Thermodynamic model investigation for S-CO_2 Brayton cycle for coal-fired power plant application

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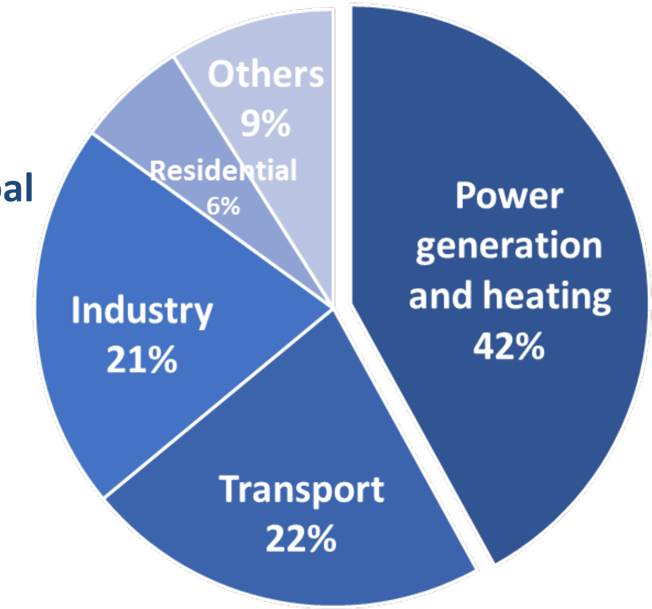
Outline

- Introduction and context
- Objectives
- Methodology
- Thermodynamics investigation (Results)
- Conclusion and future works

CONTEXT

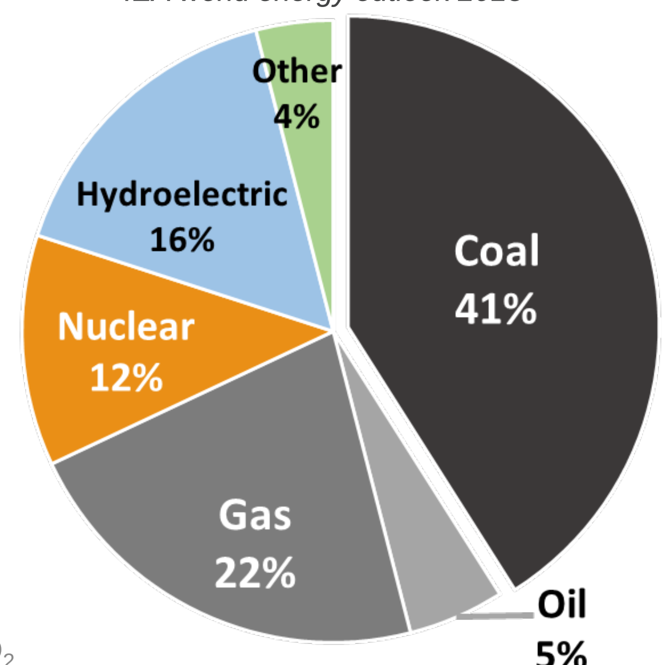
- **Challenge in energy demand and the important role of coal in energy mix**
  - Growing world energy demands :
    - 22126 TWh in 2011
    - Electricity↑ 80% from 1990 to 2010
    - ↑70% is expected by 2035
  - Coal-fired plants: 41% of world's power generation
  - Power generation: 42% of world's CO_2 emission



Word CO_2 emission in different sector – IEA world energy outlook 2013

- **Challenge in environment**
  - CO_2 emission: 31.3 Gt in 2011
  - Reduction target of 40%-70% by 2050 (post COP 21)

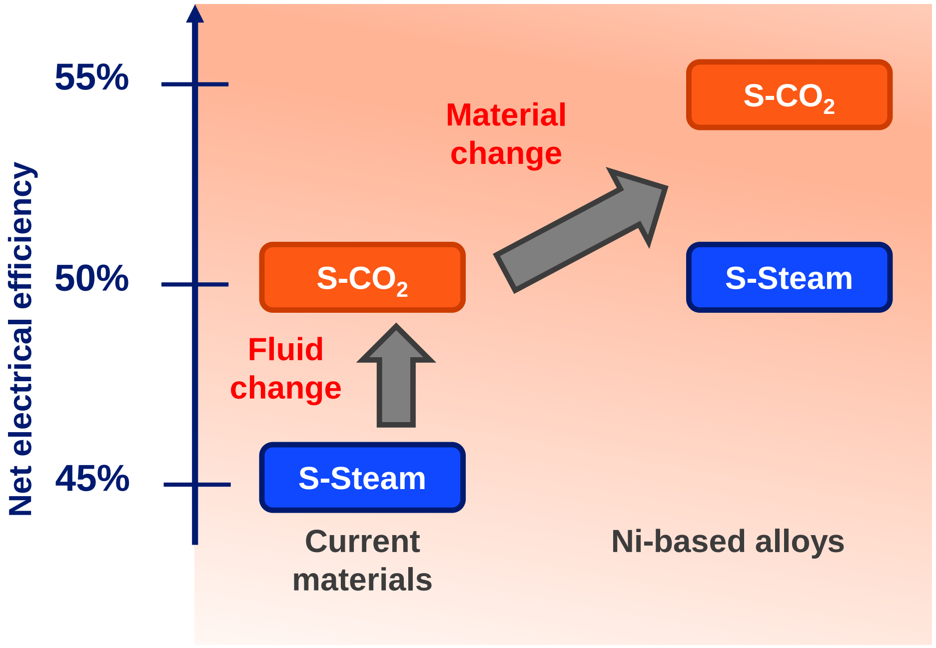
Power Plant Efficiency improvement



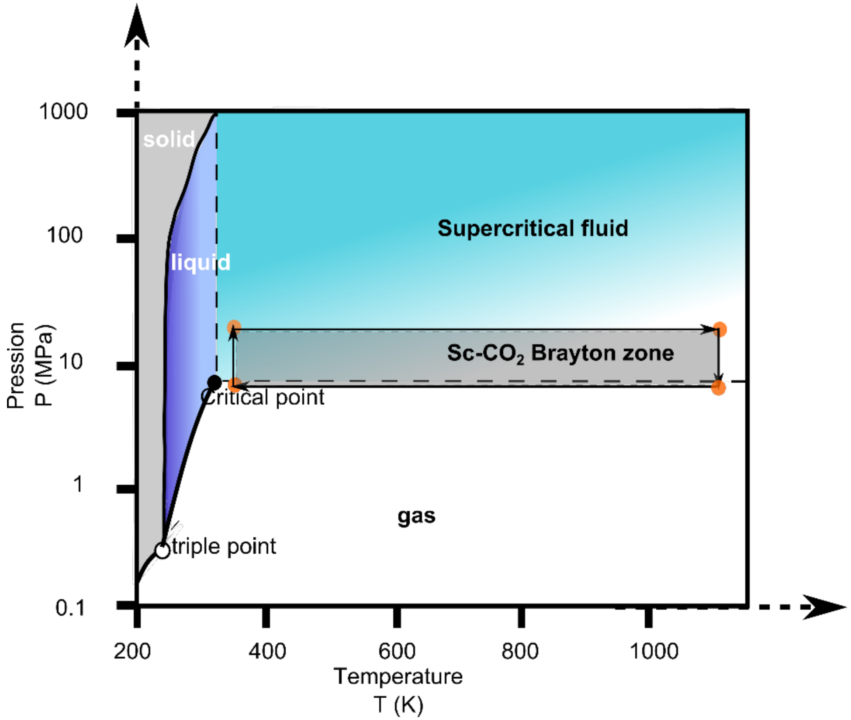
World energy production – IEA world energy outlook 2013

INTRODUCTION

- **State of the art for coal-fired plant**
  - S-Steam:46% $_{LHV}$ 30MPa/873/893 K
  - Potential of enhancement (material/architecture/working fluid?)
- **$S\text{-}CO_2$ cycle allows at least ↗ 5%pts LHV efficiency**



- **Operation condition**
  - In the vicinity of the critical point
  - High T(up to 1300K) and P(30 MPa)



Phase Diagram of CO_2

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OBJECTIVES OF THIS STUDY

Modeling and simulation of cycle
Learn more about the cycle behaviors before demonstration at industrial scale

- Cycle performance
- Machinery sizing
- Economics

Thermodynamic model (EoS) for S-CO_2
Calculations on density, speed of sound, heat capacity, transport properties

Difficulty on thermodynamic models:
Operation condition
- High T and P
- Non-classical behaviors near critical point

Objectives

- **Comparison of existing thermodynamics models (EoS) for CO_2**
- **Selection of the most accurate model for CO_2 (in the vicinity of the critical point and supercritical region)**
- **EoS sensitivity study in process simulation**

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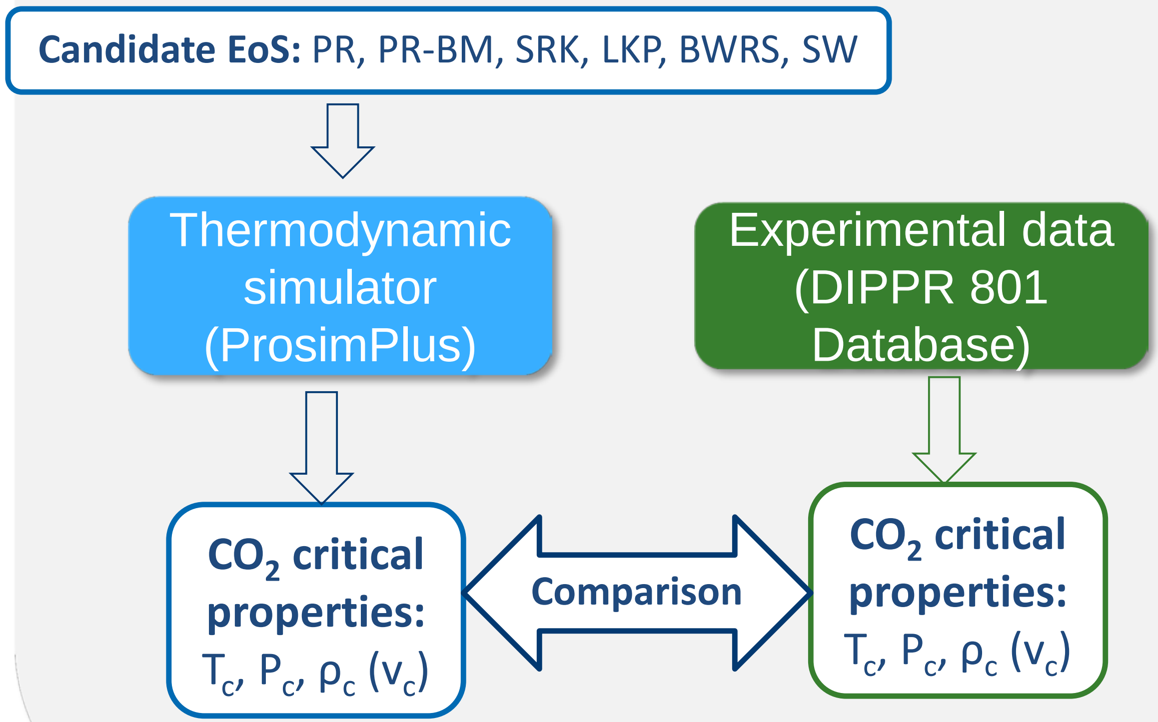
METHODOLOGY

Step 1: CO_2 critical property comparison with collected DIPPR database

Step 1: Simulated CO_2 critical properties compared with experimental data

Cubic EoS, virial type EoS, EoS expressed in terms of Helmholtz energy



Peng-Robinson (PR); Peng-Robinson with Boston-Mathias alpha function (PR-BM); Soave modified Redlich-Kwong (SRK); Lee-Kesler-Plöcker (LKP), Benedict-Webb-Rubin modified by Starling and Nushiumi (BWRS) and Span-Wagner (SW).

METHODOLOGY

Step 1: CO_2 critical property comparison with collected DIPPR database

Step 2: CO_2 criteria property comparison in the vicinity of the critical point

Step 2: CO_2 criteria property comparison in the vicinity of the critical point

- **300 K<T<310 K, P=7.38 MPa**

Candidate EoS: PR, PR-BM, SRK, LKP, BWRS, SW

Thermodynamic simulator (ProsimPlus)

Experimental data (DECHEMA Database)

criteria properties: Density(ρ), heat capacity (c_p), speed of sound(ω)

Comparison

criteria properties: Density(ρ), heat capacity (c_p), speed of sound(ω)

METHODOLOGY

Step 1: CO_2 critical property comparison with collected DIPPR database

Step 2: CO2 criteria property comparison in the vicinity of the critical point

Step 3: CO_2 criteria property comparison in the whole region of study

Step 3: CO_2 criteria property comparison in the entire region of interest

- **300 K<T<900 K, 7 MPa<P<30 MPa**

Candidate EoS: PR, PR-BM, SRK, LKP, BWRS, SW

Thermodynamic simulator (ProsimPlus)

Experimental data (DECHEMA Database)

criteria properties: Density, heat capacity, speed of sound(ω)

Comparison

criteria properties: Density, heat capacity, speed of sound(ω)

Favorable EoS

EoS leads to the smallest relative "model/measurement" deviation

METHODOLOGY

Step 1: CO_2 critical property comparison with collected DIPPR database

Step 2: CO2 criteria property comparison in the vicinity of the critical point

Step 3: CO2 criteria property comparison in the whole region of study

Step 4: EoS sensitivity study in process modeling

Step 4: EoS sensitivity in process modeling of Brayton cycle

- **Recuperated Brayton Cycle (RC)**
- **Recompression Recuperated Brayton Cycle (RRC)**

Favorable EoS

Process simulator (ProsimPlus)

Process modeling with constraints: Design parameter, cycle efficiency,…

Comparison

Other 5 EoS

Process simulator (ProsimPlus)

Process modeling with constraints: Design parameter, cycle efficiency,…

Results Analysis and Discussion

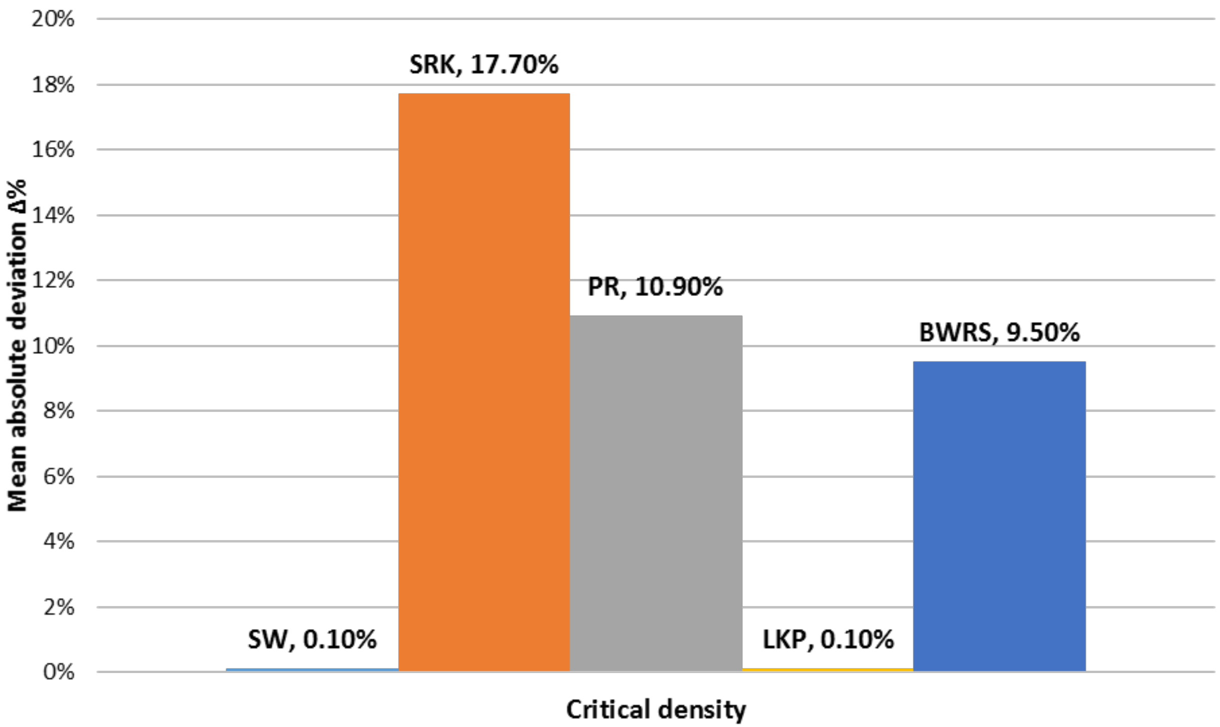
Outline

- Introduction and context
- Objectives
- Methodology
- Thermodynamics investigation
  - Step 1: CO_2 critical property comparison
  - Step 2: Criteria property comparison near the critical point
  - Step 3: Criteria property comparison in the region of interest
  - Step 4: Model Sensitivity (process simulation)
- Conclusion and future works

STEP 1) CRITICAL PROPERTIES COMPARISON

- **Experimental T_c , P_c as input parameters**
  - T_c=304.21 K, P_c=7.3830 MPa
- **Except for SW EoS**
  - T_c=304.13 K, P_c=7.3773 MPa

- **Critical density**
  - SW and LKP EoS exhibit 0.1% on ρ_c
  - SRK EoS shows the biggest deviation



Δ is defined as the absolute mean average of (Critical density$_{experimental}$ −Critical density$_{EoS\ calculated}$)/Critical density$_{experimental}$

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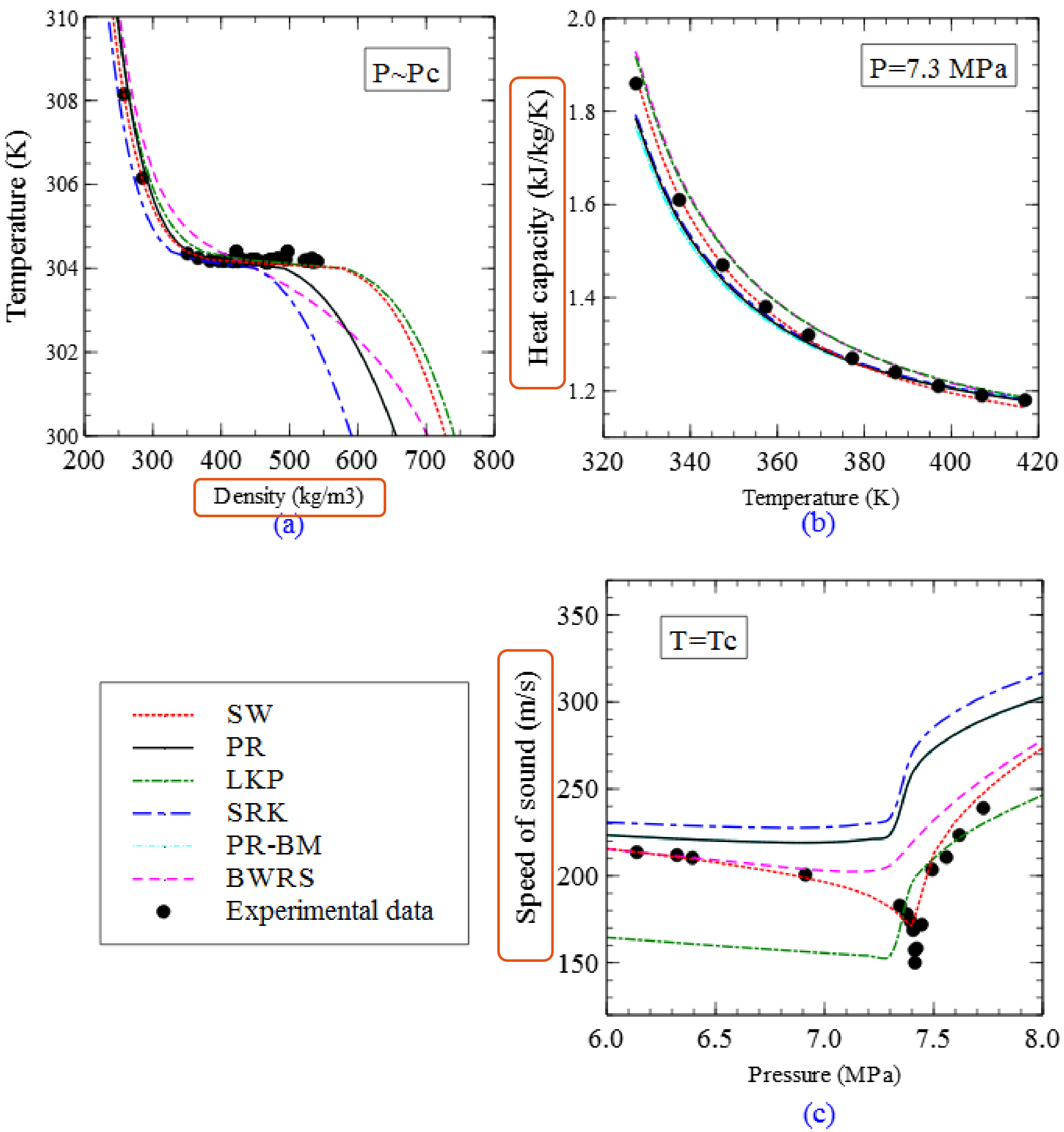
STEP 2) COMPARISON NEAR CRITICAL POINT



Representation of (a) isobaric density, (b) heat capacity, (c) isotherm speed of sound in the critical region of CO_2

- **In the vicinity of the critical point**
  - 300 K<T<310 K, P=7.38 Mpa
  - ω: T=T_c and 6 MPa<P<8 MPa
- **Density**
  - SW: Δρ around 10%
- **Heat capacity**
  - SW: Δc_p around 2%
- **Speed of sound**
  - SW: Δω around 7%
  - Severe criteria for EoS validation

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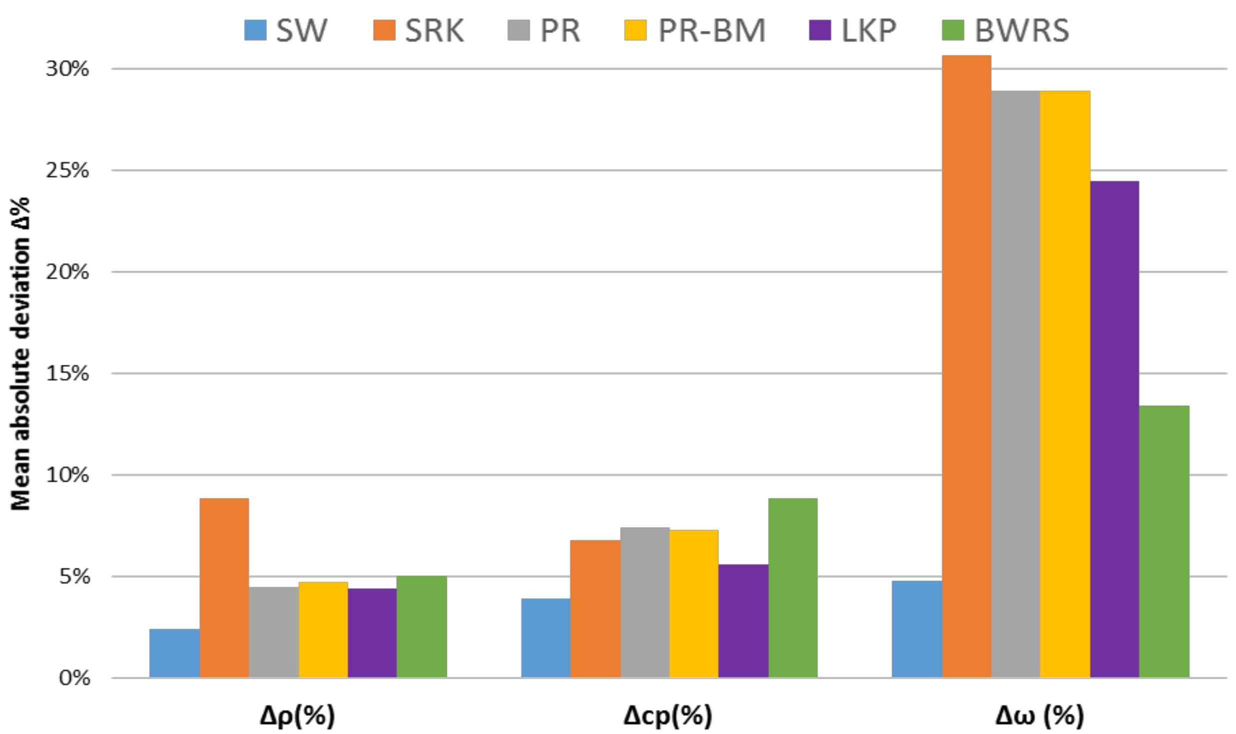
STEP 3) COMPARISON IN ENTIRE REGION OF INTEREST

- **In the entire region of interest**
  - 300K <T<900 K and 7 MPa <P<30 MPa
  - 2641 “density” pts; 359 “heat capacity” pts; 138 “speed of sound” pts



Δ is defined as the absolute mean average of (property value$_{experimental}$ −property value$_{EoS\ calculated}$)/property value$_{experimental}$

SW is the most accurate EoS in the entire region of interest

Outline

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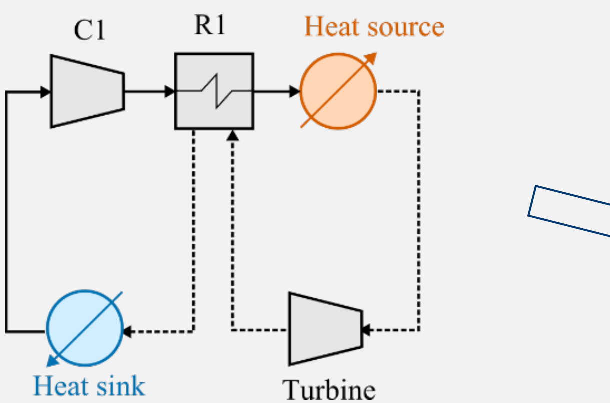
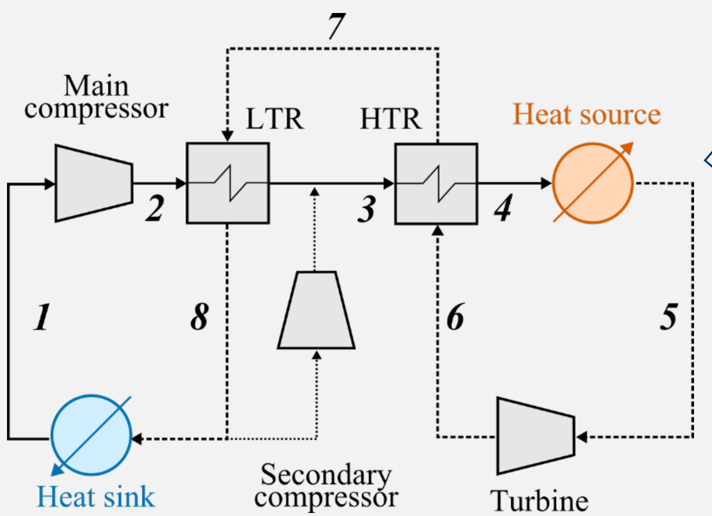
STEP 4) SENSITIVITY STUDY

EoS sensitivity in process modeling simulation

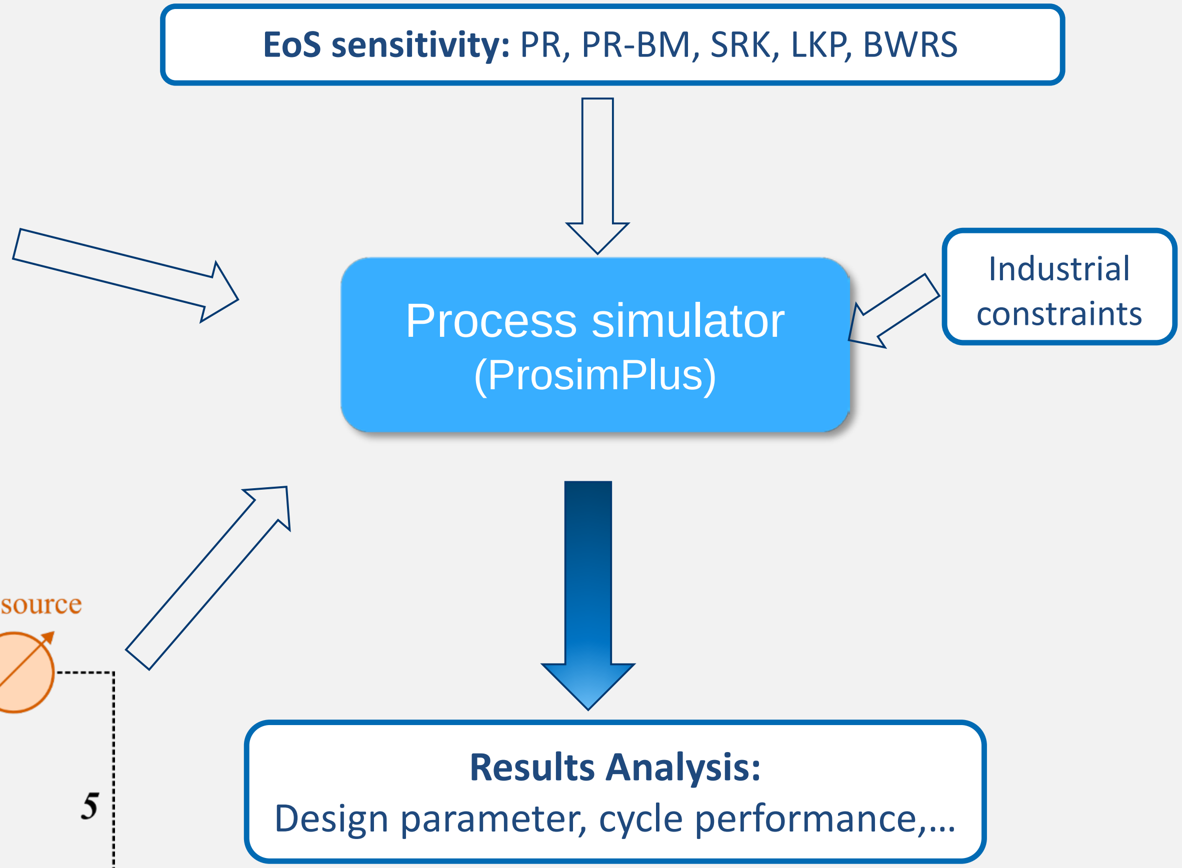
- Set SW EoS simulation as reference



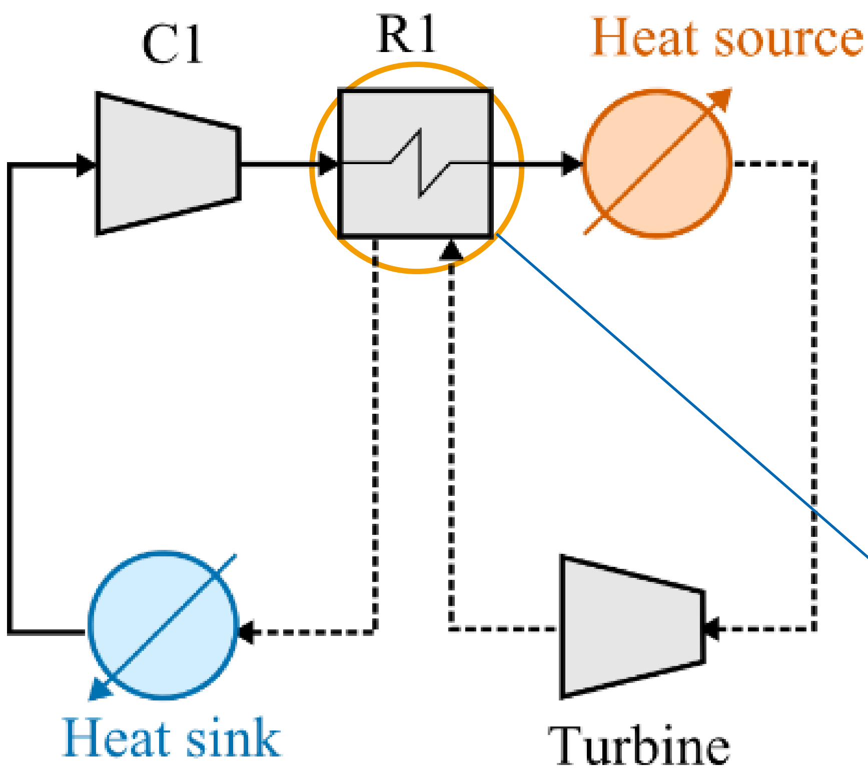
Recuperated Brayton cycle (RC)



Recompression Recuperated Brayton cycle (RRC)



STEP 4) SENSITIVITY STUDY: RC BRAYTON CYCLE

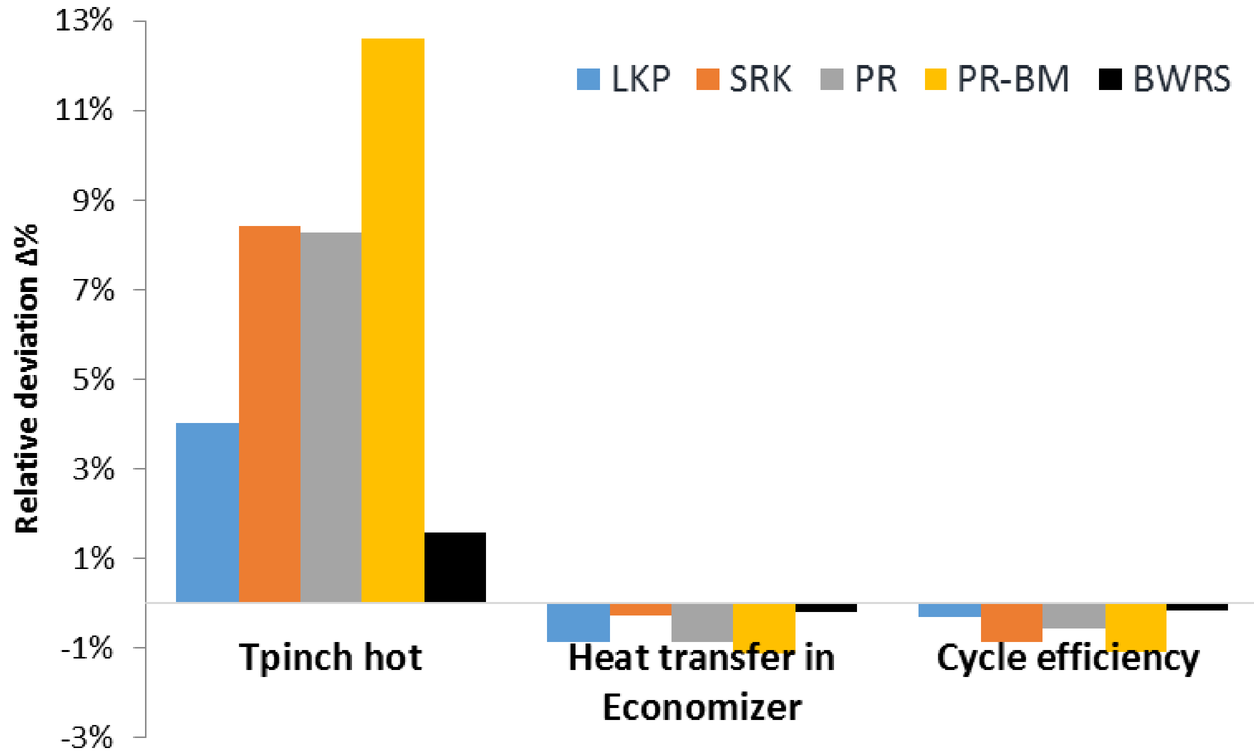


- CSP application reference to Mohagheghi and Kapat, 2013[1]
- Parameter and constraints set identical to reference
- 5 other EoS process simulation compared with SW EoS process simulation

- T_{pinch} hot
- $Q_{economizer}$
- Cycle efficiency

[1]M. Mohagheghi and J. Kapat, "Thermodynamic Optimization Of Recuperated S-CO_2 Brayton Cycles For Solar Tower Applications", *Proceedings of ASME Turbo Expo* , 2013

STEP 4) SENSITIVITY STUDY: RC BRAYTON CYCLE



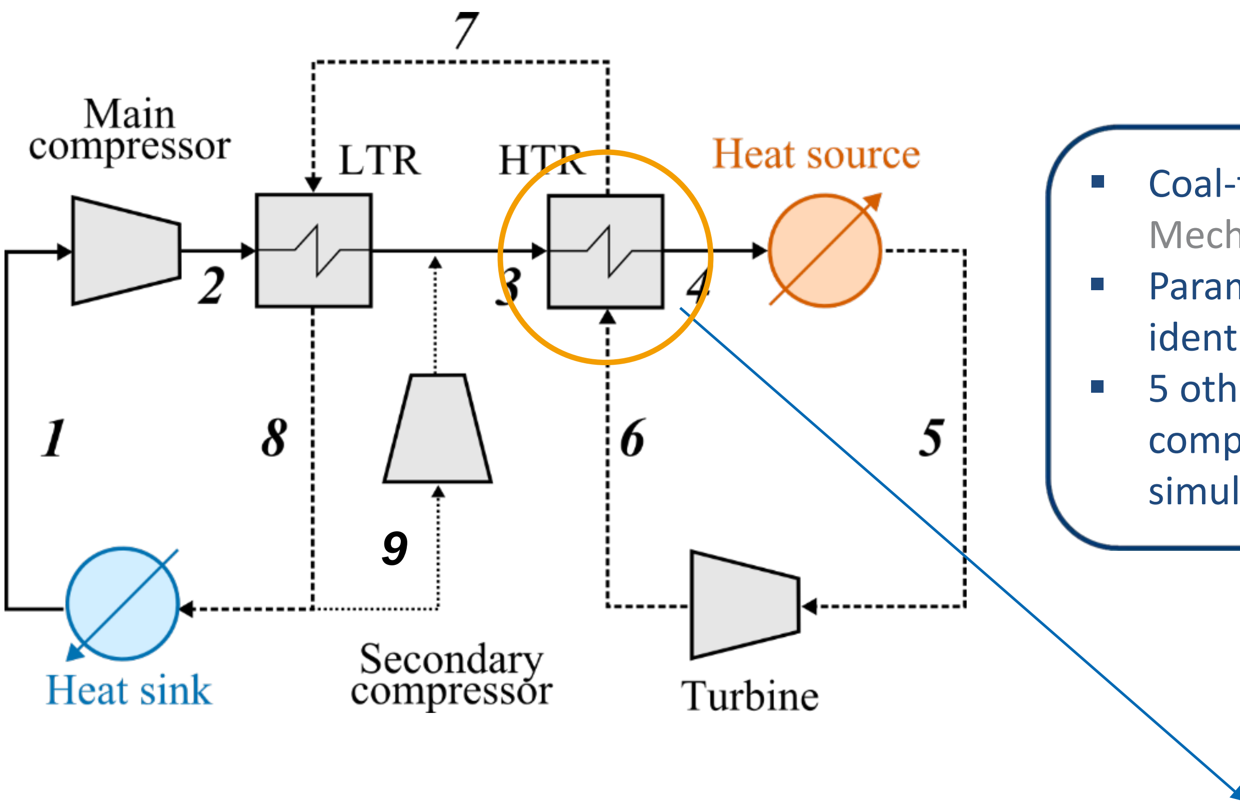
* Δ is defined as the relative deviation of (result simulated by other EoS – result simulated by SW)/result simulated by SW

Other EoS

- Hot Pinch temperature on economizer overestimated
- Heat in economizer underestimated
- Small impact on cycle efficiency

⇒ **Surface of economizer underestimated**

STEP 4) SENSITIVITY STUDY: RRC BRAYTON CYCLE

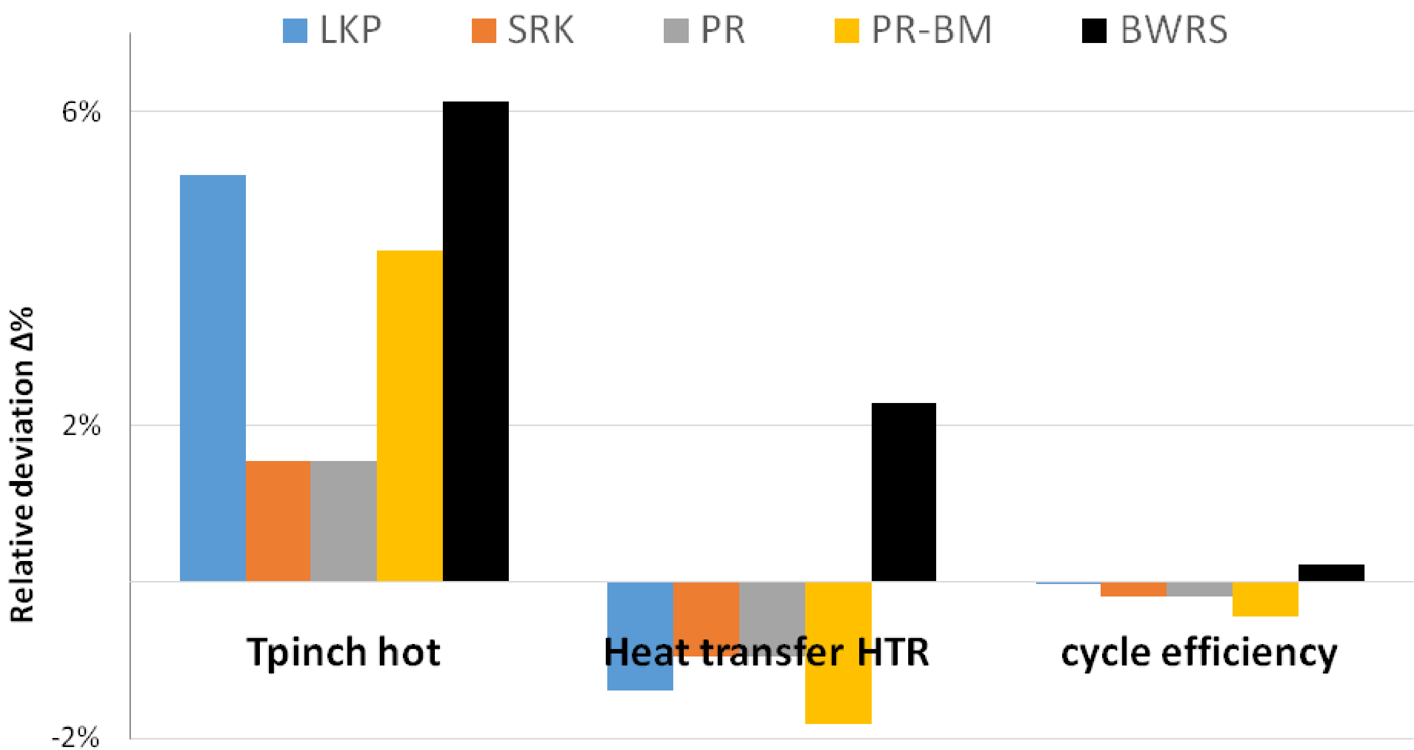


- Coal-fired application referenced to Mecheri and Le Moullec, 2016[2]
- Parameter and constraints set identical to reference
- 5 other EoS process simulation compared with SW EoS process simulation

- T_{pinch} hot
- $Q_{economizer}$
- Cycle efficiency

[2]M. Mecheri and Y. Le Moullec, "Supercritical CO_2 Brayton Cycles For Coal-fired Power Plants", accepted by *Energy* in 2016

STEP 4) SENSITIVITY STUDY: RRC BRAYTON CYCLE

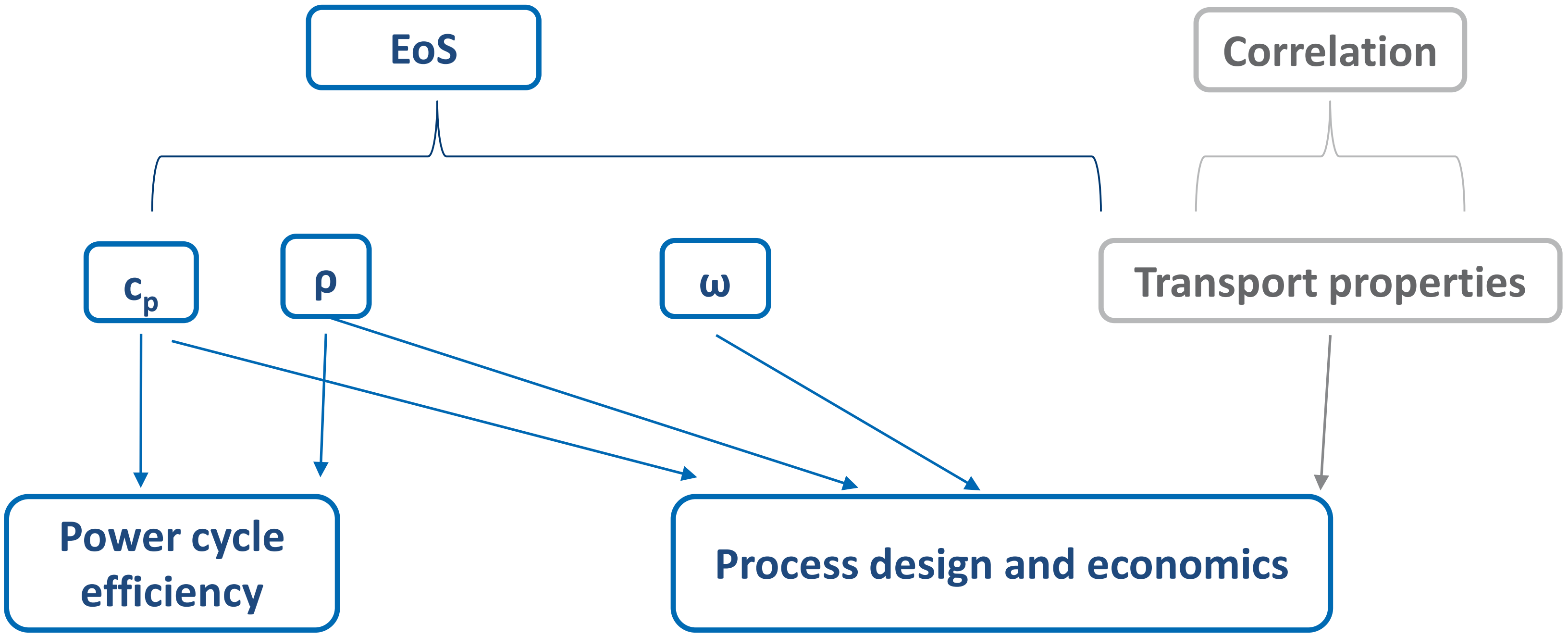


Δ is defined as the relative deviation of (result simulated by other EoS – result simulated by SW)/result simulated by SW

- Hot Pinch temperature on economizer overestimated
- Heat in economizer underestimated (except for BWRS)
- Small impact on cycle efficiency
- Influence of EoS becomes more complex when layout is more **complicate** and **number(component)** ↗

STEP 4) SENSITIVITY STUDY: DISCUSSION

- **Small effect of EoS on power cycle efficiency**
- **No involvement of speed of sound in cycle efficiency calculation** (strong involvement in machinery sizing)
- **Predictable strong dependence of EoS on Process Design and Economical Assessment**
- **Foreseen effects on Brayton cycle optimization: maximize the cycle efficiency**



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Conclusion

- **SW EoS is the most accurate model (among the 6 studied EoS) in both critical and supercritical region for CO_2**
- **Small effects of EoS observed on power cycle efficiency**
- **However process design is expected to strongly depend on EoS**
- **Precision of EoS is required for complex cycle layout**
- **Accurate EoS is required for mixture of CO_2**

Future Work

- **Process optimization with respect to energy and economics (Non-Linear Programming)**
- **Propagation of thermodynamic model uncertainty to cycle output**
- **Optimization of process structure (Flowsheet)**

Thank you for your attention

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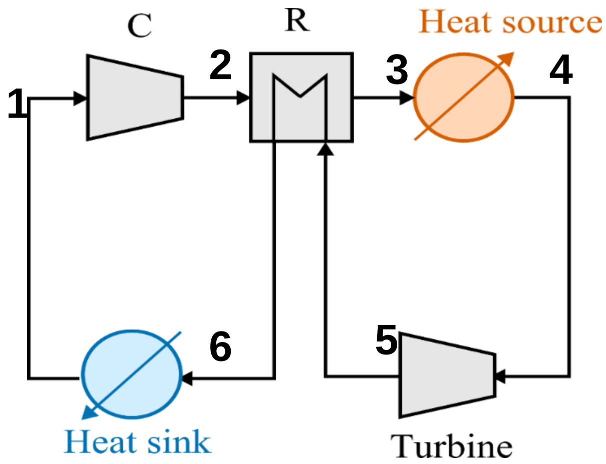
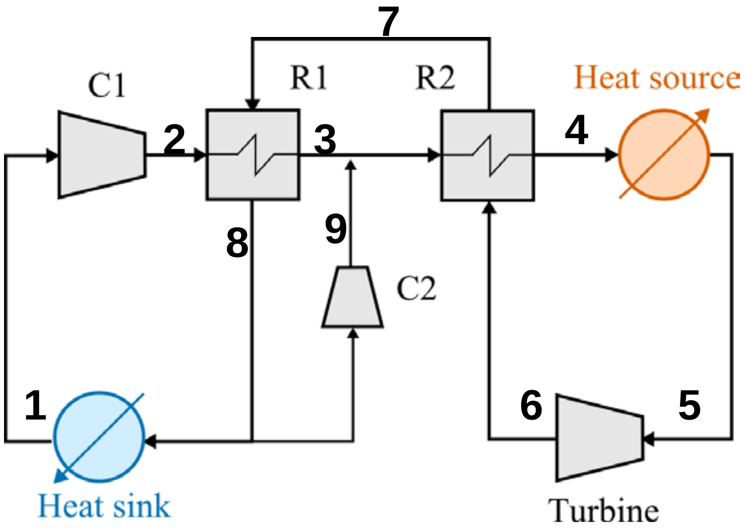
BACK UP
1) HYPOTHESIS AND CONSTRAINTS





Tin compressor (=Tcooling) (K)	320
Pin compressor (MPa)	3.274
Pout compressor (MPa)	12
T heater (K)	1373
Tpinch cold (K)	20
isentropic efficiency of turbine	0.9
isentropic efficiency of compressor	0.89
heat source (MW)	200
Pressure drop in every component (%)	1

Tin compressor (=Tcooling) (K)	308.15
Pin compressor (MPa)	75
Pout compressor (MPa)	20
Pout sec compressor (MPa)	19.9
T heater (K)	773
Tpinch cold (K)	10
isentropic efficiency of turbine	0.9
isentropic efficiency of compressor	0.89
Mechanical efficiency of compressor	0.981
heat source (MW)	200
Pressure drop in every component (MPa)	0.1

Temperature equality in Flow(9) and Flow(3)

Constant heat source (1187 MW)in the boiler

BACK UP
2) THERMODYNAMICS BASIS (HEAT CAPACITY)

$$c_p^*(T^*,\, v^*) = c_p^\bullet(T^*,\, v^*) + c_p^{res}(T^*,\, v^*)$$

$$c_p^\bullet = A + B\left(\frac{\frac{C}{T}}{sinh(\frac{C}{T})}\right)^2 + D\left(\frac{\frac{E}{T}}{cosh(\frac{E}{T})}\right)^2$$

$$\begin{cases} s^{var}(T,\, v) = -\left[\dfrac{\partial a^{var}(T,v)}{\partial T}\right]_v \\ P^{var}(T,v) = -\left[\dfrac{\partial a^{var}(T,v)}{\partial v}\right]_T \\ u^{var}(T,\, v) = a^{var}(T,\, v) + T \cdot s^{var}(T,\, v) \\ C_v^{var}(T,\, v) = \left[\dfrac{\partial u^{var}(T,v)}{\partial T}\right]_v \\ C_p^{var}(T,\, v) = C_v^{var} - T\dfrac{\left[\left(\frac{\partial P^{var}(T,v)}{\partial T}\right)\right]^2}{\left(\frac{\partial P^{var}(T,v)}{\partial v}\right)_T} \end{cases}$$

$$\begin{cases} A = 29370 \\ B = 34540 \\ C = 1428 \\ D = 26400 \\ E = 588 \end{cases}$$

SW EoS:

$$\frac{c_p}{R} = \underbrace{-\tau^2(\varphi^\circ{}_{\tau\tau} + \varphi^r_{\tau\tau})}_{\frac{c_v}{R}} + \frac{\overbrace{(1 + \delta\varphi^r_\delta - \delta\tau\varphi^r_{\delta\tau})^2}^{\approx(\frac{\partial p}{\partial T})^2_\rho}}{\underbrace{1 + 2\delta\varphi^r_\delta + \delta^2\varphi^r_{\delta\delta}}_{\approx(\frac{\partial p}{\partial \rho})_T}}$$

eDF

BACK UP
2) THERMODYNAMICS BASIS (SPEED OF SOUND)

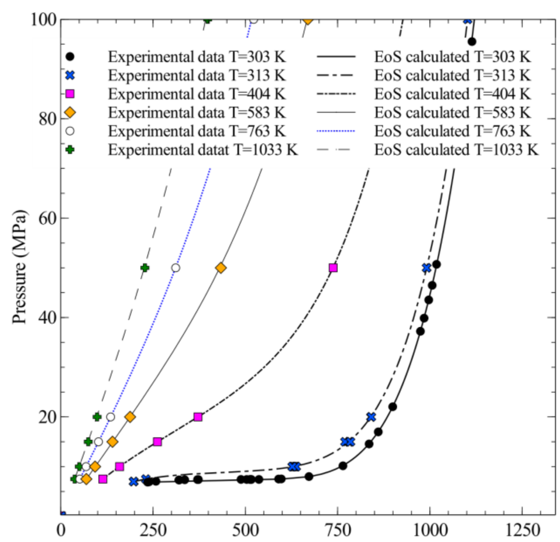
$$w = \sqrt{(\frac{\partial P}{\partial \rho})_s}$$

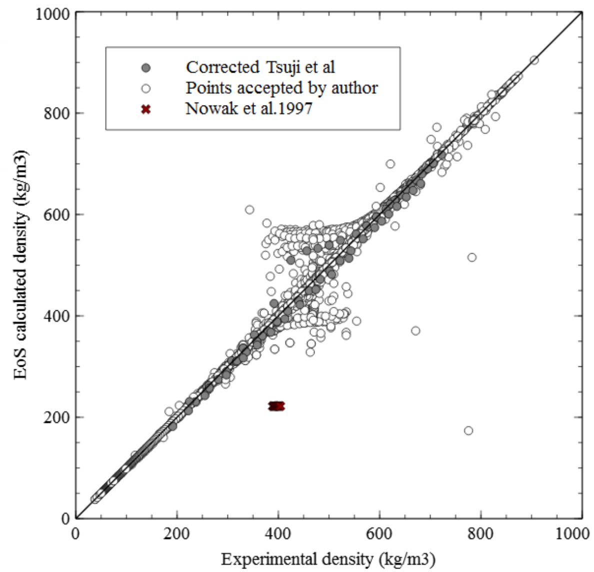
SW EoS:

$$\frac{w^2}{RT} = \underbrace{1 + 2\delta\varphi^r_\delta + \delta^2\varphi^r_{\delta\delta}}_{\approx(\frac{\partial p}{\partial \rho})_T} - \frac{\overbrace{(1 + \delta\varphi^r_\delta - \delta\tau\varphi^r_{\delta\tau})^2}^{\approx(\frac{\partial p}{\partial T})^2_\rho}}{\underbrace{\tau^2({\varphi^\circ}_{\tau\tau} + {\varphi^r}_{\tau\tau})}_{-\frac{c_v}{R}}}$$

BACK UP
STEP 3) SW EoS IN ENTIRE REGION OF INTEREST

- **Region of entire study: 300<T<900 K, 7<P<30 MPa**



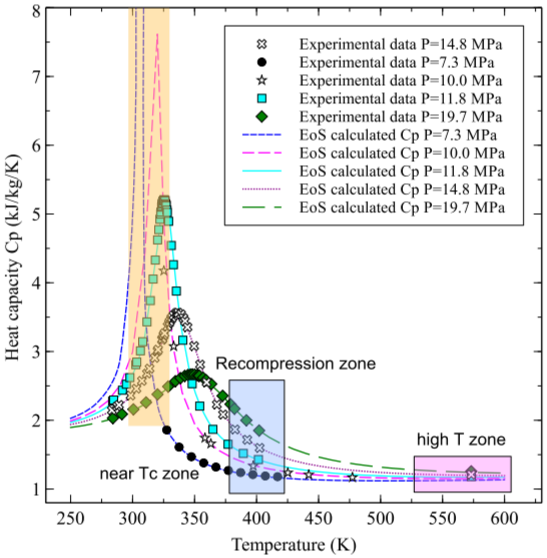


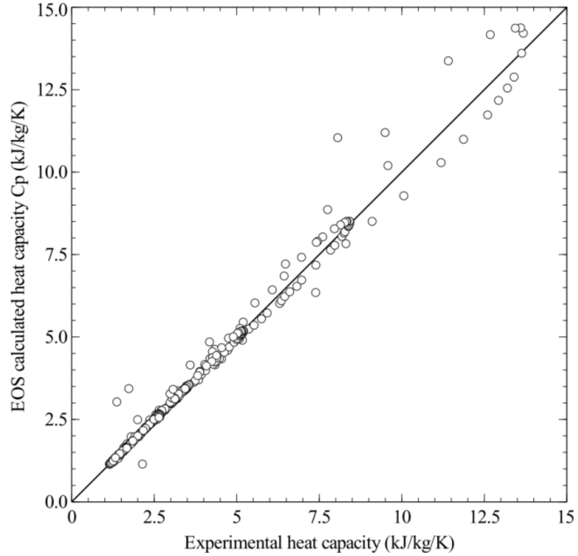
- **Satisfactory agreement between $\rho_{SW\ EoS\ calculated}$ and $\rho_{experimental}$**

- **Parity curve with all accessed experimental data**
  - Δρ=2.4 %
  - Relative important deviations (>15%) in the vicinity of the critical point

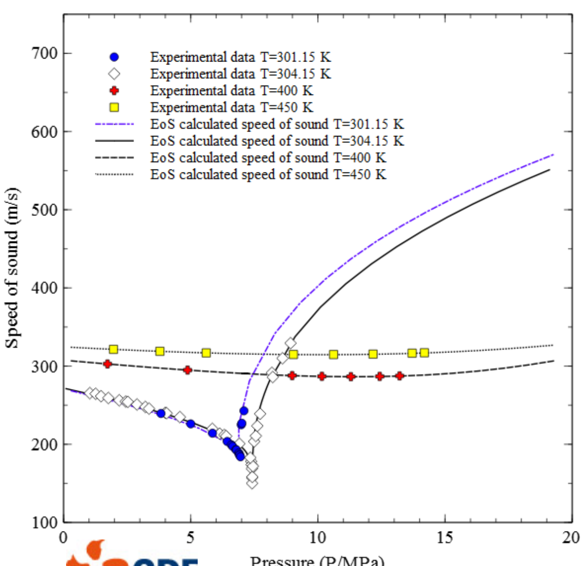
BACK UP

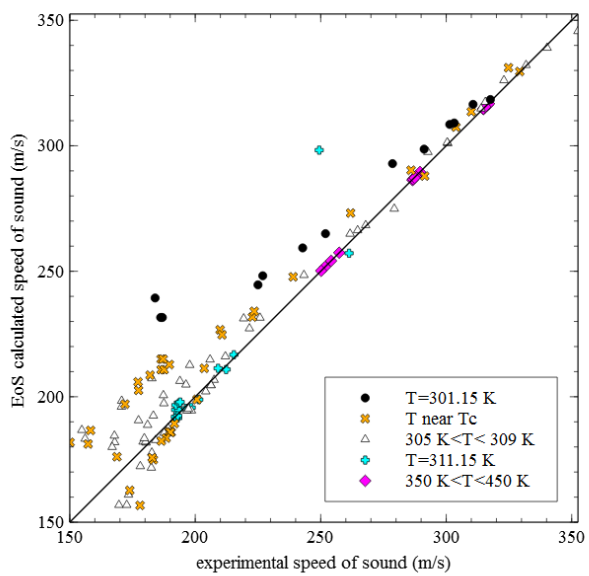
STEP 3) SW EoS IN ENTIRE REGION OF INTEREST





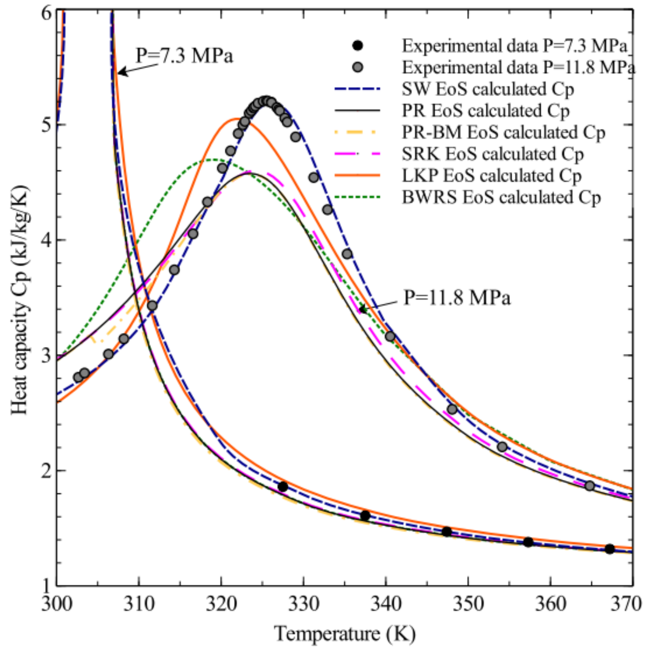
- **Satisfactory agreement between $c_{p\ \text{SW EoS calculated}}$ and $c_{p\ \text{experimental}}$**
- **Parity curve with all accessed experimental data**
  - Δc_p=4.0%



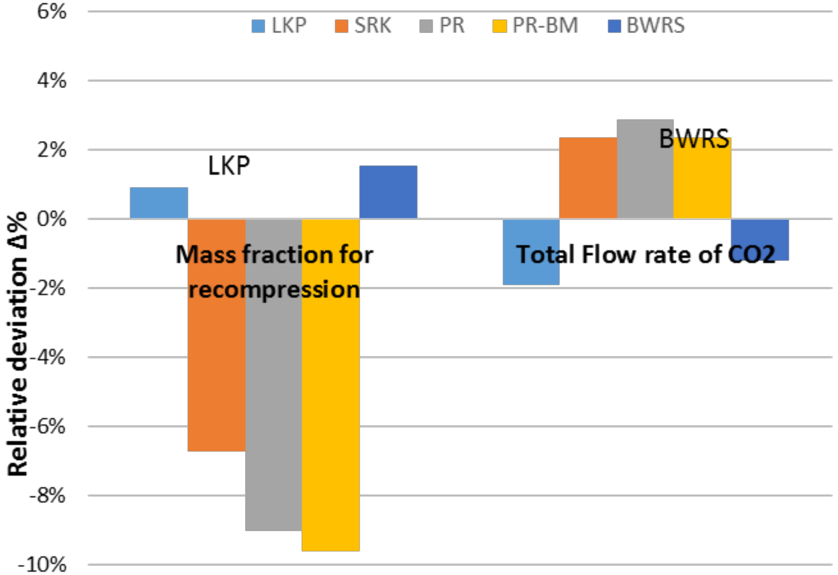


- **Satisfactory agreement between $\omega_{\text{SW EoS calculated}}$ and $\omega_{\text{experimental}}$**
- **Parity curve with all accessed experimental data**
  - $\Delta\omega$=4.8%

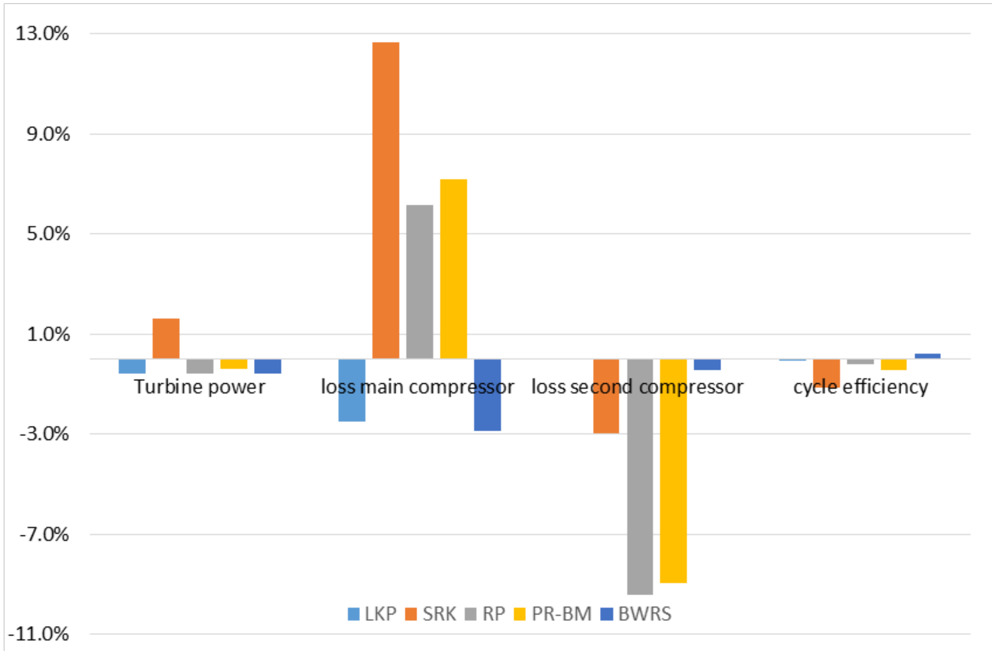
BACK UP
EoS IN ENTIRE REGION OF INTEREST



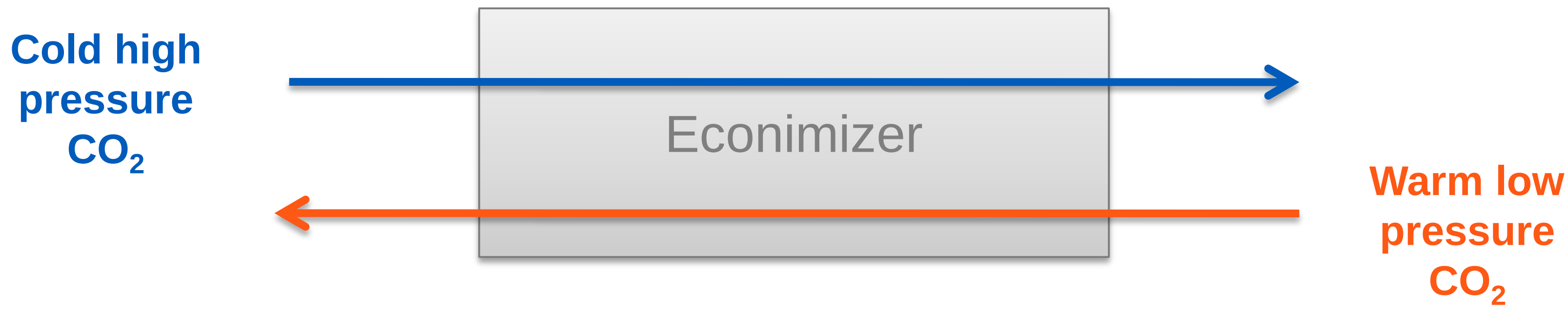
BACK UP
RRC BRAYTON CYCLE

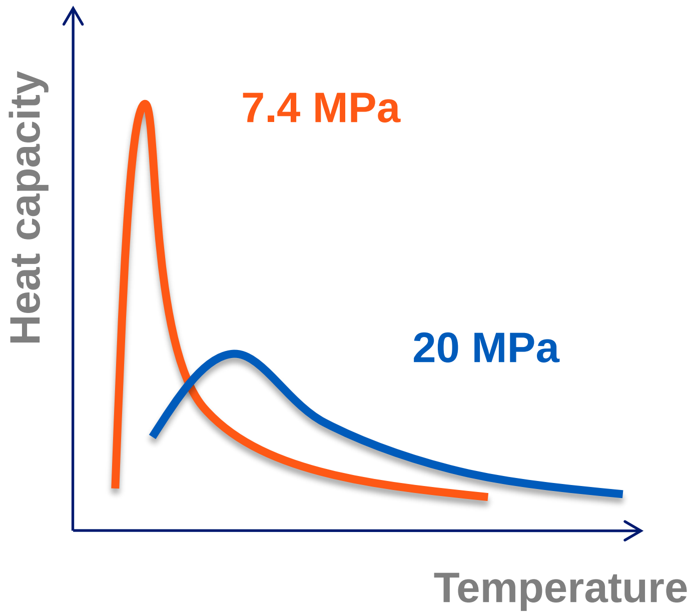


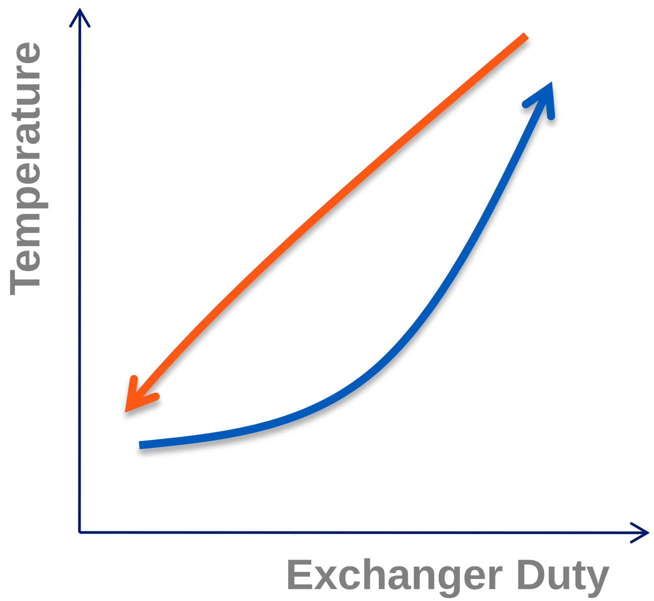
Δ is defined as the relative deviation of (result simulated by other EoS – result simulated by SW)/result simulated by SW



BACK UP
ECONOMIZER PINCH PROBLEM







BACK UP
RESULTS – Cycle economizer configuration

- **3 studied cases (all other parameters being similar with reference case):**
  - No recompression cycle
  - Single recompression cycle (ref. case)
  - Double recompression cycle

- **Significant reduction of economizer temperature difference between heat and cold side**
  → more heat is exchanged
  → cycle efficiency increases

- **Double recompression cycle efficiency gains do not justify expected material additional costs**

Economizer temperature difference as a function of cumulative duty