Fermi-Jagla Potential –A spherically symmetric potential mimics water

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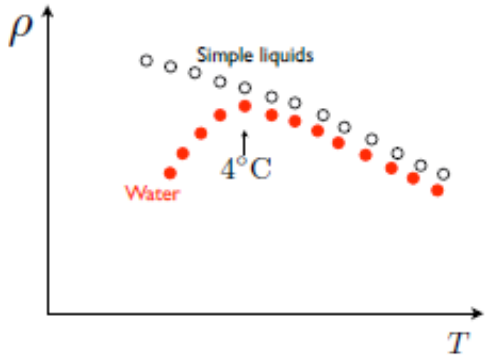
Outline

- **Introduction**
  - Water
  - Jagla model
  - Fermi-Jagla model
- **Methods**
  - Fermi-Jagla model with Discrete Molecular Dynamics (DMD)
- **Results**
  - The Liquid Liquid Critical Point (LLCP)
  - The isobaric specific heat (C_p) of Fermi-Jagla Liquid
  - Phase Flipping of Fermi-Jagla Liquid
- **Conclusion**

Intro: Water -- A Mysterious Liquid

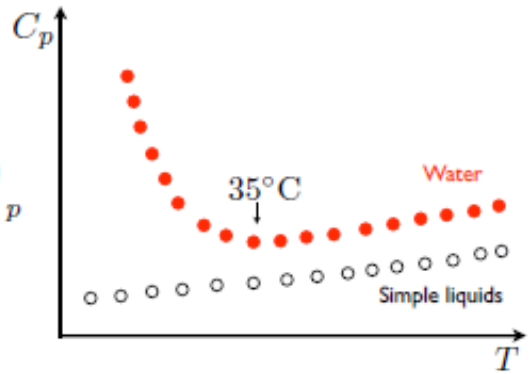
Water has more than 60 anomalies (http://www.lsbu.ac.uk/water/anmlies.html)

density



heat capacity

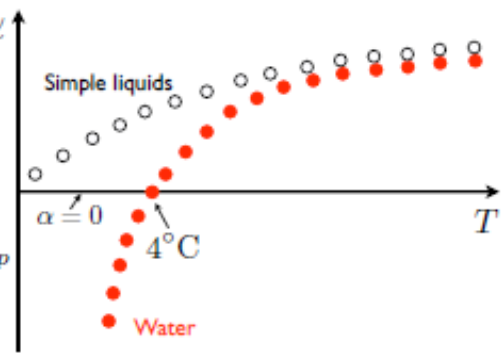
$$C_p = T\left(\frac{\partial S}{\partial T}\right)_p$$



$$< (\delta S)^2 >= N k_B C_p$$

thermal expansion coefficient

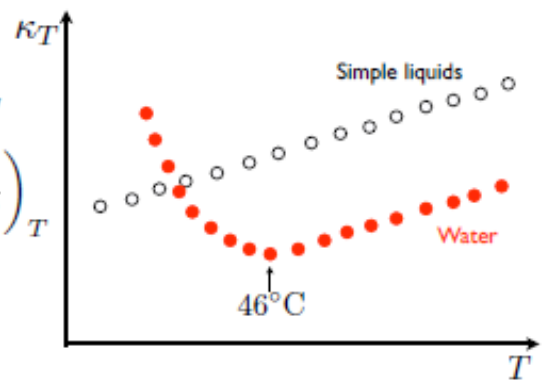
$$\alpha = -\frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_p$$



$$< (\delta S \delta V) >= V k_B T \alpha$$

isothermal compressibility

$$\kappa_T = -\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_T$$

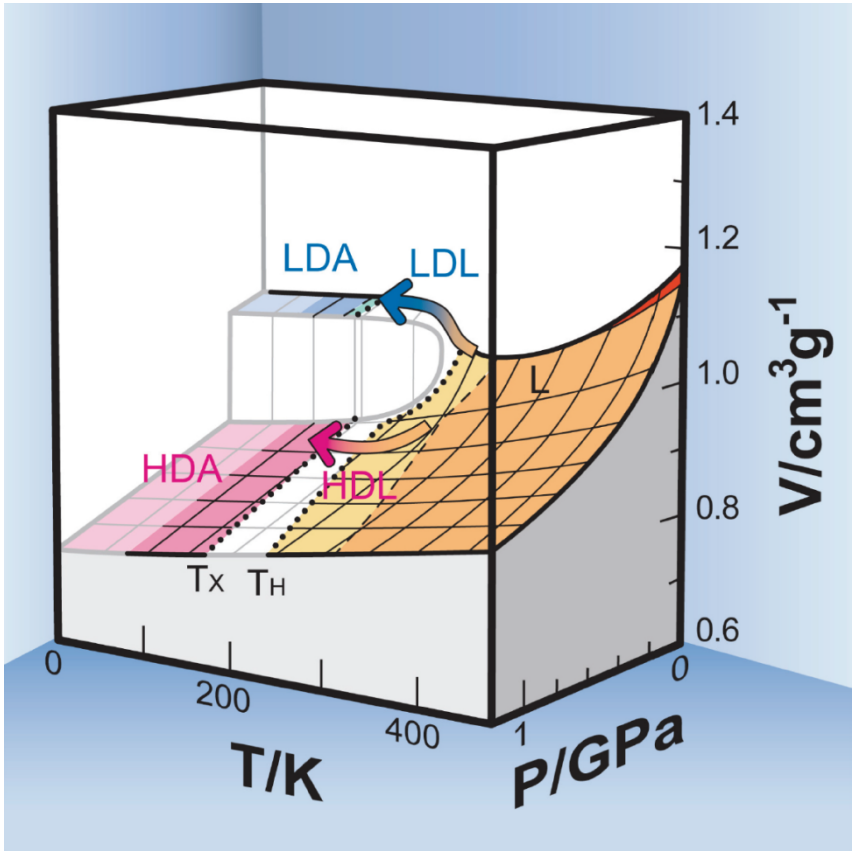


$$< (\delta V)^2 >= V k_B T \kappa_T$$

Intro: Water -- Liquid-Liquid Phase Transition

Hypothesis
(Poole/Sciortino/Essmann/Stanley, 1992)

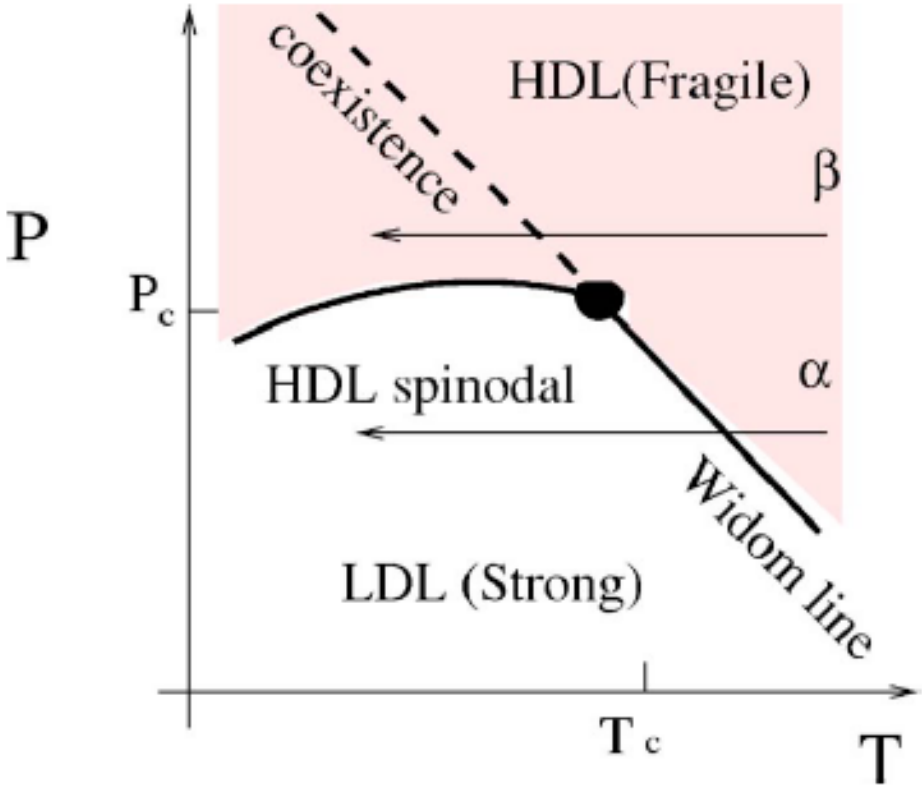
- Two liquids below nucleation temperature:
  - Low density liquid (LDL)
  - High density liquid (HDL)
  - Low density amorphous (LDA)
  - High density amorphous (HDA)
- Separated by liquid-liquid phase transition
- Ending in liquid-liquid critical point



Cover of JPC, volume 115, 8 Dec 2011

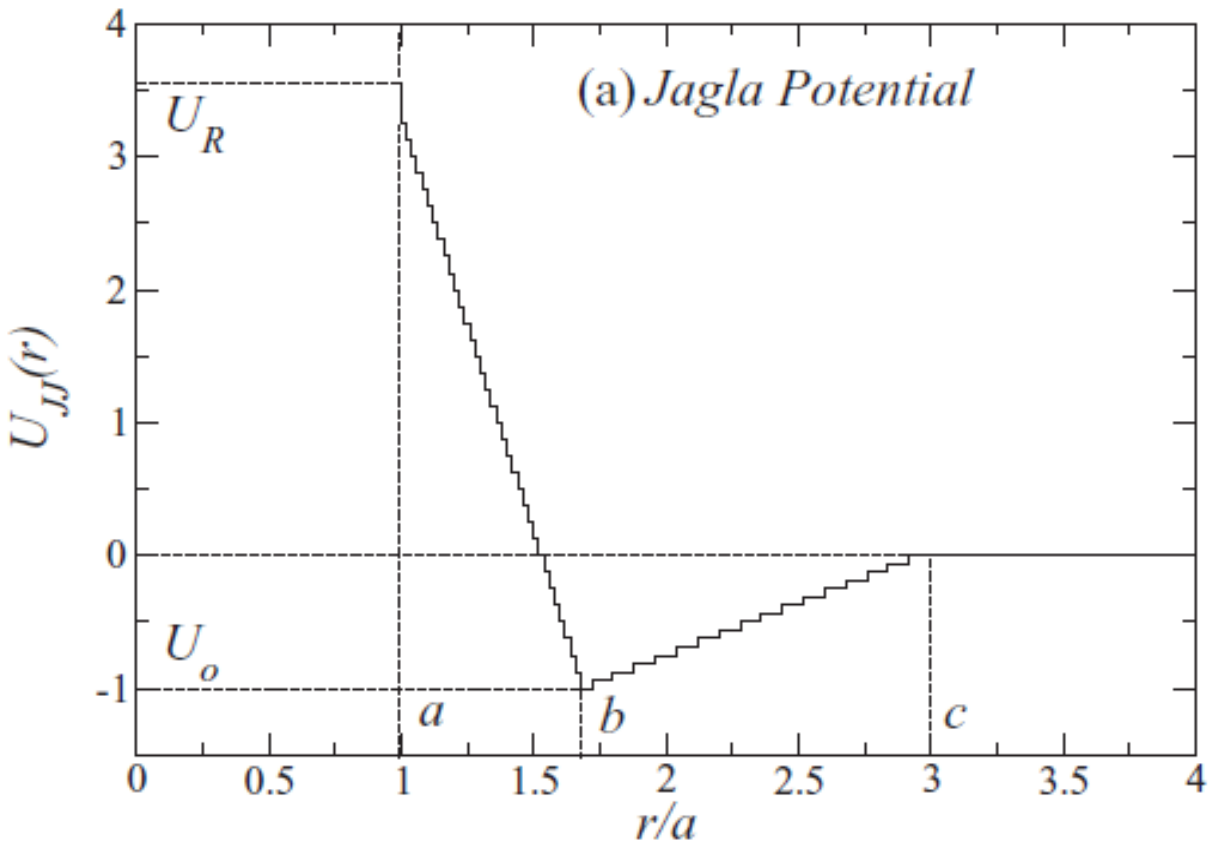
Intro: The Widom line of Real Water

In real water, the Widom Line has a negative slope.



Intro: Jagla Model

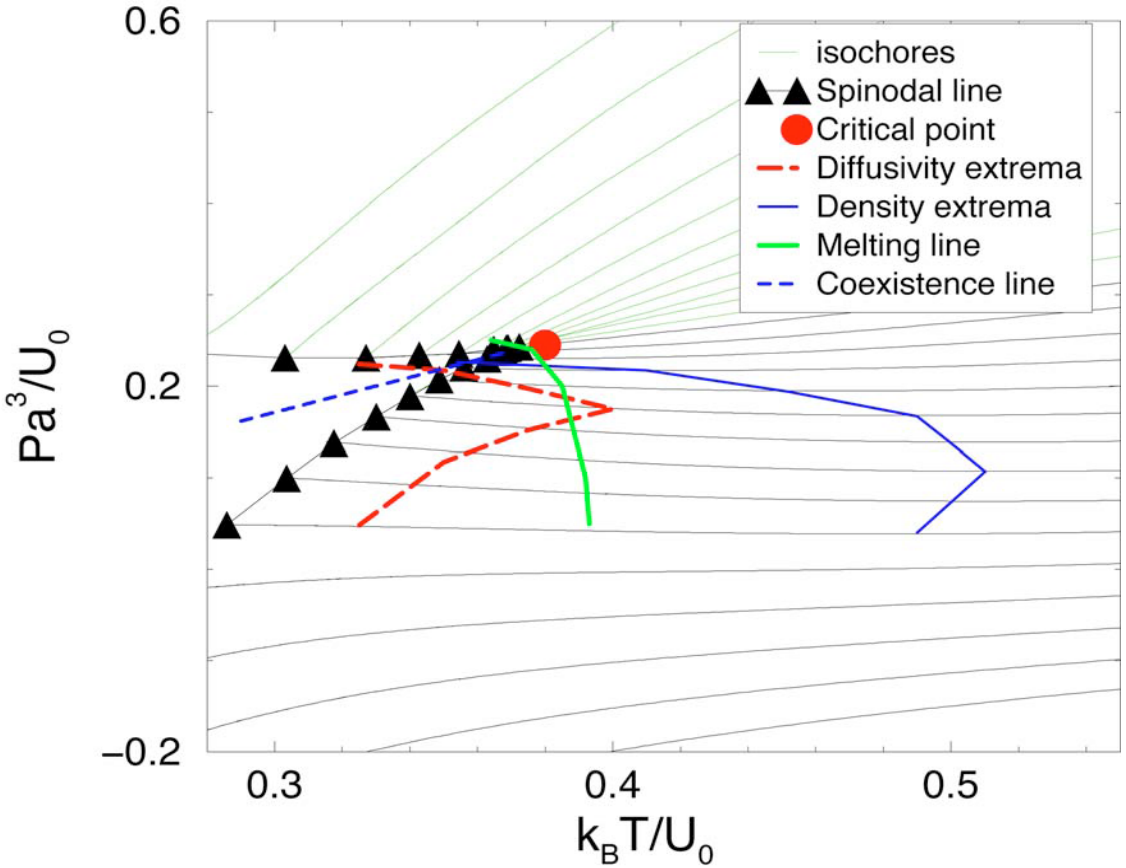
- b=1.72a, c=3a



Intro: Jagla Model -- Isochores

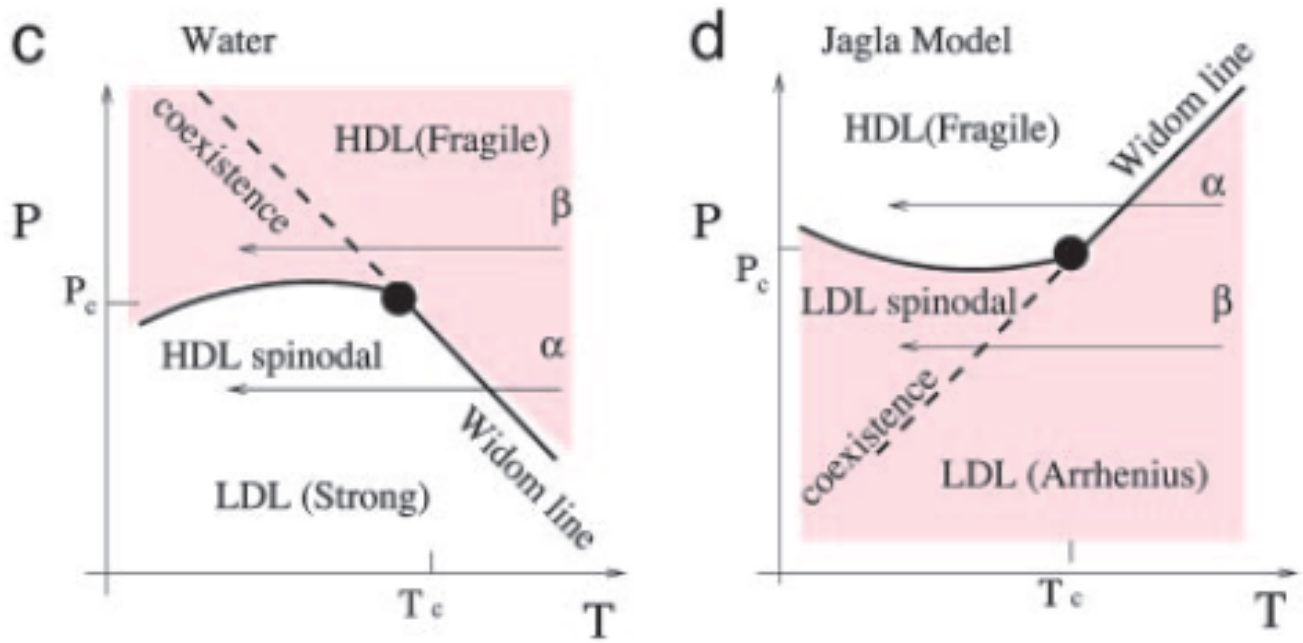
- Coexistence line has a positive slope, unlike real water.

  Limei Xu et al. J.Phys: Condens. Matter 18, 2239 (2006)

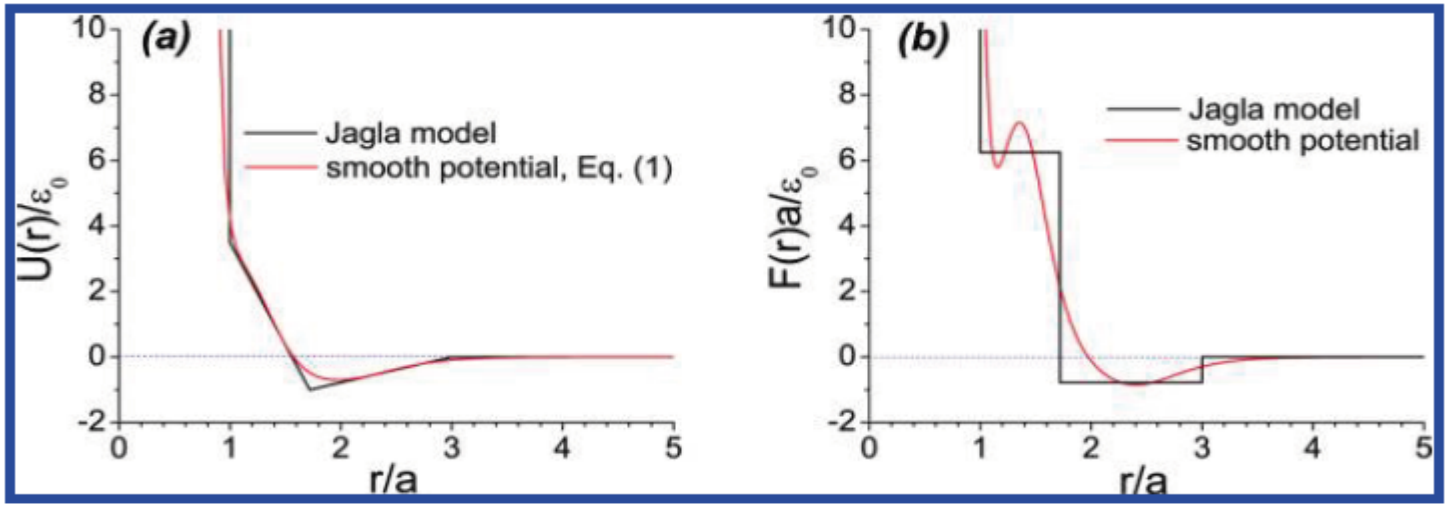


Intro: The difference between Real Water and Jagla Liquid

In real water, the Widom Line has a negative slope. Xu et al. PNAS, V102, P16558 (2005)



Intro: Fermi-Jagla Model



$$U(r) = \epsilon_0 \left[(a/r)^n + \frac{A_0}{1 + \exp\left[\frac{A_1}{A_0}(r/a - A_2)\right]} - \frac{B_0}{1 + \exp\left[\frac{B_1}{B_0}(r/a - B_2)\right]} \right] \quad (1)$$

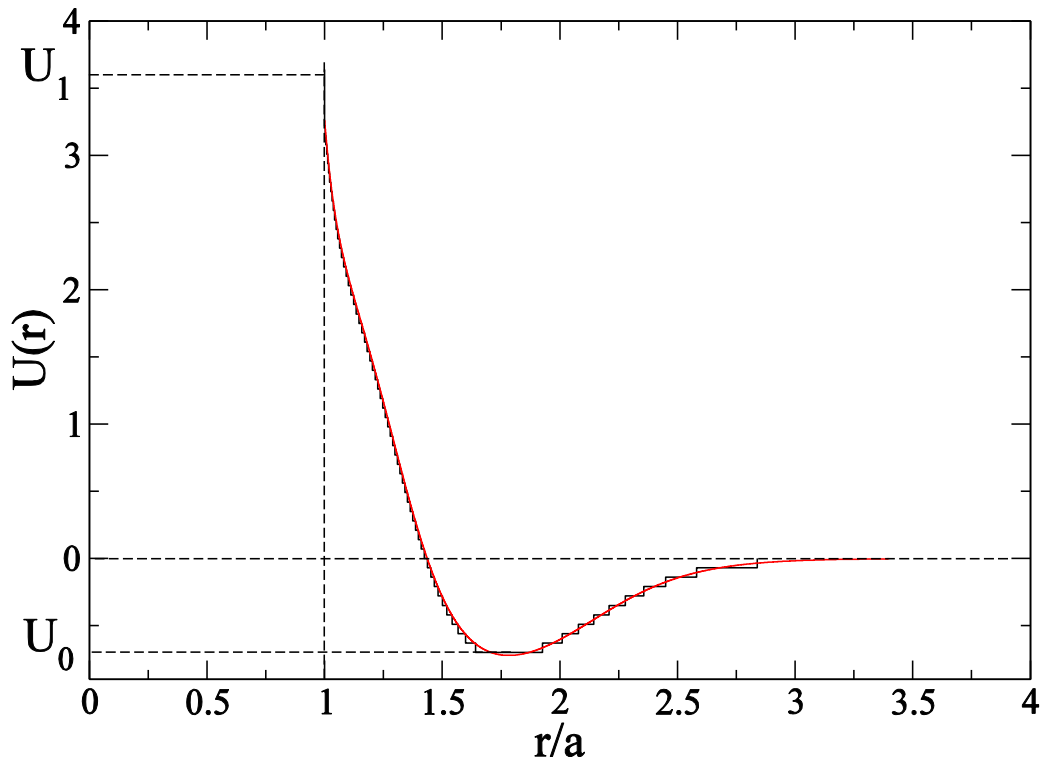
- Can reproduce the water anomalies.
- Has LLCP
- May have Widom line with a negative slope
- Temperature of $C_{\downarrow p\uparrow}$ maximum cannot be reached!!

J.Y. Abraham, S.V.Buldyrev and N. Giovambasstista, J. Phys. Chem.B 115, 14229(2011)

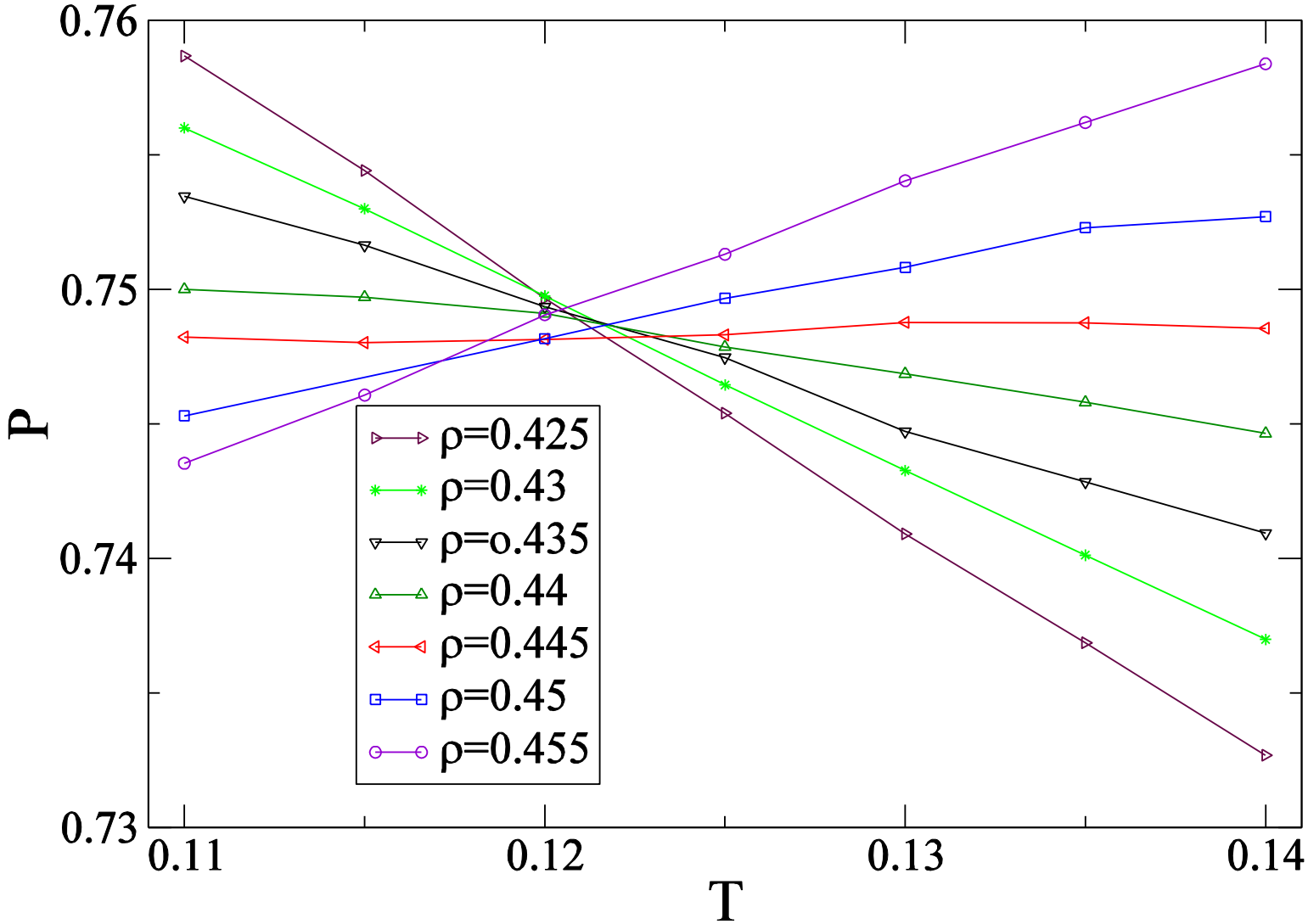
Method: Fermi-Jagla model in DMD

- Goals:
  - reach maximum of $C\downarrow p\uparrow$
  - Negative slope,

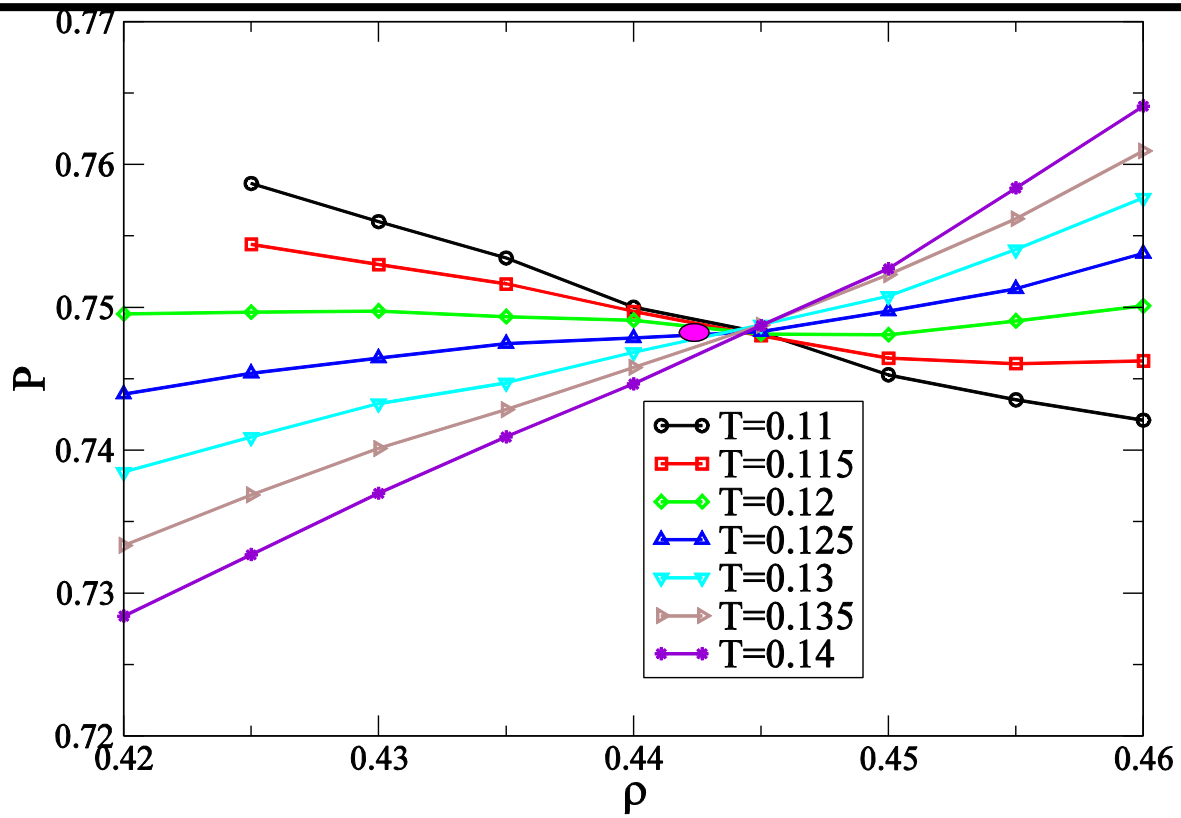
- Method:
  Fermi-Jagla model in
  Discrete molecular dynamics (DMD)



Result I: Isochores of Fermi-Jagla Liquid

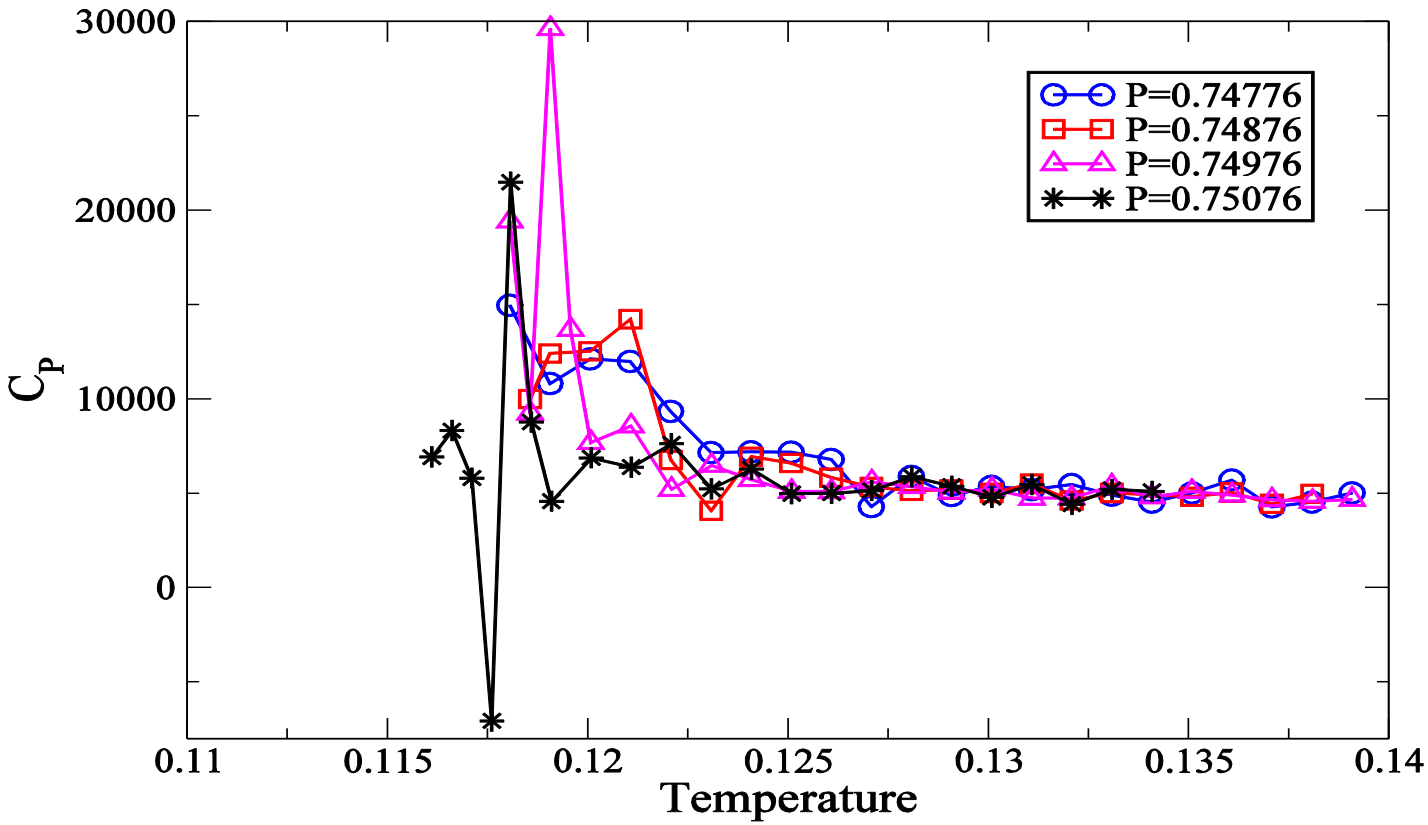


Result II: Isotherms of Fermi-Jagla Liquid



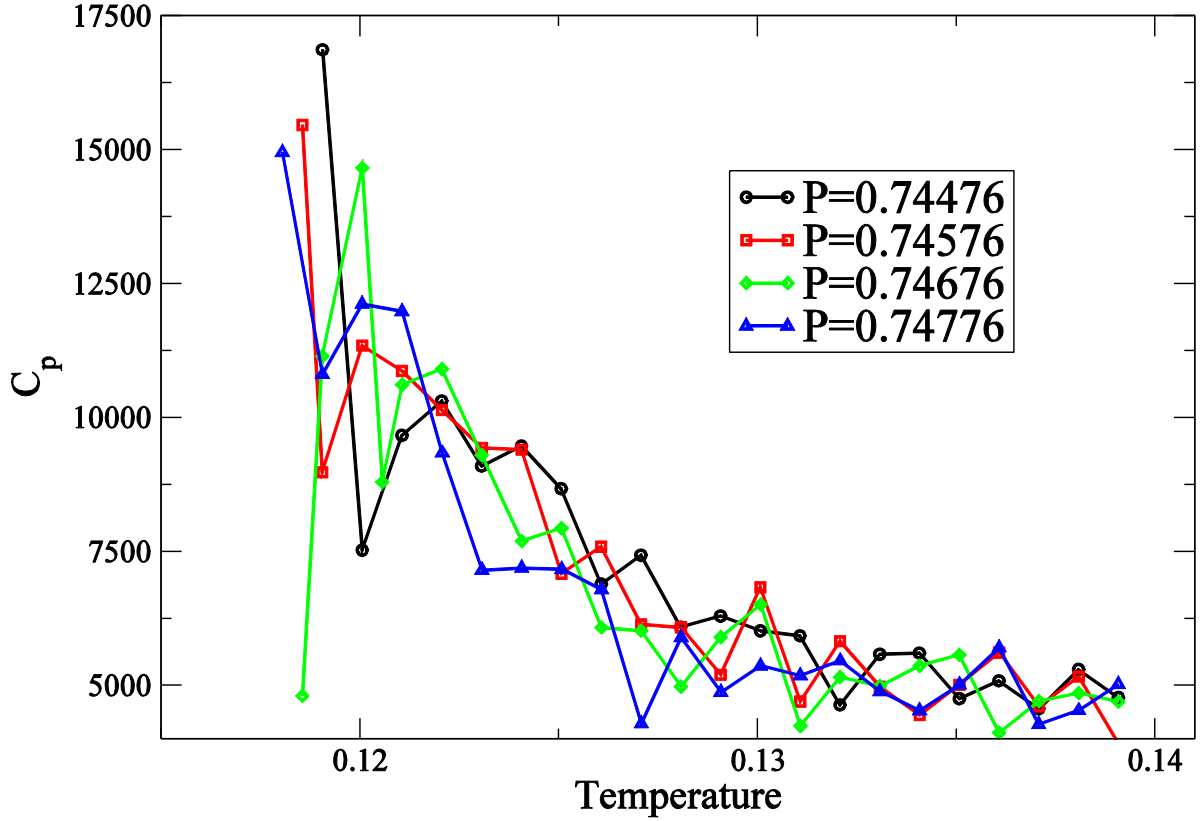
- LLPT locates at T_c=0.123, P_c=0.7481.
- The Widom line may have a negative slope.
  We calculate the maximum temperature of C_p to verify this.

Result: C_p ($P>P_c$)



As the pressure increases, the temperature of maximum C_p shifts to a lower value, which implies that the Widom line has a negative slope.

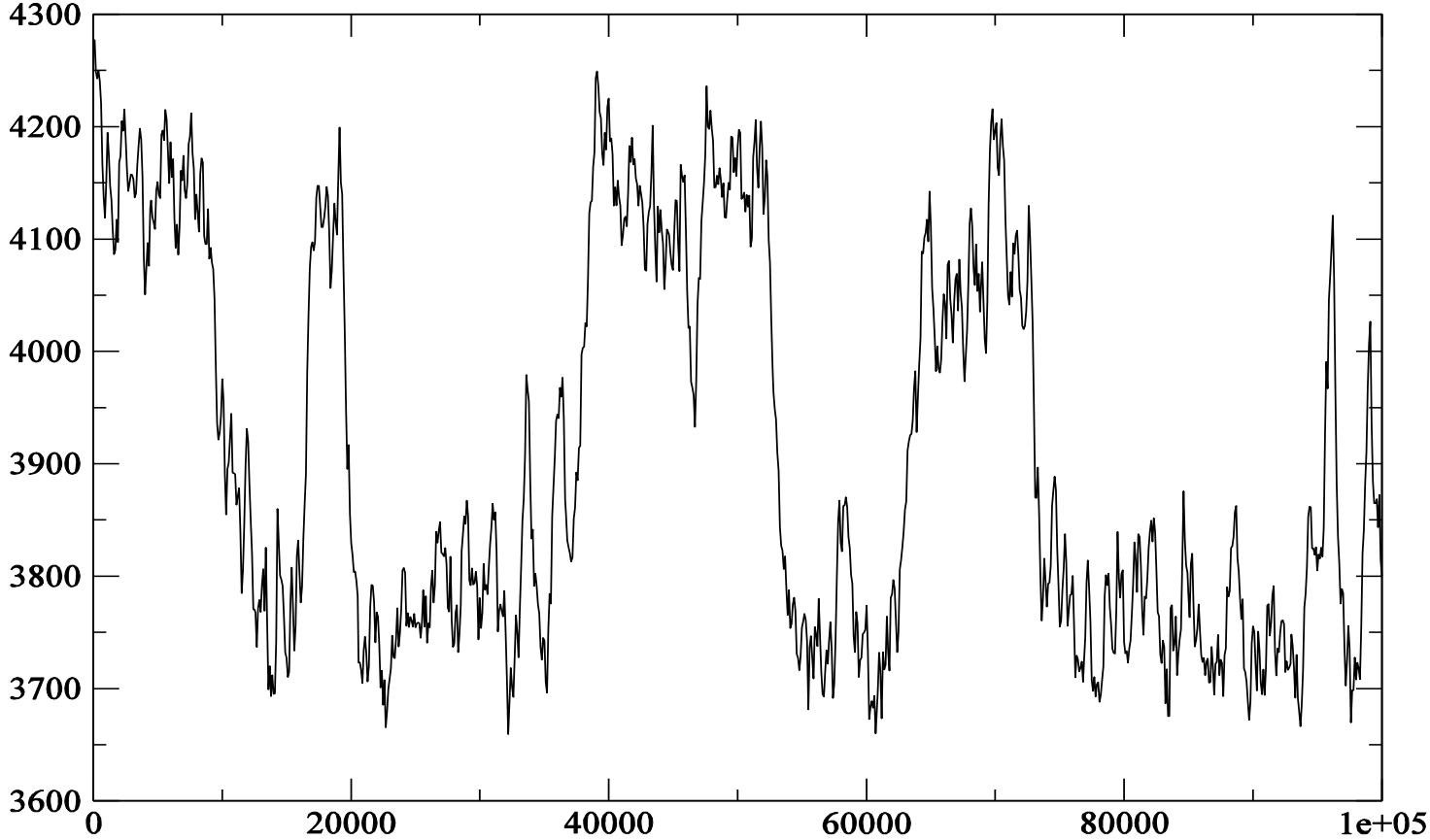
Result: C_p ($P<P_c$)



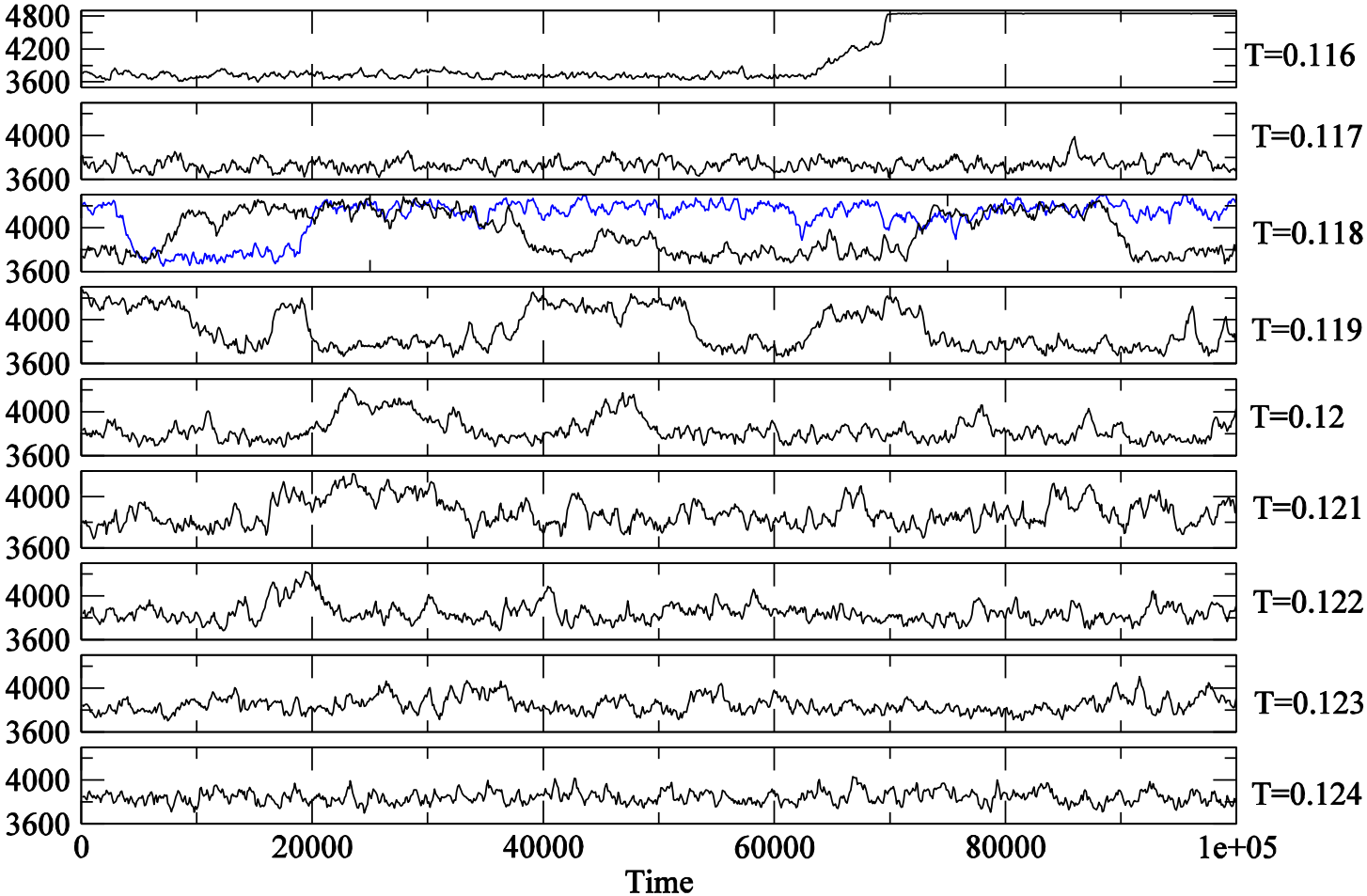
As the pressure increases, the temperature of maximum C_p shifts to a lower value, which implies that the Widom line has a negative slope.

Result: Phase flipping example

- At P=0.75076 (> P_c) and T=0.119



Result: Phase flipping region



Conclusion

- We have found a symmetric potential that can reproduce a negative-slope of the Widom line
- We found the phase flipping phenomena in the region around the LLCP

Future Work

- Decide the phase flipping region
- Using the Fermi-Jagla potential to build a dimer model for methanol

Fitting Isochores to get Temperatures of Cp_max and Kt-max