time for the adsorption bed to achieve the correct pressures. Insufficient heat is supplied, then the pressure is not high enough to allow the refrigerant to leave the adsorption bed. At 350 seconds, the adsorption bed still contains a great deal of the refrigerant, as is evident by the low COP value of 0.24. The quick rise in COP as the frequency is increased from

350 seconds to 360 seconds indicates available refrigerant. The maximum at 360 seconds indicates that all of the refrigerant has been moved. After the maximum is achieved at 360 seconds, the COP slowly decreases. Constant HTF flow rate of 0.01 m/s requires a switching frequency of 360 seconds.

4.5 Incorporation of Metal Gauze

This model demonstrated the overall benefit from incorporation of metal gauze. Optimized pin fin conditions of 0.0005m for the pin fin size and 20% volume ratio of metal gauze/adsorbent were derived from optimization . Figure 27 depicts the improvement of COP by the addition of metal gauze (pin fins). With the metal gauze, the COP response has a different response to thermal conductivity. An average COP value of 1.07 runs from the low thermal conductivity value to the upper end of the scale. COP exhibits a small amount of change when thermal conductivity is varied from 0.01 (COP = 1.04) to 10 W/m K (COP = 1.11), as compared to the original design that lacks metal gauze.

Addition of metal gauze produces a large difference at the beginning range of thermal conductivity, but quickly dissipates at the upper range. Figure 28 illustrates the differences between the two curves. COP improves by 89% at k_a equal to 0.5 and then steadily decreases to a 3% improvement at the end of the thermal conductivity scale. Incorporation of metal gauze displays an advantage over the original thesis model (without gauze).

Figure 27: Incorporation of Metal Gauze

Figure 28: Difference Between Metal Gauze Design and Original

$$\%COP_{\text{Improvement}} = \frac{COP_{\text{w/ gauze}} - COP_{\text{w/o gauze}}}{COP_{\text{w/o gauze}}} \quad (22)$$

4.6 Evaluation of Zeolite 13X

A simulation was conducted to review the Zeolite 13x as the adsorbent material. Volume ratio between the pin fin and adsorbent material was kept at 20%, while the pin fin size was held at 0.0005m. The adsorbent thermal conductivity was virtually the same for both Zeolite 13x and activated carbon. However, the adsorption ability of the two adsorbents varied for the ammonia refrigerant. Table 5 is the COP results from the activated carbon and zeolite 13X.

Table 5: Adsorbent COP results

Adsorbent	COP
Activated Carbon	1.11
Zeolite 13X	0.89

Since activated carbon was better ammonia adsorbent than zeolite 13x, activated carbon achieved a 1.11 COP and the Zeolite 13x had a 0.89 COP at a pin fin setting of 0.0005 m for the pin fin size and 20% volume ratio. As with other optimized heat pump parameters the adsorbent material must be correctly selected to achieve the best COP given a particular refrigerant.

5. Conclusion

5.1 Model Validation

The constant temperature, refrigerant flow, and thermal conductivity simulations validated the baseline model. These simulations insured the validity of the model for future comparison of the model with pin fins. Most importantly, there was good agreement between the developed model and literature (see Figure 23).

5.2 Optimal Pin Size

The results agree with expectations for a pin fin design (Figure 24). Large pin fin sizes results in too much heat allocation to the non-adsorbing mass. As a result, the COP diminishes to counter productive results (COP equals 0.33 at pin fin size of 0.01 meters). Also, the portion of the curve to the left of the maximum displays lower values of COP because there is not enough heat supplied to the adsorbent bed. The mass of the pin fin has to be able to deliver a certain amount of heat in order to achieve any effectiveness. Otherwise, a portion of the useable heat is loss to elevating the temperature of a non-adsorbing mass and not directed into the adsorbent bed.

Typical pin fin designs require an optimization of the geometry, in this case the width of the pin fin. As illustrated in Figure 24 the optimum value was at 0.1 mm, however the available metal gauze is 0.5 mm. An actual device would suffer some loss, but this size is still very close the maximum. A luxury in this design parameter is the small sensitivity to change in the pin fin size. Since this is only a factor of five change

and not ten, the COP is still close to the maximum value.

5.3 Optimal Pin Volume

The stainless steel design had an optimal volume of 20% for pin fins relative to adsorbent material (Figure 25). As with the geometry of the pin fin, the number of pin fins or volume must be optimized for each constructional material. Too many pin fins sacrifices adsorbing material, which is a similar result to the consolidated adsorbent reviews. In addition, too little mass only warms the adsorbent up in secluded pockets, and the heat is not utilized effectively.

5.4 Time Variation

When the pumping speed is held constant, there was an optimum bed frequency of 360 seconds (Figure 26). Since the available heat is held constant, there is an optimum amount of time to achieve the best COP with a dual adsorption bed design. If the bed is not given enough time to heat up, then the refrigerant will not reach a high enough pressure to flow. Once sufficient time is allowed for refrigerant flow, then the optimum COP value depends upon displacing the entire available refrigerant. Once the entire refrigerant has been displaced, then additional heat dumped into the system is for naught. There is no more refrigerant to move, so heat is wasted into a fully discharged bed. As depicted by the COP vs. Time figure (Figure 26), the COP steadily decays after achieving the maximum value for bed switching frequency. Since the COP response to change is small after the maximum, the frequency window should always guarantee the

maximum value with a slight overshoot.

5.5 Incorporation of Metal Gauze

Incorporation of metal gauze achieved a definite benefit (Figure 27). The metal gauze design exhibited a superior COP over the entire thermal conductivity range. The greatest impact was at low values of thermal conductivity. The main problem with the available adsorbents is the low thermal conductivity value. The pin fin design compensates for typical low thermal conductivity values and allows the bed to behave as though the thermal conductivity was at 10 W/m K (Figure 25: Incorporation of Metal Gauze). In fact, the COP displayed a linear response to change in thermal conductivity that ranged from 1.04 to 1.11. The metal gauze/pin fin design is an excellent alteration to allow low thermal conducting materials into the adsorption bed.

Low thermal conductivity is resolved with the metal gauze design. Other researchers indicated that thermal conductivity is one of the main barriers for most adsorbents. However, the metal gauze compensates for the low thermal conductivity. Metal gauze removes the main hindrance of low thermal conductivity and allows for the exploration of adsorbent material with better adsorptive capabilities. Other design concepts can now focus on improving the heat transfer between the heating mass and the adsorbent material without worrying about the adsorbent thermal conductivity.

5.6 Evaluation of Zeolite 13X

The results indicate the importance of adsorption properties of the adsorbent. Although Zeolite 13x had excellent adsorbing properties for water, however this thesis modeled an Ammonia based system. Activated carbon had better adsorption for Ammonia, and delivered a superior COP when compared to Zeolite 13x. Future consideration should be given to optimization for a Zeolite 13X adsorbent. This comparison was performed at optimized conditions for activated carbon. However, variation in the volume ratio for the pin fin and Zeolite 13X might reveal an improved value for COP. Thorough review of the adsorbent's potential for the desired refrigerant will benefit the overall design by attaining higher COPs.

5.7 Overall

This thesis realized the value of incorporating metal gauze. This design is not dependent upon the thermal conductivity of the adsorbent material. As with other adsorbent heat pumps, operating parameters as well as building materials require optimization to achieve the best COP.

6. Future Work

6.1 Model Refinement

Due to the restrictions of the C++ compiler, the grid was restrained to alternating rows of adsorbent and metal gauze material. The number of intermediate nodes between the metal gauze could be increased and the total number of pin fins reduced. As a result, the overall length of the adsorbent bed would decrease. This action would explore the unforeseen COP sensitivity at the lower thermal conductivity values.

6.2 Adsorbent Focus

This new metal gauze design minimizes the thermal conductivity impact on COP for low values. Future work should focus on reviewing adsorbents with high adsorption capacity, even the adsorbents with low thermal conductivity.

6.3 Contact Resistance

As indicated by Ellis and Wepfer, an increase in heat transfer from the heating medium to the adsorbent bed will increase COP. This area requires more attention to maximize the COP for adsorption heat pumps.

6.4 Experimental Device

This thesis produced simulated results, and future work in this area would benefit from an actual device. Experiments with a physical device would provide further validation of the finite difference model and the metal gauze design.

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Appendix A Mathematical Relations and Results by Zheng, Worek, and Nowakowski

Bed Switching Speed (ω)

$$\omega = \frac{M_d C_{p,d}}{\bullet m_f C_{p,f} t_{hc}}$$

M_d = weight of dry adsorbent, kg

$C_{p,d}$ = specific heat of adsorbent, kJ/kg °C

•

m_f = flow rate of heat transfer fluid, kg/s

$C_{p,f}$ = specific heat of refrigerant, kJ/kg °C

t_{hc} = time of bed in one position, s

Number of Transfer Units (NTU)

$$NTU = \frac{h_f A_f}{\bullet m_f C_{p,f}}$$

h_f = convective heat transfer coefficient, kW/m² °C

A_f = heat transfer area in bed, m²

•

m_f = flow rate of heat transfer fluid, kg/s

$C_{p,f}$ = specific heat of refrigerant, kJ/kg °C

Adsorbent Biot Number (Bi_d)

$$Bi_d = \frac{h_f D}{k_d}$$

h_f = convective heat transfer coefficient, kW/m² °C

D = half of adsorbent layer thickness, m

k_d = thermal conductivity of adsorbent, kW/m °C

Contact Biot Number (Bi_c)

$$Bi_c = \frac{h_f}{h_c}$$

h_f = convective heat transfer coefficient, kW/m² °C

h_c = contact heat transfer coefficient, kW/m² °C

Inert Alpha Number (α_{w-d})

$$\alpha_{w-d} = \frac{M_w C_{p,w}}{M_d C_{p,d}}$$

M_w = weight of inert mass, kg

$C_{p,w}$ = specific heat of tubing wall, kJ/kg °C

M_d = weight of dry adsorbent, kg

$C_{p,d}$ = specific heat of adsorbent, kJ/kg °C

Fluid Alpha Number (α_{f-d})

$$\alpha_{f-d} = \frac{M_f C_{p,f}}{M_d C_{p,d}}$$

M_f = weight of resident heat transfer fluid, kg

$C_{p,f}$ = specific heat of heat transfer fluid, kJ/kg °C

M_d = weight of dry adsorbent, kg

$C_{p,d}$ = specific heat of adsorbent, kJ/kg °C

Note: NSCC = dimensionless specific cooling capacity

Appendix B Definitions of Nondimensional Relations

Vapor specific volume (A)

Ratio of the vapor specific volume to the adsorbate specific volume.

$$A = \frac{(1 - \varepsilon)}{\varepsilon} \cdot \frac{\rho_r \omega}{\rho_v^s}$$

ε = void volume

ρ_r = adsorbate density, kg/m³

ρ_v^s = saturated refrigerant vapor, kg/m³

ω = adsorption level, kg/kg_a

Contact Biot number (Bi_c)

Ratio of the tube/adsorbent contact heat transfer coefficient to the convective coefficient.

$$Bi_c = \frac{h_o}{h_i}$$

h_o = contact heat transfer coefficient at tube/adsorbent interface, W/m² K

h_i = convective heat transfer coefficient at fluid/tube interface, W/m² K

Heat of vaporization (C_{av})

Ratio of the thermal capacitance associated with adsorption to that of the adsorbent.

$$C_{av} = \frac{\rho_r \omega h_{av}^s}{\rho_a C_a T_h}$$

ρ_r = adsorbate density, kg/m³

ρ_a = adsorbent density, kg/m³

ω = adsorption level, kg/kg_a

h_{av}^s = specific enthalpy of refrigerant, kJ/kg

C_a = specific heat of adsorbent, kJ/kg K

T_h = Highest temperature, K

HTF pipe thermal capacitance (C_{tf})

Ratio of the heat transfer tube (HTF pipe) thermal capacitance to the heat transfer fluid
(HTF) thermal capacitance

$$C_{tf} = \frac{2b\rho_t C_t}{r_t \rho_f C_f}$$

b = tube wall thickness, m

ρ_t = density of the HTF pipe, kg/m³

C_t = specific heat of the HTF pipe, kJ/kg K

r_t = inside radius of the HTF pipe, m

ρ_f = density of the heat transfer fluid, kg/m³

C_f = specific heat of the heat transfer fluid, kJ/kg K

Vapor specific heat (C_p)

Ratio of the vapor thermal capacitance to the adsorbent thermal capacitance

$$C_p = \frac{\varepsilon \rho_v^s C_{p,v}}{(1 - \varepsilon) \rho_a C_a}$$

ϵ = void volume

ρ_v^s = saturated refrigerant vapor, kg/m³

$C_{p,v}$ = specific heat of refrigerant vapor, kJ/kg °C

ρ_a = adsorbent density, kg/m³

C_a = specific heat of adsorbent, kJ/kg K

Compression Work (C_{pr})

Ratio of the compression work to the adsorbent thermal capacitance

$$C_{pr} = \frac{\epsilon P_c}{(1 - \epsilon) \rho_a C_a T_h}$$

ϵ = void volume

P_c = condenser pressure, kPa

ρ_a = adsorbent density, kg/m³

C_a = specific heat of adsorbent, kJ/kg K

T_h = high temperature, K

Fourier Number (Fo)

Ratio of the system time scale to the time scale for radial conduction

$$Fo = \frac{k_a t^s}{(1 - \epsilon) \rho_a C_a r_a^2}$$

k_a = thermal conductivity of adsorbent, W/m K

t^s = time to saturation, sec

ϵ = void volume

ρ_a = adsorbent density, kg/m³

C_a = specific heat of adsorbent, kJ/kg K

r_a = radius of adsorbent, m

Time Ratio (H_o)

Ratio of the system time to the time for fluid to traverse the length of the tube

$$H_o = \frac{V_{fl} t^s}{L}$$

V_{fl} = heat transfer fluid velocity, m/s

t^s = time to saturation, sec

L = length of the adsorbent bed, m

Aspect Ratio (N_l)

Ratio of the adsorbent length to the adsorbent radius

$$N_l = \frac{L}{r_a}$$

L = length of the adsorbent bed, m

r_a = radius of the adsorbent, m

Number of transfer units (NTU)

Ratio of the heat transfer at the tube wall to the advection of energy in the fluid

$$NTU = \frac{2\pi r_i L h_i}{\pi r_i^2 V_{fl} \rho_{fl} C_{fl}}$$

r_i = radius of the HTF pipe, m

L = length of the adsorbent bed, m

h_i = convective heat transfer coefficient at fluid/tube interface, W/m² K

V_{η} = heat transfer fluid velocity, m/s

ρ_{η} = density of heat transfer fluid, kg/m³

C_{η} = specific heat of heat transfer fluid, kJ/kg K

Peclet Number (Pe)

Ratio of axial advection to axial conduction in the fluid

$$Pe = \frac{V_{\eta} L}{k_{\eta} / \rho_{\eta} C_{\eta}}$$

V_{η} = heat transfer fluid velocity, m/s

L = length of the adsorbent bed, m

k_{η} = thermal conductivity of heat transfer fluid, W/m K

ρ_{η} = density of heat transfer fluid, kg/m³

C_{η} = specific heat of heat transfer fluid, kJ/kg K

Tube resistance (Ω_t)

Ratio of the thermal resistance of the tube to the thermal resistance of the heat transfer fluid

$$\Omega_t = \frac{r_t k_{\eta}}{2bk_t}$$

r_t = radius of the HTF pipe, m

k_f = thermal conductivity of heat transfer fluid, W/m K

b = tube wall thickness of HTF pipe, m

k_t = thermal conductivity of HTF pipe, W/m K

Appendix C C++ code for Adsorption heat pump without metal gauze

/*C program to calculate temperatures from numerical nodes*/

#include <stdio.h>

#include <math.h>

#include <stdlib.h>

#include <alloc.h>

/*Main part of program*/

float main ()

{

/*Declaration of variables*/

int i, timestep1, timestep2, k, vcheck, j;

double exptime, deltat;

double pi, zstep1, rstep[4];

double r[6]; /*radius dimensions*/

double Ap[6], Ar[8]; /*Cross section area along z direction and parallel area in r direction*/

double alphas1, alphas, alphas; /*thermal diffusion for HTF,HTF pipe, adsorbent*/

double Bi[8], Fo[10]; /*Fourier numbers*/

double kfl, kt;

float ka; /*thermal conductivity*/

```

double pfl, pt, pa, pr; /*density*/

double cfl, ct, ca, cr; /*specific heat*/

double epsilon; /*void volume*/

double omegao, omega; /*adsorption level*/

double vrfl; /*velocity of refrigerant*/

float vfl; /*velocity of HTF*/

double hav;

static double Ca, Cb, Cc, vrtot; /*constants for adosrbent layers*/

double HV; /*heat of vaporization for ammonia*/

double D; /*coefficient in Dubinin-Raduschkovich equation*/

double B; /*constant in vapor pressure curve correlation*/

double m; /*coefficient in vapor pressure curve correlation*/

double R, z, mr, vmax;

double CE, K, u;

double hfl, ha; /*convective and contact resistance coeff*/

FILE *fptr;

char *filename="therm.txt";

FILE *fptr3;

char *filename3="htemp.txt";

FILE *fptr4;

char *filename4="hparam.txt";

static float T[3501][2];

```

```

double MW; /*Molecular weight of refrigerant*/

double Press[3]; /*condenser [1] and exit pressure [2]*/

double InitBed; /*Initial Bed Temp*/

double InitHTF, InitHTF2; /*HTF temp into Bed*/


printf("\nHeating of Cold adsorption bed / Pressurization\n");


printf("Enter the bed thermal conductivity 1 W/m/K\n");

scanf("%f", &ka);


/*printf("Enter the velocity of the HTF (ie .0158 m/s)\n");

scanf("%f", &vfl);*/

for (j=1; j<2; j++){

vfl = (j/1000.0+1)*0.03;


/*Retrieve Parameters*/

/*printf("Enter the deltat time from the time step application (ie 1.0e-3 seconds)\n");

scanf("%f", &deltat);*/

deltat = 0.01;

```



```

/*printf("Enter the HTF temperature entering the adsorbent bed (ie 500 Kelvin)\n");

scanf("%f", &InitHTF);*/

InitHTF = 503.0;


/*printf("Enter the initial adsorbent bed temperature (ie 280 Kelvin)\n");

scanf("%f", &InitBed);*/

InitBed = 314.0;


/*printf("Enter the radius length for the interval spacing in the adsorbent beds (ie .03175
m)\n");

scanf("%f", &rstep[1]);*/

rstep[1] = 0.004;


/*printf("Enter the HTF pipe thickness (ie .0735 m)\n");

scanf("%f", &rstep[2]);*/

rstep[2] = 0.0006;


/*printf("Enter the inside radius of the HTF pipe (ie .0037 m)\n");

scanf("%f", &rstep[3]);*/

rstep[3] = .003;


/*printf("Enter the adsorbent spacing in the z direction (ie .0095 m)\n");

```

```
scanf("%f", &zstep1);*/
```

```
zstep1 = 0.0057143;
```

```
/*printf("Enter the contact resistance between the adsorbent and HTF pipe (ie 180 Watts /  
(m^2 K)\n");
```

```
scanf("%f", &ha);*/
```

```
ha = 180.0;
```

```
/*Assignment of variables*/
```

```
pi = 3.14159265;
```

```
/*Radius measurements in meters*/
```

```
r[1] = rstep[1]/2.0;
```

```
r[2] = r[1]+rstep[1];
```

```
r[3] = r[2]+rstep[1];
```

```
r[4] = r[3]+rstep[2];
```

```
r[5] = r[4]+rstep[3];
```

```
/*Cross section area along z axis*/
```

```
for (i=1; i<5; i=i+1){
```

```
    Ap[i] = pi * (r[6-i]*r[6-i]-r[5-i]*r[5-i]);
```

```
}
```

```
Ap[5] = pi * (r[1]*r[1]);
```

```
/*parallel area in concentric radius axis*/
```

```
Ar[1] = 2 * pi * r[4] * zstep1;
```

```
Ar[3] = 2 * pi * r[3] * zstep1;
```

```
Ar[5] = 2 * pi * r[2] * zstep1;
```

```
Ar[7] = 2 * pi * r[1] * zstep1;
```

```
/*Thermal conductivity*/
```

```
kfl = .115; /*htf thermal conductivity W /m / K at avg of 500 and 280K */
```

```
kt = 17.319; /*htf pipe thermal conductivity, AISI 1010 Carbon Steel, Incropera &  
DeWitt p 828*/
```

```
/*adsorbent thermal conductivity
```

```
printf("Enter the thermal conductivity of the adsorbent bed (ie 1 Watts / (m K)\n");
```

```
scanf("%f", &ka); */
```

```
/*density*/
```

```
pfl = 914.0; /*density of htf*/
```

```
pt = 7832.0; /*density of htf pipe kg / m^3*/
```

pa = 450.0; /*density of adsorbent*/

/*molecular weight of ammonia in g/mole */

MW = 17.03;

**R=8.314/MW*1000.0; /*R constant in terms of J/K/kg(refrigerant) or m³ * Pa / K / kg
*/**

/*specific heat*/

cfl = 1930.0; /*htf at 400K J/kg K*/

ct = 490.1; /*htf pipe at 400K*/

ca = 920.0; /*adsorbent*/

cr = 1399.2; /*refrigerant vapor*/

/*convective heat transfer for HTF*/

hfl = 4.36*kfl/(rstep[3]);

/*Fraction of Void Volume*/

epsilon = .27;

/*adsorption level*/

omegao = .55;

/*coefficient in Dubinin-Raduschkovich equation*/

$$D = 1.2e-6;$$

/*constant in vapor pressure curve correlation*/

$$B = 23.066;$$

/*Heat of Vaporization*/

$$HV = 1351.0 * 1000.0; /*J /kg */$$

/*coefficient in vapor pressure curve correlation*/

$$m = HV/R;$$

/*Constant in Ergun Equation*/

$$CE = 0.55;$$

/*Permeability*/

$$K = 1.0e-9;$$

/*Dynamic Viscosity, N s / m^2*/

$$u = 134.5e-7;$$

/*Thermal diffusivity*/

alphafl = kfl/(pfl * cfl); /*HTF*/

alphan = kt / (pt * ct); /* HTF pipe*/

alphaa = ka / (pa * ca); /*adsorbent*/

/*Biot Numbers*/

Bi[1] = (hfl * zstep1)/kfl;

Bi[3] = (hfl * zstep1) / kt;

Bi[4] = (ha * zstep1) / kt;

Bi[7] = (ha * zstep1) / ka;

/*Fourier Number*/

Fo[1] = alphafl*deltat/zstep1/zstep1;

Fo[3] = alphan*deltat/zstep1/zstep1;

Fo[9] = alphaa*deltat/zstep1/zstep1;

/*Compressibility Factor*/

z = 0.78; /*compressibility factor with Tr = .962 and Pr = .473 */

/*Header Statement on disk file*/

if ((fptr3 = fopen(filename3, "a")) == NULL)

printf("\nBad File Open");

```

        fprintf(fp3, "Time, HTF in, HTF out, ADS in, ADS out, Mass
Flow, Press in, Press out, omega, in rho, out rho\n");

        fclose(fp3);

/*Initial temp conditions*/

        for (i=1; i<3501; i=i+1){

                T[i][0] = InitBed;    /*T[#][time step] Temperature number at time t*/

        }

/*HTF initial conditions*/

        T[5][0] = InitHTF;

        InitHTF2 = 314.0;

/*vcheck will equal 1 if the amount of mass moved exceeds the initial mass of the bed*/

        vcheck = 0;

/*Initial density conditions*/

        pr = 11.2;

        vmax = ((1.0-epsilon)*pa*omegao+epsilon*pr)*pi*r[3]*r[3]*zstep1*699.0;

```

```
Cc = pr*R*z;
```

```
for (k=1; k<6; k++){
```

```
/*total refrigerant moved*/
```

```
vrtot = 1.0e-30;
```

```
vrfl = 1.0e-30;
```

```
vcheck = 0;
```

```
/*Temperature determination at each time step*/
```

```
for (timestep1=1; timestep1<3601; timestep1++){
```

```
    for (timestep2=1; timestep2<=10; timestep2++){
```

```
/*velocity of refrigerant*/
```

```
vrtot = vrtot + pi*r[3]*r[3]*vrfl*pr*deltat;
```

```
if (k==1){
```

```
    Press[1] = pr*R*T[1][0]*z;
```

```
    Press[2] = pr*R*T[3496][0]*z;
```

```
        if (Press[2]>1.603e6)
```



```

        {vrfl = (-u/K+sqrt(u*u/K/K-4.0*(Press[2]-
Press[1])*CE*pr/sqrt(K)/zstep1/699.0))/(2.0*CE*pr/sqrt(K));

        }

        if (vrtot > vmax)

            {vrfl = 1.0e-30;

            vcheck = 1;

            }

        /*Initial Temp for heating phase*/

        T[5][0] = InitHTF;

    }

    if (k==2){

        Press[1] = pr*R*T[3496][0]*z;

        Press[2] = pr*R*T[1][0]*z;

        if (Press[2]<1.38e6)

            {vrfl = (-u/K+sqrt(u*u/K/K-4.0*(Press[2]-
Press[1])*CE*pr/sqrt(K)/zstep1/699.0))/(2.0*CE*pr/sqrt(K));

            }
    }

```

```

        if (vrtot > vmax)

            {vrfl = 1.0e-30;

            vcheck = 1;

            }

        /*Initial Temp for cooling phase*/

        T[5][0] = InitHTF2;

    }

    if (k==3){

        Press[1] = pr*R*T[1][0]*z;

        Press[2] = pr*R*T[3496][0]*z;

        if (Press[2]>1.603e6)

            {vrfl = (-u/K+sqrt(u*u/K/K-4.0*(Press[2]-
Press[1])*CE*pr/sqrt(K)/zstep1/699.0))/(2.0*CE*pr/sqrt(K));

            }

        if (vrtot > vmax)

            {vrfl = 1.0e-30;

            vcheck = 1;

            }

```

```

        /*Initial Temp for heating phase*/

        T[5][0] = InitHTF;

    }

    if (k==4){

        Press[1] = pr*R*T[3496][0]*z;

        Press[2] = pr*R*T[1][0]*z;

        if (Press[2]<1.38e6)

            {vrfl = (-u/K+sqrt(u*u/K/K-4.0*(Press[2]-
Press[1])*CE*pr/sqrt(K)/zstep1/699.0))/(2.0*CE*pr/sqrt(K));

            }

        if (vrtot > vmax)

            {vrfl = 1.0e-30;

            vcheck = 1;

            }

        /*Initial Temp for cooling phase*/

        T[5][0] = InitHTF2;

    }

```

```

if (k==5){

    Press[1] = pr*R*T[1][0]*z;

    Press[2] = pr*R*T[3496][0]*z;


    if (Press[2]>1.603e6)

        {vrfl = (-u/K+sqrt(u*u/K/K-4.0*(Press[2]-
Press[1])*CE*pr/sqrt(K)/zstep1/699.0))/(2.0*CE*pr/sqrt(K));

        }


    if (vrtot > vmax)

        {vrfl = 1.0e-30;

        vcheck = 1;

        }


    /*Initial Temp for heating phase*/

    T[5][0] = InitHTF;

}


if (k==6){

    Press[1] = pr*R*T[3496][0]*z;

    Press[2] = pr*R*T[1][0]*z;

```

```

        if (Press[2]<1.358e6)

            {vrfl = (-u/K+sqrt(u*u/K/K-4.0*(Press[2]-
Press[1])*CE*pr/sqrt(K)/zstep1/699.0))/(2.0*CE*pr/sqrt(K));

            }

        if (vrtot > vmax)

            {vrfl = 1.0e-30;

            vcheck = 1;

            }

        /*Initial Temp for cooling phase*/

        T[5][0] = InitHTF2;

    }

    /*Node 5, HTF at z=0*/

    i=5;

    T[i][1] = T[i][0];

    /*Node 500, HTF at z=L*/

    i = 3500;

    T[i][1] =-Ar[1]*Fo[1]*Bi[1]/Ap[1]*T[i][0]+(-
2.0*Fo[1]*Ap[1]*zstep1*T[i][0]+Ar[1]*Fo[1]*Bi[1]*zstep1*T[i-

```

```
1][0]+T[i][0]*Ap[1]*zstep1+2.0*Fo[1]*Ap[1]*zstep1*T[i-5][0]+vfl*deltat*Ap[1]*T[i-5][0]-vfl*deltat*Ap[1]*T[i][0])/(Ap[1]*zstep1);
```

```
/*Node 10, HTF intermediate*/
```

```
for (i=10; i<3496; i=i+5){
```

```
    T[i][1] = (-vfl*deltat*Ap[1]+zstep1*Ap[1]-2.0*Fo[1]*zstep1*Ap[1])/(zstep1*Ap[1])*T[i][0]+(Fo[1]*zstep1*Ap[1]*T[i-5][0]+vfl*deltat*Ap[1]*T[i-5][0]-Ar[1]*Fo[1]*Bi[1]*zstep1*T[i][0]+Ar[1]*Bi[1]*Fo[1]*zstep1*T[i-1][0]+Fo[1]*zstep1*Ap[1]*T[i+5][0])/(zstep1*Ap[1]);

}
```

```
/*Node 4, HTF pipe - beginning*/
```

```
i =4;
```

```
    T[i][1] = (-Ar[3]*Fo[3]*Bi[4]+Ap[2]-2.0*Fo[3]*Ap[2]-Ar[1]*Fo[3]*Bi[3])/(Ap[2])*T[i][0]+(Ar[3]*Fo[3]*Bi[4]*T[i-1][0]+2.0*Fo[3]*Ap[2]*T[i+5][0]+Ar[1]*Fo[3]*Bi[3]*T[i+1][0])/(Ap[2]);
```

```
/*Node 9, HTF pipe intermediate*/
```

```
for (i=9; i<3496; i=i+5){
```

```
    T[i][1] = (Ap[2]-2.0*Fo[3]*Ap[2]-Ar[1]*Fo[3]*Bi[3]-
```

$$\frac{Ar[3]*Fo[3]*Bi[4]}{Ap[2]*T[i][0]} + (Ar[1]*Fo[3]*Bi[3]*T[i+1][0] + Fo[3]*Ap[2]*T[i-5][0] + Fo[3]*Ap[2]*T[i+5][0] + Ar[3]*Fo[3]*Bi[4]*T[i-1][0]) / Ap[2];$$

}

/*Node 499, HTF parallel to pin fin layer*/

i = 3499;

$$T[i][1] = (-Ar[3]*Fo[3]*Bi[4] + Ap[2] - 2.0*Fo[3]*Ap[2] - Ar[1]*Fo[3]*Bi[3]) / (Ap[2]*T[i][0] + (Ar[3]*Fo[3]*Bi[4]*T[i-1][0] + 2.0*Fo[3]*Ap[2]*T[i-5][0] + Ar[1]*Fo[3]*Bi[3]*T[i+1][0]) / Ap[2]);$$

/*Node 3, adsorbent node, column 3, beginning*/

i = 3;

$$\omega = \omega_{ao} * \exp(-D*T[i][0]*T[i][0]*(B-m/T[i][0] - \log(pr*R*T[i][0]*z)) * (B-m/T[i][0] - \log(pr*R*T[i][0]*z)));$$

$$Ca = (cr + 1.42/2.0*R/\sqrt{D}) * (-2.0*D*T[i][0]*(B-m/T[i][0] - \log(pr*R*T[i][0]*z)) * (B-m/T[i][0] - \log(pr*R*T[i][0]*z)) - 2.0*D*T[i][0]*T[i][0]*(B-m/T[i][0] - \log(pr*R*T[i][0]*z)) * (m/T[i][0]/T[i][0] - 1.0/T[i][0])) * \omega / \omega_{ao};$$

$$Cb = (-2.0*D*T[i][0]*(B-m/T[i][0] - \log(pr*R*T[i][0]*z)) * (B-m/T[i][0] - \log(pr*R*T[i][0]*z)) - 2.0*D*T[i][0]*T[i][0]*(B-m/T[i][0] - \log(pr*R*T[i][0]*z)) * (m/T[i][0]/T[i][0] - 1.0/T[i][0])) * \omega;$$

$$hav = (m + 1.58/\sqrt{D} - 1.42/\sqrt{D}) * \omega / \omega_{ao} * R;$$

$$\begin{aligned}
T[i][1] = & (\text{epsilon} * \text{pr} * \text{cr} * \text{alphaa} * T[i][0] * \text{Ap}[3] * \text{rstep}[1] - \\
& \text{cr} * \text{pr} * \text{vrf1} * \text{Fo}[9] * \text{zstep1} * \text{Ap}[3] * \text{rstep}[1] * T[i][0] + \text{cr} * \text{pr} * \text{vrf1} * \text{Fo}[9] * \text{zstep1} * \text{Ap}[3] * \text{rstep}[1] * T[i+5][0] + T[i][0] * \text{ka} * \text{Ap}[3] * \text{rstep}[1] - \\
& T[i][0] * \text{ka} * \text{Ap}[3] * \text{rstep}[1] * \text{epsilon} + \text{Ar}[5] * \text{Fo}[9] * \text{zstep1} * \text{ka} * T[i-1][0] - \\
& \text{Ar}[5] * \text{Fo}[9] * \text{zstep1} * \text{ka} * T[i][0] + \text{pa} * \text{omega} * \text{alphaa} * \text{Ca} * T[i][0] * \text{Ap}[3] * \text{rstep}[1] - \\
& \text{pa} * \text{omega} * \text{alphaa} * \text{Ca} * T[i][0] * \text{Ap}[3] * \text{rstep}[1] * \text{epsilon} - \\
& \text{pa} * \text{hav} * \text{alphaa} * \text{Cb} * T[i][0] * \text{Ap}[3] * \text{rstep}[1] + \text{pa} * \text{hav} * \text{alphaa} * \text{Cb} * T[i][0] * \text{Ap}[3] * \text{rstep}[1] * \\
& \text{epsilon} - \\
& \text{epsilon} * \text{alphaa} * \text{Cc} * T[i][0] * \text{Ap}[3] * \text{rstep}[1] + 2.0 * \text{Fo}[9] * \text{ka} * \text{Ap}[3] * \text{rstep}[1] * T[i+5][0] - \\
& 2.0 * \text{Fo}[9] * \text{ka} * \text{Ap}[3] * \text{rstep}[1] * T[i][0] + \text{Ar}[3] * \text{Fo}[9] * \text{Bi}[7] * \text{ka} * \text{rstep}[1] * T[i+1][0] - \\
& \text{Ar}[3] * \text{Fo}[9] * \text{Bi}[7] * \text{ka} * \text{rstep}[1] * T[i][0]) / (\text{Ap}[3] * \text{rstep}[1] * (\text{epsilon} * \text{pr} * \text{cr} * \text{alphaa} + \text{ka} - \\
& \text{epsilon} * \text{ka} + \text{pa} * \text{omega} * \text{alphaa} * \text{Ca} - \text{pa} * \text{omega} * \text{alphaa} * \text{Ca} * \text{epsilon} - \\
& \text{pa} * \text{hav} * \text{alphaa} * \text{Cb} + \text{pa} * \text{hav} * \text{alphaa} * \text{Cb} * \text{epsilon} - \text{epsilon} * \text{alphaa} * \text{Cc}));
\end{aligned}$$

/*Node 2, adsorbent node, column 2, beginning*/

i=2;

$$\begin{aligned}
\text{omega} = & \text{omegao} * \exp(-D * T[i][0] * T[i][0] * (B - m/T[i][0] - \\
& \log(\text{pr} * R * T[i][0] * z)) * (B - m/T[i][0] - \log(\text{pr} * R * T[i][0] * z)));
\end{aligned}$$

$$\begin{aligned}
\text{Ca} = & (\text{cr} + 1.42/2.0 * R / \sqrt{D}) * (-2.0 * D * T[i][0] * (B - m/T[i][0] - \\
& \log(\text{pr} * R * T[i][0] * z)) * (B - m/T[i][0] - \log(\text{pr} * R * T[i][0] * z)) - 2.0 * D * T[i][0] * T[i][0] * (B - \\
& m/T[i][0] - \log(\text{pr} * R * T[i][0] * z)) * (m/T[i][0] / T[i][0] - 1.0/T[i][0])) * \text{omega} / \text{omegao});
\end{aligned}$$

$$\begin{aligned}
Cb &= (-2.0 \cdot D \cdot T[i][0] \cdot (B - m/T[i][0] - \log(pr \cdot R \cdot T[i][0] \cdot z)) \cdot (B - \\
&m/T[i][0] - \log(pr \cdot R \cdot T[i][0] \cdot z)) - 2.0 \cdot D \cdot T[i][0] \cdot T[i][0] \cdot (B - m/T[i][0] - \\
&\log(pr \cdot R \cdot T[i][0] \cdot z)) \cdot (m/T[i][0]/T[i][0] - 1.0/T[i][0])) \cdot \omega; \\
hav &= (m + 1.58/\sqrt{D} - 1.42/\sqrt{D}) \cdot \omega / \omega_{gao} \cdot R; \\
T[i][1] &= (\epsilon \cdot pr \cdot cr \cdot \alpha_{haa} \cdot T[i][0] \cdot Ap[4] \cdot rstep[1] - \\
&cr \cdot pr \cdot vrf \cdot Fo[9] \cdot zstep[1] \cdot Ap[4] \cdot rstep[1] \cdot T[i][0] + cr \cdot pr \cdot vrf \cdot Fo[9] \cdot zstep[1] \cdot Ap[4] \cdot rstep[1] \cdot T[i+5][0] + T[i][0] \cdot ka \cdot Ap[4] \cdot rstep[1] - \\
&T[i][0] \cdot ka \cdot Ap[4] \cdot rstep[1] \cdot \epsilon + Ar[5] \cdot Fo[9] \cdot zstep[1] \cdot ka \cdot T[i+1][0] - \\
&Ar[5] \cdot Fo[9] \cdot zstep[1] \cdot ka \cdot T[i][0] + pa \cdot \omega \cdot \alpha_{haa} \cdot Ca \cdot T[i][0] \cdot Ap[4] \cdot rstep[1] - \\
&pa \cdot \omega \cdot \alpha_{haa} \cdot Ca \cdot T[i][0] \cdot Ap[4] \cdot rstep[1] \cdot \epsilon - \\
&pa \cdot hav \cdot \alpha_{haa} \cdot Cb \cdot T[i][0] \cdot Ap[4] \cdot rstep[1] + pa \cdot hav \cdot \alpha_{haa} \cdot Cb \cdot T[i][0] \cdot Ap[4] \cdot rstep[1] \cdot \epsilon - \\
&\epsilon \cdot \alpha_{haa} \cdot Cc \cdot T[i][0] \cdot Ap[4] \cdot rstep[1] + 2.0 \cdot Fo[9] \cdot ka \cdot Ap[4] \cdot rstep[1] \cdot T[i+5][0] - \\
&2.0 \cdot Fo[9] \cdot ka \cdot Ap[4] \cdot rstep[1] \cdot T[i][0] + Ar[7] \cdot Fo[9] \cdot zstep[1] \cdot ka \cdot T[i-1][0] - \\
&Ar[7] \cdot Fo[9] \cdot zstep[1] \cdot ka \cdot T[i][0]) / (Ap[4] \cdot rstep[1] \cdot (\epsilon \cdot pr \cdot cr \cdot \alpha_{haa} + ka - \\
&\epsilon \cdot ka + pa \cdot \omega \cdot \alpha_{haa} \cdot Ca - pa \cdot \omega \cdot \alpha_{haa} \cdot Ca \cdot \epsilon - \\
&pa \cdot hav \cdot \alpha_{haa} \cdot Cb + pa \cdot hav \cdot \alpha_{haa} \cdot Cb \cdot \epsilon - \epsilon \cdot \alpha_{haa} \cdot Cc));
\end{aligned}$$

/*Node 1, adsorbent node, column 1, beginning*/

$$i = 1;$$

$$\begin{aligned}
\omega &= \omega_{gao} \cdot \exp(-D \cdot T[i][0] \cdot T[i][0] \cdot (B - m/T[i][0] - \\
&\log(pr \cdot R \cdot T[i][0] \cdot z)) \cdot (B - m/T[i][0] - \log(pr \cdot R \cdot T[i][0] \cdot z)));
\end{aligned}$$

$$Ca = (cr + 1.42/2.0 * R / \sqrt{D}) * (-2.0 * D * T[i][0] * (B - m/T[i][0] - \log(pr * R * T[i][0] * z)) * (B - m/T[i][0] - \log(pr * R * T[i][0] * z)) - 2.0 * D * T[i][0] * T[i][0] * (B - m/T[i][0] - \log(pr * R * T[i][0] * z)) * (m/T[i][0]/T[i][0] - 1.0/T[i][0])) * \omega / \omega_{gao});$$

$$Cb = (-2.0 * D * T[i][0] * (B - m/T[i][0] - \log(pr * R * T[i][0] * z)) * (B - m/T[i][0] - \log(pr * R * T[i][0] * z)) - 2.0 * D * T[i][0] * T[i][0] * (B - m/T[i][0] - \log(pr * R * T[i][0] * z)) * (m/T[i][0]/T[i][0] - 1.0/T[i][0])) * \omega;$$

$$hav = (m + 1.58/\sqrt{D}) - 1.42/\sqrt{D} * \omega / \omega_{gao} * R;$$

$$T[i][1] =$$

$$\begin{aligned} & (\epsilon * pr * cr * \alpha_{aa} * T[i][0] * Ap[5] * rstep[1] + T[i][0] * ka * Ap[5] * rstep[1] - \\ & T[i][0] * ka * Ap[5] * rstep[1] * \epsilon + Ar[7] * Fo[9] * zstep[1] * ka * T[i+1][0] - \\ & Ar[7] * Fo[9] * zstep[1] * ka * T[i][0] + pa * \omega * \alpha_{aa} * Ca * T[i][0] * Ap[5] * rstep[1] - \\ & pa * \omega * \alpha_{aa} * Ca * T[i][0] * Ap[5] * rstep[1] * \epsilon - \\ & pa * hav * \alpha_{aa} * Cb * T[i][0] * Ap[5] * rstep[1] + pa * hav * \alpha_{aa} * Cb * T[i][0] * Ap[5] * rstep[1] * \\ & \epsilon - \\ & \epsilon * \alpha_{aa} * Cc * T[i][0] * Ap[5] * rstep[1] + 2.0 * Fo[9] * ka * Ap[5] * rstep[1] * T[i+5][0] - \\ & 2.0 * Fo[9] * ka * Ap[5] * rstep[1] * T[i][0] - \\ & cr * pr * vrfl * Fo[9] * zstep[1] * Ap[5] * rstep[1] * T[i][0] + cr * pr * vrfl * Fo[9] * zstep[1] * Ap[5] * rstep[1] * T[i+5][0]) / (Ap[5] * rstep[1] * (\epsilon * pr * cr * \alpha_{aa} + ka - \\ & \epsilon * ka + pa * \omega * \alpha_{aa} * Ca - pa * \omega * \alpha_{aa} * Ca * \epsilon - \\ & pa * hav * \alpha_{aa} * Cb + pa * hav * \alpha_{aa} * Cb * \epsilon - \epsilon * \alpha_{aa} * Cc)); \end{aligned}$$

/*Node 8, adsorbent node, column 3, intermediate*/

```

for (i=8; i<3496; i=i+5){

    omega = omegao*exp(-D*T[i][0]*T[i][0]*(B-
m/T[i][0]-log(pr*R*T[i][0]*z))*(B-m/T[i][0]-log(pr*R*T[i][0]*z)));

    Ca = (cr+1.42/2.0*R/sqrt(D))*(-2.0*D*T[i][0]*(B-
m/T[i][0]-log(pr*R*T[i][0]*z))*(B-m/T[i][0]-log(pr*R*T[i][0]*z))-
2.0*D*T[i][0]*T[i][0]*(B-m/T[i][0]-log(pr*R*T[i][0]*z))*(m/T[i][0]/T[i][0]-
1.0/T[i][0]))*omega/omegao);

    Cb = (-2.0*D*T[i][0]*(B-m/T[i][0]-
log(pr*R*T[i][0]*z))*(B-m/T[i][0]-log(pr*R*T[i][0]*z))-2.0*D*T[i][0]*T[i][0]*(B-
m/T[i][0]-log(pr*R*T[i][0]*z))*(m/T[i][0]/T[i][0]-1.0/T[i][0]))*omega;

    hav = (m+1.58/sqrt(D)-
1.42/sqrt(D))*omega/omegao)*R;

    T[i][1] = (-
epsilon*pr*cr*alphaa*T[i][0]*Ap[3]*rstep[1]+cr*pr*vrf1*zstep1*Fo[9]*Ap[3]*rstep[1]*
T[i][0]-cr*pr*vrf1*zstep1*Fo[9]*Ap[3]*rstep[1]*T[i+5][0]-
T[i][0]*ka*Ap[3]*rstep[1]+T[i][0]*ka*Ap[3]*rstep[1]*epsilon-
Fo[9]*ka*Ap[3]*rstep[1]*T[i-5][0]+2.0*Fo[9]*ka*Ap[3]*rstep[1]*T[i][0]-
pa*omega*alphaa*Ca*T[i][0]*Ap[3]*rstep[1]+pa*omega*alphaa*Ca*T[i][0]*Ap[3]*rste
p[1]*epsilon-Ar[5]*zstep1*Fo[9]*ka*T[i-
1][0]+Ar[5]*zstep1*Fo[9]*ka*T[i][0]+pa*hav*alphaa*Cb*T[i][0]*Ap[3]*rstep[1]-
pa*hav*alphaa*Cb*T[i][0]*Ap[3]*rstep[1]*epsilon+epsilon*alphaa*Cc*T[i][0]*Ap[3]*r
step[1]-Fo[9]*ka*Ap[3]*rstep[1]*T[i+5][0]-

```

```

Ar[3]*Fo[9]*Bi[7]*ka*rstep[1]*T[i+1][0]+Ar[3]*Fo[9]*Bi[7]*ka*rstep[1]*T[i][0])/(Ap[
3]*rstep[1]*(-ka+epsilon*ka-
pa*omega*alphaa*Ca+pa*omega*alphaa*Ca*epsilon+pa*hav*alphaa*Cb-
pa*hav*alphaa*Cb*epsilon+epsilon*alphaa*Cc-epsilon*pr*cr*alphaa));
}

```

/*Node 7, adsorbent node, column 2, intermediate*/

```

for (i=7; i<3496; i=i+5){

    omega = omegao*exp(-D*T[i][0]*T[i][0]*(B-
m/T[i][0]-log(pr*R*T[i][0]*z))*(B-m/T[i][0]-log(pr*R*T[i][0]*z)));

    Ca = (cr+1.42/2.0*R/sqrt(D))*(-2.0*D*T[i][0]*(B-
m/T[i][0]-log(pr*R*T[i][0]*z))*(B-m/T[i][0]-log(pr*R*T[i][0]*z))-
2.0*D*T[i][0]*T[i][0]*(B-m/T[i][0]-log(pr*R*T[i][0]*z))*(m/T[i][0]/T[i][0]-
1.0/T[i][0]))*omega/omegao);

    Cb = (-2.0*D*T[i][0]*(B-m/T[i][0]-
log(pr*R*T[i][0]*z))*(B-m/T[i][0]-log(pr*R*T[i][0]*z))-2.0*D*T[i][0]*T[i][0]*(B-
m/T[i][0]-log(pr*R*T[i][0]*z))*(m/T[i][0]/T[i][0]-1.0/T[i][0]))*omega;

    hav = (m+1.58/sqrt(D)-
1.42/sqrt(D)*omega/omegao)*R;

    T[i][1] = (-
epsilon*pr*cr*alphaa*T[i][0]*Ap[4]*rstep[1]-
cr*pr*vrf*zstep1*Fo[9]*Ap[4]*rstep[1]*T[i+5][0]+cr*pr*vrf*Fo[9]*zstep1*Ap[4]*rste

```

```

p[1]*T[i][0]-T[i][0]*ka*Ap[4]*rstep[1]+T[i][0]*ka*Ap[4]*rstep[1]*epsilon-
Fo[9]*ka*Ap[4]*rstep[1]*T[i+5][0]+2.0*Fo[9]*ka*Ap[4]*rstep[1]*T[i][0]-
pa*omega*alphaa*Ca*T[i][0]*Ap[4]*rstep[1]+pa*omega*alphaa*Ca*T[i][0]*Ap[4]*rste
p[1]*epsilon-Ar[7]*zstep1*Fo[9]*ka*T[i-
1][0]+Ar[7]*zstep1*Fo[9]*ka*T[i][0]+pa*hav*alphaa*Cb*T[i][0]*Ap[4]*rstep[1]-
pa*hav*alphaa*Cb*T[i][0]*Ap[4]*rstep[1]*epsilon+epsilon*alphaa*Cc*T[i][0]*Ap[4]*r
step[1]-Fo[9]*ka*Ap[4]*rstep[1]*T[i-5][0]+Ar[5]*zstep1*Fo[9]*ka*T[i][0]-
Ar[5]*zstep1*Fo[9]*ka*T[i+1][0])/(Ap[4]*rstep[1]*(-ka+epsilon*ka-
pa*omega*alphaa*Ca+pa*omega*alphaa*Ca*epsilon+pa*hav*alphaa*Cb-
pa*hav*alphaa*Cb*epsilon+epsilon*alphaa*Cc-epsilon*pr*cr*alphaa));
}

```

/*Node 6, adsorbent node, column 1, intermediate*/

```

for (i=6; i<3496; i=i+5){

    omega = omegao*exp(-D*T[i][0]*T[i][0]*(B-
m/T[i][0]-log(pr*R*T[i][0]*z))*(B-m/T[i][0]-log(pr*R*T[i][0]*z)));

    Ca = (cr+1.42/2.0*R/sqrt(D)*(-2.0*D*T[i][0]*(B-
m/T[i][0]-log(pr*R*T[i][0]*z))*(B-m/T[i][0]-log(pr*R*T[i][0]*z))-
2.0*D*T[i][0]*T[i][0]*(B-m/T[i][0]-log(pr*R*T[i][0]*z))*(m/T[i][0]/T[i][0]-
1.0/T[i][0])))*omega/omegao);

```

```

Cb = (-2.0*D*T[i][0]*(B-m/T[i][0]-
log(pr*R*T[i][0]*z))*(B-m/T[i][0]-log(pr*R*T[i][0]*z))-2.0*D*T[i][0]*T[i][0]*(B-
m/T[i][0]-log(pr*R*T[i][0]*z))*(m/T[i][0]/T[i][0]-1.0/T[i][0]))*omega;

hav = (m+1.58/sqrt(D)-
1.42/sqrt(D)*omega/omegao)*R;

T[i][1] = (-
epsilon*pr*cr*alphaa*T[i][0]*rstep[1]*Ap[5]-
cr*pr*vrfl*zstep1*Fo[9]*Ap[5]*rstep[1]*T[i+5][0]+cr*pr*vrfl*zstep1*Fo[9]*Ap[5]*rste
p[1]*T[i][0]-T[i][0]*ka*Ap[5]*rstep[1]+T[i][0]*ka*Ap[5]*rstep[1]*epsilon-
Fo[9]*ka*Ap[5]*rstep[1]*T[i-5][0]+2.0*Fo[9]*ka*rstep[1]*Ap[5]*T[i][0]-
pa*omega*alphaa*Ca*T[i][0]*rstep[1]*Ap[5]+pa*omega*alphaa*Ca*T[i][0]*rstep[1]*A
p[5]*epsilon+pa*hav*alphaa*Cb*T[i][0]*rstep[1]*Ap[5]-
pa*hav*alphaa*Cb*T[i][0]*rstep[1]*Ap[5]*epsilon+epsilon*alphaa*Cc*T[i][0]*rstep[1]
*Ap[5]-Fo[9]*ka*rstep[1]*Ap[5]*T[i+5][0]-
Ar[7]*zstep1*Fo[9]*ka*T[i+1][0]+Ar[7]*zstep1*Fo[9]*ka*T[i][0])/(rstep[1]*Ap[5]*(-
ka+epsilon*ka-
pa*omega*alphaa*Ca+pa*omega*alphaa*Ca*epsilon+pa*hav*alphaa*Cb-
pa*hav*alphaa*Cb*epsilon+epsilon*alphaa*Cc-epsilon*pr*cr*alphaa));

}

```

```

/*Node 3498, adsorbent node, column 3, ending*/

```

```

i = 3498;

```

$$\begin{aligned}
\omega &= \omega_{\text{gao}} \cdot \exp(-D \cdot T[i][0] \cdot T[i][0] \cdot (B - m/T[i][0] - \log(\text{pr} \cdot R \cdot T[i][0] \cdot z)) \cdot (B - m/T[i][0] - \log(\text{pr} \cdot R \cdot T[i][0] \cdot z))))); \\
C_a &= (cr + 1.42/2.0 \cdot R/\sqrt{D}) \cdot (-2.0 \cdot D \cdot T[i][0] \cdot (B - m/T[i][0] - \log(\text{pr} \cdot R \cdot T[i][0] \cdot z)) \cdot (B - m/T[i][0] - \log(\text{pr} \cdot R \cdot T[i][0] \cdot z)) - 2.0 \cdot D \cdot T[i][0] \cdot T[i][0] \cdot (B - m/T[i][0] - \log(\text{pr} \cdot R \cdot T[i][0] \cdot z)) \cdot (m/T[i][0]/T[i][0] - 1.0/T[i][0])) \cdot \omega/\omega_{\text{gao}}); \\
C_b &= (-2.0 \cdot D \cdot T[i][0] \cdot (B - m/T[i][0] - \log(\text{pr} \cdot R \cdot T[i][0] \cdot z)) \cdot (B - m/T[i][0] - \log(\text{pr} \cdot R \cdot T[i][0] \cdot z)) - 2.0 \cdot D \cdot T[i][0] \cdot T[i][0] \cdot (B - m/T[i][0] - \log(\text{pr} \cdot R \cdot T[i][0] \cdot z)) \cdot (m/T[i][0]/T[i][0] - 1.0/T[i][0])) \cdot \omega); \\
hav &= (m + 1.58/\sqrt{D} - 1.42/\sqrt{D}) \cdot \omega/\omega_{\text{gao}} \cdot R; \\
T[i][1] &= (\epsilon \cdot \text{pr} \cdot cr \cdot \alpha_{\text{haa}} \cdot T[i][0] \cdot A_p[3] \cdot r_{\text{step}}[1] - cr \cdot \text{pr} \cdot v_{\text{rfl}} \cdot F_o[9] \cdot z_{\text{step}}[1] \cdot A_p[3] \cdot r_{\text{step}}[1] \cdot T[i][0] + cr \cdot \text{pr} \cdot v_{\text{rfl}} \cdot F_o[9] \cdot z_{\text{step}}[1] \cdot A_p[3] \cdot r_{\text{step}}[1] \cdot T[i-5][0] + T[i][0] \cdot ka \cdot A_p[3] \cdot r_{\text{step}}[1] - T[i][0] \cdot ka \cdot A_p[3] \cdot r_{\text{step}}[1] \cdot \epsilon + Ar[5] \cdot F_o[9] \cdot z_{\text{step}}[1] \cdot ka \cdot T[i-1][0] - Ar[5] \cdot F_o[9] \cdot z_{\text{step}}[1] \cdot ka \cdot T[i][0] + pa \cdot \omega \cdot \alpha_{\text{haa}} \cdot C_a \cdot T[i][0] \cdot A_p[3] \cdot r_{\text{step}}[1] - pa \cdot \omega \cdot \alpha_{\text{haa}} \cdot C_a \cdot T[i][0] \cdot A_p[3] \cdot r_{\text{step}}[1] \cdot \epsilon - pa \cdot hav \cdot \alpha_{\text{haa}} \cdot C_b \cdot T[i][0] \cdot A_p[3] \cdot r_{\text{step}}[1] + pa \cdot hav \cdot \alpha_{\text{haa}} \cdot C_b \cdot T[i][0] \cdot A_p[3] \cdot r_{\text{step}}[1] \cdot \epsilon - \epsilon - \epsilon \cdot \alpha_{\text{haa}} \cdot C_c \cdot T[i][0] \cdot A_p[3] \cdot r_{\text{step}}[1] - 2.0 \cdot F_o[9] \cdot ka \cdot A_p[3] \cdot r_{\text{step}}[1] \cdot T[i][0] + 2.0 \cdot F_o[9] \cdot ka \cdot A_p[3] \cdot r_{\text{step}}[1] \cdot T[i-5][0] + Ar[3] \cdot F_o[9] \cdot Bi[7] \cdot ka \cdot r_{\text{step}}[1] \cdot T[i+1][0] - Ar[3] \cdot F_o[9] \cdot Bi[7] \cdot ka \cdot r_{\text{step}}[1] \cdot T[i][0]) / (A_p[3] \cdot r_{\text{step}}[1] \cdot (\epsilon \cdot \text{pr} \cdot cr \cdot \alpha_{\text{haa}} + ka - \epsilon \cdot ka + pa \cdot \omega \cdot \alpha_{\text{haa}} \cdot C_a - pa \cdot \omega \cdot \alpha_{\text{haa}} \cdot C_a \cdot \epsilon - pa \cdot hav \cdot \alpha_{\text{haa}} \cdot C_b + pa \cdot hav \cdot \alpha_{\text{haa}} \cdot C_b \cdot \epsilon - \epsilon \cdot \alpha_{\text{haa}} \cdot C_c));
\end{aligned}$$

/*Node 3497, adsorbent node, column 2, ending*/

i = 3497;

omega = omegao*exp(-D*T[i][0]*T[i][0]*(B-m/T[i][0]-
log(pr*R*T[i][0]*z))*(B-m/T[i][0]-log(pr*R*T[i][0]*z)));

Ca = (cr+1.42/2.0*R/sqrt(D))*(-2.0*D*T[i][0]*(B-m/T[i][0]-
log(pr*R*T[i][0]*z))*(B-m/T[i][0]-log(pr*R*T[i][0]*z))-2.0*D*T[i][0]*T[i][0]*(B-
m/T[i][0]-log(pr*R*T[i][0]*z))*(m/T[i][0]/T[i][0]-1.0/T[i][0]))*omega/omegao;

Cb = (-2.0*D*T[i][0]*(B-m/T[i][0]-log(pr*R*T[i][0]*z))*(B-
m/T[i][0]-log(pr*R*T[i][0]*z))-2.0*D*T[i][0]*T[i][0]*(B-m/T[i][0]-
log(pr*R*T[i][0]*z))*(m/T[i][0]/T[i][0]-1.0/T[i][0]))*omega;

hav = (m+1.58/sqrt(D)-1.42/sqrt(D))*omega/omegao)*R;

T[i][1] =

(epsilon*pr*cr*alphaa*T[i][0]*Ap[4]*rstep[1]+cr*pr*vrfl*Fo[9]*zstep1*Ap[4]*rstep[1]
*T[i-5][0]-cr*pr*vrfl*Fo[9]*zstep1*Ap[4]*rstep[1]*T[i][0]+T[i][0]*ka*Ap[4]*rstep[1]-
T[i][0]*ka*Ap[4]*rstep[1]*epsilon+Ar[5]*Fo[9]*zstep1*ka*T[i+1][0]-
Ar[5]*Fo[9]*zstep1*ka*T[i][0]+pa*omega*alphaa*Ca*T[i][0]*Ap[4]*rstep[1]-
pa*omega*alphaa*Ca*T[i][0]*Ap[4]*rstep[1]*epsilon-
pa*hav*alphaa*Cb*T[i][0]*Ap[4]*rstep[1]+pa*hav*alphaa*Cb*T[i][0]*Ap[4]*rstep[1]*
epsilon-epsilon*alphaa*Cc*T[i][0]*Ap[4]*rstep[1]+2.0*Fo[9]*ka*Ap[4]*rstep[1]*T[i-
5][0]-2.0*Fo[9]*ka*Ap[4]*rstep[1]*T[i][0]+Ar[7]*Fo[9]*zstep1*ka*T[i-1][0]-
Ar[7]*Fo[9]*zstep1*ka*T[i][0])/(Ap[4]*rstep[1]*(epsilon*pr*cr*alphaa+ka-

epsilon*ka+pa*omega*alphaa*Ca-pa*omega*alphaa*Ca*epsilon-
pa*hav*alphaa*Cb+pa*hav*alphaa*Cb*epsilon-epsilon*alphaa*Cc));

/*Node 3496, adsorbent node, column 1, ending*/

i = 3496;

omega = omegao*exp(-D*T[i][0]*T[i][0]*(B-m/T[i][0]-
log(pr*R*T[i][0]*z))*(B-m/T[i][0]-log(pr*R*T[i][0]*z)));

Ca = (cr+1.42/2.0*R/sqrt(D)*(-2.0*D*T[i][0]*(B-m/T[i][0]-
log(pr*R*T[i][0]*z))*(B-m/T[i][0]-log(pr*R*T[i][0]*z))-2.0*D*T[i][0]*T[i][0]*(B-
m/T[i][0]-log(pr*R*T[i][0]*z))*(m/T[i][0]/T[i][0]-1.0/T[i][0]))*omega/omegao);

Cb = (-2.0*D*T[i][0]*(B-m/T[i][0]-log(pr*R*T[i][0]*z))*(B-
m/T[i][0]-log(pr*R*T[i][0]*z))-2.0*D*T[i][0]*T[i][0]*(B-m/T[i][0]-
log(pr*R*T[i][0]*z))*(m/T[i][0]/T[i][0]-1.0/T[i][0]))*omega;

hav = (m+1.58/sqrt(D)-1.42/sqrt(D)*omega/omegao)*R;

T[i][1] =

(epsilon*pr*cr*alphaa*T[i][0]*Ap[5]*rstep[1]+T[i][0]*ka*Ap[5]*rstep[1]-
T[i][0]*ka*Ap[5]*rstep[1]*epsilon+Ar[7]*Fo[9]*zstep1*ka*T[i+1][0]-
Ar[7]*Fo[9]*zstep1*ka*T[i][0]+pa*omega*alphaa*Ca*T[i][0]*Ap[5]*rstep[1]-
pa*omega*alphaa*Ca*T[i][0]*Ap[5]*rstep[1]*epsilon-
pa*hav*alphaa*Cb*T[i][0]*Ap[5]*rstep[1]+pa*hav*alphaa*Cb*T[i][0]*Ap[5]*rstep[1]*
epsilon-epsilon*alphaa*Cc*T[i][0]*Ap[5]*rstep[1]+2.0*Fo[9]*ka*Ap[5]*rstep[1]*T[i-
5][0]-

```

2.0*Fo[9]*ka*Ap[5]*rstep[1]*T[i][0]+cr*pr*vrfl*Fo[9]*zstep1*Ap[5]*rstep[1]*T[i-
5][0]-
cr*pr*vrfl*Fo[9]*zstep1*Ap[5]*rstep[1]*T[i][0])/(Ap[5]*rstep[1]*(epsilon*pr*cr*alphaa
+ka-epsilon*ka+pa*omega*alphaa*Ca-pa*omega*alphaa*Ca*epsilon-
epsilon*alphaa*Cb-pa*hav*alphaa*Cb+pa*hav*alphaa*Cb*epsilon));

```

```

/*Convert Data from T[x][1] to T[x][0]*/

```

```

    for (i=1; i<3501; i=i+1){

```

```

        T[i][0]=T[i][1];

```

```

    }

```

```

/*close first loop*/

```

```

    }

```

```

/*Calculate expired time*/

```

```

exptime = deltat*(timestep1)*(timestep2-1);

```

```

printf("\ntimestep2 = %i", timestep2-1);

```

```

printf("\ntimestep1 = %i\n", timestep1);

```

```

printf("\nk = %i", k);

```

```

mr = pi*r[3]*r[3]*vrfl*pr*1.0e9;

```

```

if (k==5){

/*Record Time and temperature of exit HTF and refrigerant into text file
c:\\htemp00.txt*/

    if ((fptr3 = fopen(filename3, "a")) == NULL)

        printf("\nBad File Open");

        fprintf(fptr3, "%f, %f, %f, %f, %f, %f, %f, %f, %f\n", exptime,
T[5][0], T[3500][0], T[1][0], T[3496][0], mr, Press[1], Press[2], omega);

        fclose(fptr3);

}

/*close last loop*/

}

/*Record Temp at each node into text file c:\\thermal00.txt*/

    if ((fptr = fopen(filename, "a")) == NULL)

        printf("\nBad File Open");

        fprintf(fptr, "Final Temperature\n");

        for (i=1; i<3501; i=i+5){

            fprintf(fptr, "%f, %f, %f, %f, %f\n", T[i+4][0], T[i+3][0],
T[i+2][0], T[i+1][0], T[i][0]);

        }

```

```
fclose(fptr);
```

```
/*Convert Data from T[x][1] to T[x][0]*/
```

```
for (i=1; i<3501; i=i+5){  
    T[i][0]=T[3497-i][1];  
    T[i+1][0]=T[3498-i][1];  
    T[i+2][0]=T[3499-i][1];  
    T[i+3][0]=T[3500-i][1];  
    T[i+4][0]=T[3501-i][1];  
}
```

```
/*Close the heating phase of the bed and begin the cooling phase*/
```

```
}
```

```
/*Record parameters a:\\hparam.txt*/
```

```
if ((fptr4 = fopen(filename4, "a")) == NULL)
```

```
printf("\nBad File Open");
```

```
fprintf(fptr4, "Heating Parameters\n");
```

```
fprintf(fptr4, "delta time          =\t%f\n", deltat);
```

```

fprintf(fp4, "adsorbent ka      =\t%f\n", ka);
fprintf(fp4, "contact resis    =\t%f\n", ha);
fprintf(fp4, "HTF conv coef        =\t%f\n", hfl);
fprintf(fp4, "HTF velocity          =\t%f\n", vfl);
fprintf(fp4, "HTF spec heat           =\t%f\n", cfl);
fprintf(fp4, "zstep1                  =\t%f\n", zstep1);
fprintf(fp4, "rstep1                  =\t%f\n", rstep[1]);
fprintf(fp4, "rstep2                  =\t%f\n", rstep[2]);
fprintf(fp4, "rstep3                  =\t%f\n", rstep[3]);
fprintf(fp4, "r[1]                   =\t%f\n", r[1]);
fprintf(fp4, "r[2]                   =\t%f\n", r[2]);
fprintf(fp4, "r[3]                   =\t%f\n", r[3]);
fprintf(fp4, "r[4]                   =\t%f\n", r[4]);
fprintf(fp4, "r[5]                   =\t%f\n", r[5]);
fprintf(fp4, "vcheck                  =\t%i\n", vcheck);
fprintf(fp4, "Bi[1]                   =\t%f\n", Bi[1]);
fprintf(fp4, "Bi[3]                   =\t%f\n", Bi[3]);
fprintf(fp4, "Bi[4]                   =\t%f\n", Bi[4]);
fprintf(fp4, "Bi[7]                   =\t%f\n", Bi[7]);
fprintf(fp4, "Fo[1]                   =\t%e\n", Fo[1]);
fprintf(fp4, "Fo[3]                   =\t%f\n", Fo[3]);
fprintf(fp4, "Fo[9]                   =\t%f\n", Fo[9]);

```

```

        fprintf(fp4, "Ar[1]           =\t%f\n", Ar[1]);
        fprintf(fp4, "Ar[3]           =\t%f\n", Ar[3]);
        fprintf(fp4, "Ar[5]           =\t%f\n", Ar[5]);
        fprintf(fp4, "Ar[7]           =\t%f\n", Ar[7]);

    fprintf(fp4, "Ap[1]               =\t%f\n", Ap[1]);

        fprintf(fp4, "Ap[2]           =\t%f\n", Ap[2]);
        fprintf(fp4, "Ap[3]           =\t%f\n", Ap[3]);
        fprintf(fp4, "Ap[4]           =\t%f\n", Ap[4]);
        fprintf(fp4, "Ap[5]           =\t%f\n", Ap[5]);
        fprintf(fp4, "HTF Flow           =\t%f\n",
Ap[1]*vfl*pfl);

        fprintf(fp4, "Max Refrig           =\t%f\n", vmax);
        fprintf(fp4, "vrtot           =\t%f\n", vrtot);
        fclose(fp4);

}

printf("Finished Modeling");

return 0;

}

```

Appendix D C++ code for Adsorption heat pump with metal gauze

```
/*C program to calculate temperatures from numerical nodes*/

#include <stdio.h>

#include <math.h>

#include <stdlib.h>

#include <alloc.h>


/*Main part of program*/

float main ()

{


/*Declaration of variables*/

    int i, timestep1, timestep2, k, vcheck;

    float exptime, deltat;

    float pi, zstep1, zstep2, zstep3, rstep[5];

    float r[6]; /*radius dimensions*/

    float Ap[6], Ar[9]; /*Cross section area along z direction and parallel area in r
direction*/

    float alphafl, alphas, alphaa; /*thermal diffusion for HTF,HTF pipe, adsorbent*/

    float Bi[8], Fo[10]; /*Fourier numbers*/

    float kfl, kt, ka;

    float pfl, pt, pa, pr; /*density*/
```

```

float cfl, ct, ca, cr; /*specific heat*/

float epsilon; /*void volume*/

float omegao, omega; /*adsorption level*/

float vrfl; /*velocity of refrigerant*/

float vfl; /*velocity of HTF*/

float hav;

static double Ca, Cb, Cc, vrtot; /*constants for adsorbent layers*/

float HV; /*heat of vaporization for ammonia*/

float D; /*coefficient in Dubinin-Radushkevich equation*/

float B; /*constant in vapor pressure curve correlation*/

float m; /*coefficient in vapor pressure curve correlation*/

float R, z, mr, vmax;

float CE, K, u;

float hfl, ha; /*convective and contact resistance coef*/

FILE *fptr;

char *filename="therm.txt";

FILE *fptr3;

char *filename3="htemp.txt";

FILE *fptr4;

char *filename4="hparam.txt";

static float T[4666][2];

float MW; /*Molecular weight of refrigerant*/

```



```

float Press[3]; /*condenser [1] and exit pressure [2]*/

float InitBed; /*Initial Bed Temp*/

float InitHTF, InitHTF2; /*HTF temp into Bed*/


printf("\nHeating of Cold adsorption bed / Pressurization\n");


/*printf("Enter the bed thermal conductivity 5 W/m/K\n");

scanf("%f", &ka); */

ka = 5.0;


printf("Enter the velocity of the HTF (ie .0158 m/s)\n");

scanf("%f", &vfl);


/*Retrieve Parameters*/

/*printf("Enter the deltat time from the time step application (ie 1.0e-3 seconds)\n");

scanf("%f", &deltat);*/

deltat = 0.006;


/*printf("Enter the HTF temperature entering the adsorbent bed (ie 500 Kelvin)\n");

scanf("%f", &InitHTF);*/

```

InitHTF = 503.0;

/*printf("Enter the initial adsorbent bed temperature (ie 280 Kelvin)\n");

scanf("%f", &InitBed);*/

InitBed = 314.0;

/*printf("Enter the radius length for the interval spacing in the adsorbent beds (ie .03175 m)\n");

scanf("%f", &rstep[1]);*/

rstep[1] = 0.004;

/*printf("Enter the HTF pipe thickness (ie .0735 m)\n");

scanf("%f", &rstep[2]);*/

rstep[2] = 0.0006;

/*printf("Enter the inside radius of the HTF pipe (ie .0037 m)\n");

scanf("%f", &rstep[3]);*/

rstep[3] = .003;

/*printf("Enter the pin fin spacing in the z direction (ie .0005 m)\n");

scanf("%f", &zstep2); */

zstep2 = 0.0003;

```
/*printf("Enter the adsorbent spacing in the z direction (ie .0095 m)\n");
```

```
scanf("%f", &zstep1);*/
```

```
zstep1 = 0.0035;
```

```
/*printf("Enter the contact resistance between the adsorbent and HTF pipe (ie 180 Watts /  
(m^2 K)\n");
```

```
scanf("%f", &ha);*/
```

```
ha = 180.0;
```

```
/*Assignment of variables*/
```

```
pi = 3.14159265;
```

```
/*zstep3 calculation*/
```

```
zstep3 = (zstep1+zstep2)/2.0;
```

```
/*rstep4 calculation*/
```

```
rstep[4] = (rstep[1]+rstep[2])/2.0;
```

```
/*Radius measurements in meters*/
```

```
r[1] = rstep[1]/2.0;
```

```
r[2] = r[1]+rstep[1];
```

$r[3] = r[2] + rstep[1];$

$r[4] = r[3] + rstep[2];$

$r[5] = r[4] + rstep[3];$

*/*Cross section area along z axis*/*

for (i=1; i<5; i=i+1){

$Ap[i] = \pi * (r[6-i] * r[6-i] - r[5-i] * r[5-i]);$

}

$Ap[5] = \pi * (r[1] * r[1]);$

*/*parallel area in concentric radius axis*/*

$Ar[1] = 2 * \pi * r[4] * zstep1;$

$Ar[2] = 2 * \pi * r[4] * zstep2;$

$Ar[3] = 2 * \pi * r[3] * zstep1;$

$Ar[4] = 2 * \pi * r[3] * zstep2;$

$Ar[5] = 2 * \pi * r[2] * zstep1;$

$Ar[6] = 2 * \pi * r[2] * zstep2;$

$Ar[7] = 2 * \pi * r[1] * zstep1;$

$Ar[8] = 2 * \pi * r[1] * zstep2;$

*/*Thermal conductivity*/*

$k_{fl} = .115$; /*htf thermal conductivity W /m / K at avg of 500 and 280K */

$k_t = 186.0$; /*htf pipe thermal conductivity, AISI 1010 Carbon Steel, Incropera & DeWitt

p_{828} */

/*density*/

$\rho_{fl} = 914.0$; /*density of htf*/

$\rho_t = 2770.0$; /*density of htf pipe kg / m³*/

$\rho_a = 450.0$; /*density of adsorbent*/

/*molecular weight of ammonia in g/mole */

$MW = 17.03$;

$R = 8.314/MW * 1000.0$; /*R constant in terms of J/K/kg(refrigerant) or m³ * Pa / K / kg

*/

/*specific heat*/

$c_{fl} = 1930.0$; /*htf at 400K J/kg K*/

$c_t = 930.0$; /*htf pipe at 400K*/

$c_a = 920.0$; /*adsorbent*/

$c_r = 1399.2$; /*refrigerant vapor*/

/*convective heat transfer for HTF*/

hfl = 4.36*kfl/(rstep[3]);

/*Fraction of Void Volume*/

epsilon = .27;

/*adsorption level*/

omegao = .55;

/*coefficient in Dubinin-Raduschkovich equation*/

D = 1.2e-6;

/*constant in vapor pressure curve correlation*/

B = 23.066;

/*Heat of Vaporization*/

HV =1351.0*1000.0; /*J /kg */

/*coefficient in vapor pressure curve correlation*/

m = HV/R;

/*Constant in Ergun Equation*/

CE = 0.55;

/*Permeability*/

K = 1.0e-9;

/*Dynamic Viscosity, N s / m^2*/

u = 134.5e-7;

/*Thermal diffusivity*/

alphafl = kfl/(pfl * cfl); /*HTF*/

alphanat = kt / (pt * ct); /* HTF pipe*/

alphaa = ka / (pa * ca); /*adsorbent*/

/*Biot Numbers*/

Bi[1] = (hfl * zstep1)/kfl;

Bi[2] = (hfl * zstep3)/kfl;

Bi[3] = (hfl * zstep1) / kt;

Bi[4] = (ha * zstep1) / kt;

Bi[5] = (hfl * zstep3) / kt;

Bi[6] = (ha * zstep3) / kt;

Bi[7] = (ha * zstep1) / ka;

/*Fourier Number*/

Fo[1] = alphaf1*deltat/zstep1/zstep1;

Fo[2] = alphaf1*deltat/zstep1/zstep3;

Fo[3] = alphasat*deltat/zstep1/zstep1;

Fo[4] = alphasat*deltat/zstep1/zstep3;

Fo[5] = alphaf1*deltat/zstep2/zstep3;

Fo[6] = alphasat*deltat/zstep2/zstep3;

Fo[7] = alphaa*deltat/zstep3/zstep1;

Fo[9] = alphaa*deltat/zstep1/zstep1;

/*Compressibility Factor*/

z = 0.78; /*compressibility factor with Tr = .962 and Pr = .473 */

/*Header Statement on disk file*/

if ((fptr3 = fopen(filename3, "a")) == NULL)

printf("\nBad File Open");

fprintf(fptr3, "Time, HTF in, HTF out, ADS in, ADS out, Mass

Flow, Press in, Press out, omega, in rho, out rho\n");

fclose(fptr3);

/*Initial temp conditions*/

for (i=1; i<4666; i=i+1){


```

        T[i][0] = InitBed;    /*T[#][time step] Temperature number at time t*/
    }

/*HTF initial conditions*/

    T[5][0] = InitHTF;

    InitHTF2 = 314.0;

/*vcheck will equal 1 if the amount of mass moved exceeds the initial mass of the bed*/

vcheck = 0;

/*Initial density conditions*/

pr = 11.2;

vmax = ((1.0-epsilon)*pa*omegao+epsilon*pr)*pi*r[3]*r[3]*zstep1*466.0;

Cc = pr*R*z;

for (k=1; k<6; k++){

/*total refrigerant moved*/

vrtot = 1.0e-30;

vrfl = 1.0e-30;

```

```
vcheck = 0;
```

```
/*Temperature determination at each time step*/
```

```
for (timestep1=1; timestep1<3001; timestep1++){
```

```
    for (timestep2=1; timestep2<=20; timestep2++){
```

```
/*velocity of refrigerant*/
```

```
vrtot = vrtot + pi*r[3]*r[3]*vrfl*pr*deltat;
```

```
if (k==1){
```

```
    Press[1] = pr*R*T[1][0]*z;
```

```
    Press[2] = pr*R*T[4661][0]*z;
```

```
        if (Press[2]>1.603e6)
```

```
            {vrfl = (-u/K+sqrt(u*u/K/K-4.0*(Press[2]-
```

```
Press[1]))*CE*pr/sqrt(K)/zstep1/466.0))/(2.0*CE*pr/sqrt(K));
```

```
        }
```

```
        if (vrtot > vmax)
```

```
            {vrfl = 1.0e-30;
```

```
            vcheck = 1;
```

```
        }
```

```

        /*Initial Temp for heating phase*/

        T[5][0] = InitHTF;

    }

    if (k==2){

        Press[1] = pr*R*T[4661][0]*z;

        Press[2] = pr*R*T[1][0]*z;

        if (Press[2]<1.358e6)

            {vrfl = (-u/K+sqrt(u*u/K/K-4.0*(Press[2]-
Press[1])*CE*pr/sqrt(K)/zstep1/466.0))/(2.0*CE*pr/sqrt(K));

            }

        if (vrtot > vmax)

            {vrfl = 1.0e-30;

            vcheck = 1;

            }

        /*Initial Temp for cooling phase*/

        T[5][0] = InitHTF2;

    }

```

```

if (k==3){

    Press[1] = pr*R*T[1][0]*z;

    Press[2] = pr*R*T[4661][0]*z;


    if (Press[2]>1.603e6)

        {vrfl = (-u/K+sqrt(u*u/K/K-4.0*(Press[2]-
Press[1])*CE*pr/sqrt(K)/zstep1/466.0))/(2.0*CE*pr/sqrt(K));

        }


    if (vrtot > vmax)

        {vrfl = 1.0e-30;

        vcheck = 1;

        }


    /*Initial Temp for heating phase*/

    T[5][0] = InitHTF;

}


if (k==4){

    Press[1] = pr*R*T[4661][0]*z;

    Press[2] = pr*R*T[1][0]*z;

```

```

        if (Press[2]<1.358e6)

            {vrfl = (-u/K+sqrt(u*u/K/K-4.0*(Press[2]-
Press[1])*CE*pr/sqrt(K)/zstep1/466.0))/(2.0*CE*pr/sqrt(K));

            }

        if (vrtot > vmax)

            {vrfl = 1.0e-30;

            vcheck = 1;

            }

        /*Initial Temp for cooling phase*/

        T[5][0] = InitHTF2;

    }

    if (k==5){

        Press[1] = pr*R*T[1][0]*z;

        Press[2] = pr*R*T[4661][0]*z;

        if (Press[2]>1.603e6)

            {vrfl = (-u/K+sqrt(u*u/K/K-4.0*(Press[2]-
Press[1])*CE*pr/sqrt(K)/zstep1/466.0))/(2.0*CE*pr/sqrt(K));

            }

```

```

if (vrtot > vmax)

    {vrfl = 1.0e-30;

    vcheck = 1;

    }

/*Initial Temp for heating phase*/

T[5][0] = InitHTF;

}

/*Node 5, HTF at z=0*/

i=5;

T[i][1] = T[i][0];

/*Node 1330, HTF at z=L*/

i = 4665;

T[i][1] = -Ar[1]*Fo[2]*Bi[2]/Ap[1]*T[i][0]+(-
2.0*Fo[2]*Ap[1]*zstep3*T[i][0]+Ar[1]*Fo[2]*Bi[2]*zstep3*T[i-
1][0]+T[i][0]*Ap[1]*zstep3+2.0*Fo[2]*Ap[1]*zstep3*T[i-5][0]+vfl*deltat*Ap[1]*T[i-
5][0]-vfl*deltat*Ap[1]*T[i][0])/(Ap[1]*zstep3);

/*Node 10, HTF intermediate adjacent to pin fin*/

```

```

for (i=10; i<4661; i=i+10){

    T[i][1] = (zstep1*Ap[1]-Fo[3]*zstep1*Ap[1]-
Fo[1]*zstep1*Ap[1]-
vfl*deltat*Ap[1])/(zstep1*Ap[1])*T[i][0]+(Fo[1]*zstep1*Ap[1]*T[i-
5][0]+vfl*deltat*Ap[1]*T[i-5][0]-
Ar[1]*Fo[1]*Bi[1]*zstep1*T[i][0]+Ar[1]*Bi[1]*Fo[1]*zstep1*T[i-
1][0]+Fo[3]*zstep1*Ap[1]*T[i+5][0])/(zstep1*Ap[1]);

}

```

/*Node 15, HTF intermediate adjacent to adsorbent*/

```

for (i=15; i<4661; i=i+10){

    T[i][1] = (-2.0*Fo[2]*zstep3*Ap[1]-
vfl*deltat*Ap[1]+zstep3*Ap[1])/(zstep3*Ap[1])*T[i][0]+(vfl*deltat*Ap[1]*T[i-
5][0]+Fo[2]*zstep3*Ap[1]*T[i+5][0]-
Ar[1]*Fo[2]*Bi[2]*zstep3*T[i][0]+Fo[2]*zstep3*Ap[1]*T[i-
5][0]+Ar[1]*Fo[2]*Bi[2]*zstep3*T[i-1][0])/(zstep3*Ap[1]);

}

```

/*Node 4, HTF pipe - beginning*/

```

i =4;

```

$$T[i][1] = (-Ar[3]*Fo[3]*Bi[4]+Ap[2]-2.0*Fo[4]*Ap[2]-Ar[1]*Fo[3]*Bi[3])/Ap[2]*T[i][0]+(Ar[3]*Fo[3]*Bi[4]*T[i-1][0]+2.0*Fo[4]*Ap[2]*T[i+5][0]+Ar[1]*Fo[3]*Bi[3]*T[i+1][0])/(Ap[2]);$$

/*Node 9, HTF pipe intermediate adjacent to pin fin*/

for (i=9; i<4661; i=i+10){

$$T[i][1] = (-2.0*Fo[6]*Ap[2]*rstep[4]-Ar[2]*Fo[6]*Bi[5]*rstep[4]+Ap[2]*rstep[4]-Ar[4]*Fo[6]*zstep3)/Ap[2]/rstep[4]*T[i][0]+(Ar[2]*Fo[6]*Bi[5]*rstep[4]*T[i+1][0]+Fo[6]*Ap[2]*rstep[4]*T[i+5][0]+Ar[4]*Fo[6]*zstep3*T[i-1][0]+Fo[6]*Ap[2]*rstep[4]*T[i-5][0])/Ap[2]/rstep[4];$$

}

/*Node 14, HTF pipe intermediate adjacent to adsorbent*/

for (i=14; i<4661; i=i+10){

$$T[i][1] = (Ap[2]-Ar[1]*Fo[3]*Bi[3]-Ar[3]*Fo[3]*Bi[4]-2.0*Fo[4]*Ap[2])/Ap[2]*T[i][0]+(Ar[1]*Fo[3]*Bi[3]*T[i+1][0]+Fo[4]*Ap[2]*T[i+5][0]+Ar[3]*Fo[3]*Bi[4]*T[i-1][0]+Fo[4]*Ap[2]*T[i-5][0])/Ap[2];$$

}

/*Node 1329, HTF pipe at the end*/

i = 4664;

$$T[i][1] = (-Ar[3]*Fo[3]*Bi[4]+Ap[2]-2.0*Fo[4]*Ap[2]-Ar[1]*Fo[3]*Bi[3])/Ap[2]*T[i][0]+(Ar[3]*Fo[3]*Bi[4]*T[i-1][0]+2.0*Fo[4]*Ap[2]*T[i-5][0]+Ar[1]*Fo[3]*Bi[3]*T[i+1][0])/(Ap[2]);$$

/*Node 3, adsorbent node, column 3, beginning*/

i = 3;

$$\omega = \omega_{gao} \exp(-D*T[i][0]*T[i][0]*(B-m/T[i][0]-\log(pr*R*T[i][0]*z))*(B-m/T[i][0]-\log(pr*R*T[i][0]*z)));$$

$$Ca = (cr+1.42/2.0*R/\sqrt{D})*(-2.0*D*T[i][0]*(B-m/T[i][0]-\log(pr*R*T[i][0]*z))*(B-m/T[i][0]-\log(pr*R*T[i][0]*z))-2.0*D*T[i][0]*T[i][0]*(B-m/T[i][0]-\log(pr*R*T[i][0]*z))*(m/T[i][0]/T[i][0]-1.0/T[i][0]))*\omega/\omega_{gao};$$

$$Cb = (-2.0*D*T[i][0]*(B-m/T[i][0]-\log(pr*R*T[i][0]*z))*(B-m/T[i][0]-\log(pr*R*T[i][0]*z))-2.0*D*T[i][0]*T[i][0]*(B-m/T[i][0]-\log(pr*R*T[i][0]*z))*(m/T[i][0]/T[i][0]-1.0/T[i][0]))*\omega;$$

$$hav = (m+1.58/\sqrt{D}-1.42/\sqrt{D})*\omega/\omega_{gao}*R;$$

$$T[i][1] = (-\epsilon*pr*cr*\alpha_{aa}*T[i][0]*Ap[3]*rstep[1]-cr*pr*vrf1*Fo[7]*zstep1*Ap[3]*rstep[1]*T[i+5][0]+cr*pr*vrf1*Fo[7]*zstep1*Ap[3]*rstep[1]*T[i][0]-T[i][0]*ka*Ap[3]*rstep[1]+T[i][0]*ka*Ap[3]*rstep[1]*\epsilon-Ar[5]*Fo[9]*zstep1*ka*T[i-1][0]+Ar[5]*Fo[9]*zstep1*ka*T[i][0]-pa*\omega*\alpha_{aa}*Ca*T[i][0]*Ap[3]*rstep[1]+pa*\omega*\alpha_{aa}*Ca*T[i][0]*Ap[3]*rstep[1]*\epsilon+pa*hav*\alpha_{aa}*Cb*T[i][0]*Ap[3]*rstep[1]-$$

```

pa*hav*alphaa*Cb*T[i][0]*Ap[3]*rstep[1]*epsilon+epsilon*alphaa*Cc*T[i][0]*Ap[3]*r
step[1]-
2.0*Fo[9]*Bi[7]*ka*Ap[3]*rstep[1]*T[i+5][0]+2.0*Fo[9]*Bi[7]*ka*Ap[3]*rstep[1]*T[i]
[0]-
Ar[3]*Fo[9]*Bi[7]*ka*rstep[1]*T[i+1][0]+Ar[3]*Fo[9]*Bi[7]*ka*rstep[1]*T[i][0])/(Ap[
3]*rstep[1]*(-epsilon*pr*cr*alphaa-ka+epsilon*ka-
pa*omega*alphaa*Ca+pa*omega*alphaa*Ca*epsilon+pa*hav*alphaa*Cb-
pa*hav*alphaa*Cb*epsilon+epsilon*alphaa*Cc));

```

/*Node 2, adsorbent node, column 2, beginning*/

```
i=2;
```

```

omega = omegao*exp(-D*T[i][0]*T[i][0]*(B-m/T[i][0]-
log(pr*R*T[i][0]*z))*(B-m/T[i][0]-log(pr*R*T[i][0]*z)));

```

```

Ca = (cr+1.42/2.0*R/sqrt(D)*(-2.0*D*T[i][0]*(B-m/T[i][0]-
log(pr*R*T[i][0]*z))*(B-m/T[i][0]-log(pr*R*T[i][0]*z))-2.0*D*T[i][0]*T[i][0]*(B-
m/T[i][0]-log(pr*R*T[i][0]*z))*(m/T[i][0]/T[i][0]-1.0/T[i][0]))*omega/omegao);

```

```

Cb = (-2.0*D*T[i][0]*(B-m/T[i][0]-log(pr*R*T[i][0]*z))*(B-
m/T[i][0]-log(pr*R*T[i][0]*z))-2.0*D*T[i][0]*T[i][0]*(B-m/T[i][0]-
log(pr*R*T[i][0]*z))*(m/T[i][0]/T[i][0]-1.0/T[i][0]))*omega;

```

```
hav = (m+1.58/sqrt(D)-1.42/sqrt(D)*omega/omegao)*R;
```

```

T[i][1] = (-epsilon*pr*cr*alphaa*T[i][0]*Ap[4]*rstep[1]-
cr*pr*vrfl*Fo[7]*zstep1*Ap[4]*rstep[1]*T[i+5][0]+cr*pr*vrfl*Fo[7]*zstep1*Ap[4]*rste

```

p[1]*T[i][0]-

T[i][0]*ka*Ap[4]*rstep[1]+T[i][0]*ka*Ap[4]*rstep[1]*epsilon+Ar[5]*Fo[9]*zstep1*ka*
T[i][0]-Ar[5]*Fo[9]*zstep1*ka*T[i+1][0]-

pa*omega*alphaa*Ca*T[i][0]*Ap[4]*rstep[1]+pa*omega*alphaa*Ca*T[i][0]*Ap[4]*rste
p[1]*epsilon+pa*hav*alphaa*Cb*T[i][0]*Ap[4]*rstep[1]-

pa*hav*alphaa*Cb*T[i][0]*Ap[4]*rstep[1]*epsilon+epsilon*alphaa*Cc*T[i][0]*Ap[4]*r
step[1]-

2.0*Fo[9]*Bi[7]*ka*Ap[4]*rstep[1]*T[i+5][0]+2.0*Fo[9]*Bi[7]*ka*Ap[4]*rstep[1]*T[i]
[0]-Ar[7]*Fo[9]*zstep1*ka*T[i]-

1][0]+Ar[7]*Fo[9]*zstep1*ka*T[i][0])/(Ap[4]*rstep[1]*(-epsilon*pr*cr*alphaa-
ka+epsilon*ka-

pa*omega*alphaa*Ca+pa*omega*alphaa*Ca*epsilon+pa*hav*alphaa*Cb-
pa*hav*alphaa*Cb*epsilon+epsilon*alphaa*Cc));

/*Node 1, adsorbent node, column 1, beginning*/

i = 1;

omega = omegao*exp(-D*T[i][0]*T[i][0]*(B-m/T[i][0]-
log(pr*R*T[i][0]*z))*(B-m/T[i][0]-log(pr*R*T[i][0]*z)));

Ca = (cr+1.42/2.0*R/sqrt(D))*(-2.0*D*T[i][0]*(B-m/T[i][0]-
log(pr*R*T[i][0]*z))*(B-m/T[i][0]-log(pr*R*T[i][0]*z))-2.0*D*T[i][0]*T[i][0]*(B-
m/T[i][0]-log(pr*R*T[i][0]*z))*(m/T[i][0]/T[i][0]-1.0/T[i][0]))*omega/omegao);

```

        Cb = (-2.0*D*T[i][0]*(B-m/T[i][0]-log(pr*R*T[i][0]*z))*(B-
m/T[i][0]-log(pr*R*T[i][0]*z))-2.0*D*T[i][0]*T[i][0]*(B-m/T[i][0]-
log(pr*R*T[i][0]*z))*(m/T[i][0]/T[i][0]-1.0/T[i][0]))*omega;

        hav = (m+1.58/sqrt(D)-1.42/sqrt(D)*omega/omegao)*R;

        T[i][1] = (-epsilon*pr*cr*alphaa*T[i][0]*Ap[5]*rstep[1]-
T[i][0]*ka*Ap[5]*rstep[1]+T[i][0]*ka*Ap[5]*rstep[1]*epsilon-
Ar[7]*Fo[9]*zstep1*ka*T[i+1][0]+Ar[7]*Fo[9]*zstep1*ka*T[i][0]-
pa*omega*alphaa*Ca*T[i][0]*Ap[5]*rstep[1]+pa*omega*alphaa*Ca*T[i][0]*Ap[5]*rste
p[1]*epsilon+pa*hav*alphaa*Cb*T[i][0]*Ap[5]*rstep[1]-
pa*hav*alphaa*Cb*T[i][0]*Ap[5]*rstep[1]*epsilon+epsilon*alphaa*Cc*T[i][0]*Ap[5]*r
step[1]-
2.0*Fo[9]*Bi[7]*ka*Ap[5]*rstep[1]*T[i+5][0]+2.0*Fo[9]*Bi[7]*ka*Ap[5]*rstep[1]*T[i
][0]-
cr*pr*vrfl*Fo[7]*zstep1*Ap[5]*rstep[1]*T[i+5][0]+cr*pr*vrfl*Fo[7]*zstep1*Ap[5]*rste
p[1]*T[i][0])/(Ap[5]*rstep[1]*(-epsilon*pr*cr*alphaa-ka+epsilon*ka-
pa*omega*alphaa*Ca+pa*omega*alphaa*Ca*epsilon+pa*hav*alphaa*Cb-
pa*hav*alphaa*Cb*epsilon+epsilon*alphaa*Cc));

```

```

/*Node 13, adsorbent node, column 3, intermediate adjacent to
adsorbent*/

```

```

for (i=13; i<4661; i=i+10){

```

$$\omega = \omega_0 \cdot \exp(-D \cdot T[i][0] \cdot T[i][0] \cdot (B - m/T[i][0] - \log(pr \cdot R \cdot T[i][0] \cdot z)) \cdot (B - m/T[i][0] - \log(pr \cdot R \cdot T[i][0] \cdot z)));$$

$$C_a = (cr + 1.42/2.0 \cdot R/\sqrt{D}) \cdot (-2.0 \cdot D \cdot T[i][0] \cdot (B - m/T[i][0] - \log(pr \cdot R \cdot T[i][0] \cdot z)) \cdot (B - m/T[i][0] - \log(pr \cdot R \cdot T[i][0] \cdot z)) - 2.0 \cdot D \cdot T[i][0] \cdot T[i][0] \cdot (B - m/T[i][0] - \log(pr \cdot R \cdot T[i][0] \cdot z)) \cdot (m/T[i][0]/T[i][0] - 1.0/T[i][0])) \cdot \omega/\omega_0);$$

$$C_b = (-2.0 \cdot D \cdot T[i][0] \cdot (B - m/T[i][0] - \log(pr \cdot R \cdot T[i][0] \cdot z)) \cdot (B - m/T[i][0] - \log(pr \cdot R \cdot T[i][0] \cdot z)) - 2.0 \cdot D \cdot T[i][0] \cdot T[i][0] \cdot (B - m/T[i][0] - \log(pr \cdot R \cdot T[i][0] \cdot z)) \cdot (m/T[i][0]/T[i][0] - 1.0/T[i][0])) \cdot \omega;$$

$$hav = (m + 1.58/\sqrt{D}) - 1.42/\sqrt{D} \cdot \omega/\omega_0 \cdot R;$$

$$T[i][1] = (-\epsilon \cdot pr \cdot cr \cdot \alpha_{aa} \cdot T[i][0] \cdot Ap[3] \cdot rstep[1] + cr \cdot pr \cdot vrfl \cdot zstep1 \cdot Fo[7] \cdot Ap[3] \cdot rstep[1] \cdot T[i][0] - cr \cdot pr \cdot vrfl \cdot zstep1 \cdot Fo[7] \cdot Ap[3] \cdot rstep[1] \cdot T[i+5][0] - T[i][0] \cdot ka \cdot Ap[3] \cdot rstep[1] + T[i][0] \cdot ka \cdot Ap[3] \cdot rstep[1] \cdot \epsilon - Fo[9] \cdot Bi[7] \cdot ka \cdot Ap[3] \cdot rstep[1] \cdot T[i-5][0] + 2.0 \cdot Bi[7] \cdot Fo[9] \cdot ka \cdot Ap[3] \cdot rstep[1] \cdot T[i][0] - pa \cdot \omega \cdot \alpha_{aa} \cdot Ca \cdot T[i][0] \cdot Ap[3] \cdot rstep[1] + pa \cdot \omega \cdot \alpha_{aa} \cdot Ca \cdot T[i][0] \cdot Ap[3] \cdot rstep[1] \cdot \epsilon - Ar[5] \cdot Fo[9] \cdot zstep1 \cdot ka \cdot T[i-1][0] + Ar[5] \cdot zstep1 \cdot Fo[9] \cdot ka \cdot T[i][0] + pa \cdot hav \cdot \alpha_{aa} \cdot Cb \cdot T[i][0] \cdot Ap[3] \cdot rstep[1] - pa \cdot hav \cdot \alpha_{aa} \cdot Cb \cdot T[i][0] \cdot Ap[3] \cdot rstep[1] \cdot \epsilon + \epsilon \cdot \alpha_{aa} \cdot Cc \cdot T[i][0] \cdot Ap[3] \cdot rstep[1] - Fo[9] \cdot Bi[7] \cdot ka \cdot Ap[3] \cdot rstep[1] \cdot T[i+5][0] - Ar[3] \cdot Fo[9] \cdot Bi[7] \cdot ka \cdot rstep[1] \cdot T[i+1][0] + Ar[3] \cdot Fo[9] \cdot Bi[7] \cdot ka \cdot rstep[1] \cdot T[i][0]) / (Ap[$$

```

3]*rstep[1]*(-ka+epsilon*ka-
pa*omega*alphaa*Ca+pa*omega*alphaa*Ca*epsilon+pa*hav*alphaa*Cb-
pa*hav*alphaa*Cb*epsilon+epsilon*alphaa*Cc-epsilon*pr*cr*alphaa));
}

```

```

/*Node 12, adsorbent node, column 2, intermediate adjacent to
adsorbent*/

```

```

for (i=12; i<4661; i=i+10){

    omega = omegao*exp(-D*T[i][0]*T[i][0]*(B-
m/T[i][0]-log(pr*R*T[i][0]*z))*(B-m/T[i][0]-log(pr*R*T[i][0]*z)));

    Ca = (cr+1.42/2.0*R/sqrt(D)*(-2.0*D*T[i][0]*(B-
m/T[i][0]-log(pr*R*T[i][0]*z))*(B-m/T[i][0]-log(pr*R*T[i][0]*z))-
2.0*D*T[i][0]*T[i][0]*(B-m/T[i][0]-log(pr*R*T[i][0]*z))*(m/T[i][0]/T[i][0]-
1.0/T[i][0]))*omega/omegao);

    Cb = (-2.0*D*T[i][0]*(B-m/T[i][0]-
log(pr*R*T[i][0]*z))*(B-m/T[i][0]-log(pr*R*T[i][0]*z))-2.0*D*T[i][0]*T[i][0]*(B-
m/T[i][0]-log(pr*R*T[i][0]*z))*(m/T[i][0]/T[i][0]-1.0/T[i][0]))*omega;

    hav = (m+1.58/sqrt(D)-
1.42/sqrt(D)*omega/omegao)*R;

    T[i][1] = (-
epsilon*pr*cr*alphaa*T[i][0]*Ap[4]*rstep[1]-
cr*pr*vrfl*zstep1*Fo[7]*Ap[4]*rstep[1]*T[i+5][0]+cr*pr*vrfl*zstep1*Fo[7]*Ap[4]*rste

```

```

p[1]*T[i][0]-T[i][0]*ka*Ap[4]*rstep[1]+T[i][0]*ka*Ap[4]*rstep[1]*epsilon-
Bi[7]*Fo[9]*ka*Ap[4]*rstep[1]*T[i-5][0]+2.0*Bi[7]*Fo[9]*ka*Ap[4]*rstep[1]*T[i][0]-
pa*omega*alphaa*Ca*T[i][0]*Ap[4]*rstep[1]+pa*omega*alphaa*Ca*T[i][0]*Ap[4]*rste
p[1]*epsilon-Ar[7]*zstep1*Fo[9]*ka*T[i-
1][0]+Ar[7]*Fo[9]*zstep1*ka*T[i][0]+pa*hav*alphaa*Cb*T[i][0]*Ap[4]*rstep[1]-
pa*hav*alphaa*Cb*T[i][0]*Ap[4]*rstep[1]*epsilon+epsilon*alphaa*Cc*T[i][0]*Ap[4]*r
step[1]-Fo[9]*Bi[7]*ka*Ap[4]*rstep[1]*T[i+5][0]-
Fo[9]*ka*Ar[5]*zstep1*T[i+1][0]+Ar[5]*zstep1*Fo[9]*ka*T[i][0])/(Ap[4]*rstep[1]*(-
ka+epsilon*ka-
pa*omega*alphaa*Ca+pa*omega*alphaa*Ca*epsilon+pa*hav*alphaa*Cb-
pa*hav*alphaa*Cb*epsilon+epsilon*alphaa*Cc-epsilon*pr*cr*alphaa));

```

```

}
```

```

/*Node 11, adsorbent node, column 1, intermediate adjacent to adsorbent*/

```

```

for (i=11; i<4661; i=i+10){

```

```

    omega = omegao*exp(-D*T[i][0]*T[i][0]*(B-
m/T[i][0]-log(pr*R*T[i][0]*z))*(B-m/T[i][0]-log(pr*R*T[i][0]*z)));

    Ca = (cr+1.42/2.0*R/sqrt(D)*(-2.0*D*T[i][0]*(B-
m/T[i][0]-log(pr*R*T[i][0]*z))*(B-m/T[i][0]-log(pr*R*T[i][0]*z))-
2.0*D*T[i][0]*T[i][0]*(B-m/T[i][0]-log(pr*R*T[i][0]*z))*(m/T[i][0]/T[i][0]-
1.0/T[i][0])))*omega/omegao);

```

```

Cb = (-2.0*D*T[i][0]*(B-m/T[i][0]-
log(pr*R*T[i][0]*z))*(B-m/T[i][0]-log(pr*R*T[i][0]*z))-2.0*D*T[i][0]*T[i][0]*(B-
m/T[i][0]-log(pr*R*T[i][0]*z))*(m/T[i][0]/T[i][0]-1.0/T[i][0]))*omega;

hav = (m+1.58/sqrt(D)-
1.42/sqrt(D)*omega/omegao)*R;

T[i][1] = (-
epsilon*pr*cr*alphaa*T[i][0]*Ap[5]*rstep[1]-
cr*pr*vrf1*zstep1*Fo[7]*Ap[5]*rstep[1]*T[i+5][0]+cr*pr*vrf1*zstep1*Fo[7]*Ap[5]*rste
p[1]*T[i][0]-T[i][0]*ka*Ap[5]*rstep[1]+T[i][0]*ka*Ap[5]*rstep[1]*epsilon-
Bi[7]*Fo[9]*ka*Ap[5]*rstep[1]*T[i-5][0]+2.0*Bi[7]*Fo[9]*ka*Ap[5]*rstep[1]*T[i][0]-
pa*omega*alphaa*Ca*T[i][0]*rstep[1]*Ap[5]+pa*omega*alphaa*Ca*T[i][0]*rstep[1]*A
p[5]*epsilon+pa*hav*alphaa*Cb*T[i][0]*rstep[1]*Ap[5]-
pa*hav*alphaa*Cb*T[i][0]*rstep[1]*Ap[5]*epsilon+epsilon*alphaa*Cc*T[i][0]*rstep[1]
*Ap[5]-Fo[9]*Bi[7]*ka*rstep[1]*Ap[5]*T[i+5][0]-
Ar[7]*Fo[9]*ka*zstep1*T[i+1][0]+Ar[7]*zstep1*Fo[9]*ka*T[i][0])/(rstep[1]*Ap[5]*(-
ka+epsilon*ka-
pa*omega*alphaa*Ca+pa*omega*alphaa*Ca*epsilon+pa*hav*alphaa*Cb-
pa*hav*alphaa*Cb*epsilon+epsilon*alphaa*Cc-epsilon*pr*cr*alphaa));

}

/*Node 4663, adsorbent node, column 3, ending*/

i = 4663;

```


$$\omega = \omega_0 \cdot \exp(-D \cdot T[i][0] \cdot T[i][0] \cdot (B - m/T[i][0] - \log(pr \cdot R \cdot T[i][0] \cdot z)) \cdot (B - m/T[i][0] - \log(pr \cdot R \cdot T[i][0] \cdot z)));$$

$$Ca = (cr + 1.42/2.0 \cdot R/\sqrt{D}) \cdot (-2.0 \cdot D \cdot T[i][0] \cdot (B - m/T[i][0] - \log(pr \cdot R \cdot T[i][0] \cdot z)) \cdot (B - m/T[i][0] - \log(pr \cdot R \cdot T[i][0] \cdot z)) - 2.0 \cdot D \cdot T[i][0] \cdot T[i][0] \cdot (B - m/T[i][0] - \log(pr \cdot R \cdot T[i][0] \cdot z)) \cdot (m/T[i][0]/T[i][0] - 1.0/T[i][0])) \cdot \omega/\omega_0);$$

$$Cb = (-2.0 \cdot D \cdot T[i][0] \cdot (B - m/T[i][0] - \log(pr \cdot R \cdot T[i][0] \cdot z)) \cdot (B - m/T[i][0] - \log(pr \cdot R \cdot T[i][0] \cdot z)) - 2.0 \cdot D \cdot T[i][0] \cdot T[i][0] \cdot (B - m/T[i][0] - \log(pr \cdot R \cdot T[i][0] \cdot z)) \cdot (m/T[i][0]/T[i][0] - 1.0/T[i][0])) \cdot \omega;$$

$$hav = (m + 1.58/\sqrt{D} - 1.42/\sqrt{D}) \cdot \omega/\omega_0 \cdot R;$$

$$T[i][1] =$$

$$\begin{aligned} & (\epsilon \cdot pr \cdot cr \cdot \alpha_{aa} \cdot T[i][0] \cdot Ap[3] \cdot rstep[1] + cr \cdot pr \cdot vrf1 \cdot Fo[7] \cdot zstep1 \cdot Ap[3] \cdot rstep[1] \\ & \cdot T[i-5][0] - cr \cdot pr \cdot vrf1 \cdot Fo[7] \cdot zstep1 \cdot Ap[3] \cdot rstep[1] \cdot T[i][0] + T[i][0] \cdot ka \cdot Ap[3] \cdot rstep[1] - \\ & T[i][0] \cdot ka \cdot Ap[3] \cdot rstep[1] \cdot \epsilon + Ar[5] \cdot Fo[9] \cdot zstep1 \cdot ka \cdot T[i-1][0] - \\ & Ar[5] \cdot Fo[9] \cdot zstep1 \cdot ka \cdot T[i][0] + pa \cdot \omega \cdot \alpha_{aa} \cdot Ca \cdot T[i][0] \cdot Ap[3] \cdot rstep[1] - \\ & pa \cdot \omega \cdot \alpha_{aa} \cdot Ca \cdot T[i][0] \cdot Ap[3] \cdot rstep[1] \cdot \epsilon - \\ & pa \cdot hav \cdot \alpha_{aa} \cdot Cb \cdot T[i][0] \cdot Ap[3] \cdot rstep[1] + pa \cdot hav \cdot \alpha_{aa} \cdot Cb \cdot T[i][0] \cdot Ap[3] \cdot rstep[1] \cdot \epsilon - \\ & \epsilon \cdot \alpha_{aa} \cdot Cc \cdot T[i][0] \cdot Ap[3] \cdot rstep[1] + 2.0 \cdot Fo[9] \cdot Bi[7] \cdot ka \cdot Ap[3] \cdot rstep[1] \cdot T[i-5][0] - \\ & 2.0 \cdot Fo[9] \cdot Bi[7] \cdot ka \cdot Ap[3] \cdot rstep[1] \cdot T[i][0] + Ar[3] \cdot Fo[9] \cdot Bi[7] \cdot ka \cdot rstep[1] \cdot T[i+1][0] - \\ & Ar[3] \cdot Fo[9] \cdot Bi[7] \cdot ka \cdot rstep[1] \cdot T[i][0]) / (Ap[3] \cdot rstep[1] \cdot (\epsilon \cdot pr \cdot cr \cdot \alpha_{aa} + pa \cdot \omega \cdot \alpha_{aa} \cdot Ca \cdot T[i][0] \cdot Ap[3] \cdot rstep[1] - \\ & pa \cdot \omega \cdot \alpha_{aa} \cdot Ca \cdot T[i][0] \cdot Ap[3] \cdot rstep[1] \cdot \epsilon - pa \cdot hav \cdot \alpha_{aa} \cdot Cb \cdot T[i][0] \cdot Ap[3] \cdot rstep[1] + pa \cdot hav \cdot \alpha_{aa} \cdot Cb \cdot T[i][0] \cdot Ap[3] \cdot rstep[1] \cdot \epsilon - \\ & \epsilon \cdot \alpha_{aa} \cdot Cc \cdot T[i][0] \cdot Ap[3] \cdot rstep[1] + 2.0 \cdot Fo[9] \cdot Bi[7] \cdot ka \cdot Ap[3] \cdot rstep[1] \cdot T[i-5][0] - 2.0 \cdot Fo[9] \cdot Bi[7] \cdot ka \cdot Ap[3] \cdot rstep[1] \cdot T[i][0] + \\ & Ar[3] \cdot Fo[9] \cdot Bi[7] \cdot ka \cdot rstep[1] \cdot T[i+1][0] - Ar[3] \cdot Fo[9] \cdot Bi[7] \cdot ka \cdot rstep[1] \cdot T[i][0]) \end{aligned}$$

ga*alphaa*Ca-pa*omega*alphaa*Ca*epsilon+ka-epsilon*ka-
 pa*hav*alphaa*Cb+pa*hav*alphaa*Cb*epsilon-epsilon*alphaa*Cc));

/*Node 4662, adsorbent node, column 2, ending*/

i = 4662;

omega = omegao*exp(-D*T[i][0]*T[i][0]*(B-m/T[i][0]-
 log(pr*R*T[i][0]*z))*(B-m/T[i][0]-log(pr*R*T[i][0]*z)));

Ca = (cr+1.42/2.0*R/sqrt(D)*(-2.0*D*T[i][0]*(B-m/T[i][0]-
 log(pr*R*T[i][0]*z))*(B-m/T[i][0]-log(pr*R*T[i][0]*z))-2.0*D*T[i][0]*T[i][0]*(B-
 m/T[i][0]-log(pr*R*T[i][0]*z))*(m/T[i][0]/T[i][0]-1.0/T[i][0]))*omega/omegao);

Cb = (-2.0*D*T[i][0]*(B-m/T[i][0]-log(pr*R*T[i][0]*z))*(B-
 m/T[i][0]-log(pr*R*T[i][0]*z))-2.0*D*T[i][0]*T[i][0]*(B-m/T[i][0]-
 log(pr*R*T[i][0]*z))*(m/T[i][0]/T[i][0]-1.0/T[i][0]))*omega;

hav = (m+1.58/sqrt(D)-1.42/sqrt(D)*omega/omegao)*R;

T[i][1] = (epsilon*pr*cr*alphaa*T[i][0]*Ap[4]*rstep[1]-
 cr*pr*vrfl*Fo[7]*zstep1*Ap[4]*rstep[1]*T[i][0]+cr*pr*vrfl*Fo[7]*zstep1*Ap[4]*rstep[1]*T[i-5][0]+T[i][0]*ka*Ap[4]*rstep[1]-
 T[i][0]*ka*Ap[4]*rstep[1]*epsilon+Ar[5]*Fo[9]*zstep1*ka*T[i+1][0]-
 Ar[5]*Fo[9]*zstep1*ka*T[i][0]+pa*omega*alphaa*Ca*T[i][0]*Ap[4]*rstep[1]-
 pa*omega*alphaa*Ca*T[i][0]*Ap[4]*rstep[1]*epsilon-
 pa*hav*alphaa*Cb*T[i][0]*Ap[4]*rstep[1]+pa*hav*alphaa*Cb*T[i][0]*Ap[4]*rstep[1]*
 epsilon-epsilon*alphaa*Cc*T[i][0]*Ap[4]*rstep[1]-

$2.0 \cdot \text{Fo}[9] \cdot \text{Bi}[7] \cdot \text{ka} \cdot \text{Ap}[4] \cdot \text{rstep}[1] \cdot \text{T}[i][0] + 2.0 \cdot \text{Fo}[9] \cdot \text{Bi}[7] \cdot \text{ka} \cdot \text{Ap}[4] \cdot \text{rstep}[1] \cdot \text{T}[i-5][0] + \text{Ar}[7] \cdot \text{Fo}[9] \cdot \text{zstep}[1] \cdot \text{ka} \cdot \text{T}[i-1][0] -$
 $\text{Ar}[7] \cdot \text{Fo}[9] \cdot \text{zstep}[1] \cdot \text{ka} \cdot \text{T}[i][0]) / (\text{Ap}[4] \cdot \text{rstep}[1] \cdot (\text{epsilon} \cdot \text{pr} \cdot \text{cr} \cdot \text{alphaa} + \text{pa} \cdot \text{omega} \cdot \text{alphaa} \cdot \text{Ca} - \text{pa} \cdot \text{omega} \cdot \text{alphaa} \cdot \text{Ca} \cdot \text{epsilon} + \text{ka} \cdot \text{epsilon} - \text{ka} \cdot \text{epsilon} \cdot \text{alphaa} \cdot \text{Cc} - \text{pa} \cdot \text{hav} \cdot \text{alphaa} \cdot \text{Cb} + \text{pa} \cdot \text{hav} \cdot \text{alphaa} \cdot \text{Cb} \cdot \text{epsilon}));$

/*Node 4661, adsorbent node, column 1, ending*/

i = 4661;

$\text{omega} = \text{omegao} \cdot \exp(-D \cdot \text{T}[i][0] \cdot \text{T}[i][0] \cdot (B - m / \text{T}[i][0] - \log(\text{pr} \cdot \text{R} \cdot \text{T}[i][0] \cdot z)) \cdot (B - m / \text{T}[i][0] - \log(\text{pr} \cdot \text{R} \cdot \text{T}[i][0] \cdot z)));$

$\text{Ca} = (\text{cr} + 1.42 / 2.0 \cdot \text{R} / \sqrt{D}) \cdot (-2.0 \cdot D \cdot \text{T}[i][0] \cdot (B - m / \text{T}[i][0] - \log(\text{pr} \cdot \text{R} \cdot \text{T}[i][0] \cdot z)) \cdot (B - m / \text{T}[i][0] - \log(\text{pr} \cdot \text{R} \cdot \text{T}[i][0] \cdot z)) - 2.0 \cdot D \cdot \text{T}[i][0] \cdot \text{T}[i][0] \cdot (B - m / \text{T}[i][0] - \log(\text{pr} \cdot \text{R} \cdot \text{T}[i][0] \cdot z)) \cdot (m / \text{T}[i][0] / \text{T}[i][0] - 1.0 / \text{T}[i][0])) \cdot \text{omega} / \text{omegao};$

$\text{Cb} = (-2.0 \cdot D \cdot \text{T}[i][0] \cdot (B - m / \text{T}[i][0] - \log(\text{pr} \cdot \text{R} \cdot \text{T}[i][0] \cdot z)) \cdot (B - m / \text{T}[i][0] - \log(\text{pr} \cdot \text{R} \cdot \text{T}[i][0] \cdot z)) - 2.0 \cdot D \cdot \text{T}[i][0] \cdot \text{T}[i][0] \cdot (B - m / \text{T}[i][0] - \log(\text{pr} \cdot \text{R} \cdot \text{T}[i][0] \cdot z)) \cdot (m / \text{T}[i][0] / \text{T}[i][0] - 1.0 / \text{T}[i][0])) \cdot \text{omega};$

$\text{hav} = (m + 1.58 / \sqrt{D}) - 1.42 / \sqrt{D} \cdot \text{omega} / \text{omegao} \cdot \text{R};$

T[i][1] =

$(\text{epsilon} \cdot \text{pr} \cdot \text{cr} \cdot \text{alphaa} \cdot \text{T}[i][0] \cdot \text{Ap}[5] \cdot \text{rstep}[1] + \text{T}[i][0] \cdot \text{ka} \cdot \text{Ap}[5] \cdot \text{rstep}[1] - \text{T}[i][0] \cdot \text{ka} \cdot \text{Ap}[5] \cdot \text{rstep}[1] \cdot \text{epsilon} + 2.0 \cdot \text{Ar}[7] \cdot \text{Fo}[9] \cdot \text{zstep}[1] \cdot \text{ka} \cdot \text{T}[i+1][0] - 2.0 \cdot \text{Ar}[7] \cdot \text{Fo}[9] \cdot \text{zstep}[1] \cdot \text{ka} \cdot \text{T}[i][0] + \text{pa} \cdot \text{omega} \cdot \text{alphaa} \cdot \text{Ca} \cdot \text{T}[i][0] \cdot \text{Ap}[5] \cdot \text{rstep}[1] - \text{pa} \cdot \text{omega} \cdot \text{alphaa} \cdot \text{Ca} \cdot \text{T}[i][0] \cdot \text{Ap}[5] \cdot \text{rstep}[1] \cdot \text{epsilon} -$

```

pa*hav*alphaa*Cb*T[i][0]*Ap[5]*rstep[1]+pa*hav*alphaa*Cb*T[i][0]*Ap[5]*rstep[1]*
epsilon-
epsilon*alphaa*Cc*T[i][0]*Ap[5]*rstep[1]+2.0*Fo[9]*Bi[7]*ka*Ap[5]*rstep[1]*T[i-
5][0]-
2.0*Fo[9]*Bi[7]*ka*Ap[5]*rstep[1]*T[i][0]+cr*pr*vrf1*Fo[7]*zstep1*Ap[5]*rstep[1]*T
[i-5][0]-
cr*pr*vrf1*Fo[7]*zstep1*Ap[5]*rstep[1]*T[i][0])/(Ap[5]*rstep[1]*(epsilon*pr*cr*alphaa
+pa*omega*alphaa*Ca-pa*omega*alphaa*Ca*epsilon+ka-epsilon*ka-
pa*hav*alphaa*Cb+pa*hav*alphaa*Cb*epsilon-epsilon*alphaa*Cc));

```

```

/*Node 8, pin fin, column 3*/

```

```

for (i=8; i<4661; i=i+10){

```

```

    T[i][1] = (-

```

```

2.0*Bi[6]*Fo[6]*Ap[3]*rstep[4]*rstep[1]+Ap[3]*rstep[4]*rstep[1]-

```

```

Ar[4]*Fo[6]*zstep3*rstep[1]-

```

```

Ar[6]*Fo[6]*zstep3*rstep[4])/(Ap[3]*rstep[4]*rstep[1]*T[i][0]+(Bi[6]*Fo[6]*Ap[3]*rst
ep[4]*rstep[1]*T[i-

```

```

5][0]+Ar[4]*Fo[6]*zstep3*rstep[1]*T[i+1][0]+Ar[6]*Fo[6]*zstep3*rstep[4]*T[i-

```

```

1][0]+Bi[6]*Fo[6]*Ap[3]*rstep[4]*rstep[1]*T[i+5][0])/(Ap[3]*rstep[4]*rstep[1]);

```

```

    }

```

```

/*Node 7, pin fin, column 3*/

```

```

        for (i=7; i<4661; i=i+10){
            T[i][1] = (-2.0*Bi[6]*Fo[6]*Ap[4]*rstep[1]-
Ar[6]*Fo[6]*zstep3+Ap[4]*rstep[1]-
Ar[8]*Fo[6]*zstep3)/(Ap[4]*rstep[1])*T[i][0]+(Bi[6]*Fo[6]*Ap[4]*rstep[1]*T[i-
5][0]+Ar[6]*Fo[6]*zstep3*T[i+1][0]+Ar[8]*Fo[6]*zstep3*T[i-
1][0]+Bi[6]*Fo[6]*Ap[4]*rstep[1]*T[i+5][0])/(Ap[4]*rstep[1]);
        }

```

/*Node 6, pin fin, column 3*/

```

        for (i=6; i<4661; i=i+10){
            T[i][1] = (Ap[5]*rstep[1]-
2.0*Bi[6]*Fo[6]*Ap[5]*rstep[1]-
Ar[6]*Fo[6]*zstep3)/(Ap[5]*rstep[1])*T[i][0]+(Bi[6]*Fo[6]*Ap[5]*rstep[1]*T[i-
5][0]+Ar[6]*Fo[6]*zstep3*T[i+1][0]+Bi[6]*Fo[6]*Ap[5]*rstep[1]*T[i+5][0])/(Ap[5]*rst
ep[1]);
        }

```

/*Convert Data from T[x][1] to T[x][0]*/

```

        for (i=1; i<4666; i=i+1){
            T[i][0]=T[i][1];
        }

```

```

/*close first loop*/

    }

/*Calculate expired time*/

exptime = deltat*(timestep1)*(timestep2-1);

printf("\ntimestep2 = %i", timestep2-1);

printf("\ntimestep1 = %i\n", timestep1);

printf("k = %i\n", k);

mr = pi*r[3]*r[3]*vrfl*pr*1.0e9;

if (k==5){

/*Record Time and temperature of exit HTF and refrigerant into text file

c:\\htemp00.txt*/

    if ((fptr3 = fopen(filename3, "a")) == NULL)

        printf("\nBad File Open");

        fprintf(fptr3, "%f, %f, %f, %f, %f, %f, %f, %f, %f\n", exptime,
T[5][0], T[4665][0], T[1][0], T[4661][0], mr, Press[1], Press[2], omega);

        fclose(fptr3);

}

```

```

/*close last loop*/

}

/*Record Temp at each node into text file c:\\thermal00.txt*/

if ((fptr = fopen(filename, "a")) == NULL)

    printf("\nBad File Open");


    fprintf(fptr, "Final Temperature\n");

    for (i=1; i<4666; i=i+5){

        fprintf(fptr, "%f, %f, %f, %f, %f\n", T[i+4][0], T[i+3][0],
T[i+2][0], T[i+1][0], T[i][0]);

    }


    fclose(fptr);


/*Convert Data from T[x][1] to T[x][0]*/

    for (i=1; i<4666; i=i+5){

        T[i][0]=T[4662-i][1];

        T[i+1][0]=T[4663-i][1];

        T[i+2][0]=T[4664-i][1];

        T[i+3][0]=T[4665-i][1];

        T[i+4][0]=T[4666-i][1];

    }

```

```
/*Close the heating phase of the bed and begin the cooling phase*/
```

```
}
```

```
/*Record parameters a:\\hparam.txt*/
```

```
if ((fptr4 = fopen(filename4, "a")) == NULL)
```

```
printf("\nBad File Open");
```

```
fprintf(fptr4, "Heating Parameters\n");
```

```
fprintf(fptr4, "delta time           =\t%f\n", deltat);
```

```
fprintf(fptr4, "adsorbent ka           =\t%f\n", ka);
```

```
fprintf(fptr4, "contact resis          =\t%f\n", ha);
```

```
fprintf(fptr4, "HTF conv coef          =\t%f\n", hfl);
```

```
fprintf(fptr4, "HTF velocity           =\t%f\n", vfl);
```

```
fprintf(fptr4, "HTF spec heat          =\t%f\n", cfl);
```

```
fprintf(fptr4, "zstep1                 =\t%f\n", zstep1);
```

```
fprintf(fptr4, "zstep2                 =\t%f\n", zstep2);
```

```
fprintf(fptr4, "rstep1                 =\t%f\n", rstep[1]);
```

```
fprintf(fptr4, "rstep2                 =\t%f\n", rstep[2]);
```

```
fprintf(fptr4, "rstep3                 =\t%f\n", rstep[3]);
```

```
fprintf(fptr4, "r[1]                  =\t%f\n", r[1]);
```


<code>fprintf(fp4, "r[2]</code>	<code>=\t%f\n", r[2]);</code>
<code>fprintf(fp4, "r[3]</code>	<code>=\t%f\n", r[3]);</code>
<code>fprintf(fp4, "r[4]</code>	<code>=\t%f\n", r[4]);</code>
<code>fprintf(fp4, "r[5]</code>	<code>=\t%f\n", r[5]);</code>
<code>fprintf(fp4, "vcheck</code>	<code>=\t%i\n", vcheck);</code>
<code>fprintf(fp4, "Bi[1]</code>	<code>=\t%f\n", Bi[1]);</code>
<code>fprintf(fp4, "Bi[3]</code>	<code>=\t%f\n", Bi[3]);</code>
<code>fprintf(fp4, "Bi[4]</code>	<code>=\t%f\n", Bi[4]);</code>
<code>fprintf(fp4, "Bi[7]</code>	<code>=\t%f\n", Bi[7]);</code>
<code>fprintf(fp4, "Fo[1]</code>	<code>=\t%e\n", Fo[1]);</code>
<code>fprintf(fp4, "Fo[3]</code>	<code>=\t%f\n", Fo[3]);</code>
<code>fprintf(fp4, "Fo[9]</code>	<code>=\t%f\n", Fo[9]);</code>
<code>fprintf(fp4, "Ar[1]</code>	<code>=\t%f\n", Ar[1]);</code>
<code>fprintf(fp4, "Ar[3]</code>	<code>=\t%f\n", Ar[3]);</code>
<code>fprintf(fp4, "Ar[5]</code>	<code>=\t%f\n", Ar[5]);</code>
<code>fprintf(fp4, "Ar[7]</code>	<code>=\t%f\n", Ar[7]);</code>
<code>fprintf(fp4, "Ap[1]</code>	<code>=\t%f\n", Ap[1]);</code>
<code>fprintf(fp4, "Ap[2]</code>	<code>=\t%f\n", Ap[2]);</code>
<code>fprintf(fp4, "Ap[3]</code>	<code>=\t%f\n", Ap[3]);</code>
<code>fprintf(fp4, "Ap[4]</code>	<code>=\t%f\n", Ap[4]);</code>
<code>fprintf(fp4, "Ap[5]</code>	<code>=\t%f\n", Ap[5]);</code>

```

        fprintf(fp4, "HTF Flow           =\t%f\n",
Ap[1]*vfl*pfl);

        fprintf(fp4, "Max Refrig           =\t%f\n", vmax);
        fprintf(fp4, "vrtot           =\t%f\n", vrtot);
        fclose(fp4);

printf("Finished Modeling");

return 0;

}

```