*Joint Institute for High Temperatures of the Russian Academy of Sciences*
*Izhorskaya st. 13 Bd.2, Moscow, Russia 125412*

# THE CALCULATION OF MULTICOMPONENT MIXTURE PHASE DIAGRAM, USING THE EQUATIONS OF STATE OF THE VAN DER WAALS TYPE

D.A. Molchanov, V.N. Sokotushchenko,

V.M. Torchinsky, V.M. Zaichenko.

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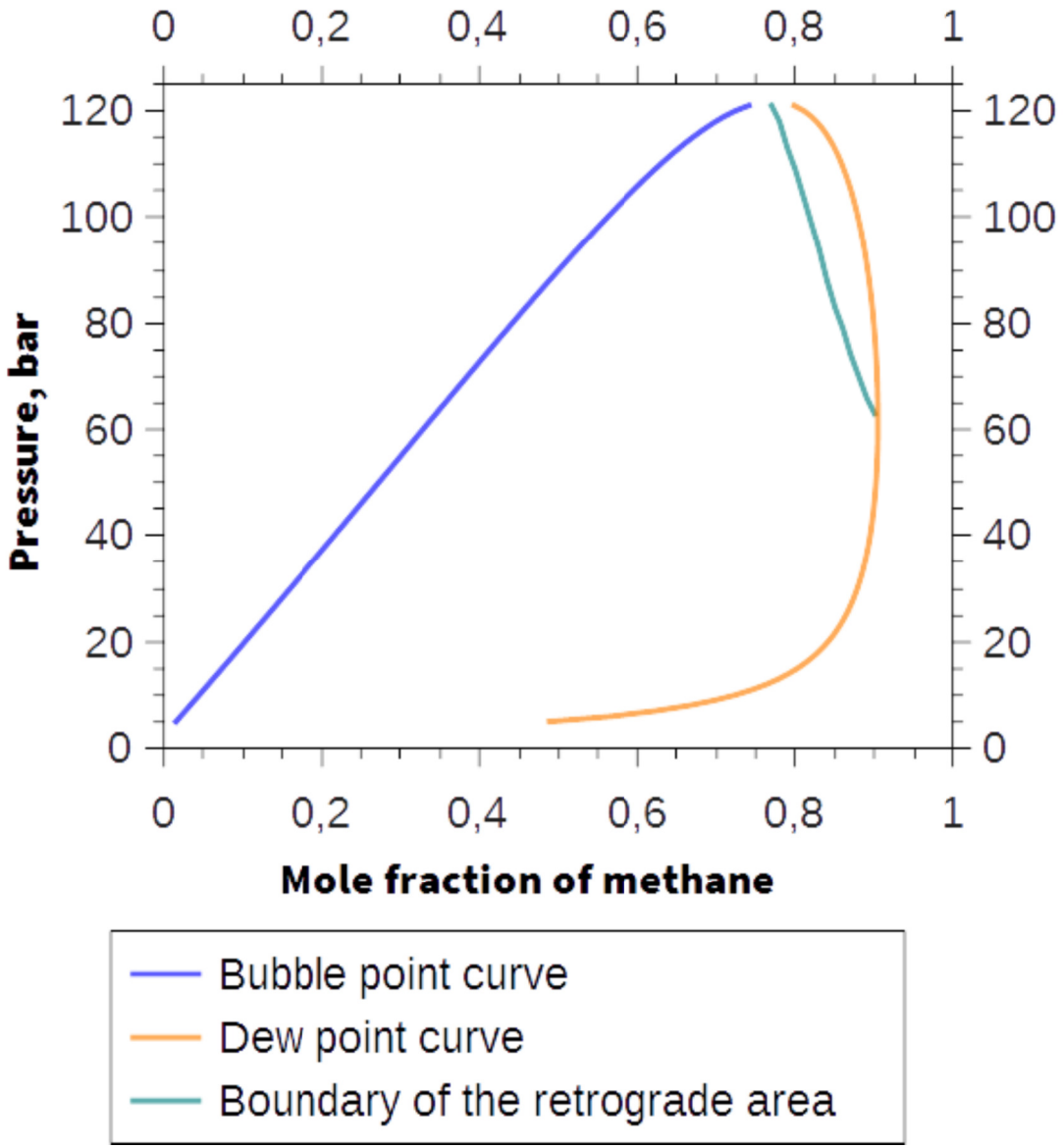
# Phase diagram of a gas-condensate mixture




**Phase diagram of methane-n-butane mixture at 293 K**

# Equation of state

$$p + \frac{a}{(v+c)(v+d)} = \frac{RT}{(v-b)},$$

Where: p — pressure, T — temperature, R — gas constant, V — mole volume,

a, b, c, d — coefficients of the equation of state

$$a = a_c \varphi(T), \qquad a_c = \alpha \frac{R^2 T_c^2}{P_c}, \qquad \varphi(T) = \left(1 + \psi\left(1 - \left(\frac{T}{T_c}\right)^{0,5}\right)\right)^2,$$

$$b = \beta \frac{RT_c}{P_c}, \qquad c = \sigma \frac{RT_c}{P_c}, \qquad d = \delta \frac{RT_c}{P_c}.$$

$$\alpha = \Omega_c^3, \qquad \beta = Z'_c + \Omega_c - 1,$$

$$\delta = -Z'_c + \Omega_c\left(0,5 - (\Omega_c - 0.75)^{1/2}\right). \qquad \sigma = -Z'_c + \Omega_c\left(0,5 + (\Omega_c - 0.75)^{1/2}\right)$$

# Algorithm

System of the equations

$$f_{Li} - f_{Vi} = 0$$
$$x_i L + y_i V - \eta_i = 0$$
$$\sum_{i=1}^{N} y_i - 1 = 0$$
$$L + V = 0$$

Initial data for the mixture:

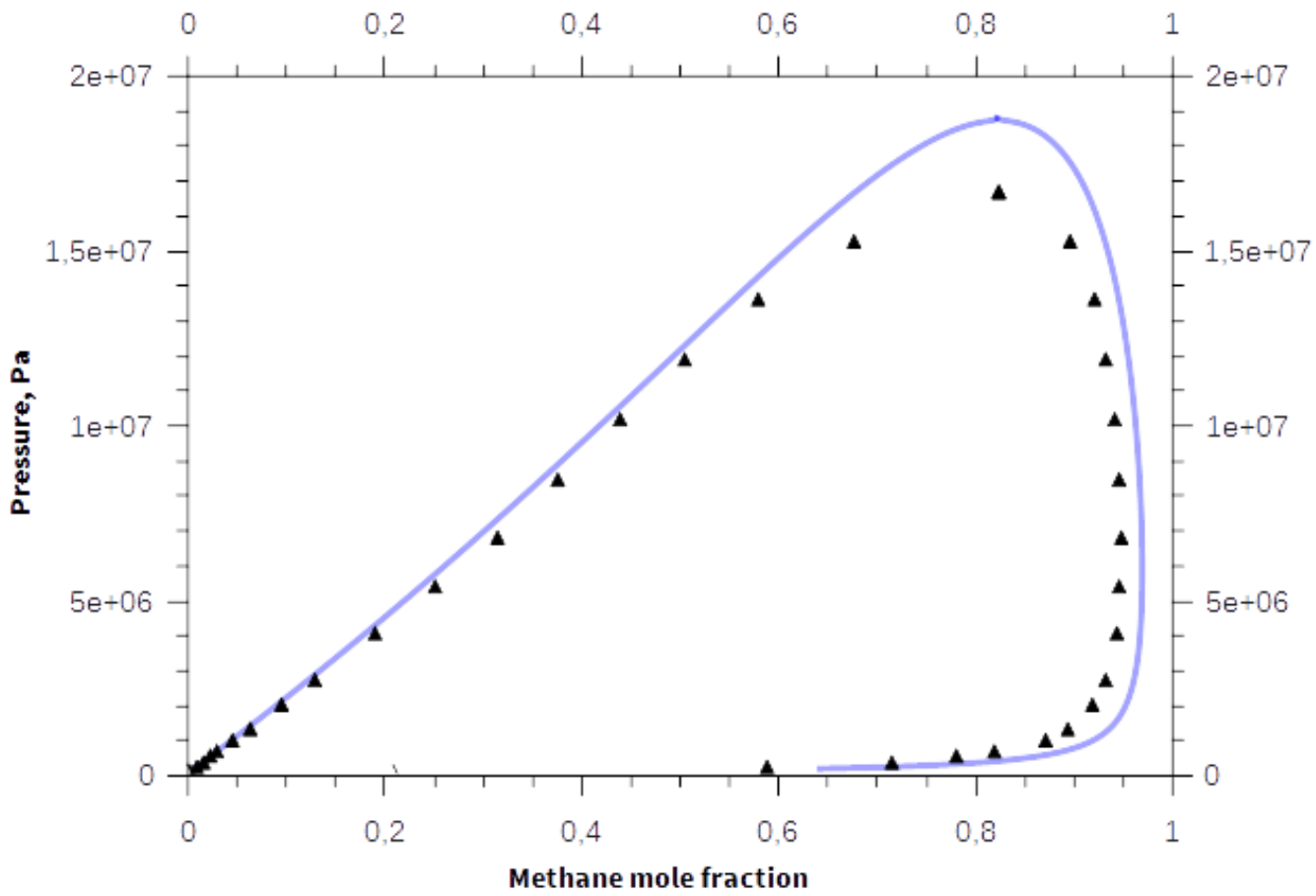
- Composition,
- Pair coefficietnts,
- P — pressure,
- T — temperature,

Initial data for components:

- $P_c$ — critical pressure,
- $T_c$ — critical temperature,
- ω — acentric factor,
- $\Omega_c$, $Z'_c$, ψ — parameters of the equation of state

| Component | $\Omega_c$ | $Z'_c$ | ψ |
|---|---|---|---|
| $N_2$ | 0.75001 | 0.34626 | 0.37182 |
| $CO_2$ | 0.75282 | 0.31933 | 0.74212 |
| $H_2S$ | 0.78524 | 0.30418 | 0.38203 |
| $CH_4$ | 0.7563 | 0.33294 | 0.37447 |
| $C_2H_6$ | 0.77698 | 0.31274 | 0.4955 |
| $C_3H_8$ | 0.76974 | 0.31508 | 0.53248 |
| i-$C_4H_{10}$ | 0.78017 | 0.30663 | 0.63875 |
| n-$C_4H_{10}$ | 0.76921 | 0.31232 | 0.57594 |

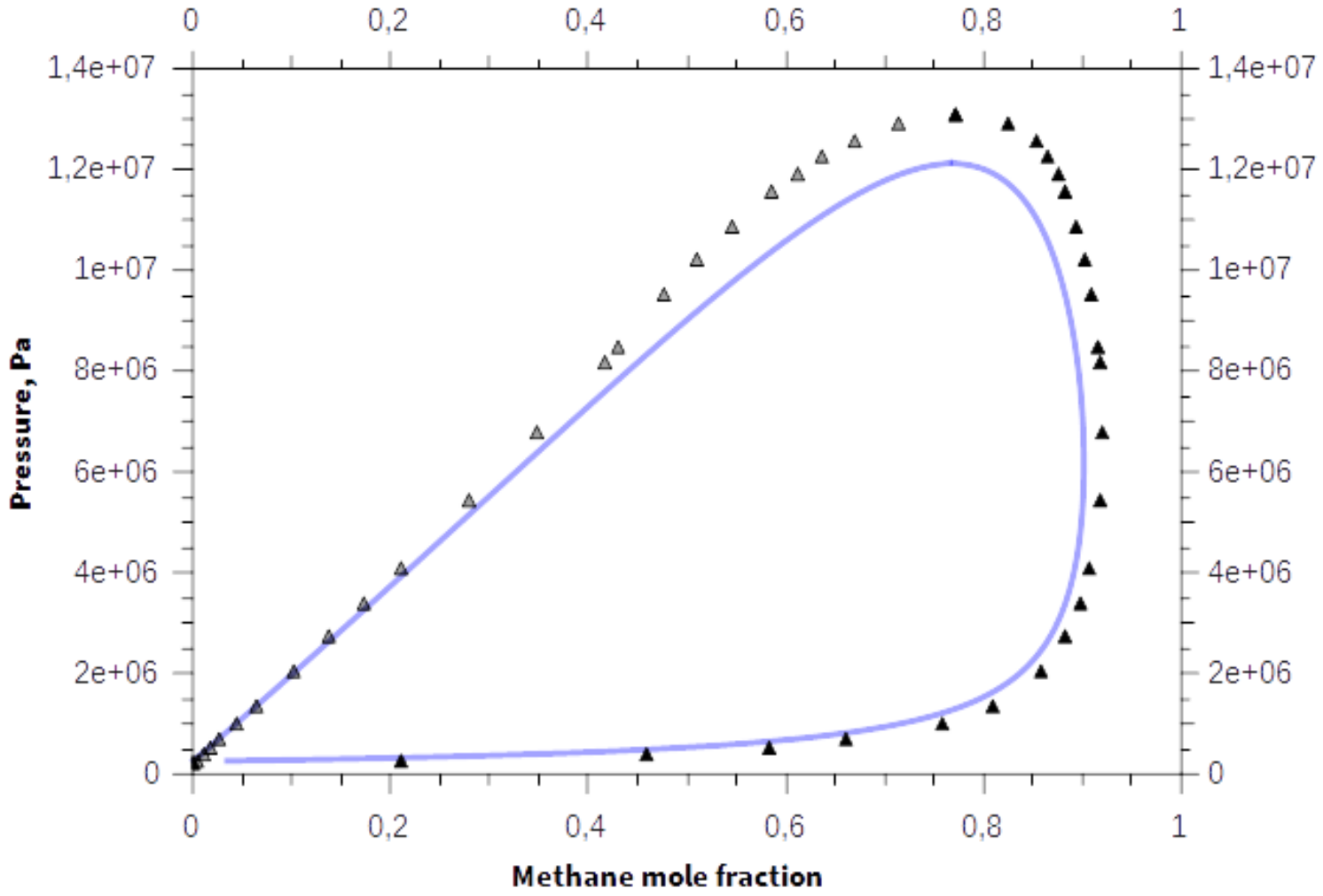
# Calculated phase diagrams




**Phase diagramm of the methane-n-pentane mixture at 311 K**

Blue line — calculation, black points — experimental data by Kogan V.B., Fridman V.M., Kafarov V.V. Liquid-vapour equilibrium. Volume 1 // M.: "Nauka", 1966, 646 p.

# Calculated phase diagrams




**Phase diagramm of the methane-n-butane mixture at 294 K**

Blue line — calculation, black points — experimental data by Kogan V.B., Fridman V.M., Kafarov V.V. Liquid-vapour equilibrium. Volume 1 // M.: "Nauka", 1966, 646 p.

# Conclusions

- **Software package to calculate the vapor-liquid equilibrium of multicomponent systems has been created.**
- **The possiblity to calculate phase equilibrium via cubic equation of state of the Wan der Waals type is shown.**

Thank you for your attention!