Thermodynamic model investigation for S-CO$_2$ Brayton cycle for coal-fired power plant application

5th International Supercritical CO$_2$ Power Cycles Symposium
San Antonio, Texas

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March 31st, 2016
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 up 80% from 1990 to 2010
    - Up 70% is expected by 2035
  - Coal-fired plants: 41% of world’s power generation
  - Power generation: 42% of world’s CO₂ emission

- **Challenge in environment**
  - CO₂ emission: 31.3 Gt in 2011
  - Reduction target of 40%-70% by 2050 (post COP 21)

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*Power Plant Efficiency improvement*
**INTRODUCTION**

- **State of the art for coal-fired plant**
  - S-Steam: 46% \(_{\text{LHV}}\) 30MPa/873/893 K
  - Potential of enhancement (material/architecture/working fluid?)

- **S-CO\(_2\)** cycle allows at least \(\uparrow 5\text{%pts}\) LHV efficiency

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

Objectives

- Comparison of existing thermodynamics models (EoS) for CO₂
- Selection of the most accurate model for CO₂ (in the vicinity of the critical point and supercritical region)
- EoS sensitivity study in process simulation

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

Thermodynamic model (EoS) for S-CO₂
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
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**METHODOLOGY**

**Step 1: CO\textsubscript{2} critical property comparison with collected DIPPR database**

**Step 1: Simulated CO\textsubscript{2} critical properties compared with experimental data**

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

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

- Thermodynamic simulator (ProsimPlus)
- Experimental data (DIPPR 801 Database)

**CO\textsubscript{2} critical properties:** $T_c, P_c, \rho_c (v_c)$

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: CO₂ critical property comparison with collected DIPPR database

Step 2: CO₂ 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 (DECHHEMA Database)

criteria properties: Density(\(\rho\)), heat capacity (\(c_p\)), speed of sound(\(\omega\))

Comparison
METHODOLOGY

Step 1: CO₂ 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 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

Favorable EoS
EoS leads to the smallest relative “model/measurement” deviation
METHODOLOGY

Step 1: CO₂ 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 of Brayton cycle
  - Recuperated Brayton Cycle (RC)
  - Recompression Recuperated Brayton Cycle (RRC)

Process simulator (ProsimPlus)

Favorable EoS

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

Comparison

Other 5 EoS

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

Results Analysis and Discussion
Outline

- Introduction and context
- Objectives
- Methodology
- Thermodynamics investigation
  - Step 1: CO₂ 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 \(\rho_c\)
  - SRK EoS shows the biggest deviation

\[
\Delta \text{ is defined as the absolute mean average of } \left(\frac{\text{Critical density}_{\text{experimental}} - \text{Critical density}_{\text{EoS calculated}}}{\text{Critical density}_{\text{experimental}}}\right)
\]
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STEP 2) COMPARISON NEAR CRITICAL POINT

- In the vicinity of the critical point
  - 300 K < T < 310 K, P = 7.38 Mpa
  - \( \omega \): T = T_c and 6 MPa < P < 8 MPa

- Density
  - SW: \( \Delta \rho \) around 10%

- Heat capacity
  - SW: \( \Delta c_p \) around 2%

- Speed of sound
  - SW: \( \Delta \omega \) around 7%
  - Severe criteria for EoS validation

Representation of (a) isobaric density, (b) heat capacity, (c) isotherm speed of sound in the critical region of CO\(_2\).
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  - Step 3: Criteria property comparison in the region of interest
  - Step 4: Model Sensitivity (process simulation)
- Conclusion and future works
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

\[
\Delta \text{defined as } \frac{\text{property value}_{\text{EoS calculated}} - \text{property value}_{\text{experimental}}}{\text{property value}_{\text{experimental}}}
\]

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

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  - Step 3: Criteria property comparison in region of interest
  - Step 4: Model Sensitivity (process simulation)
- Conclusion and future works
STEP 4) SENSITIVITY STUDY

EoS sensitivity in process modeling simulation
- Set SW EoS simulation as reference

EoS sensitivity: PR, PR-BM, SRK, LKP, BWRS

Process simulator (ProsimPlus)

Industrial constraints

Results Analysis:
Design parameter, cycle performance,...
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

- $T_{\text{pinch, hot}}$
- $Q_{\text{economizer}}$
- Cycle efficiency

STEP 4) SENSITIVITY STUDY: RC BRAYTON CYCLE

Other EoS

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

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

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

STEP 4) SENSITIVITY STUDY: RRC BRAYTON CYCLE

- 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 complex and number(component) increases

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

- Introduction and context
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Conclusion

- SW EoS is the most accurate model (among the 6 studied EoS) in both critical and supercritical region for CO2
- 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 CO2

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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1) HYPOTHESIS AND CONSTRAINTS

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tin compressor (=Tcooling) (K)</td>
<td>320</td>
</tr>
<tr>
<td>Pin compressor (MPa)</td>
<td>3.274</td>
</tr>
<tr>
<td>Pout compressor (MPa)</td>
<td>12</td>
</tr>
<tr>
<td>T heater (K)</td>
<td>1373</td>
</tr>
<tr>
<td>Tpinch cold (K)</td>
<td>20</td>
</tr>
<tr>
<td>isentropic efficiency of turbine</td>
<td>0.9</td>
</tr>
<tr>
<td>isentropic efficiency of compressor</td>
<td>0.89</td>
</tr>
<tr>
<td>heat source (MW)</td>
<td>200</td>
</tr>
<tr>
<td>Pressure drop in every component (%)</td>
<td>1</td>
</tr>
</tbody>
</table>

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

Constant heat source (1187 MW) in the boiler
2) THERMODYNAMICS BASIS (HEAT CAPACITY)

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

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

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

\[
\frac{c_p}{R} \approx -T^2\left(\varphi^{\tau\tau} + \varphi^{\tau\tau}_{\tau}\right) + \left(\frac{c_v}{R}\right)^2 \left(1 + \delta^2 \varphi^\tau_{\delta} + \delta^2 \varphi^\tau_{\delta\delta}\right)
\]

\[
A = 29370 \\
B = 34540 \\
C = 1428 \\
D = 26400 \\
E = 588
\]
BACK UP

2) THERMODYNAMICS BASIS (SPEED OF SOUND)

\[ w = \sqrt{\left( \frac{\partial P}{\partial \rho} \right)_s} \]

\[
\frac{w^2}{RT} = 1 + 2\delta \varphi^r_\delta + \delta^2 \varphi^r_{\delta \delta} - \frac{\left( \frac{\partial^2 P}{\partial T^2} \right)_\rho}{\tau^2 (\varphi^r_{TT} + \varphi^r_{TT})} - \frac{c^2}{R}
\]
STEP 3) SW EoS IN ENTIRE REGION OF INTEREST

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

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

- Parity curve with all accessed experimental data
  - $\Delta \rho = 2.4\%$
  - Relative important deviations (>15%) in the vicinity of the critical point
Satisfactory agreement between $c_p$ SW EoS calculated and $c_p$ experimental

Parity curve with all accessed experimental data

$\Delta c_p = 4.0\%$

Satisfactory agreement between $\omega$ SW EoS calculated and $\omega$ 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

Cold high pressure CO₂

Econimizer

Warm low pressure CO₂

Heat capacity

Temperature

20 MPa

7.4 MPa

Temperature

Exchanger Duty

Exchanger Duty
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