Appendix A

Matlab codes for the R-744 transcritical ejector refrigeration cycles

---

```
%Simulation code for single ejector R744 transcritical refrigeration cycle

clear all
clc
Pgco=[9000]  % Input value for PGCO
Tgco=[308]   % Input value for TGCO
Tevap=[268]  % Input value for TEVAP
snpd=[0]     % Input value for SNPD
To=[303]     % environmental temperature
fluid='CO2'  % Selecting refrigerant as Carbon dioxide
Qfrc=0;      % dry ness fraction for liquid
Qfrc1=1;     % dry ness fraction for vapour
loopcnt1=0;
loopcnt2=0;
En=0.8;      % Motive nozzle efficiency
Esuc=0.8;    % Suction nozzle efficiency
Ed=0.8;      % Diffuser efficiency
numb=0;

% Input matrix %

for i=1:1;
    for j=1:1;
          for k=1:1;
              numb=numb+1;
```

```
              TI1(numb,:)=[Pgco(i) Tgco(j) Tevap(k)];
          end
       end
    end

% simulation %

numb=0;
for i=1:1;
    numb=numb+1;
        PGCO=TI1(i,1);
    TGCO=TI1(i,2);
    TEVAP=TI1(i,3);
        Pgco=[PGCO];   % Inlet pressure for motive nozzle
    Tgco=[TGCO];   % Inlet temperature for motive nozzle
Tevap=[TEVAP];          % Evaporator temperature
SNPD=[snpd]        % Suction nozzle pressure drop

U=0.1;           % Initial value for entrainment ratio
U1=0.001;        % Incremental value for entrainment ratio
while(true);
if(U>=1)
 error ('entrainment ratio goes beyond limit')  % throwing error
end
Tref=Tevap+5;    % refrigerated object temperature
H3=refpropm('H','T',Tgco,'P',Pgco,fluid);
S3=refpropm('S','T',Tgco,'P',Pgco,fluid);
rho3=refpropm('D','T',Tgco,'P',Pgco,fluid);
Pevap=refpropm('P','T',Tevap,'Q',Qfrc1,fluid);
Psuc=Pevap-SNPD      % Suction nozzle pressure after pressure drop
H31s=refpropm('H','P',Psuc,'S',S3,fluid);
H31=H3-((H3-H31s)*En);
S31=refpropm('S','P',Psuc,'H',H31,fluid);
V31=(2*(H3-H31))^(1/2);
H7=refpropm('H','P',Pevap,'Q',Qfrc1,fluid);
S7=refpropm('S','P',Pevap,'Q',Qfrc1,fluid);
rho7=refpropm('D','P',Pevap,'Q',Qfrc1,fluid);
S8=S7;   % entropy at suction nozzle outlet
% isentropic efficiency at suction nozzle outlet
H8s=refpropm('H','P',Psuc,'S',S8,fluid);
H8=H7-((H7-H8s)*Esuc); % from efficiency of suction nozzle
S8=refpropm('S','P',Psuc,'H',H8,fluid);
V8=(2*(H7-H8))^(1/2);  % velocity at suction nozzle outlet
V4=(V31+(U*V8))/(U+1); % fluid momentum is conserved in mixing section
```

```
H5x=((H3)/(1+U))+((H7*U)/(1+U)); % overall energy balance
H4=H5x-((V4^2)/2);
H4s=((H5x-H4)*Ed)+H4;
S4=refpropm(’S’,’P’,Psuc,’H’,H4,fluid);
S4s=S4;
Ps=refpropm(’P’,’H’,H4s,’S’,S4s,fluid)
Ha=refpropm(’H’,’P’,Ps,’S’,S3,fluid);
Hb=refpropm(’H’,’P’,Ps,’S’,S7,fluid);
Hc=refpropm(’H’,’P’,Psuc,’S’,S3,fluid);
S5x=refpropm(’S’,’P’,Ps,’H’,H5x,fluid);
T5x=refpropm(’T’,’H’,H5x,’S’,S5x,fluid)
Q5x=refpropm(’Q’,’P’,Ps,’H’,H5x,fluid)
Q=1/(1+U)
loopcnt1=loopcnt1+1;
Ecomp=1.003-0.121*(Pgco/Ps);
H5L=refpropm(’H’,’P’,Ps,’Q’,Qfrc,fluid);
S5L=refpropm(’S’,’P’,Ps,’Q’,Qfrc,fluid);
H6=H5L;
S6=refpropm(’S’,’P’,Pevap,’H’,H6,fluid)
T6=refpropm(’T’,’P’,Pevap,’H’,H6,fluid);
H1=refpropm(’H’,’P’,Ps,’Q’,Qfrc1,fluid);
S1=refpropm(’S’,’P’,Ps,’Q’,Qfrc1,fluid)
S2S=S1;
H2S=refpropm(’H’,’P’,Pgco,’S’,S2S,fluid);
H2=((H2S-H1)/Ecomp)+H1
T2=refpropm(’T’,’P’,Pgco,’H’,H2,fluid);
S2=refpropm(’S’,’P’,Pgco,’H’,H2,fluid)
PR=Ps-Pevap
PRR=Ps/Pevap
RE=(U/(U+1))*(H7-H6);
WD=(H2-H1)/(1+U);
COP=RE/WD
VCC=(H7-H6)*rho7
Eeje=U*((Hb-H7)/(H3-Ha))

% % calculation for entropy %%
Icomp=To*(S2-S1)/(1+U)
Igc=(H2-H3-To*(S2-S3))/(1+U)
Iejc=To*(S5x-S3/(1+U)-S7*(U/(1+U)))
Iexp=To*(S6-S5L)*U/(1+U)
Ievap=To*((S7-S6)+((H6-H7)/Tref))*U/(1+U);
Io=Icomp+Igc+Iejc+Iexp+Ievap;
ICOMP1=(Icomp/Io)*100;
IGC1=(Igc/Io)*100;
```

```
IEJC1=(Iejc/Io)*100;
IEXP1=(Iexp/Io)*100;
IEVAP1=(Ievap/Io)*100;

WR=WD-Io
Eff2=WR/WD; % Second law efficiency

% Calculation for 10 kW load

Ms=10000/(H7-H6)
Mp=Ms/U
WD1=Mp*(H2-H1);
RE1=Ms*(H7-H6);
COP1=RE1/WD1
Mt=Ms+Mp

% Storing results
Result(loopcnt1,:)=[Psuc SNPD Tevap Pevap Tgco Pgco COP Ps
PR PRR Q5x Q U Icomp Igc Iejc Iexp Ievap Io Eff2 Eeje RE WD WR VCC];

if (Q5x-Q>=0.0001)  % Checking dryness fraction at outlet of ejector
    break
else
    U=U+U1
end
end

x(i,:)=Result(end,:)
end

% Simulation code for multi ejector R744 transcritical refrigeration cycle


close all
clear all
clc
load h1.mat
load h2.mat
Tlt=[248]  % Lower Temperature Evaporator temperature
Tmt=[273]  % Medium Temperature Evaporator temperature
Tgco=[313]  % Input value for TGCO
Pgco=[10000] % Input value for PGCO
To=[303]   % Environmental temperature
Phi=0.5
```

```
fluid='CO2'  % Selecting refrigerant as Carbon dioxide
Qfrc=0;      % dry ness fraction for liquid
Qfrc1=1      % dry ness fraction for liquid

Q6=0.5;      % Quality at MT evap exit
loopcnt1=0;
loopcnt2=0;
En=0.8;      % motive nozzle efficiency
Emix=0.85    % mixing efficiency
Ed=0.8;      % diffuser efficiency
numb=0;
Beta=0.5

% Input matrix %

for i=1:1;
    for j=1:1;
          for k=1:1;
              for l=1:1;
              numb=numb+1;
              TI1(numb,:)=[Pgco(i) Tgco(j) Tlt(k) Tmt(l)];
          end
       end
    end
end

% simulation %

numb=0;
for i=1:1;
   numb=numb+1;
    PGCO=TI1(i,1);
   TGCO=TI1(i,2);
   TLT=TI1(i,3);
   TMT=TI1(i,4);
   Tlt=[TLT]; % Lower evaporator temperature
   Tmt=[TMT]; % medium evaporator temperature
   Tgco=[TGCO]; % Inlet temperature for motive nozzle of ejector 1
   Pgco=[PGCO]; % Inlet pressure for motive nozzle of ejector 1
   U1=0.4;  % Initial value for entrainment ratio of ejector 1
U1d=0.0001; % Increment in entrainment ratio of ejector 1
U2d=0.0001; % Increment in entrainment ratio of ejector 2
Tref1=Tlt+5;    % refrigerated object temperature

```

```

while(true);
%throwing error
if(U1>=1)
 error ('entrainment ratio goes beyond limit')
end

% % calculation for Ejector 2 %%

H3=refpropm('H','T',Tgco,'P',Pgco,fluid);
S3=refpropm('S','T',Tgco,'P',Pgco,fluid);
rho3=refpropm('D','T',Tgco,'P',Pgco,fluid);
Plt=refpropm('P','T',Tlt,'Q',Qfrc1,fluid);

H31s=refpropm('H','P',Plt,'S',S3,fluid);
H31=H3-((H3-H31s)*En);
S31=refpropm('S','P',Plt,'H',H31,fluid);
V31=(2*(H3-H31))^(1/2);
H12=refpropm('H','P',Plt,'Q',Qfrc1,fluid);
S12=refpropm('S','P',Plt,'Q',Qfrc1,fluid);
rho12=refpropm('D','P',Plt,'Q',Qfrc1,fluid);
% momentum conservation in mixing section
V13=(V31*(Emix^0.5))/(U1+1);
% overall energy balance
H14=((H3)/(1+U1))+((H12*U1)/(1+U1));
H13=H14-((V13^2)/2);
H14s=((H14-H13)*Ed)+H13;
S13=refpropm('S','P',Plt,'H',H13,fluid);
S14s=S13;
Ps1=refpropm('P','H',H14s,'S',S14s,fluid)
S14=refpropm('S','P',Ps1,'H',H14,fluid);
T14=refpropm('T','H',H14,'S',S14,fluid)
Q14=refpropm('Q','P',Ps1,'H',H14,fluid)
Q=1/(1+U1)
loopcnt1=loopcnt1+1;
H10=refpropm('H','P',Ps1,'Q',Qfrc,fluid);
S10=refpropm('S','P',Ps1,'Q',Qfrc,fluid);
H11=H10;
S11=refpropm('S','P',Plt,'H',H11,fluid)
T11=refpropm('T','P',Plt,'H',H11,fluid);
H9=refpropm('H','P',Ps1,'Q',Qfrc1,fluid);
S9=refpropm('S','P',Ps1,'Q',Qfrc1,fluid);
% Checking dryness fraction at outlet of ejector
if abs((Q14-Q))<=0.001
```

```
    break
else
    U1=U1+U1d;
end

end

%  calculation for Ejector 2

while(true);
U2=Beta/(1-Beta);
% refrigerated object temperature
Tref2=Tmt+5;
T4=Tgco-10;
H4=refpropm(’H’,’T’,T4,’P’,Pgco,fluid);
S4=refpropm(’S’,’T’,T4,’P’,Pgco,fluid);
Pmt=refpropm(’P’,’T’,Tmt,’Q’,Qfrc,fluid);
H5=H4;
S5=refpropm(’S’,’P’,Pmt,’H’,H5,fluid);
H6=refpropm(’H’,’P’,Pmt,’Q’,Q6,fluid);
Phi1=((1-Beta)*(Q14)*(H6-H5))/((Beta)*(1-Q14)*(H12-H11))
S6=refpropm(’S’,’P’,Pmt,’H’,H6,fluid);
S61s=S6;
H61s=refpropm(’H’,’P’,Ps1,’S’,S61s,fluid);
H61=H6-((H6-H61s)*En);
S61=refpropm(’S’,’P’,Ps1,’H’,H61,fluid);
V61=(2*(H6-H61))^(1/2);
% momentum conservation in mixing section
V7=(V61*(Emix^0.5))/(U2+1);
% overall energy balance
H8=((H6)/(1+U2))+((H9*U2)/(1+U2));
H7=H8-((V7^2)/2);
% diffuser efficiency=0.8
H7s=((H8-H7)*Ed)+H7;
S7=refpropm(’S’,’P’,Ps1,’H’,H7,fluid);
S7s=S7;
Ps2=refpropm(’P’,’H’,H7s,’S’,S7s,fluid);

H1=H8+((H3-H4)*(U1)/(1+U1));
S1=refpropm(’S’,’P’,Ps2,’H’,H1,fluid);
Mp1=1/(1+U1)
Mp2=1-Mp1
Ms2=Mp1
Ms1=U1*Mp1
```

```
Qref1=Ms1*(H12-H11);
Qref2=Mp2*(H6-H5);
S8=refpropm('S','P',Ps2,'H',H8,fluid);
T8=refpropm('T','H',H8,'S',S8,fluid)
Q8=refpropm('Q','P',Ps2,'H',H8,fluid)
loopcnt2=loopcnt2+1;
%Checking dryness fraction at outlet of ejector
if abs((Phi1-Phi))<=0.01
    break
else
    Beta=Beta+0.001;
end
end
Ecomp=0.815+(0.022*(Pgco/Ps2))-(0.0041*((Pgco/Ps2)^2))+(0.0001*((Pgco/Ps2)^3))
S2S=S1;
H2S=refpropm('H','P',Pgco,'S',S2S,fluid);
H2=((H2S-H1)/Ecomp)+H1
T2=refpropm('T','P',Pgco,'H',H2,fluid);
S2=refpropm('S','P',Pgco,'H',H2,fluid);
W=(H2-H1)*(Mp2+Ms2);
Qref=Qref1+Qref2;
COP=Qref/W

% calculation for entropy
Icomp=To*(S2-S1)
Igc=((H2-H3)-(To*(S2-S3)))
Iejc1=To*(((Mp1+Ms1)*(S14))-((Mp1)*S3)-((Ms1)*S12))
Iejc2=To*((S8)-((Mp2)*S6)-((Ms2)*S9))
Iexp1=(To*(S11-S10)*Ms1)
Iexp2=To*(S5-S4)*Mp2
Ievap1=Ms1*((To*(S12-S11))-((H12-H11)*((To)/(Tref1))))
Ievap2=(Mp2*((To*(S6-S5))-((H6-H5)*((To)/(Tref2)))))
Iihx=(To)*(((Mp2)*(S4-S3))+(S1-S8))
Io=Icomp+Igc+Iihx+Iejc1+Iejc2+Iexp1+Iexp2+Ievap1+Ievap2;
ICOMP=Icomp/Io
IGC=Igc/Io
IEJC1=Iejc1/Io
IEJC2=Iejc2/Io
IEXP1=Iexp1/Io
IEXP2=Iexp2/Io
IEVAP1=Ievap1/Io
IEVAP2=Ievap2/Io
IIHX=Iihx/Io

```

```
WR=W-Io;
Eff2=WR/W
PR1=Ps1/Plt
PR2=Ps2/Ps1;
PR=Ps2/Plt;
% Storing results
Result(numb,:)=[Tgco Pgco Tmt Tlt Phi Phi1 COP PR1 PR2 PR Q14 Q U1 U2 Beta
Icomp Igc Iihx Iejc1 Iejc2 Iexp1 Iexp2 Ievap1 Ievap2 Io Eff2 W Qref Qref1
Qref2 ICOMP IGC IIHX IEJC1 IEJC2 IEXP1 IEXP2 IEVAP1 IEVAP2];
x(i,:)=Result(end,:)
end
```

Appendix B

CEL Expressions

B.1 CEL expressions used in Ansys CFX Pre for implementing surface tension of CO_2 as a function of temperature

```
LIBRARY:
  CEL:
    EXPRESSIONS:
      oneByTc = 3.288067e-3 [K^(-1)]
      tFactor = if(vaporCO2.Temperature<304.13 [K], (1.0-vaporCO2.Temperature*oneByT
      factor1 = 7.7841389751381843e-2
      factor2 = tFactor^1.26
      factor3 = 1.0 + 0.19*(tFactor^0.5) - 0.25*tFactor
      factor4 = factor1*factor2*factor3
      rampTime = 0.001 [s]
      surTen = if(factor4<0.0158912, factor4, 0.0158912) [N/m]
    END
  END
END
```

B.2 Options used in Ansys CFX for spatial and temporal discretization

```
Temporal scheme        : Implicit Euler
Advection scheme       : High resolution
Turbulence model       : k − Ω SST
Turbulence numerics    : First order
Pressure interpolation : Trilinear
```

```
Velocity interpolation :  Trilinear
Rhie-Chow option       :  High resolution
Volume fraction        :  Segregated
Residual target        :  10^-4
Conservation target    :  10^-4
```

B.3 Options used in Ansys CFX for phase change with the non-equilibrium solver

```
Vapor morphology       : Continuous fluid
Liquid morphology      : Droplets
Heat transfer          : Fluid dependent
Liquid heat transfer   : Small droplets
Nucleation model       : Homogeneous
Vapor heat transfer    : Total energy
Surface tension        : Vapor temp. based
Interphase transfer    : Particle model
Mass transfer          : Phase change
Phase change           : Small droplets
```

B.4 CEL expressions used in Ansys CFX Pre for varying boundary pressure with time

```
LIBRARY:
  CEL:
    EXPRESSIONS:
      inletInitialP = 56 [bar]
      inletFinalP = 80 [bar]
      inletPressure = if(t < rampTime, (inletInitialP + (inletFinalP -
                              inletInitialP)*t/rampTime), inletFinalP )
      outletInitialP = 54 [bar]
      outletFinalP = 28 [bar]
      outletPressure = if(t < rampTime, (outletInitialP + (outletFinalP -
                              outletInitialP)*t/rampTime), outletFinalP )
    END
  END
END
```

B.5 CEL expressions used in Ansys CFX Pre for varying boundary pressure with iterations of the steady solver

```
LIBRARY:
  CEL:
    EXPRESSIONS:
      rampIter = 5000
      inletInitialP = 56 [bar]
      inletFinalP = 80 [bar]
      inletPressure = if(aitern < rampIter, (inletInitialP + (inletFinalP -
                                inletInitialP)*aitern/rampIter), inletFinalP )
      outletFinalP = 28 [bar]
      outletInitialP = 54 [bar]
      outletPressure = if(aitern < rampIter, (outletInitialP + (outletFinalP
        - outletInitialP)*aitern/rampIter), outletFinalP )
    END
  END
END
```

Appendix C

List of Publications

The following publications were obtained based on the work performed in this thesis:

Proceedings

- Choudhary K.D., Dasgupta M.S., Shyam Sunder., “Energetic and Exergetic Investigation of a N2O ejector expansion transcritical refrigeration cycle”, Energy Procedia.
- Choudhary K.D., Dasgupta M.S., Shyam Sunder., “Investigation of effect of suction nozzle pressure drop and degree of sub-cooling on CO2 transcritical ejector system.”, ISHMT digital library. DOI: 10.1615/IHMTC-2017.1670

International Conferences

- Choudhary K.D., Shyam Sunder, Dasgupta M.S., “A thermodynamic analysis of various ejector expansions in R-744 transcritical cycles at warm weather condition”, The 12th Gustav Lorentzen Natural Working Fluids Conference, Edinburgh, U.K.
- Choudhary K.D., Dasgupta M.S., Shyam Sunder, “Comparative study on a dual temperature transcritical refrigeration cycle with two cascade ejectors”, 13th IIR-Gustav Lorentzen conference on natural refrigerants, Valencia, Spain.
- Choudhary K.D., Dasgupta M.S., Shyam Sunder, “Energetic and Exergetic investigation of a modified dual temperature transcritical refrigeration cycle with two cascade ejectors”, 5th IIR conference on sustainability and the cold chain, Beijing, China.
- Choudhary K.D., Dasgupta M.S., Shyam Sunder., “Effect of motive nozzle exit position in a R-744 two phase ejector”, ICRACEM 2020, IIT Kharagpur.
- Choudhary K.D., Shyam Sunder, Dasgupta M.S., “Simulation of the Phase Change Process of Carbon Dioxide Inside an Ejector Geometry”, 2nd International Conference on Recent Advances in Fluid and Thermal Sciences, 19-21 March 2021, BITS Dubai.
- Choudhary K.D., Dasgupta M.S., Shyam Sunder., “Ejector Expansion Transcritical R744 Refrigeration System Analysed for Various Climate Zones of India”, 2nd International Conference on Recent Advances in Fluid and Thermal Sciences, 19-21 March 2021, BITS Dubai.

- Choudhary K.D., Shyam Sunder, Dasgupta M.S., “Classical Nucleation Theory Based Simulations of Non-equilibrium Condensation of Carbon Dioxide inside Converging–Diverging Nozzles” ASTFE 5th Thermal and Fluids Engineering Conference (TFEC), May 26–28, 2021, New Orleans, LA, USA (Virtual Mode).

National Conferences

- Choudhary K.D., Dasgupta M.S., Shyam Sunder., “Energetic and Exergetic Investigation of a N2O ejector expansion transcritical refrigeration cycle”, Conference: International Conference on Recent Advancement in Air Conditioning and Refrigeration, Bhubaneswar, India.
- Choudhary K.D., Dasgupta M.S., Shyam Sunder., “Investigation of effect of suction nozzle pressure drop and degree of sub-cooling on CO2 transcritical ejector system”. 24th National and 2nd International ISHMT-ASTFE heat and mass transfer conference (IHMTC-2017), BITS-Pilani, Hyderabad campus.

Journal Papers

- Choudhary K.D., Shyam Sunder, Dasgupta M.S., “A Comparison of the Equilibrium and the Droplets Based Non-Equilibrium Compressible Phase Change Solvers for Condensation of Carbon Dioxide Inside Nozzles”, Frontiers in Heat and Mass Transfer (Scopus Indexed).
- Choudhary K.D., Shyam Sunder, Dasgupta M.S., “Simulation of the Phase Change of CO_2 Inside an Ejector Geometry Using the Equilibrium and the Droplets Based Non-equilibrium Flow Solvers”, **Yet to be submitted**.