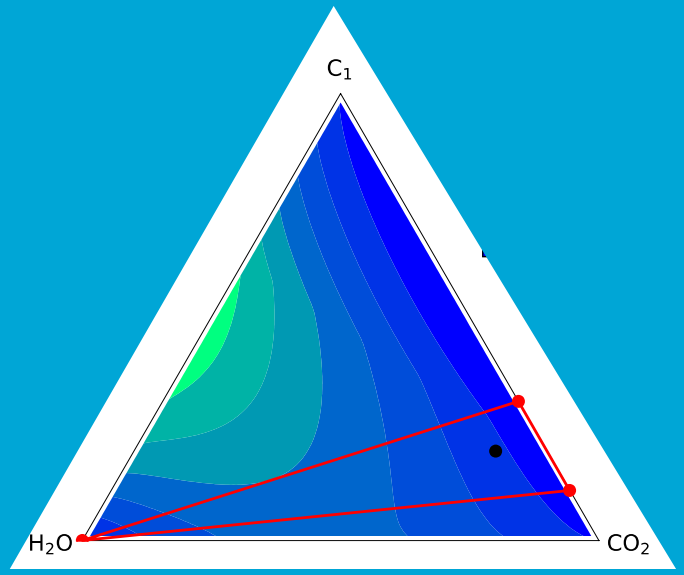
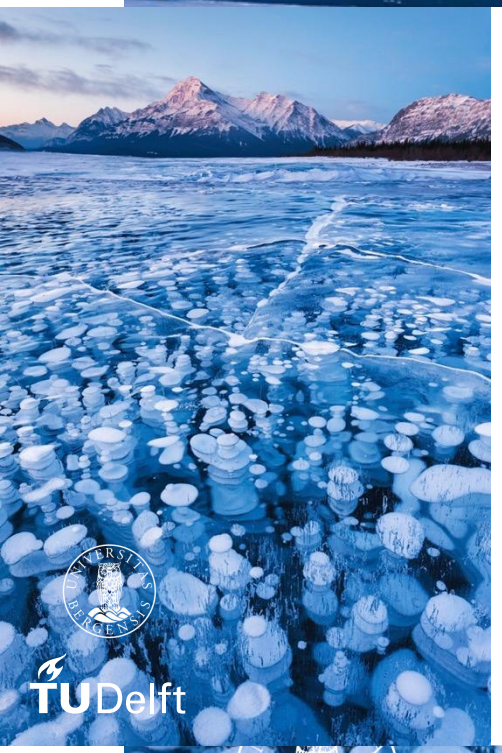
Multiphase equilibrium calculations with DARTS-flash

DARTS-thermodynamics workshop, 12 November 2024

Michiel Wapperom, Juan Heringer, Dan Nichita and Denis Voskov



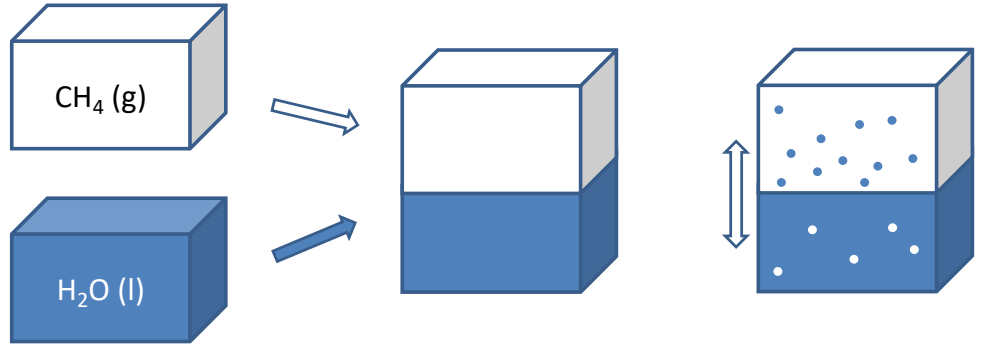


Predictive Modelling of Hydrate Formation and Dissociation

Michiel Wapperom
Under supervision of:
Dr. Denis Voskov, Xiaocong Lyu & Dr. Geir Ersland

Delft, 25 November 2019

3.3 Thermodynamics I



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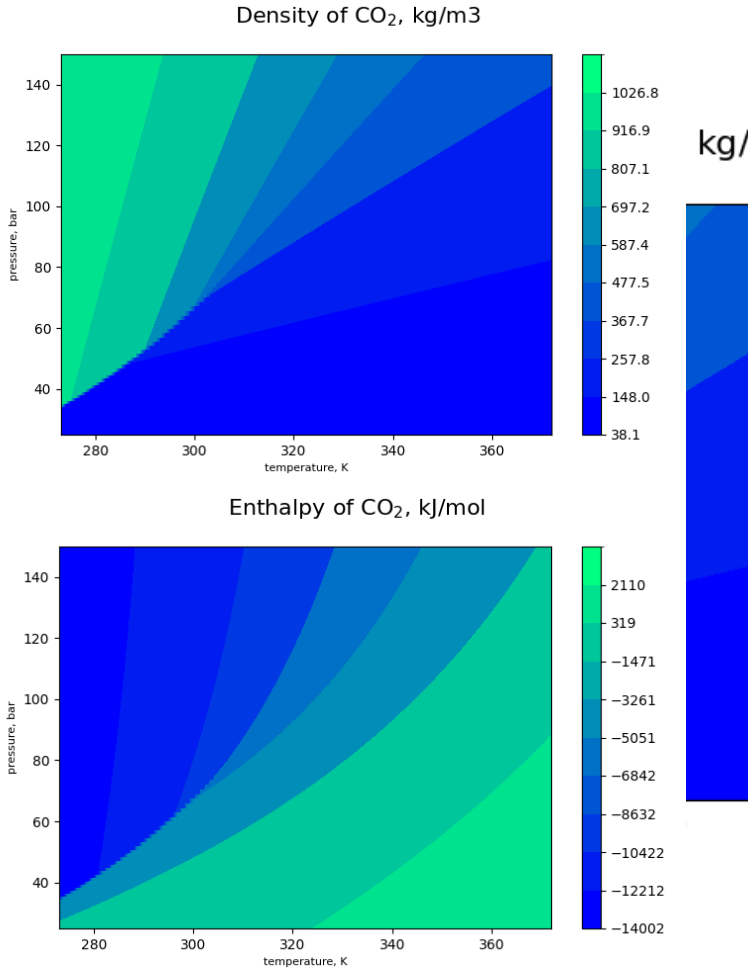
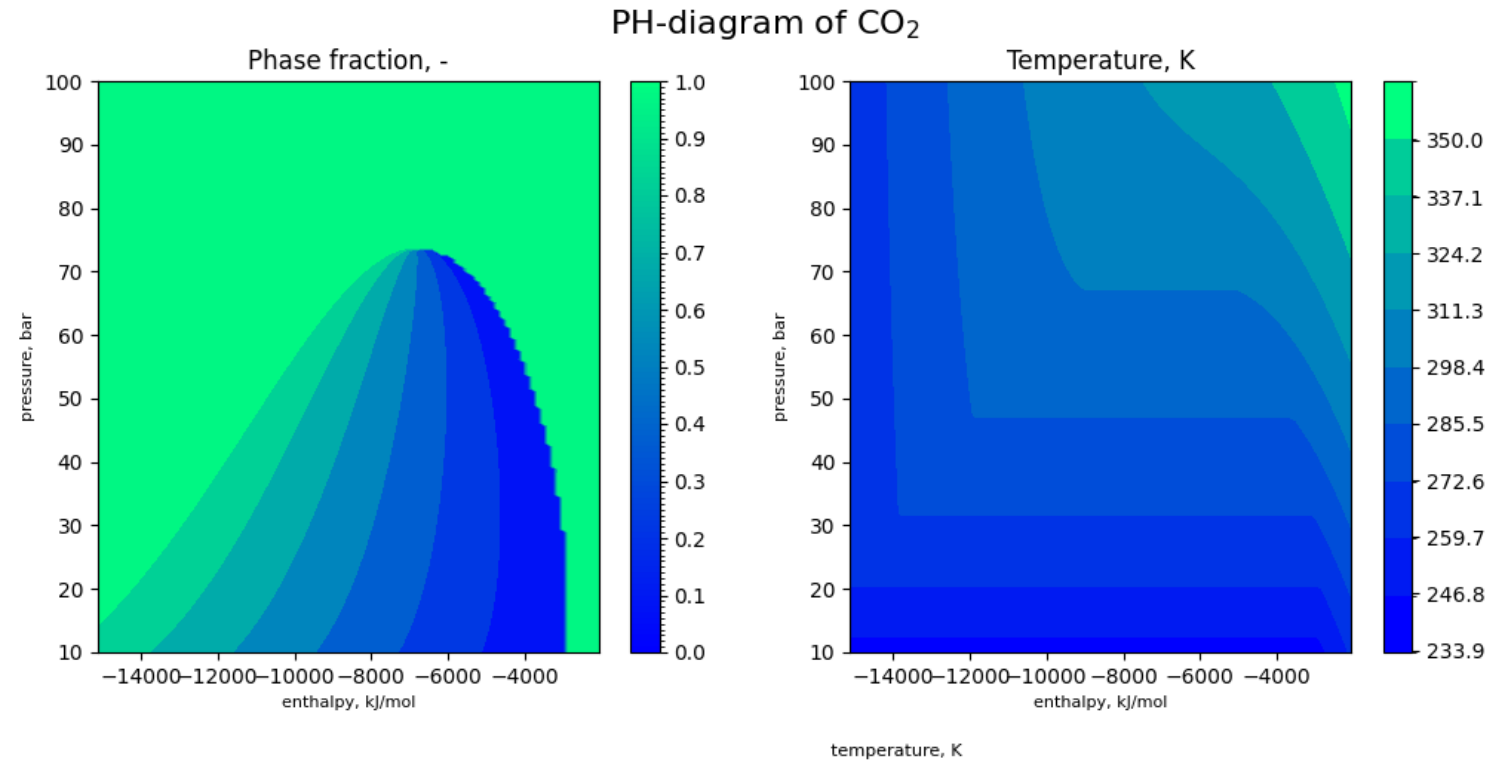
When we inject CO_2





Thermodynamic equilibrium

- Equilibrium state:
  - T, P, μ_i are uniform
  - Entropy S is at global maximum
  - State completely described by surfaces:

    (U,S,V,n), (H,S,P,n), (G,T,P,n) or (A,T,V,n)

- State specifications

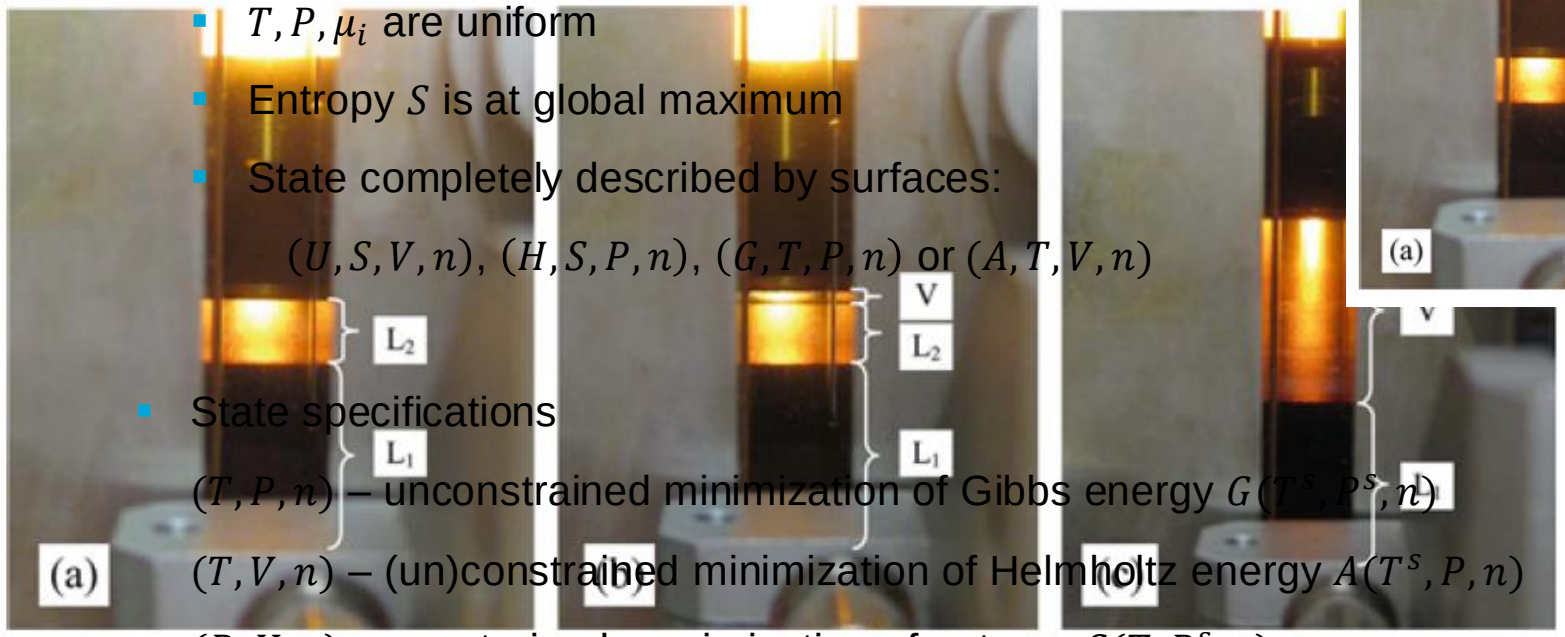
  (T,P,n) – unconstrained minimization of Gibbs energy $G(T^s,P^s,n)$

  (T,V,n) – (un)constrained minimization of Helmholtz energy $A(T^s,P,n)$

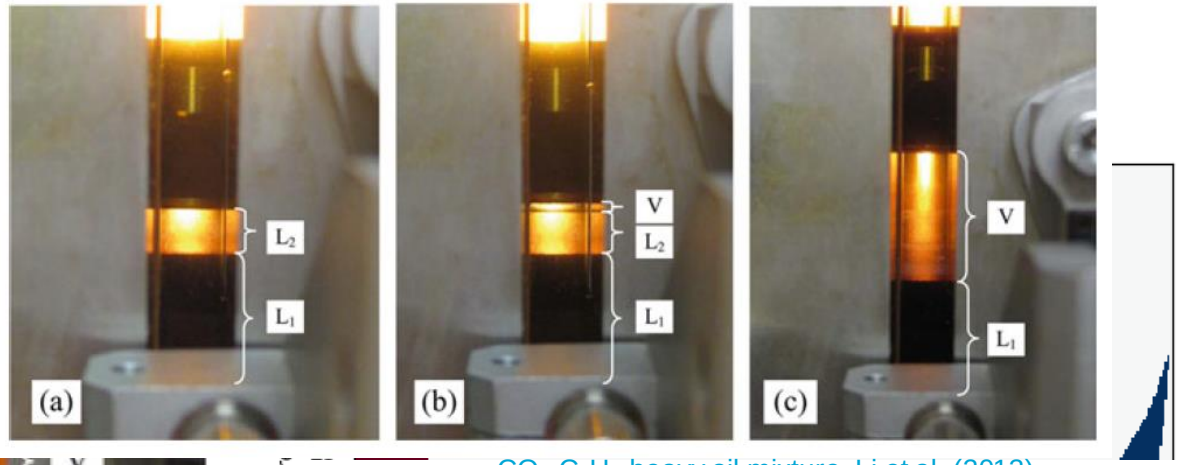
  (P,H,n) – constrained maximization of entropy $S(T,P^s,n)$

  s.t. $H(T,P^s,n)=H^s$

  (U,V,n) and (P,S,n) – constrained minimization of $-S$ and H



CO_2-C_3H_8-heavy oil mixture, Li et al. (2013)



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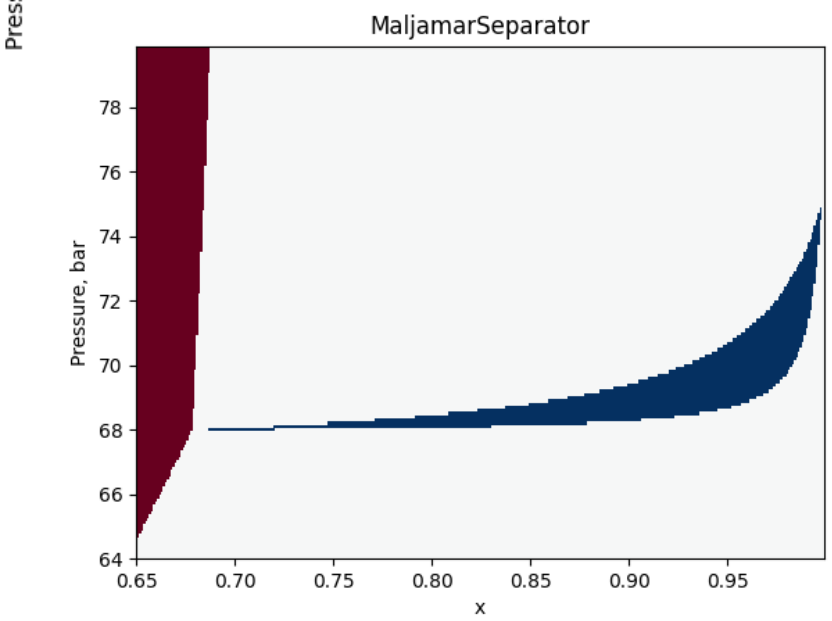


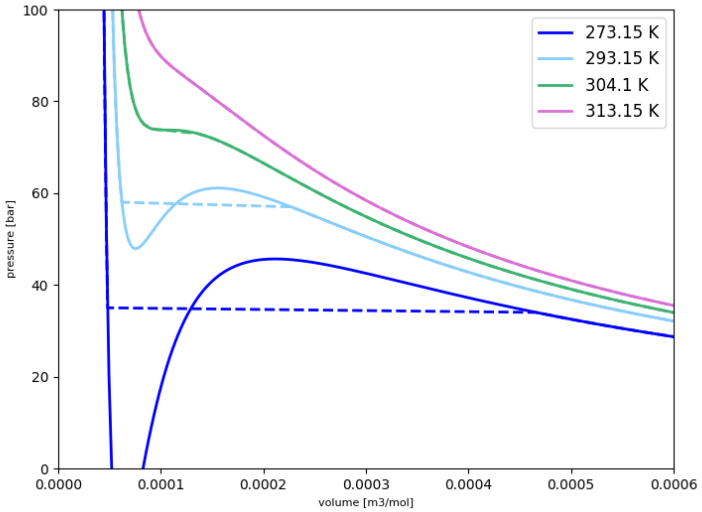
Thermodynamic models for fluid phases

- Van der Waals family EoS

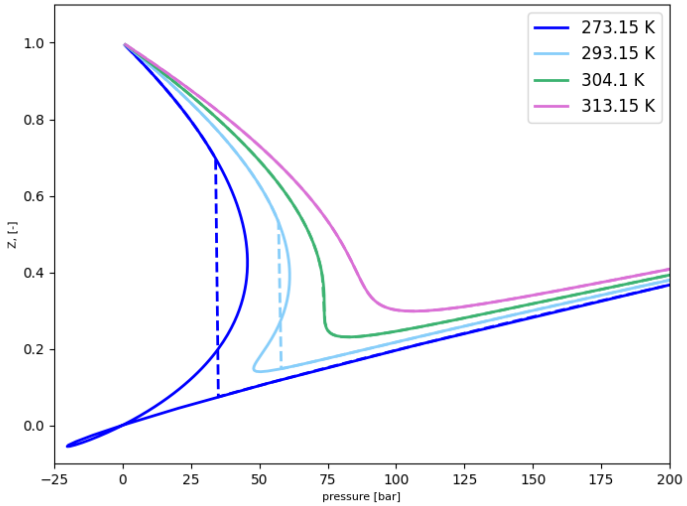
$$P = \frac{RT}{\bar{V} - b} - \frac{\alpha(T)a}{(\bar{V} + \delta_1 b)(\bar{V} + \delta_2 b)}$$

- In aqueous phase:
  - Polar and associating molecules
  - Ionic and coulombic interactions
  - Adequate alternative?

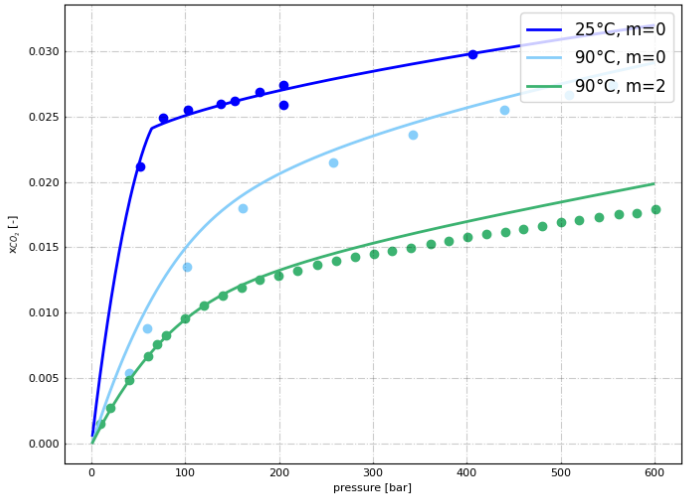
P-V diagram of CO_2



Compressibility factor Z of CO_2



CO_2 solubility in brine



Multiphase equilibrium

$$D = \left(1 - \sum_{i=1}^{n_c} Y_i\right) + \sum_{i=1}^{n_c} Y_i(\ln Y_i + \ln \varphi_i(\boldsymbol{Y}) - d_i)$$

- Stability test with $\boldsymbol{Y}$, $\ln \boldsymbol{Y}$ or $\boldsymbol{\alpha}$

$$g_i = \frac{\partial D}{\partial Y_i} = \ln Y_i + \ln \varphi_i(\boldsymbol{Y}) - d_i$$

  - Problem size: NC

$$\mathbf{H}\Delta\mathbf{n} = -\mathbf{g}$$

$$H_{ij} = \frac{\partial^2 G}{\partial n_{iL}\partial n_{jL}} = U_{ij} + \Phi_{ij}$$

Mass balance derivatives

Fugacity derivatives

  - SPD: Cholesky decomposition of $\boldsymbol{H}$
  - Not PD: perform SSI step

$$G = \sum_{i=1}^{n_c}\sum_{k=1}^{n_p} n_{ik} \ln f_{ik}$$

- Multiphase split with $\boldsymbol{n}$ or $\ln \boldsymbol{K}$

$$(g_i)_k = \frac{\partial G}{\partial n_{ik}} = \ln f_{ik} - \ln f_{iR} = \ln K_{ik} + \ln \varphi_{ik} - \ln \varphi_{iR}$$

  - Problem size: (NP-1)NC

$$\Delta\mathbf{n} = \mathbf{U}^{-1}\Delta\ln\mathbf{K}$$

$$\mathbf{J}\Delta\ln\mathbf{K} = -\mathbf{g}$$

$$\boldsymbol{J} = \mathbf{H}\mathbf{U}^{-1} = \boldsymbol{I} + \boldsymbol{\Phi}\mathbf{U}^{-1}$$

  - Better scaled, condition number improved in $\boldsymbol{J}$
  - Non-symmetric: LU factorization of $\boldsymbol{J}$
  - Or: solve $\boldsymbol{\Delta n}$ and update $\boldsymbol{\Delta \ln K = U \Delta n}$

Petitfrere and Nichita (2015, 2016)

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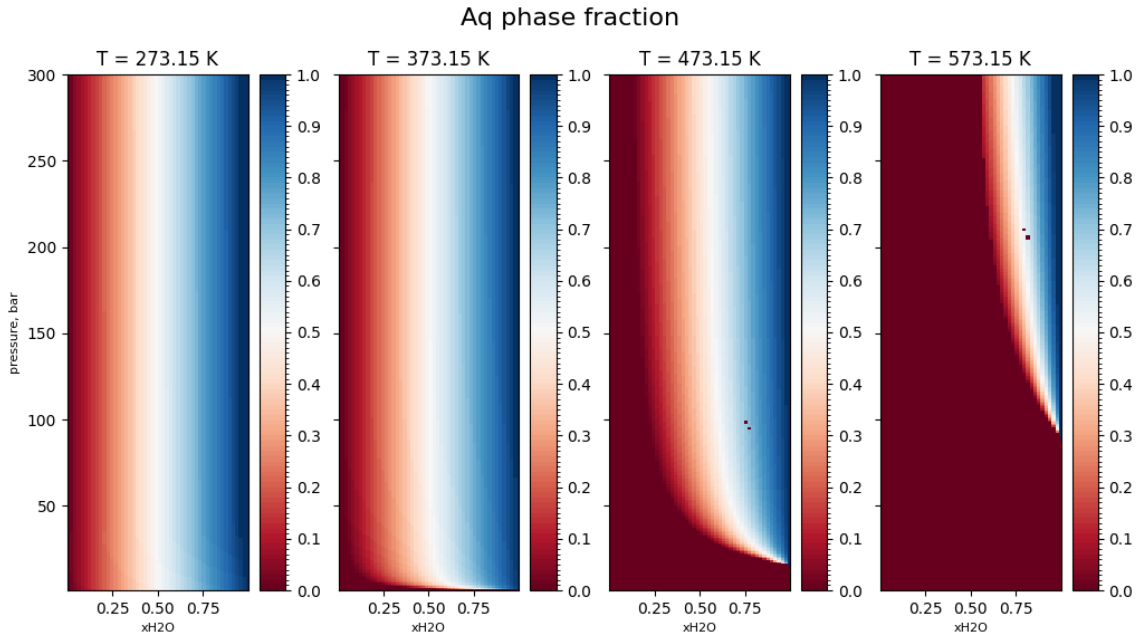
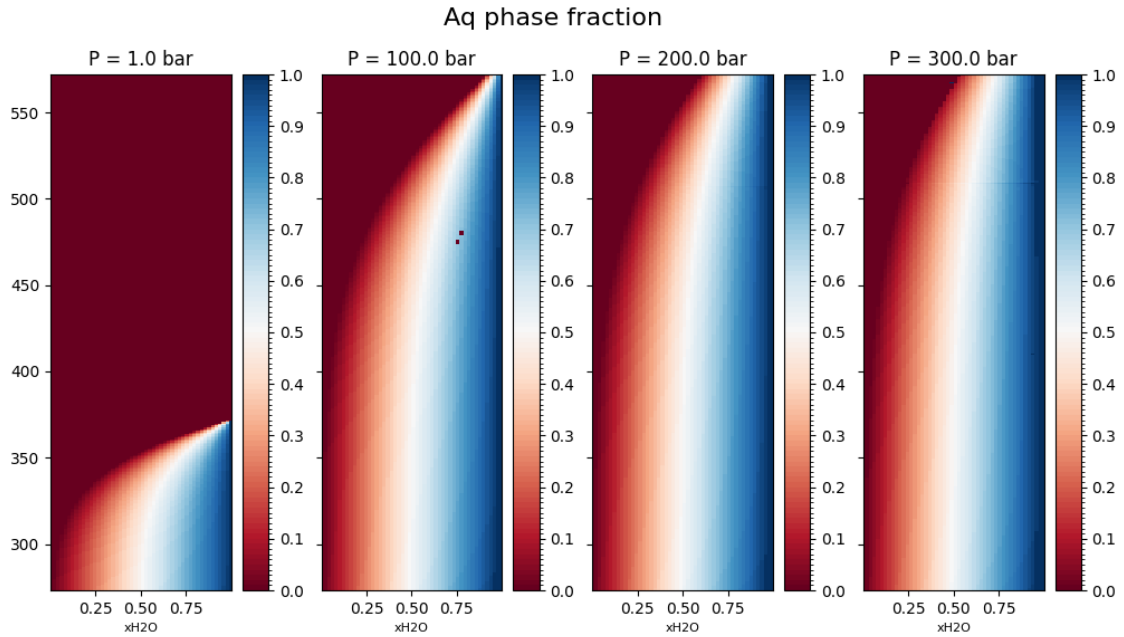
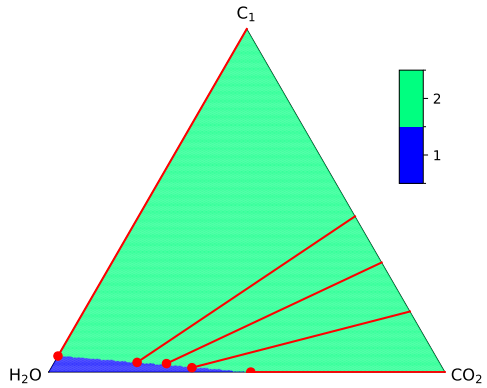
Gibbs energy analysis of H_2O-CO_2 system



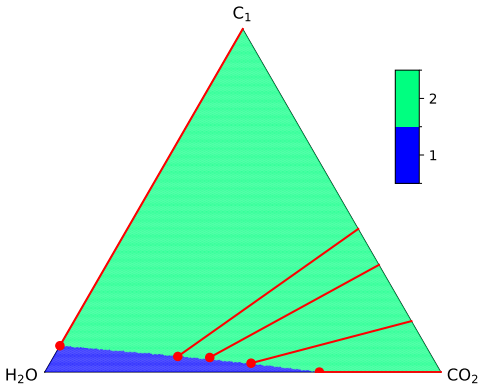


Multicomponent systems: depleted gas field

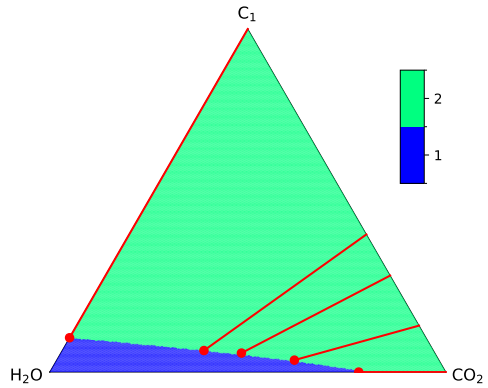
Number of phases for H_2O-CO_2-C_1 at P = 107.0 bar and T = 375.6 K



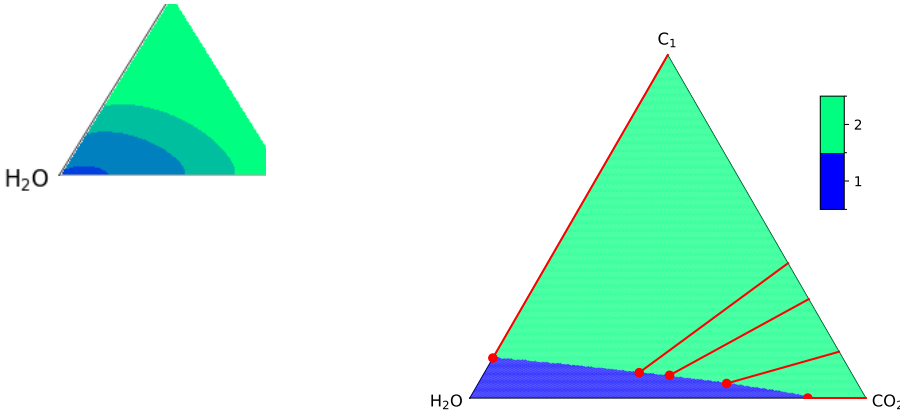
Number of phases for H_2O-CO_2-C_1 at P = 205.0 bar and T = 375.6 K



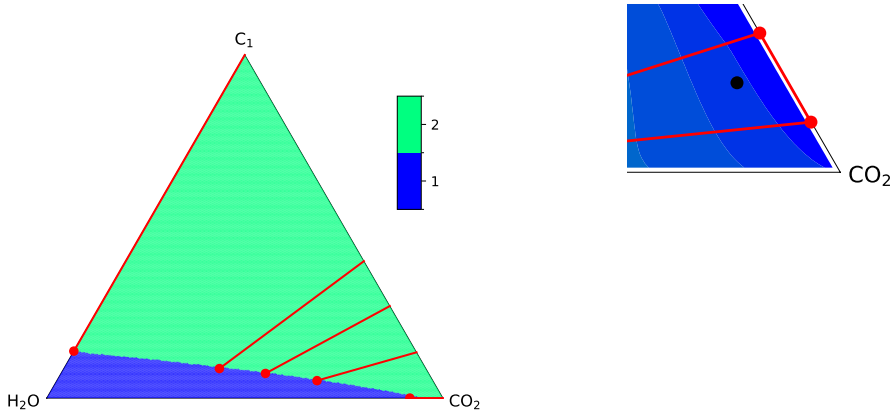
Number of phases for H_2O-CO_2-C_1 at P = 303.0 bar and T = 375.6 K



Number of phases for H_2O-CO_2-C_1 at P = 402.0 bar and T = 375.6 K

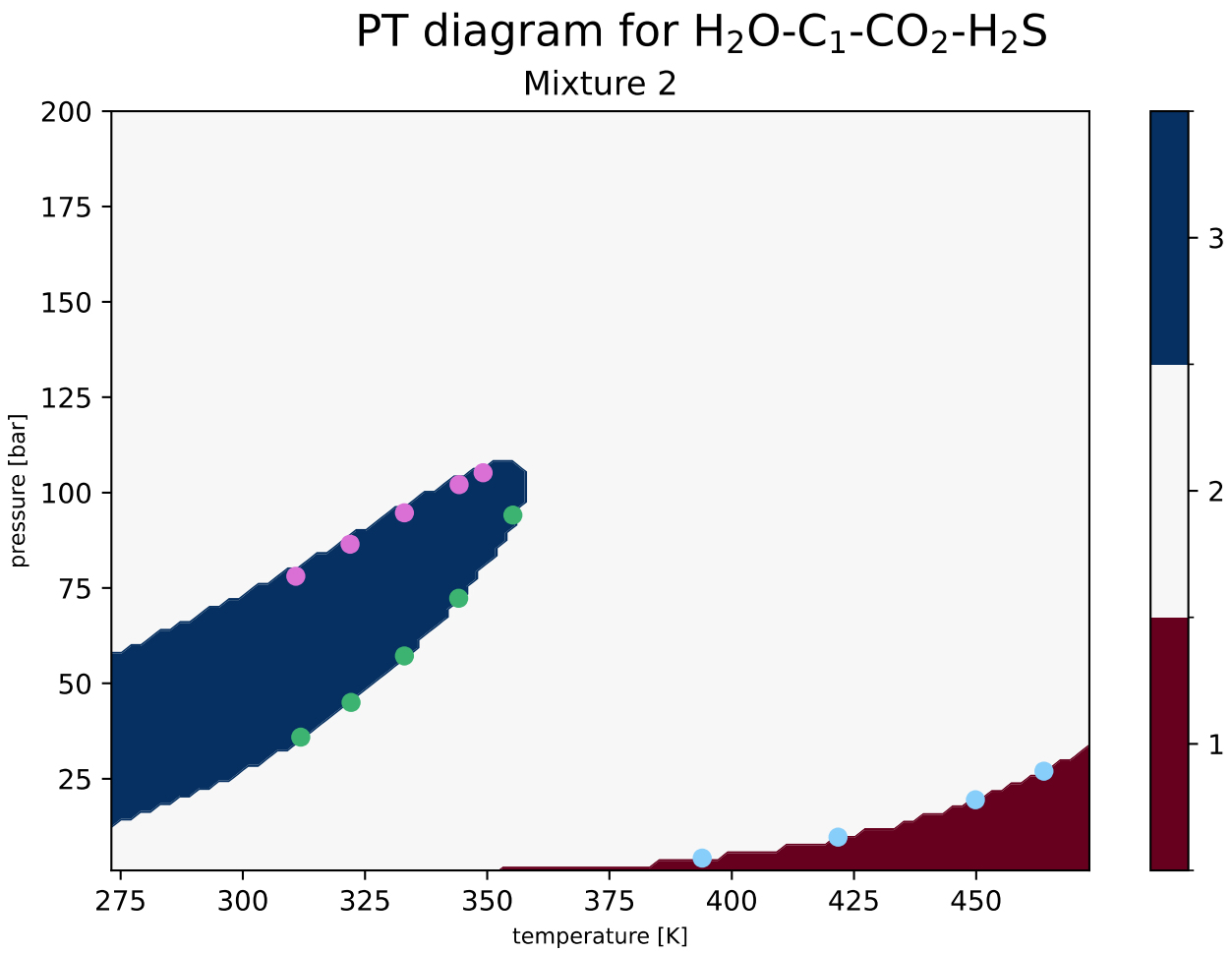


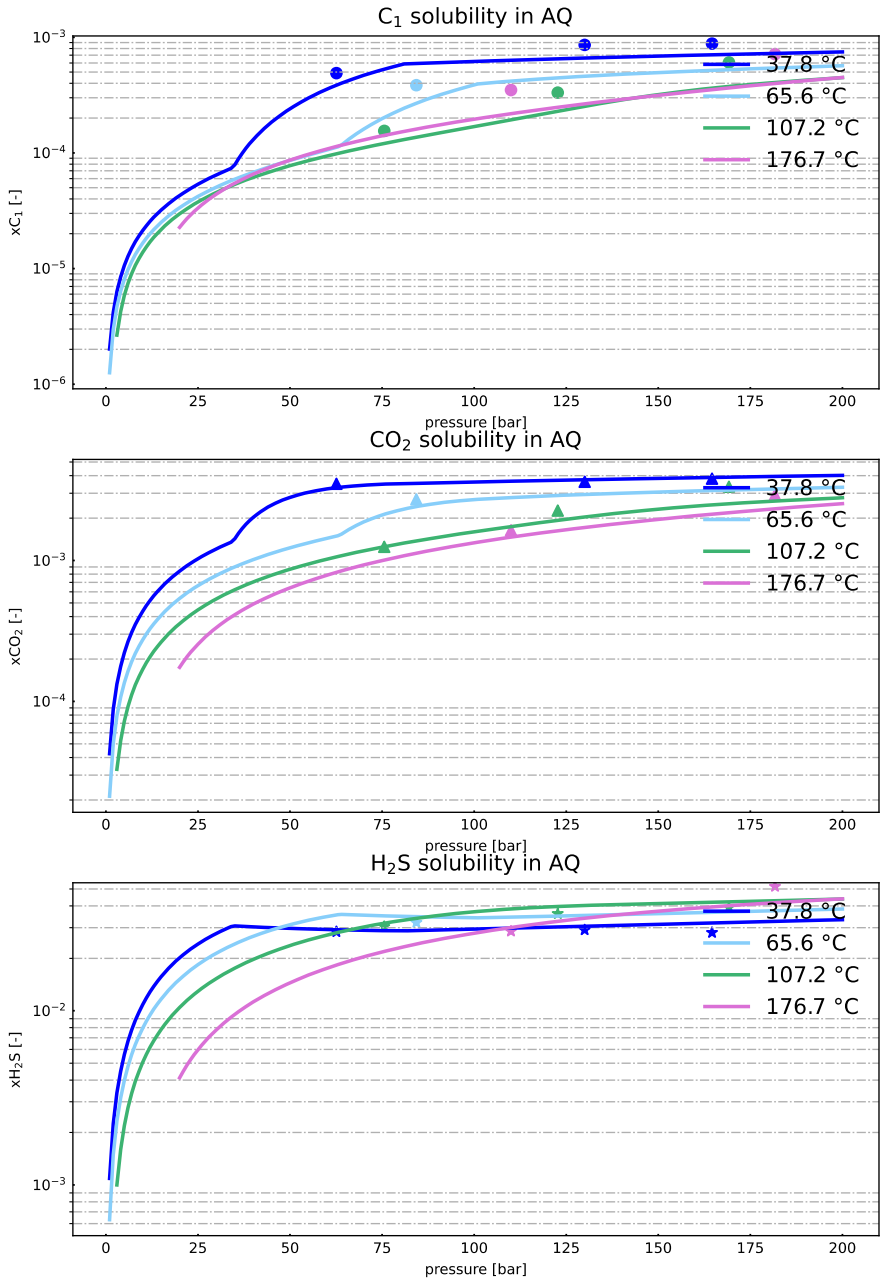
Number of phases for H_2O-CO_2-C_1 at P = 499.0 bar and T = 375.6 K



Data from Qin et al. (2008)

Multiphase equilibria





Data from Huang et al. (1985)

Thermodynamic models for hydrates

- Van der Waals and Platteeuw (1958)
  - Chemical potential change upon cage filling

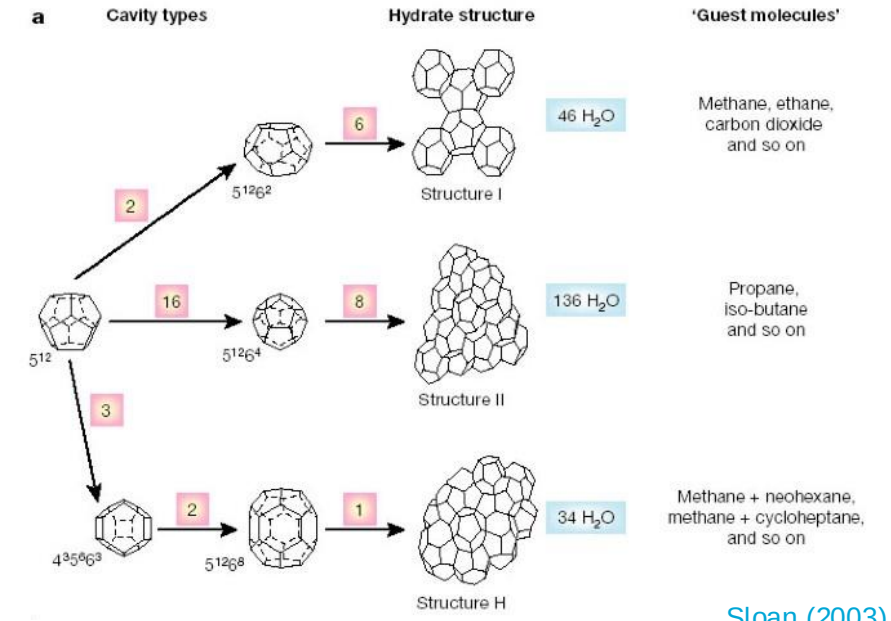
$$\frac{\Delta\mu_{w,H}}{RT} = \frac{\mu_{w,H}}{RT} - \frac{g_{w,\beta}}{RT} = \sum_m \nu_m \ln\left(1 - \sum_j \theta_{jm}\right)$$

  - Fugacity related to reference phase

$$f_{w,H} = f_{w,A} \exp\left[\frac{\Delta\mu_{w,H} - \Delta\mu_{w,A}}{RT}\right]$$

  - Langmuir 'adsorption'

$$\theta_{jm} = \frac{C_{jm} f_j}{1 + \sum_k C_{km} f_k}$$



Sloan (2003)

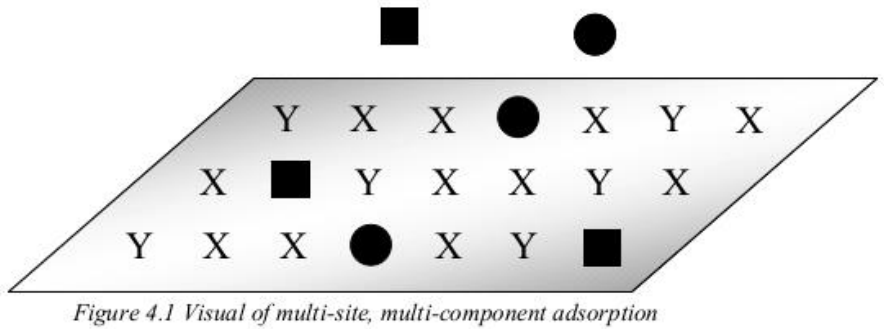
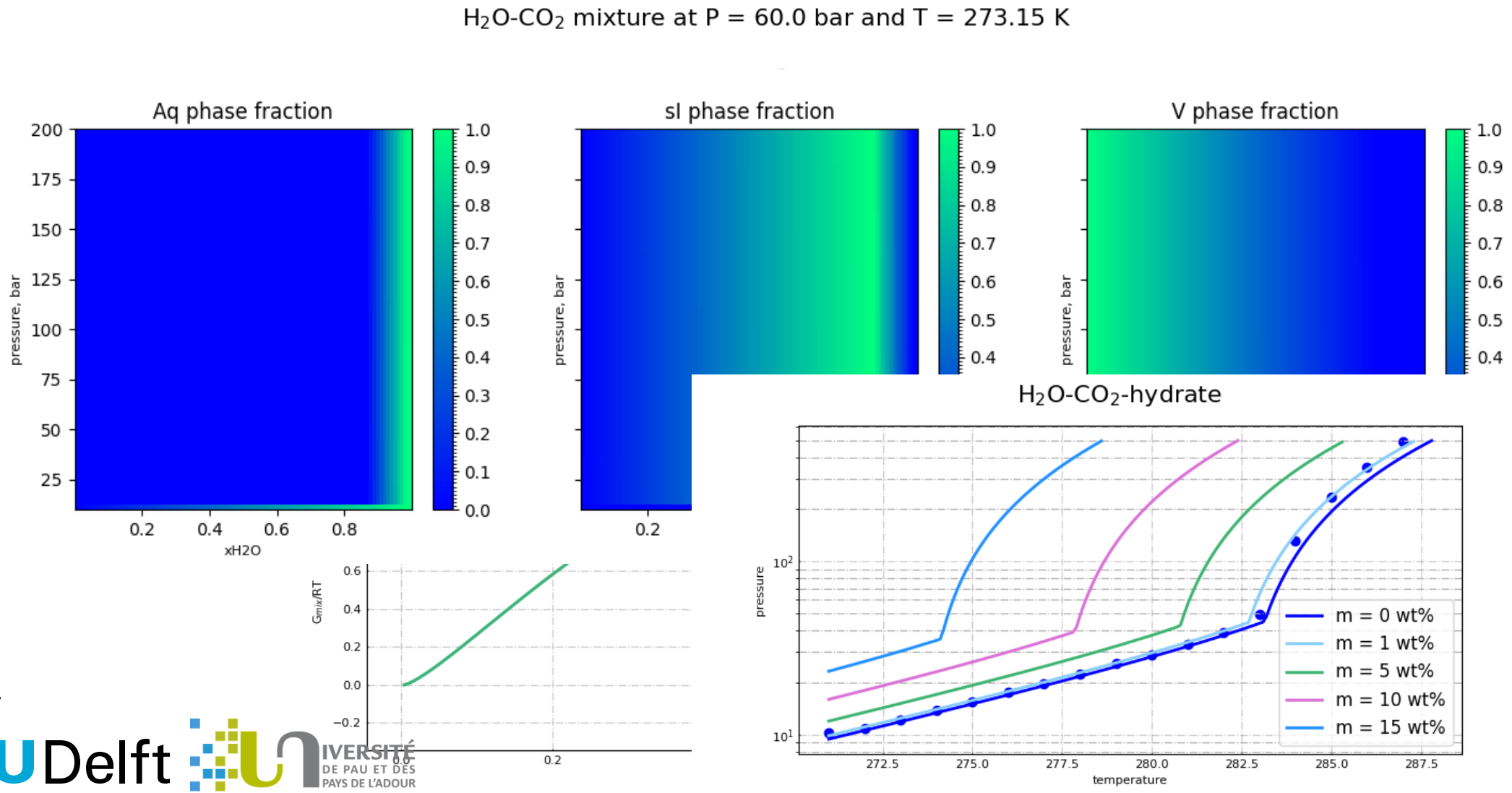


Figure 4.1 Visual of multi-site, multi-component adsorption

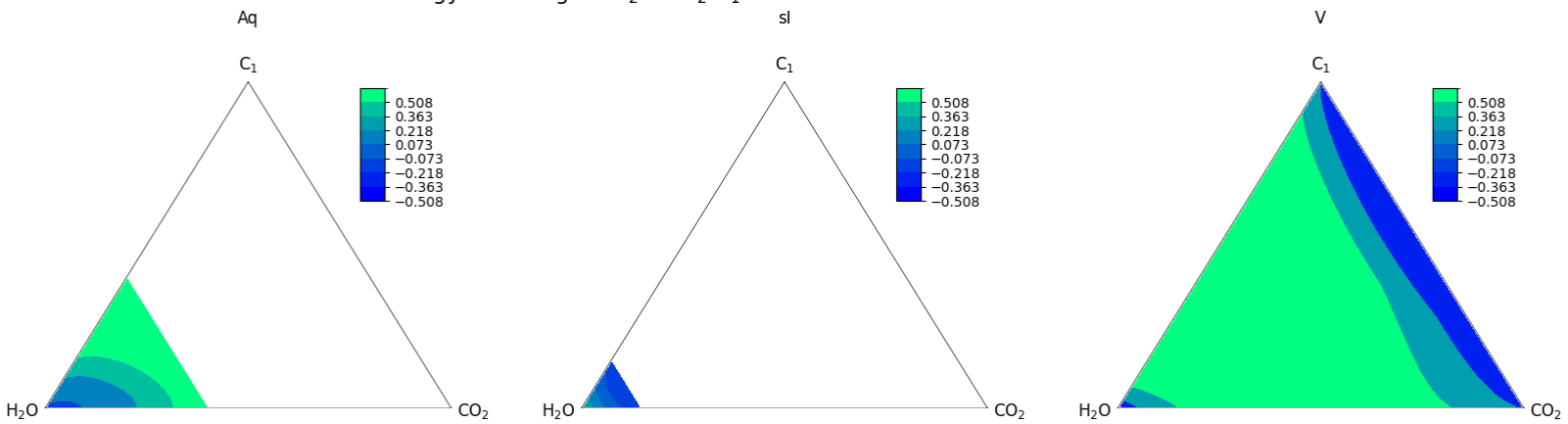
Ballard (2002)

At hydrate formation conditions

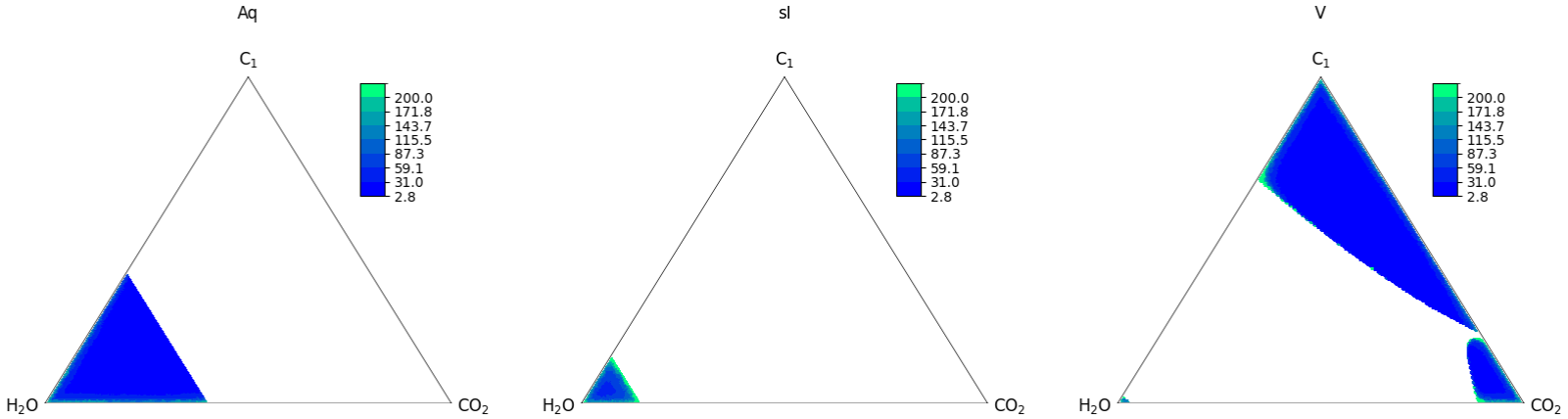


Multicomponent hydrates

Gibbs energy of mixing for H_2O-CO_2-C_1 mixture at P = 60.0 bar and T = 273.15 K



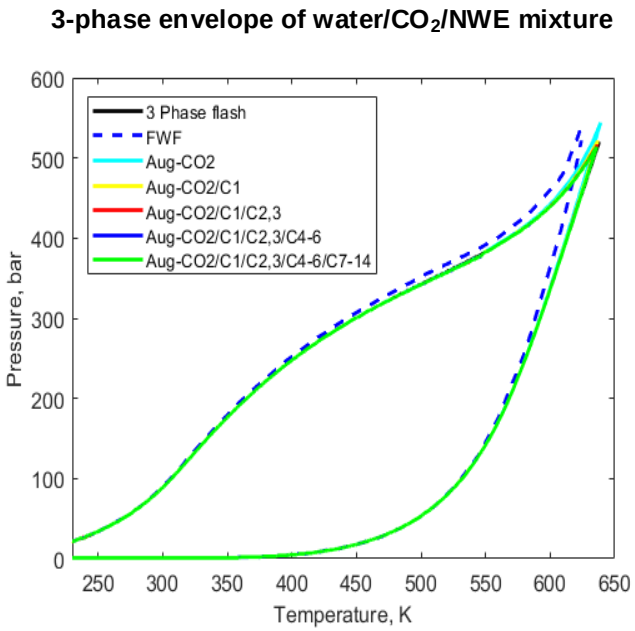
Hessian condition number for H_2O-CO_2-C_1 mixture at P = 60.0 bar and T = 273.15 K

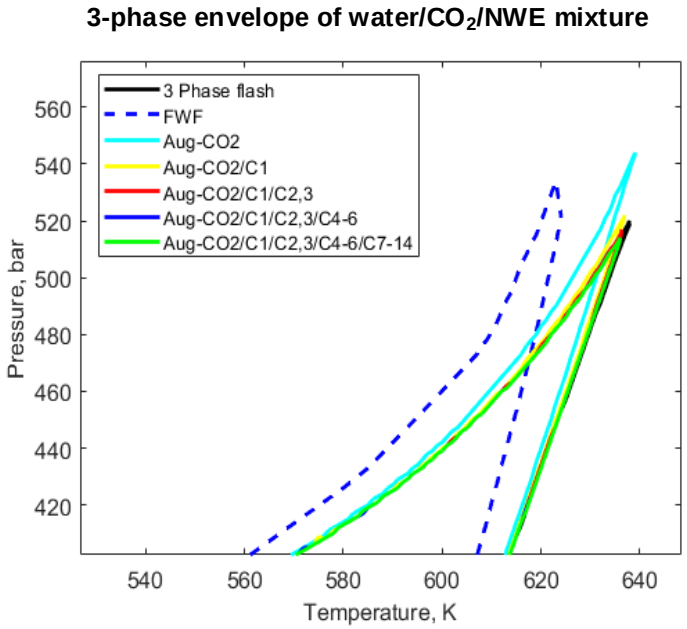


Free-water flash – selective solubility

- Not every chemical species is present in every phase
  - Brine – H_2O, ions, CH_4, CO_2, others?
  - Hydrates – H_2O and CH_4, CO_2, N_2, etc.
  - Ice – H_2O
  - Salt – NaCl, $CaCl_2$, etc.
  - Wax, asphaltenes
  - Solid solutions

- More details by Juan!





Multiphase equilibrium at other state specifications

- PT – Isobaric-isothermal
  - Both stability and flash are formulated as unconstrained optimization problem
  - ***PT*-flash not able to capture phase transitions**
- PHN – Isobaric-isenthalpic
  - **Able to capture phase transitions**
  - Suitable for thermal-compositional simulation of isenthalpic processes like in CO_2 injection
- PSN – Isobaric-isentropic
  - Compressor and turbines design
- VTN – Isochoric-isothermal
  - Phase equilibrium in closed vessels
- UVN – Isoenergetic-isochoric
  - Simulating two-phase pipe flow

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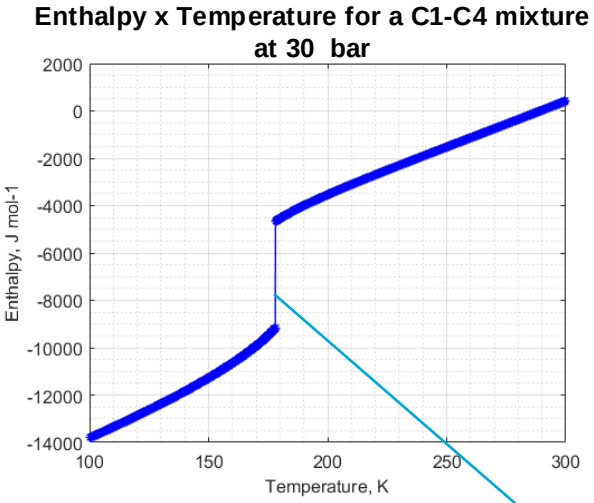
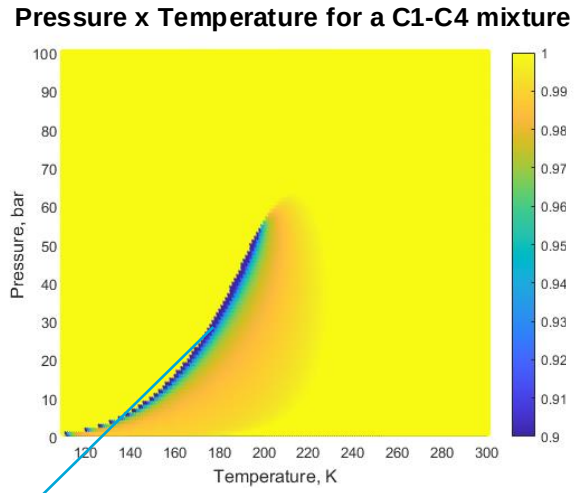
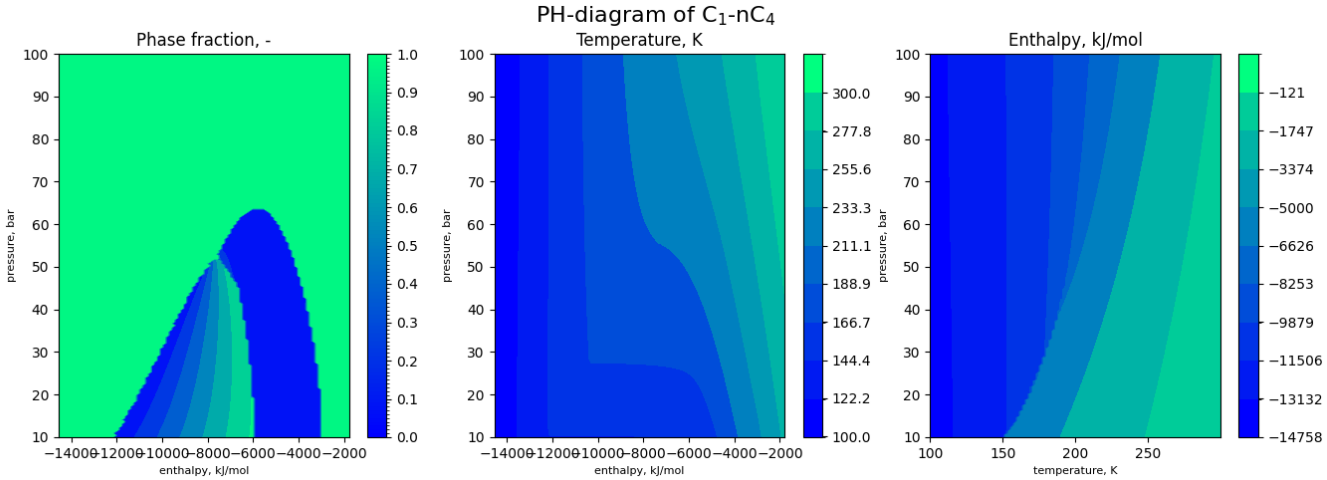
Isenthalpic flash

- Used to avoid convergence issues in thermal-compositional reservoir simulator
- Nested loop – a root-finding method (Brent, 1973) that uses PT-flash to update enthalpy $H(P, T, \boldsymbol{n})$
- More details by Lingfei!





Narrow-boiling behaviour



DARTS-flash v1.0.0

- Features
  - Robust and efficient multiphase PT/PH-flash with hybrid-EoS
  - Augmented free-water flash/Selective solubility methods
  - Solubility curves, phase diagrams, EoS computations, hydrate equilibrium curves
  - (derivatives of flash for process and reservoir simulation)

- Interface
  - C++
  - Python
  - GUI

  - gitlab.com/open-darts/darts-flash
  - pip install open-darts-flash

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Acknowledgements

- We acknowledge TotalEnergies for financial support