Simulation of Pipeline Transport of Carbon Dioxide with Impurities

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Carbon dioxide Capture and Storage (CCS) systems

- the purpose: to reduce greenhouse gas emissions into the atmosphere

- CCS systems consist of 3 parts:
  (1) capturing carbon dioxide (CO2) at its source
  (2) transporting CO2 through pipelines to special storage sites
  (3) injecting CO2 into wells, when underground storage is used

- transport in the liquid or supercritical phase is to be preferred, to support high flow rates
- transport must stay in that phase, without transitioning to gaseous state, to avoid cavitation
- precise transport simulation with indication of phase transition is required
Pipe transport variables

- mass density $\rho$, velocity $v$, pipe cross section area $S$
- mass flow: $m = \rho \cdot v \cdot S$
- density of momentum: $\rho \cdot v$, momentum flow: $\rho \cdot v^2 \cdot S$
- density of energy: $\rho \cdot e$, energy flow: $\rho \cdot e \cdot v \cdot S$
- where $e$ is specific energy (per unit mass)
- $e = u + \frac{v^2}{2} + gh$ with kinetic and gravity terms
- $u$ is specific internal energy
Pipe transport equations

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho v)}{\partial x} &= 0, \\
\frac{\partial (\rho v)}{\partial t} + \frac{\partial (\rho v^2)}{\partial x} + \frac{P}{\partial x} &= -\lambda \rho v|v|/(2D) - \rho g \frac{\partial h}{\partial x}, \\
\frac{\partial (\rho e)}{\partial t} + \frac{\partial (\rho ev)}{\partial x} + \frac{Pv}{\partial x} &= -4c_h(T - T_s)/D
\end{align*}
\]

change of (mass, momentum, energy) in dx-element
flow of (mass, momentum, energy) through boundaries
pressure contribution at the boundaries (PS=force, PSvdt=work)
can be unified to specific enthalpy
\[H_s = u + P/\rho\]
Pipe transport equations

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho v)}{\partial x} &= 0, \\
\frac{\partial (\rho v)}{\partial t} + \frac{\partial (\rho v^2 + P)}{\partial x} &= -\frac{\lambda \rho v|v|}{(2D)} - \rho g \frac{\partial h}{\partial x}, \\
\frac{\partial (\rho e)}{\partial t} + \frac{\partial (\rho e v + P v)}{\partial x} &= -\frac{4c_h(T - T_s)}{D}
\end{align*}
\]

stationary process considered: \( \partial/\partial t = 0 \)
proper discretization applied

dependence of lam on other parameters via Nikuradse/Hofer formula
Darcy-Weisbach friction term
gravity force contribution (g-free fall accel., h-height)
heat transfer to soil or other environment (T-temperature, D-pipe diameter)
Equation of state (EOS) and enthalpy definition

- EOS: \( z = z(T,P,x) \), with \( P = \rho \frac{RTz}{\mu} \) as definition of compressibility factor \( z \); 
  - \( R \) - universal gas constant, \( \mu \) - molar mass, \( x \) - vector describing fluid composition
- enthalpy, similarly: \( H = H(T,P,x) \)
- there are a lot of empirical approximations to the real fluid EOS and \( H \)
- we use the most complex ones provided by \textbf{GERG2008} thermodynamical module (ISO standard)
- Homogeneous Equilibrium Model (HEM): different phases of a fluid are homogeneously mixed and have the same speed, pressure, temperature and chemical potential
- implemented in our software \textbf{MYNTS} (Multi-phYsics NeTwork Simulator)
Phase transitions

- GERG2008 properly computes phase transitions
- for pure substances - phase transition line (transition at const T,P)
- for fluids with impurities - phase envelope (transition at const T, variable P)
Phase transitions

- $\text{frac}(T,P,x)$ – fraction of gaseous phase
- $\text{frac}=0$ liquid, $\text{frac}=1$ gas, $0<\text{frac}<1$ two-phase
- spurious jump in supercritical region (where gas and liquid states are indistinguishable)
- simple algorithm testing for phase transition in vicinity of a given $(T,P,x)$

Algorithm (proximity-alarm):

given $(T_0, P_0, x, dT, dP, \text{val})$
for $T$ in $(T_0-dT, T_0, T_0+dT)$
  for $P$ in $(P_0-dP, P_0, P_0+dP)$
    if $\text{frac}(T,P,x) != \text{val}$ return true
return false.
Numerical experiments

- 95% CO2, 3% N2, 2% O2
- single pipe, laid horizontally
- two scenarios: scen1 without phase transition, scen2 – with phase transition
- result: scen1 converges, scen2 diverges (cycling)
- the same pattern for other scenarios, phase transition leads to divergence
- the reason – too sharp change in EOS and H at phase transition

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol [units]</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>total pipe length</td>
<td>$L_{tot}$ [km]</td>
<td>150</td>
</tr>
<tr>
<td>pipe internal diameter</td>
<td>$D$ [m]</td>
<td>0.5</td>
</tr>
<tr>
<td>pipe roughness</td>
<td>$k$ [mm]</td>
<td>0.5</td>
</tr>
<tr>
<td>heat transfer coefficient</td>
<td>$e_h$ [W/(m²K)]</td>
<td>4</td>
</tr>
<tr>
<td>fluid composition</td>
<td>$x(CO_2, N_2, O_2)$</td>
<td>(0.95, 0.03, 0.02)</td>
</tr>
<tr>
<td>inlet pressure</td>
<td>$p_{set}$ [bar]</td>
<td>100</td>
</tr>
<tr>
<td>outlet norm.vol.flow, scen1</td>
<td>$q_{set1}$ [10³m³/h]</td>
<td>200</td>
</tr>
<tr>
<td>outlet norm.vol.flow, scen2</td>
<td>$q_{set2}$ [10³m³/h]</td>
<td>310</td>
</tr>
</tbody>
</table>
Numerical experiments

details

prec

convergence

iter

T, K

convergence

86 88 90 92 94 96 98 100

scen1 P, bar

 scen2 P, bar

0 20 40 60 80 100

cycling

convergent region

80 60 40 20 0

phase envelope

cycling

scen2

Spurious transition

Proximity alarm

P, bar

divergence

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Conclusion

- numerical simulation of stationary CO2 transport with impurities and phase transitions is considered
- homogeneous equilibrium model and GERG-2008 thermodynamic module are used
- the algorithms solve scenarios of CO2 transport in the liquid or supercritical phase and detect the approaching phase transition region
- convergence of the algorithms is analyzed in connection with abrupt changes of EOS and enthalpy function in the region of phase transitions
Conclusion

- numerical experiments show that the scenarios with CO2 transport in a single phase converge
- a conservative algorithm for detecting proximity of phase transitions gives the solution to the technical problem posed
- divergences can occur in scenarios with phase transitions due to the abrupt change of thermodynamic parameters
- questions about possible suppression of divergences and improved detection of phase transitions are the subject of our further work
Thank you for your attention