INFOCOMP 2023, June 26-30, Nice, Saint-Laurent-du-Var, France

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Simulation of Pipeline Transport of Carbon Dioxide with Impurities

Mehrnaz Anvari, Anton Baldin, Tanja Clees,
Bernhard Klaassen, Igor Nikitin, Lialia Nikitina, Sabine Pott

Fraunhofer Institute for Algorithms and Scientific Computing

Sankt Augustin, Germany

Contact email: lialia.nikitina@scai.fraunhofer.de

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- pipe transport modeling
- equation of state
- phase transitions
- numerical experiments

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 (CO_2) at its source
  (2) transporting CO_2 through pipelines to special storage sites
  (3) injecting CO_2 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 the 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 ρ, velocity v, pipe cross section area S
- mass flow: $m=\rho\ v\ S$
- density of momentum: $\rho\ v$, momentum flow: $\rho\ v^2\ S$
- density of energy: $\rho\ e$, energy flow: $\rho\ e\ v\ S$
- where e is specific energy (per unit mass)
- $e=u+v^2/2+gh$ with kinetic and gravity terms
- u is specific internal energy

Pipe transport equations

$$
\begin{aligned}
&\partial\rho/\partial t + \partial(\rho v)/\partial x = 0,\\
&\partial(\rho v)/\partial t + \partial(\rho v^2 + P)/\partial x = -\lambda\rho v|v|/(2D) - \rho g\,\partial h/\partial x,\\
&\partial(\rho e)/\partial t + \partial(\rho e v + P v)/\partial x = -4c_h(T - T_s)/D
\end{aligned}
$$

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

dependence of lam
on other
parameters via
Nikuradse/Hofer
formula

Darcy-
Weisbach
friction
term

gravity force
contribution
(g-free fall accel.,
h-height)

$$\partial\rho/\partial t + \partial(\rho v)/\partial x = 0,$$
$$\partial(\rho v)/\partial t + \partial(\rho v^2 + P)/\partial x = \boxed{-\lambda \rho v|v|/(2D)} \boxed{-\,\rho g\,\partial h/\partial x,}$$
$$\partial(\rho e)/\partial t + \partial(\rho e v + P v)/\partial x = \boxed{-4 c_h (T - T_s)/D}$$

heat transfer to soil
or other environment
(T-temperature,
D-pipe diameter)

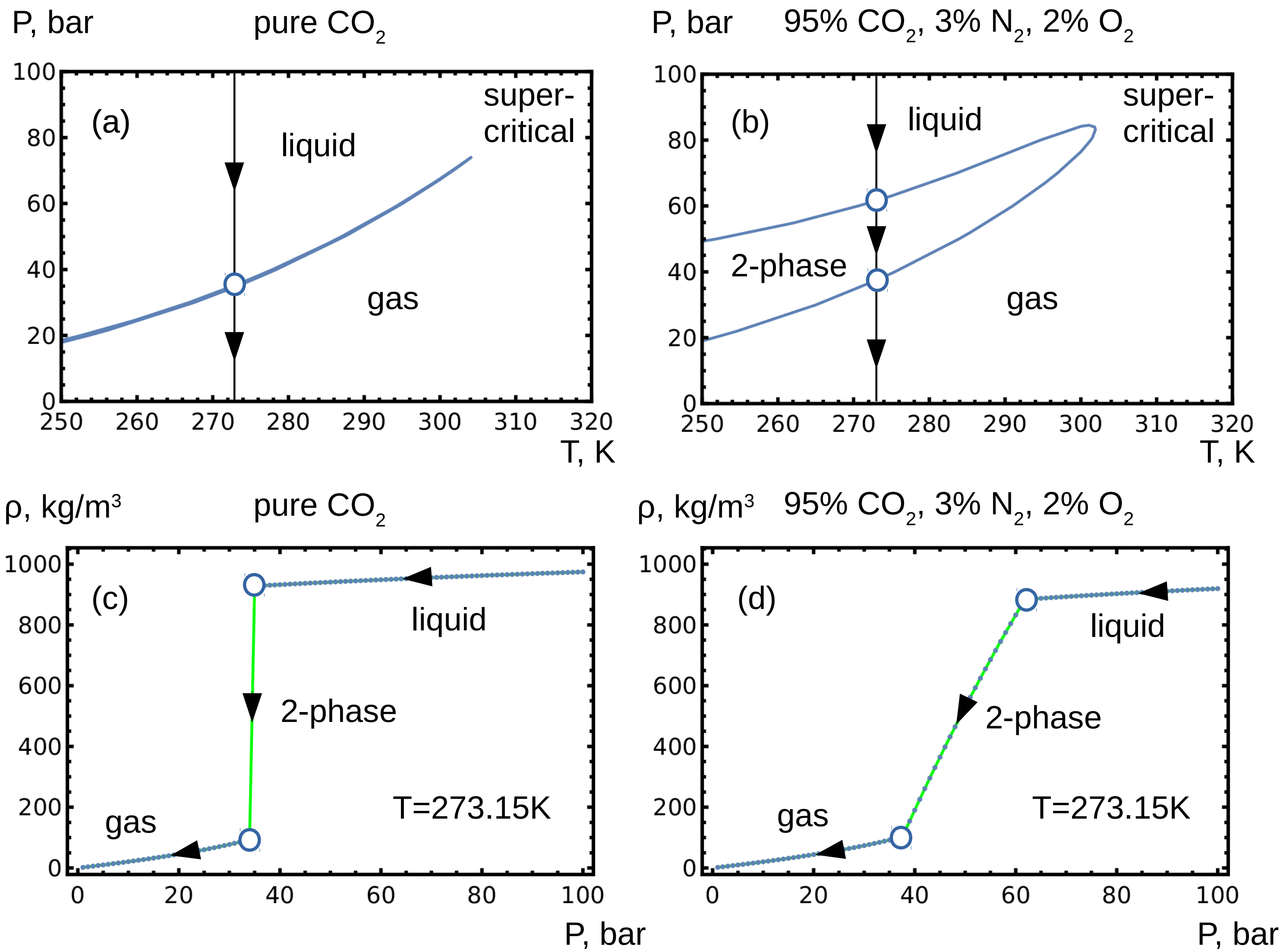
stationary process considered: *∂/∂t = 0*
proper discretization applied

Equation of state (EOS) and enthalpy definition

- EOS: $z=z(T,P,x)$, with $P=\rho\, RTz/\mu$ as definition of compressibility factor z; R - universal gas const, μ - 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 **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 **MYNTS** (Multi-phYsics NeTwork Simulator)

Phase transitions

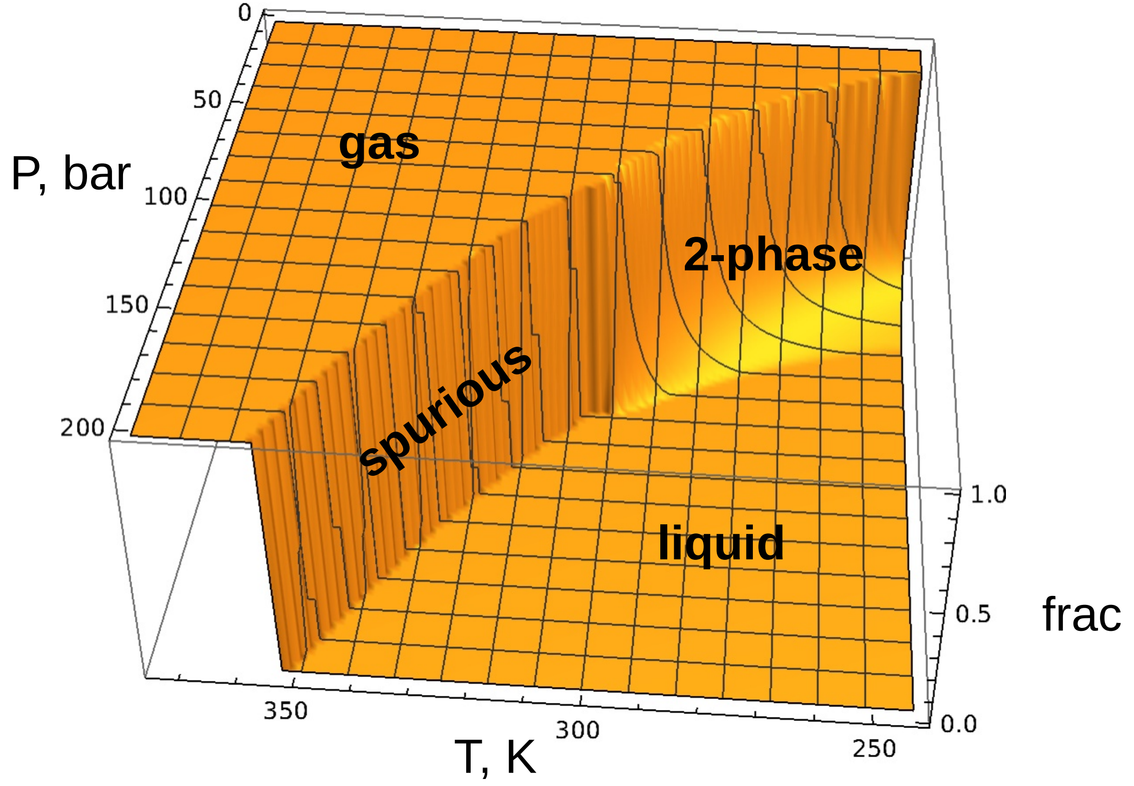
- GERG2008 properly computes phase transitions
- for pure substances – phase transition line (transition at const T,P)
- for fluids with impurities – phase envelope (transition at const T, variable P)



Phase transitions

- frac(T,P,x) – fraction of gaseous phase
- frac=0 liquid, frac=1 gas, 0<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)

95% CO2, 3% N2, 2% O2



Algorithm (proximity-alarm):

```
given (T0,P0,x,dT,dP,val)
for T in (T0-dT,T0,T0+dT)
    for P in (P0-dP,P0,P0+dP)
        if frac(T,P,x)!=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

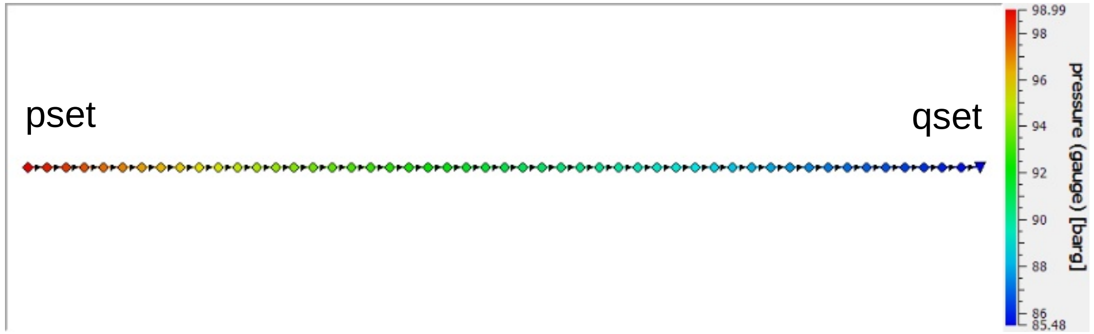
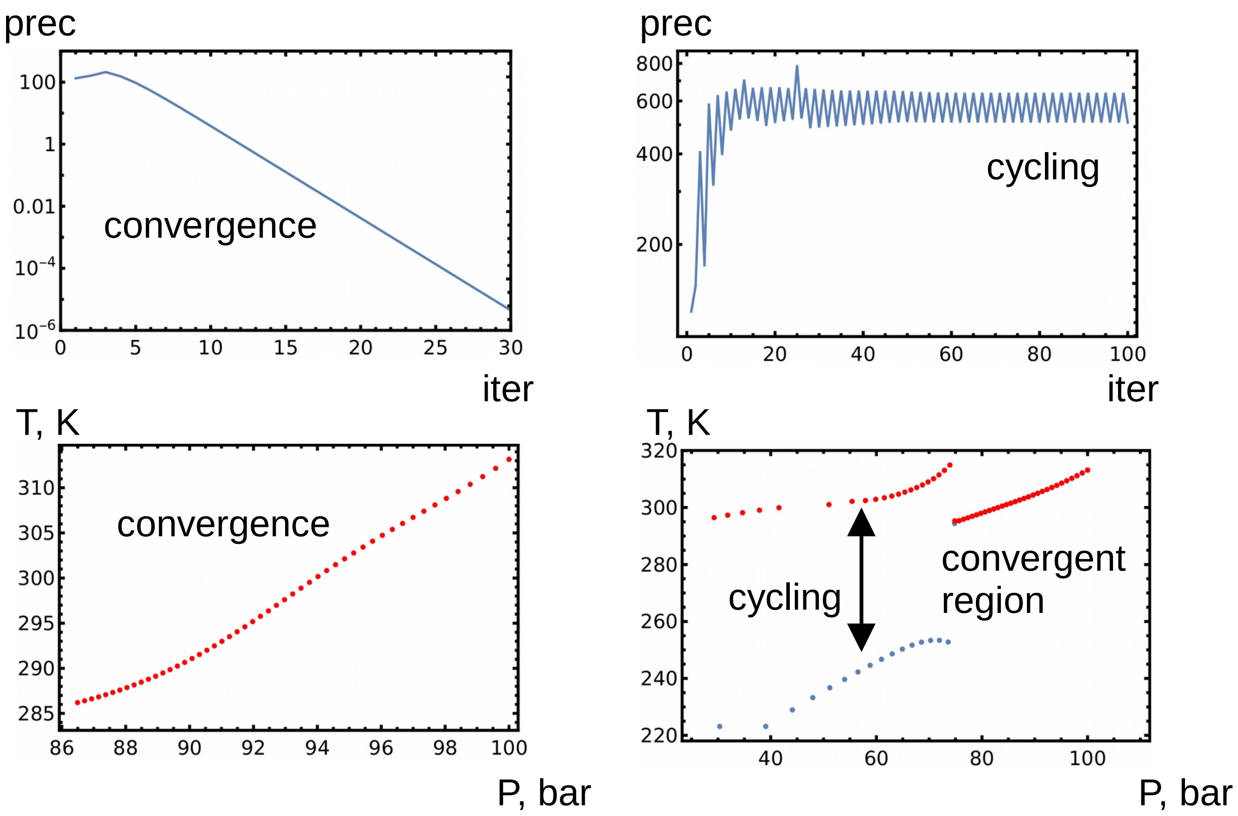


TABLE I
PARAMETERS OF TEST SCENARIOS

parameter	symbol [units]	value
total pipe length	$L_{tot}[km]$	150
pipe internal diameter	$D[m]$	0.5
pipe roughness	$k[mm]$	0.5
heat transfer coefficient	$c_h[W/(m^2K)]$	4
fluid composition	$x(CO_2, N_2, O_2)$	(0.95,0.03,0.02)
inlet pressure	pset [bar]	100
outlet norm.vol.flow, scen1	qset1 $[10^3 m^3/h]$	200
outlet norm.vol.flow, scen2	qset2 $[10^3 m^3/h]$	310

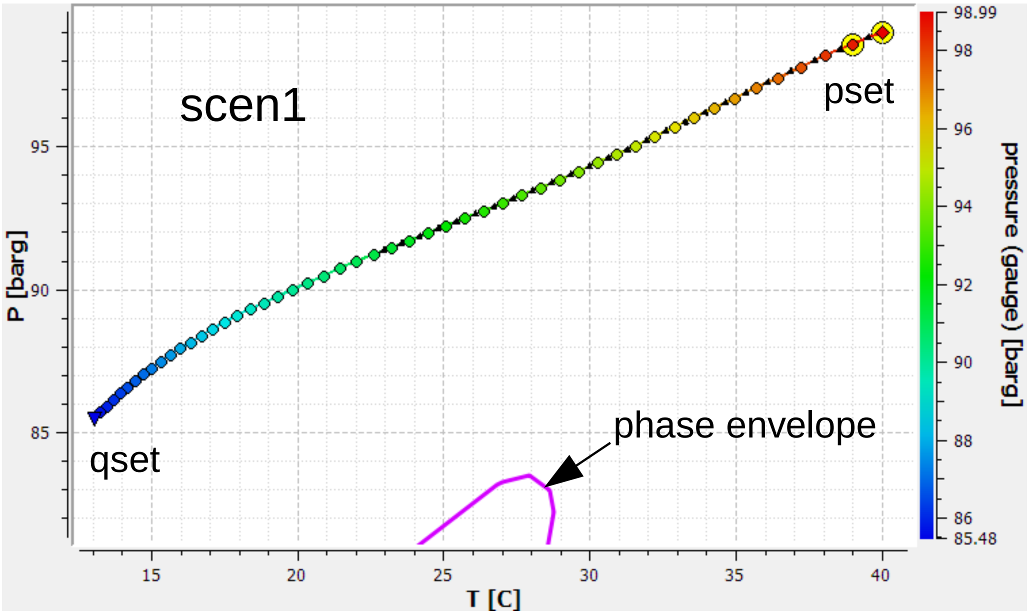
Numerical experiments

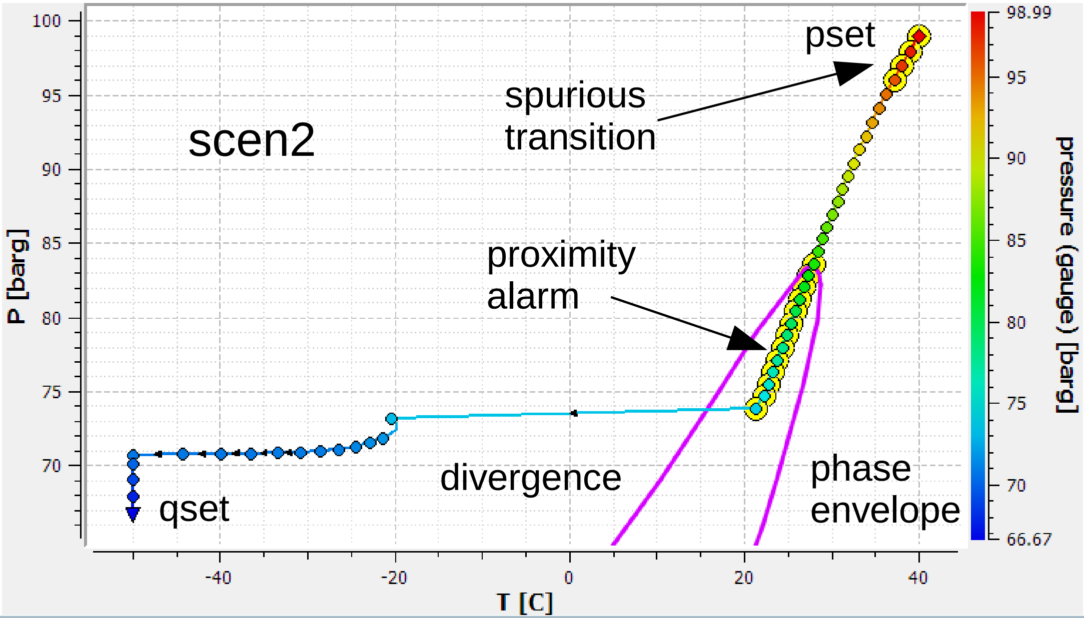
details



scen1

scen2





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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 CO_2 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