

Computationally Efficient Numerical Modelling of LiBr-H₂O and H₂O-NH₃ in Single Effect, Double Effect and Double Lift Absorption Refrigeration Configurations Using Open-Source Tools

Ludwig IRRGANG, Christopher SCHIFFLECHNER, Steffen KESTLER, Christoph WIELAND, Hartmut SPLIETHOFF

- (a) Technical University of Munich
- (b) University Duisburg-Essen

Overview

- Motivation
- Working principle
- Fluid properties
- Solution procedure
- Model behavior and validation
- Open-Source access

Motivation

- **Deep geothermal energy** offers a huge potential for absorption chillers
- **“Bathtub” heat demand** – access heat in summer month accompanied with high cold demand
- ACs can be placed in geothermal CCHP behind processes like organic Rankine cycle or district heating
- **Low driving temperature** is beneficial for both use cases
- Basic AC models are not available as Open-Source code
- Publications for numerical investigation of ACs often leave out important cycle characteristics or lack validation

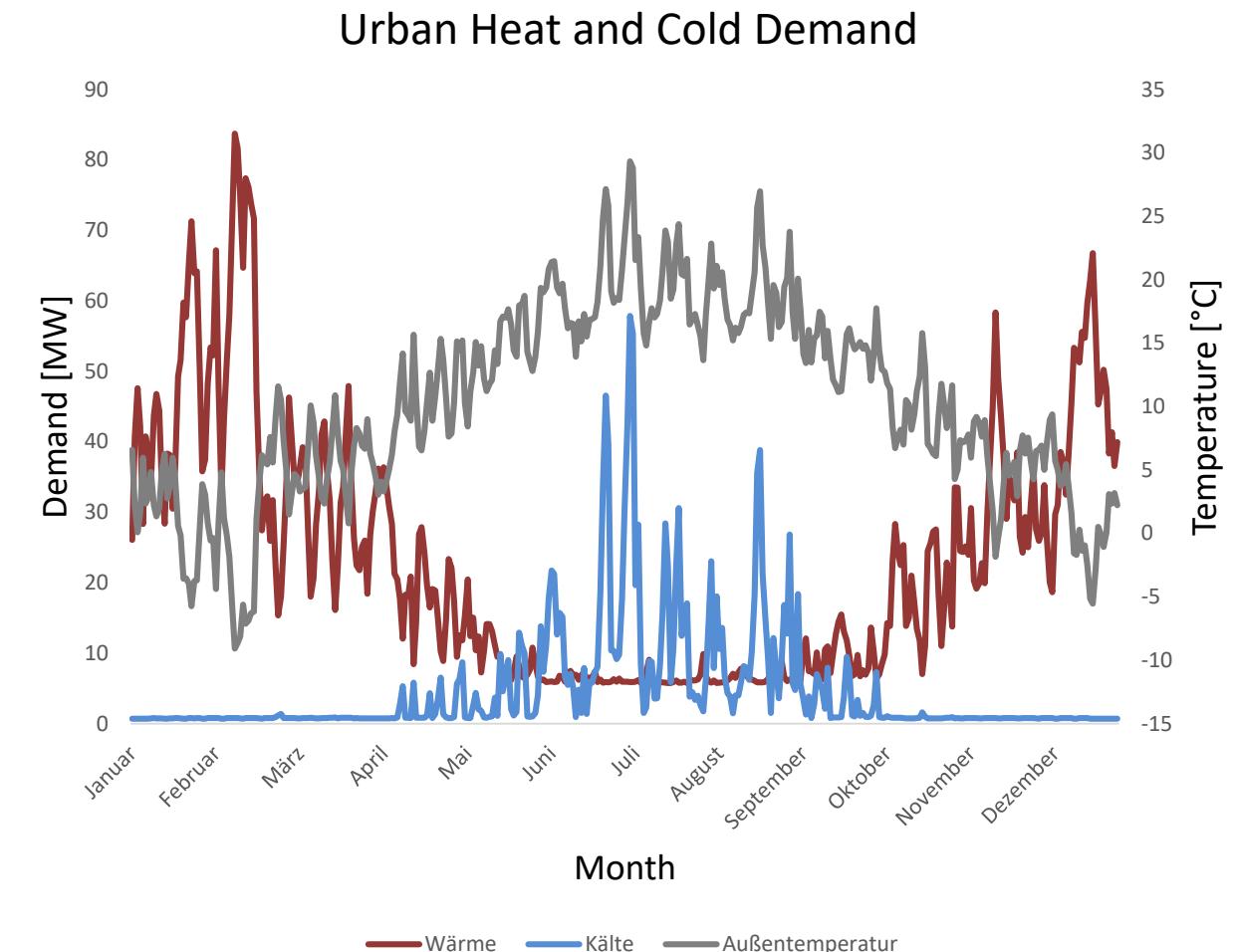


Figure 1: Typical urban heat and cold demand in the state of Bavaria, Germany

The Absorption Chiller Principle

Working principle:

- Solution cycle with absorption and desorption of refrigerant at different pressure levels
- “Thermal compressor” instead of mechanical compressor
- Cold production from thermal energy with very little electrical energy input

Basic absorption cycle:

- Two pressure levels, three temperature levels
- Most prominent working fluids: LiBr- H_2O , H_2O-NH_3

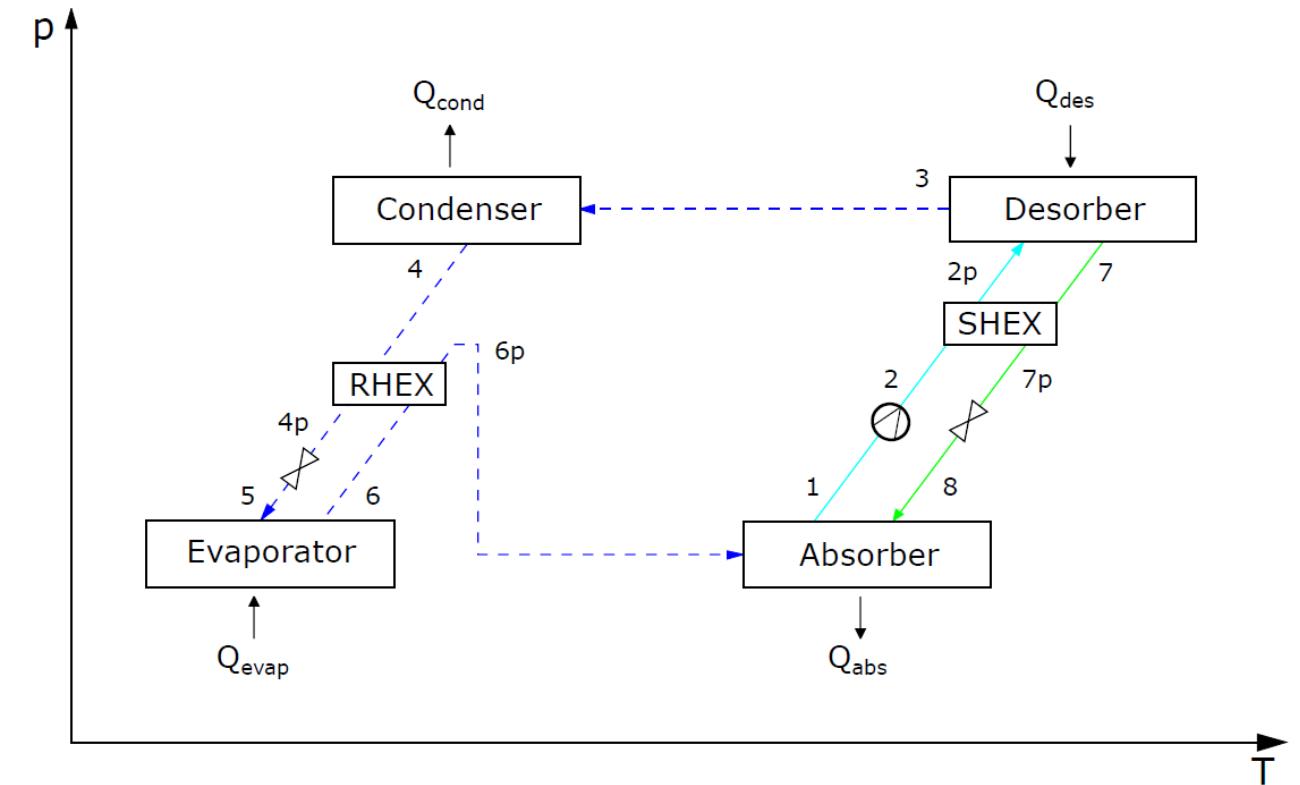


Figure 2: Schematic representation of the basic single effect absorption cycle model in a pT-diagram, including all relevant state points.

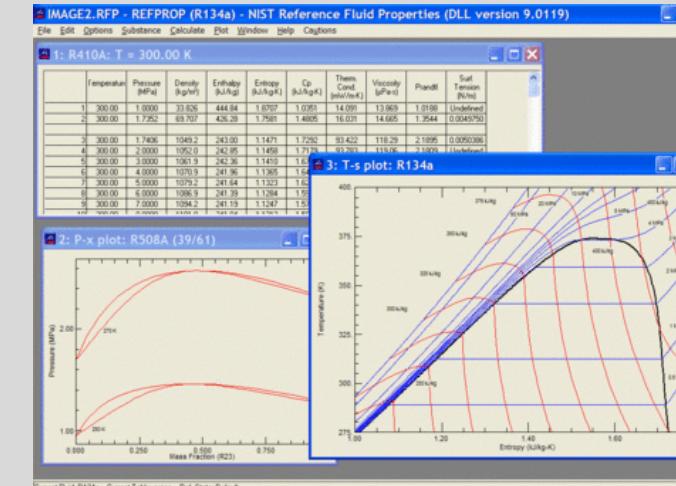
Fluid Property Calculation

CoolProp



- Open Source
- Used for **pure fluid** calculations in the models

REFPROP



- Licensed
- Used for calculation of **NH₃-H₂O solution states**

Patek and Klomfar 2006



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A computationally effective formulation of the thermodynamic properties of LiBr-H₂O solutions from 273 to 500 K over full composition range

J. Pátek*, J. Klomfar

Institute of Thermomechanics, Academy of Sciences of the Czech Republic, Dolejškova 5, CZ 182 00 Prague 8, Czech Republic

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Abstract

A set of computationally efficient formulations of thermodynamic properties of LiBr-H₂O solutions at vapor-liquid equilibrium is presented in the form of explicit separate functions of temperature and mixture composition. The set includes pressure, density, isobaric heat capacity, enthalpy, and entropy. The description of these properties is valid from 273 K or from the crystallization line up to 500 K in temperatures and for mixture composition from 0 to 75 wt% of LiBr in the solution. The equations are based upon a body of experimental data that have been critically assessed. Gaps in the database are shown to give experimenters orientation for future research. The structure of the equations guarantees an explicit transition to the properties of pure water for lithium bromide concentration approaching zero. The uncertainties associated with correlation are estimated to

- Numerically effective formulations for the calculation of **H₂O-LiBr solution states**
- Saturated solution states only

Calculation Procedure (Single Effect)

Input Structs

- Heat source temperature
- Heat sink temperature
- Cold output temperature
- Heat Input/ cold output
- Pump efficiency
- Refrigerant superheating
- Internal HX PP temperature difference



Model Assumptions

- Steady state
- Saturated vapor at evaporator outlet
- Saturated liquid at condenser outlet
- Saturated solution at desorber and absorber outlet
- No pressure losses
- No temperature losses

System pressures

Check for Crystallization

Calculate minimal necessary condenser pressure

Solution Concentrations

Refrigerant States

Solution States

Energy and Mass Balances

- $m_{ref} = m_{sol}^{rich} w_{rich} - m_{sol}^{poor} w_{poor}$
- $m_{ref} = m_{sol}^{rich} - m_{sol}^{poor}$
- $Q_{heat\ source} = m_{sol}^{poor} h_{sol}^{des,out} + m_{ref} h_{ref}^{des,out} - m_{sol}^{rich} h_{sol}^{pump,out}$
- $Q_{cold} = m_{ref} (h_{ref}^{evap,out} - h_{ref}^{evap,in})$

Post Processing

- $m_{sol}^{rich} h_{sol}^{des,in} = m_{sol}^{poor} h_{sol}^{des,out} + m_{sol}^{rich} h_{sol}^{pump,out} - m_{sol}^{poor} h_{sol}^{valve,in}$
- $Q_{cond} = m_{ref} (h_{ref}^{cond,out} - h_{ref}^{cond,in})$
- $Q_{abs} = m_{sol}^{rich} h_{sol}^{abs,out} - m_{sol}^{poor} h_{sol}^{abs,in} - m_{ref} h_{ref}^{abs,in}$
- $h_{SHEX}^{ideal} = f_{sol}(p_{cond}, T_{sol}^{pump,out})$
- $h_{RHEX}^{ideal} = f_{ref}(p_{evap}, T_{ref}^{cond,out})$
- $\eta_{SHEX} = \frac{h_{sol}^{des,in} - h_{sol}^{pump,out}}{h_{sol}^{des,out} - h_{SHEX}^{ideal}}$
- $\eta_{RHEX} = \frac{h_{ref}^{abs,in} - h_{ref}^{evap,out}}{h_{ref}^{ideal} - h_{ref}^{evap,out}}$
- $COP = \frac{Q_{evap}}{W_{pump} + Q_{des}}$

Checks

- Mass balance
- Energy balance
- Concentrations
- Crystallization
- Mass flows
- Minimal concentration difference
- Temperatures where Patek is used

Output Structs

- Temperatures
- Pressures
- Enthalpies
- Concentrations
- Mass flows
- Energy flows
- Post Process

Double Effect Cycle Solution Procedure

Middle pressure desorber temperature as low as possible:

- $T_{sol}^{des,out,min} = f_{sol}^{sat}(p_{cond}, w_{rich} + \Delta w_{min})$

Upper pressure condensation temperature:

- $T_{cond,I} = T_{sol}^{des,out,min} + \Delta T_{PP}^{cond,I}$

Energy balances:

- $Q_{cond,I} = m_{ref,I}(h_{ref}^{cond,I,out} - h_{ref}^{cond,I,in})$
- $Q_{des} = -Q_{cond,I}$
- $Q_{des} = m_{sol}^{poor} h_{sol}^{des,out} + m_{ref} h_{ref}^{des,out} - m_{sol}^{rich} h_{sol}^{pump,out}$

Additionally, desorber or evaporator energy balance:

- $Q_{heat\ source} = m_{sol}^{poor,I} h_{sol}^{des,I,out} + m_{ref,I} h_{ref}^{des,I,out} - m_{sol}^{rich,I} h_{sol}^{pump,I,out}$
- $Q_{cold\ output} = (m_{ref} + m_{ref,I})(h_{ref}^{evap,out} - h_{ref}^{evap,in})$

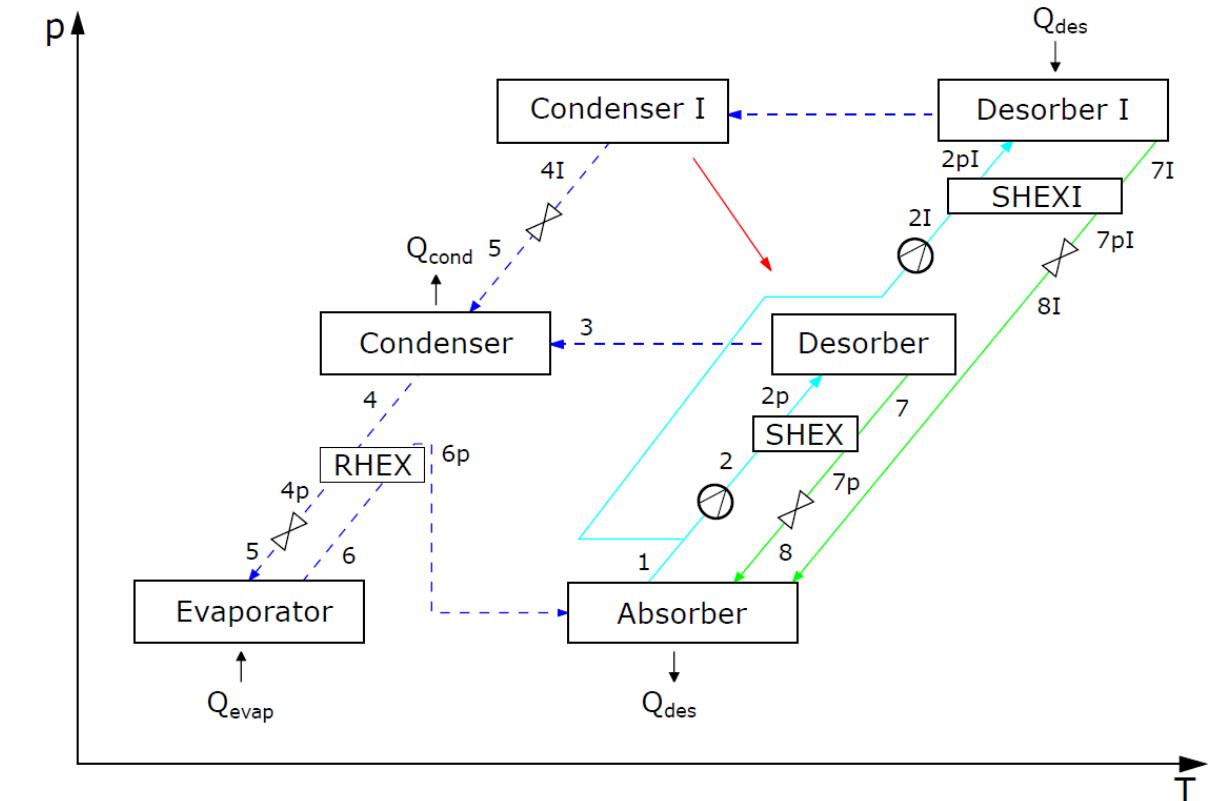


Figure 3: Schematic representation of the double effect absorption cycle model in a pT-diagram, including all relevant state points.

Double Lift Cycle Solution Procedure

Middle pressure level for maximum efficiency
(Venegas et al. (2002)):

- $p_{mid} = \sqrt{p_{evap} p_{cond}}$

Steady state mass flow equilibrium:

- $m_{ref} = m_{ref,I}$

Energy balances:

- $Q_{des} = m_{sol}^{poor} h_{sol}^{des,out} + m_{ref} h_{ref}^{des,out} - m_{sol}^{rich} h_{sol}^{pump,out}$
- $Q_{des,I} = m_{sol}^{poor,I} h_{sol}^{des,out,I} + m_{ref,I} h_{ref}^{des,out,I} - m_{sol}^{rich,I} h_{sol}^{pump,out,I}$

Additionally desorber or evaporator energy balance:

- $Q_{heat\ source} = Q_{des} + Q_{des,I}$
- $Q_{cold\ output} = m_{ref,I} (h_{ref}^{evap,out} - h_{ref}^{evap,in})$

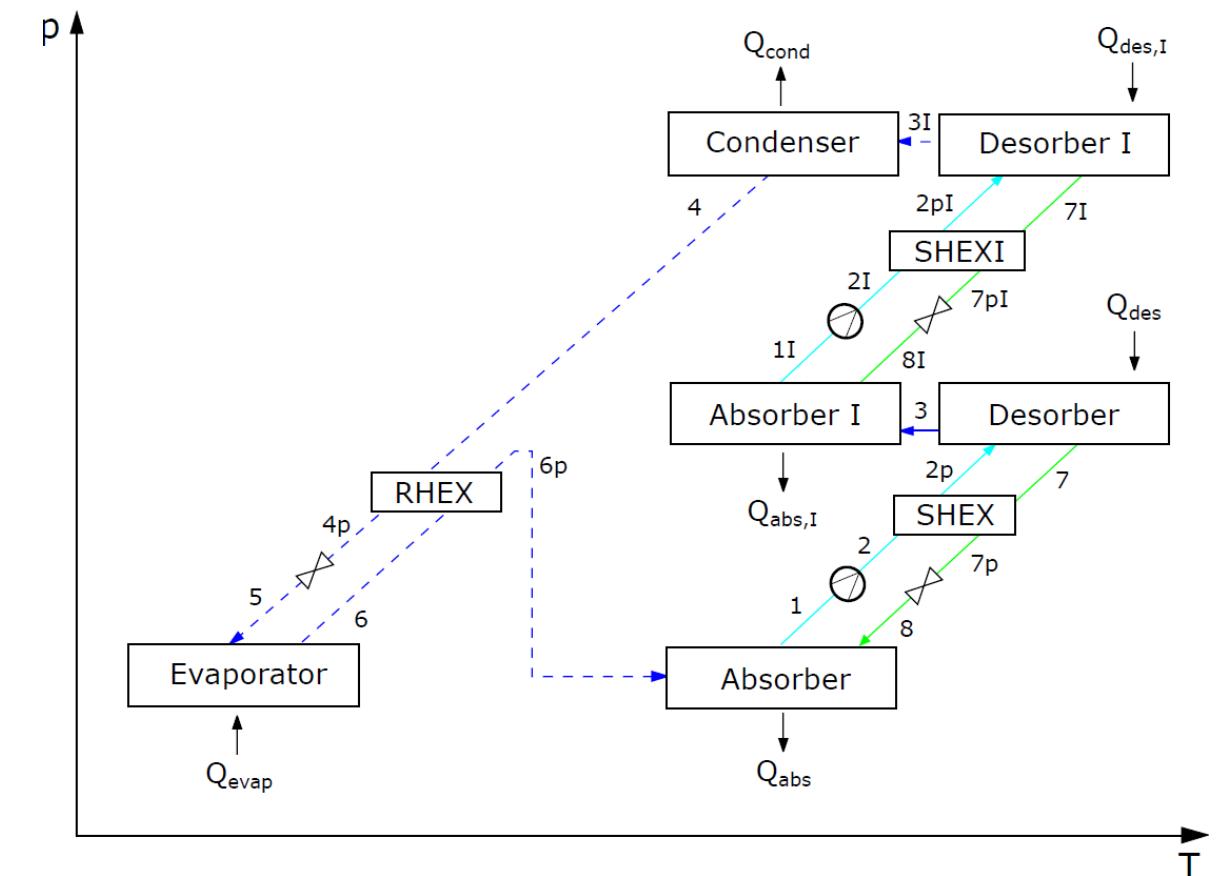


Figure 4: Schematic representation of the double effect absorption cycle model in a pT-diagram, including all relevant state points.

COPs for Heat Sink and Heat Source Temperatures

- Double effect model with significantly higher efficiencies and activation temperatures
- Double lift model opposite to double effect model
- LiBr-H₂O has generally higher COP
- Validation with experimental and simulative data from the literature
- Stable and robust calculation for wide range of boundary conditions

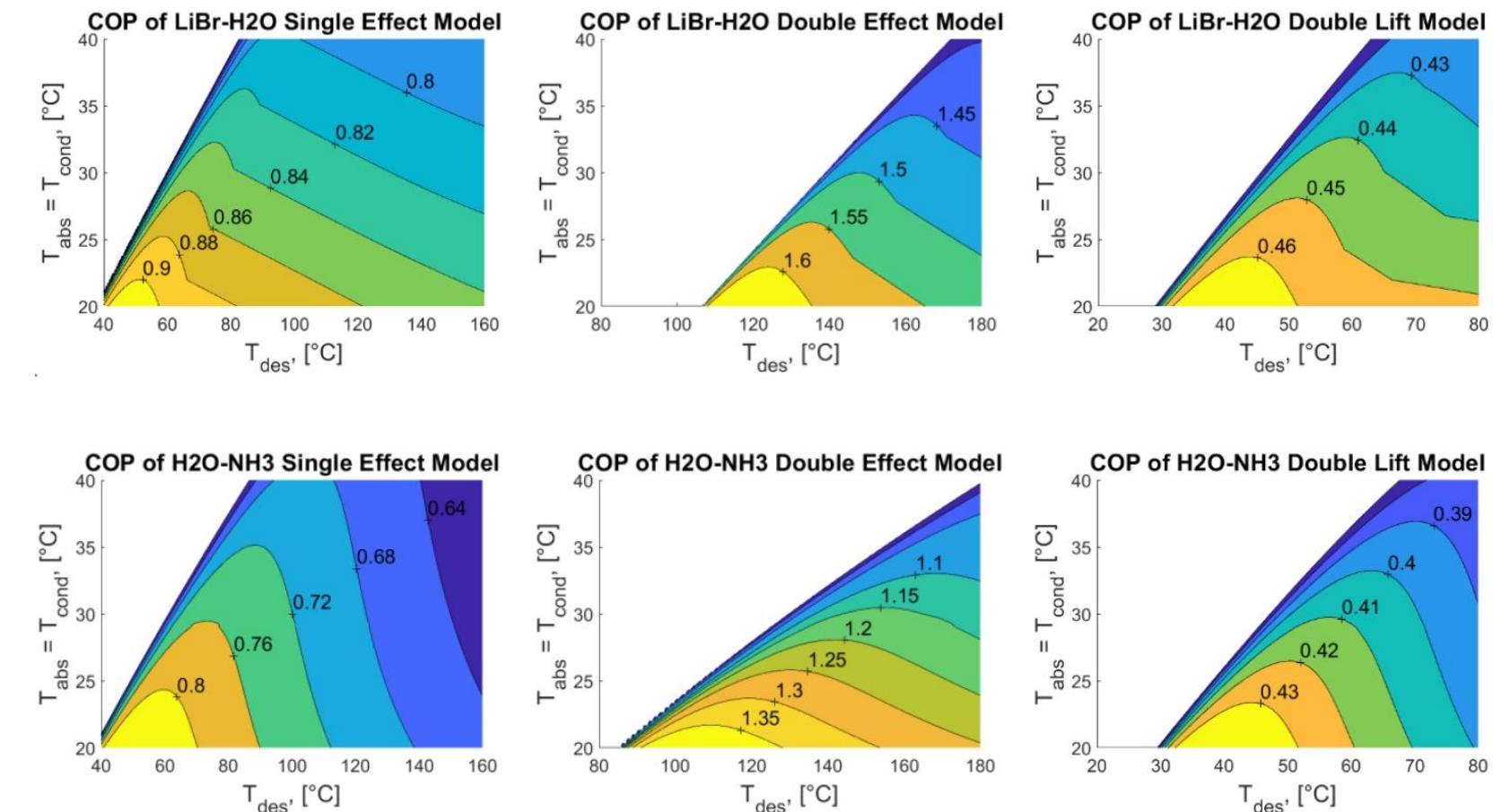


Figure 5: COPs for all model configurations and working fluids evaluated over a range of heat source and heat sink temperatures.

Influence of Solution Heat Exchanger Efficiency

Solution heat exchanger pinch point temperature difference has major influence on absorption chiller performance.

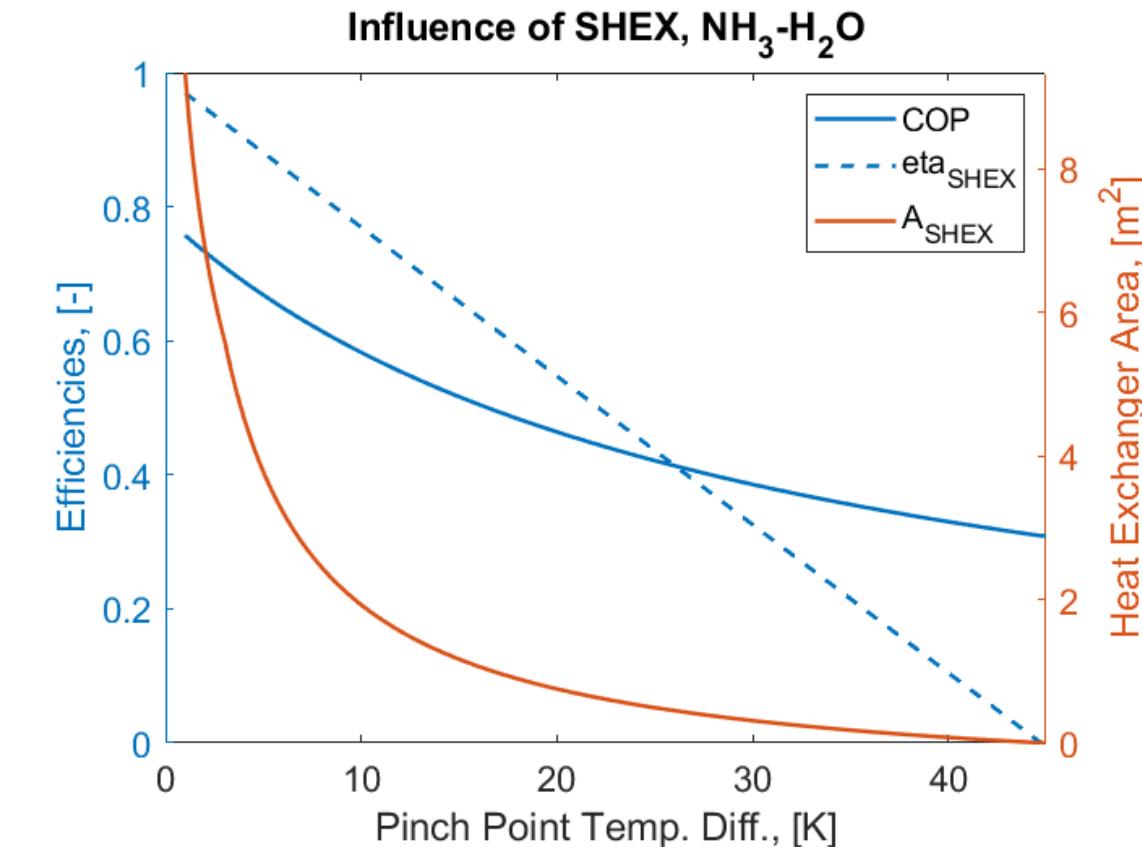
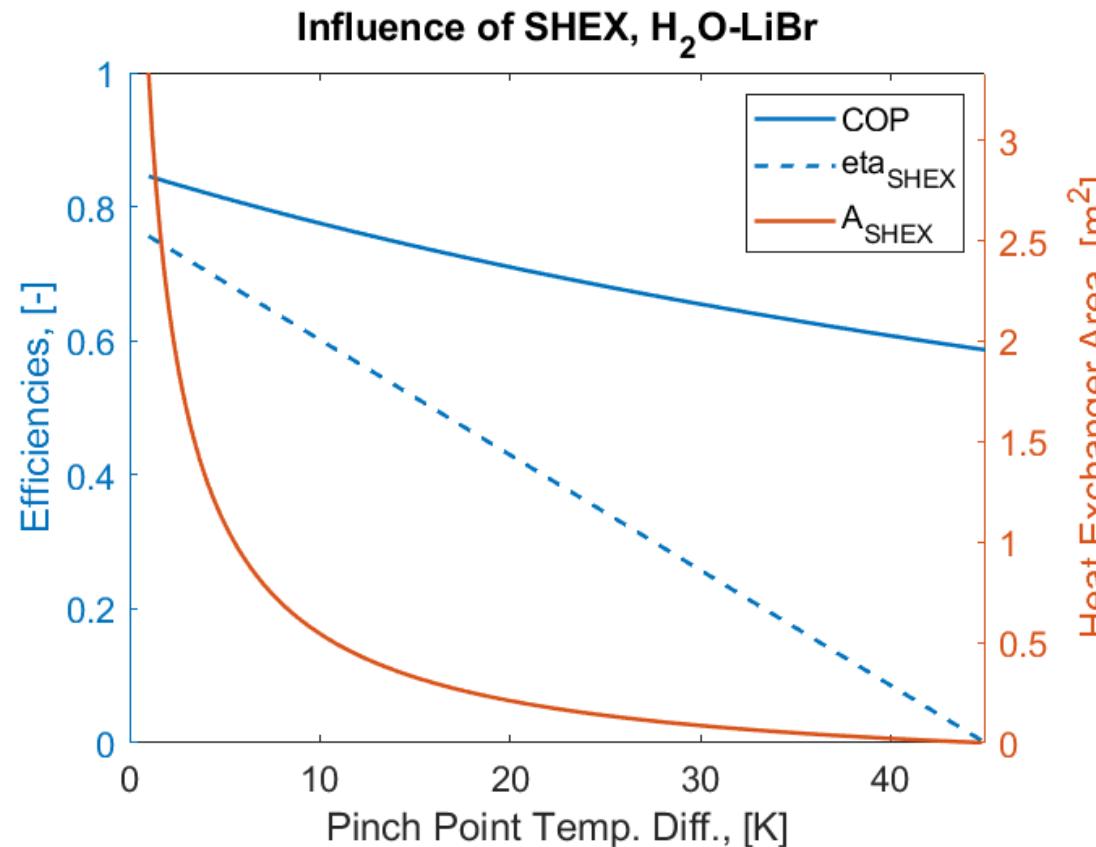


Figure 6: Influence of SHEX pinch point temperature difference on absorption chiller performance; Temperatures: $T_{des} = 80^\circ\text{C}$, $T_{cond} = 25^\circ\text{C}$, $T_{abs} = 25^\circ\text{C}$, $T_{evap} = 3^\circ\text{C}$

Influence of Refrigerant Heat Exchanger Efficiency

Only minor influence of refrigerant heat exchanger in absorption chiller performance.

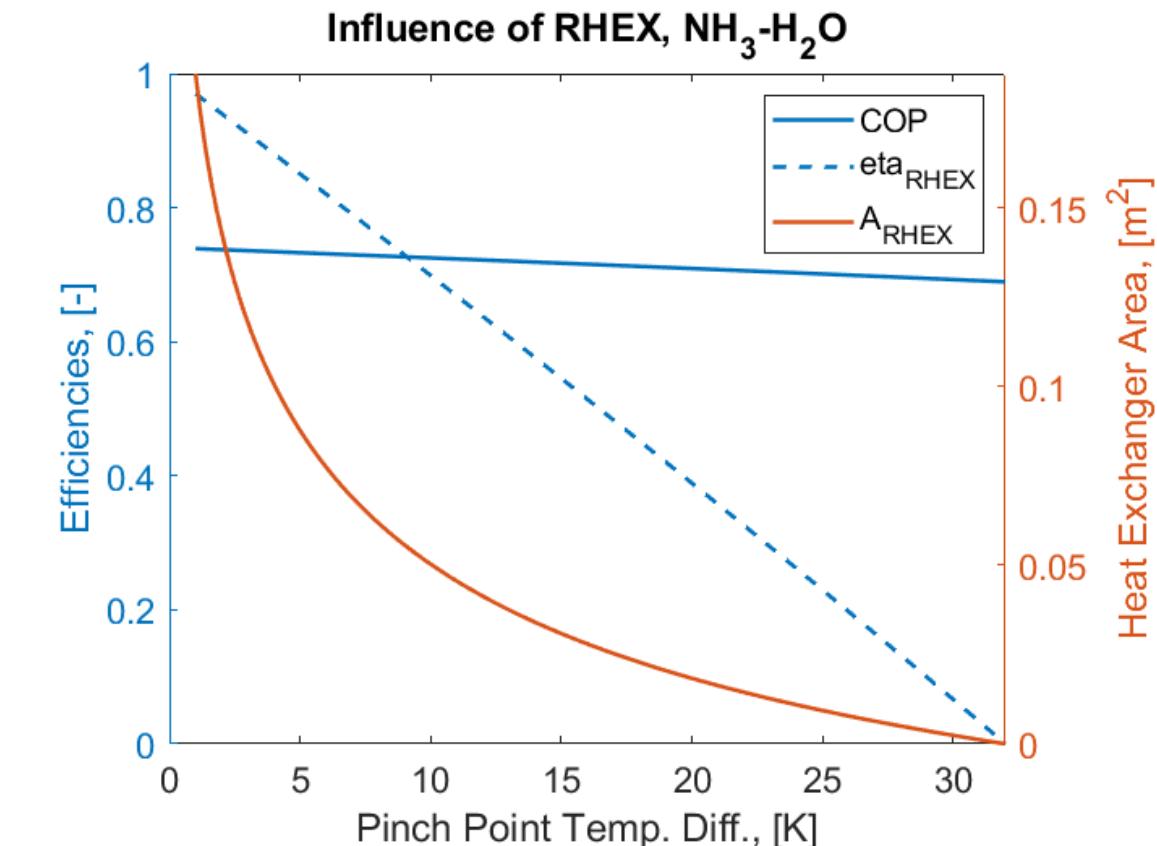
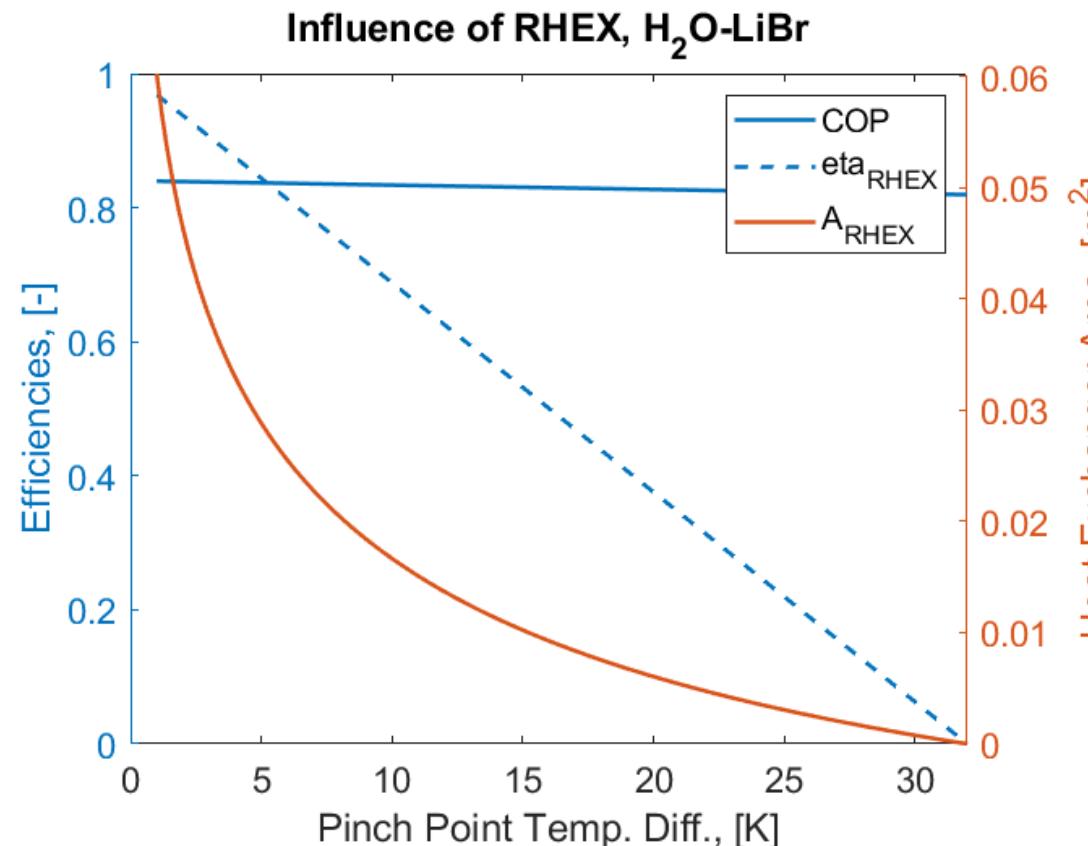


Figure 7: Influence of RHEX pinch point temperature difference on absorption chiller performance; Temperatures: $T_{des} = 80^\circ\text{C}$, $T_{cond} = 25^\circ\text{C}$, $T_{abs} = 25^\circ\text{C}$, $T_{evap} = 3^\circ\text{C}$

GitHub Repository

- Model code available via the GitHub platform
- Matlab and Python implementation
- Documentation of use and example scripts for use
- More configurations will be available in the future
- Currently changing the fluid state calculations to Open-Source where REFPROP is used
- Link:
<https://github.com/LudwigIrrgang/SorpPump>

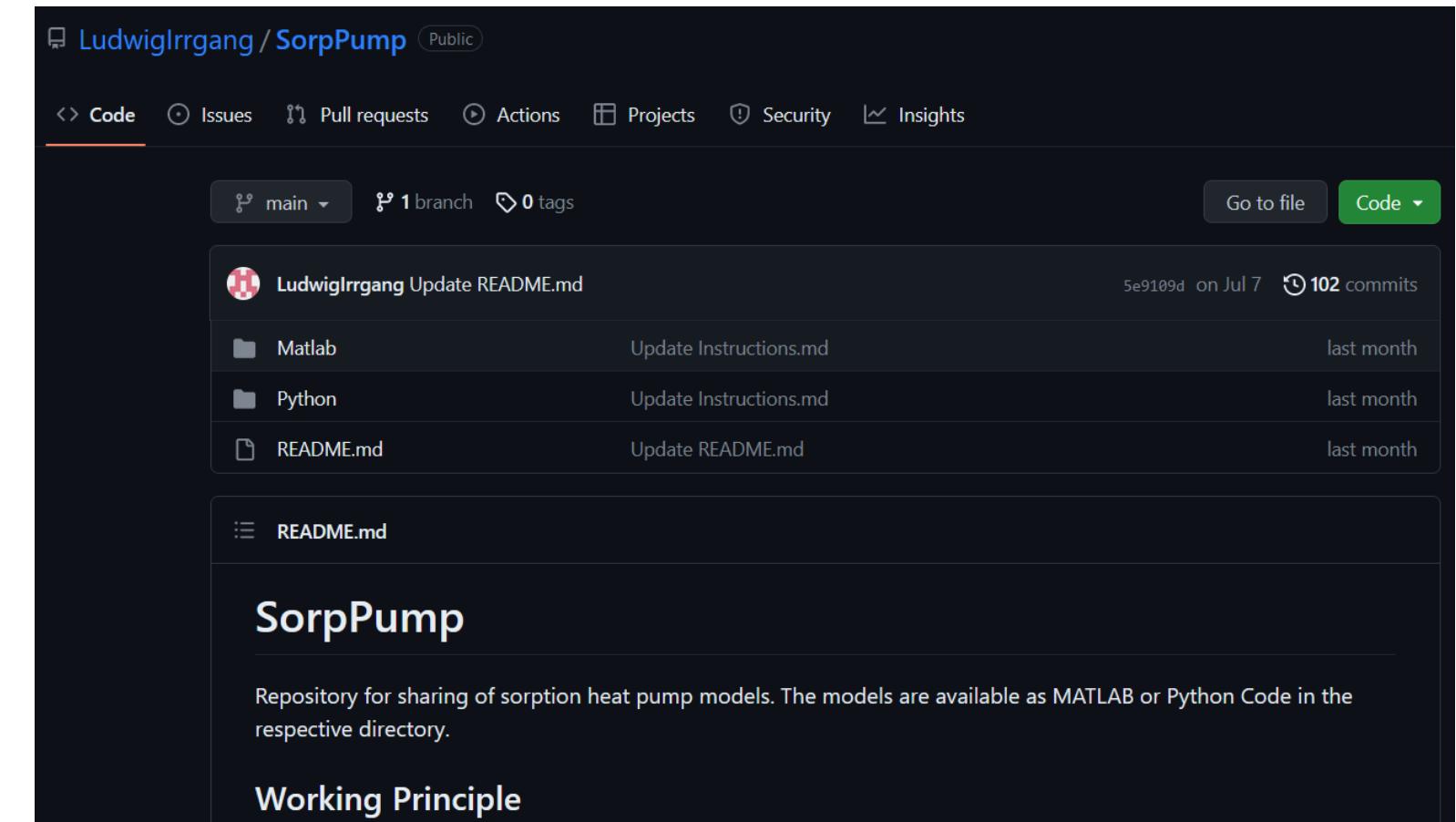


Figure 7: Screenshot of the GitHub repository

Ludwig Irrgang

Technische Universität München

ludwig.irrgang@tum.de



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GitHub Repository:



Calculation Procedure

System Pressures

$$p_{evap} = f_{ref}^{sat}(T_{evap})$$

$$p_{cond} = f_{ref}^{sat}(T_{cond})$$

Check for Crystallization

Calculate minimal necessary condenser pressure

$$w_{poor} = f_{sol}^{sat}(p_{cond}, T_{sol}^{des,out})$$

$$p_{cond,min} = f_{sol}^{cryst}(T_{des}, w_{poor})$$

Solution Concentrations

$$w_{rich} = f_{sol}^{sat}(p_{evap}, T_{sol}^{abs,out})$$

$$w_{poor} = f_{sol}^{sat}(p_{cond}, T_{sol}^{des,out})$$

Refrigerant States

$$T_{ref}^{des,out} = T_{sol}^{des,out} - \Delta T_{ref}^{des,out}$$

$$h_{ref}^{des,out} = f_{ref}(p_{cond}, T_{ref}^{des,out})$$

$$h_{ref}^{cond,out} = f_{ref}(p_{cond}, sat. liquid)$$

$$h_{ref}^{evap,out} = f_{ref}(p_{evap}, sat. vapour)$$

$$T_{ref}^{abs,in} = T_{ref}^{cond,out} - \Delta T_{PP}$$

$$h_{ref}^{abs,in} = f_{ref}(p_{evap}, T_{ref}^{abs,in})$$

$$h_{ref}^{valve,in} = h_{ref}^{cond,out} - (h_{ref}^{abs,in} - h_{ref}^{evap,out})$$

$$T_{ref}^{valve,in} = f_{ref}(p_{cond}, h_{ref}^{valve,in})$$

Solution States

$$h_{sol}^{abs,out} = f_{sol}^{sat}(w_{rich}, T_{sol}^{abs,out})$$

$$v_{sol}^{pump,in} = f_{sol}^{sat}(w_{rich}, T_{sol}^{abs,out})$$

$$w_{pump} = v_{sol}^{pump,in}(p_{cond} - p_{evap})$$

$$h_{sol}^{pump,out} = h_{sol}^{abs,out} + \frac{w_{pump}}{\eta_{pump}}$$

$$T_{sol}^{valve,in} = T_{sol}^{pump,out} + \Delta T_{SHEX}$$

$$h_{sol}^{valve,in} = h_{sol}^{des,out} + c_{p,sol}^{des,out}(T_{sol}^{valve,in} - T_{sol}^{des,out})$$

$$h_{sol}^{abs,in} = h_{sol}^{valve,in}$$

Energy and Mass Balances

$$m_{ref} = m_{sol}^{rich} w_{rich} - m_{sol}^{poor} w_{poor}$$

$$m_{ref} = m_{sol}^{rich} - m_{sol}^{poor}$$

$$Q_{des} = m_{sol}^{poor} h_{sol}^{des,out} + m_{ref} h_{ref}^{des,out} - m_{sol}^{rich} h_{sol}^{pump,out}$$

$$Q_{evap} = m_{ref} (h_{ref}^{evap,out} - h_{ref}^{evap,in})$$

Post Processing

$$m_{sol}^{rich} h_{sol}^{des,in}$$

$$= m_{sol}^{poor} h_{sol}^{des,out} + m_{sol}^{rich} h_{sol}^{pump,out} - m_{sol}^{poor} h_{sol}^{valve,in}$$

$$Q_{cond} = m_{ref} (h_{ref}^{cond,out} - h_{ref}^{cond,in})$$

$$Q_{abs} = m_{sol}^{rich} h_{sol}^{abs,out} - m_{sol}^{poor} h_{sol}^{abs,in} - m_{ref} h_{ref}^{abs,in}$$

$$h_{SHEX}^{ideal} = f_{sol}(p_{cond}, T_{sol}^{pump,out})$$

$$h_{RHEX}^{ideal} = f_{ref}(p_{evap}, T_{ref}^{cond,out})$$

$$\eta_{SHEX} = \frac{h_{sol}^{des,in} - h_{sol}^{pump,out}}{h_{sol}^{des,out} - h_{SHEX}^{ideal}}$$

$$\eta_{RHEX} = \frac{h_{ref}^{abs,in} - h_{ref}^{evap,out}}{h_{RHEX}^{ideal} - h_{ref}^{evap,out}}$$

$$COP = \frac{Q_{evap}}{W_{pump} + Q_{des}}$$

Influence of Internal Condenser Efficiency

- Pinch point temperature difference of internal condenser has major influence on double effect cycle efficiency
- Higher heat source temperature does not lead to higher efficiencies
- Amount of internal heat recovery depends on upper condenser pressure level

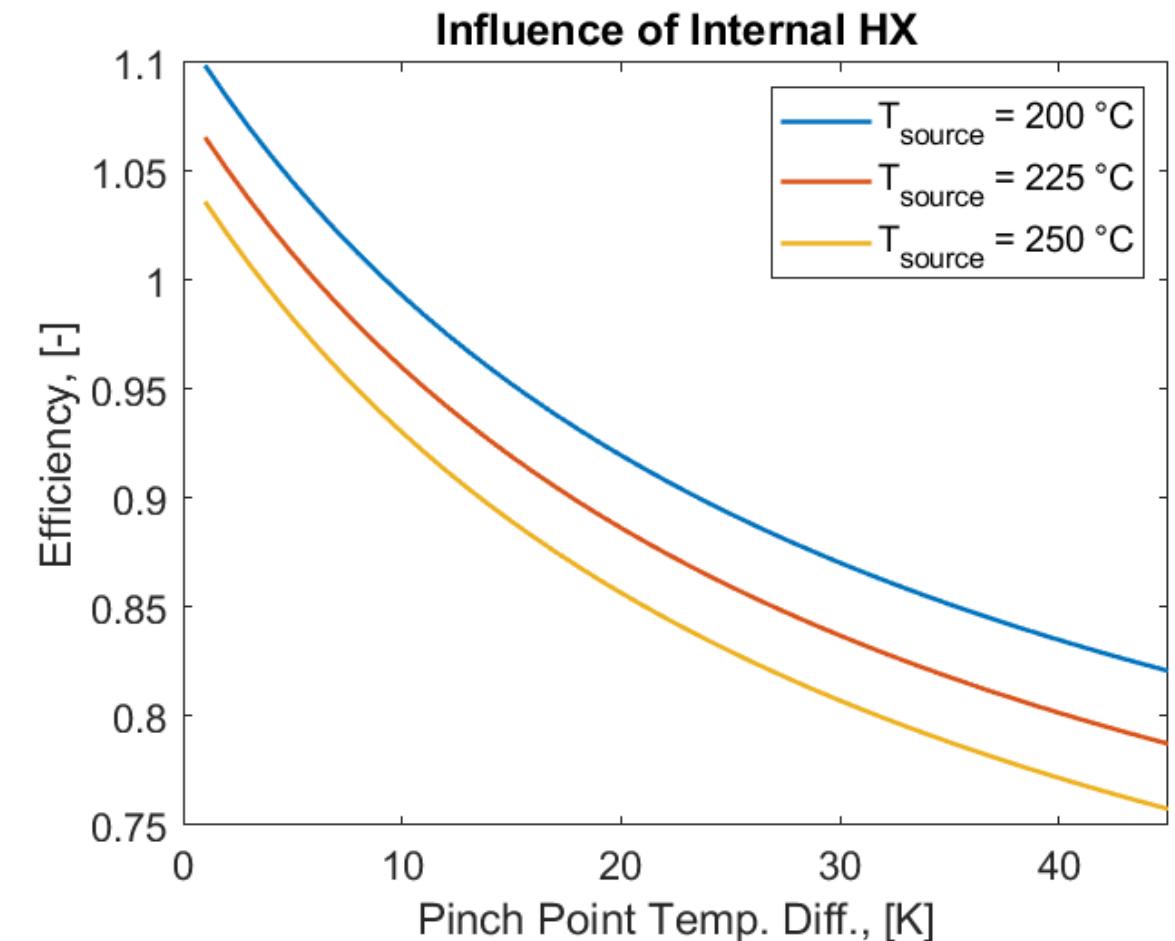


Figure 7: Influence of internal heat exchanger pinch point temperature difference on double effect absorption chiller performance

Backup

Backup

