

## Abstract Submission

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Topic : / ECCE10 / Industrial use of thermodynamics (symposium) / Fluid phase equilibria

### VAPOR–LIQUID–LIQUID EQUILIBRIUM MEASUREMENTS AND MODELING OF METHANETHIOL OR ETHANETHIOL OR OR 1-BUTANETHIOL IN METHANE + WATER TERNARY SYSTEMS AT 303, 335, AND 365 K AND PRESSURE UP TO 9 MPa

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**Submit your abstract below (400 words):** Abstract: New vapor–liquid–liquid equilibrium (VLLE) data for methanethiol + methane + water, ethanethiol + methane + water, 1-propanethiol + methane + water, and 1-butanethiol + methane + water ternary systems have been measured at three temperatures (303, 335, and 365 K) and pressures up to 9 MPa. A “static-analytic” method was used for performing all the measurements. The total system pressure was maintained by CH<sub>4</sub>. The objective of this work is to provide experimental VLLE data with thermodynamic modeling for mixtures of mercaptans (thiols) with other natural gas contents at its crude form, for which no data are available in the open literature. Such data will help the industrial modeling of processes relevant to reduction of sulfur emissions. The Cubic-Plus-Association (CPA) equation of state was applied to describe the phase behavior of the investigated systems. It is shown that the CPA EoS satisfactorily describes the solubilities of mercaptans (thiols) in all phases. It is observed from the experimental data that the solubility of CH<sub>4</sub> in the aqueous and organic phases increases with an increase of the total system pressure and decreases with an increase of the temperature. However, the solubility of CH<sub>3</sub>SH in the aqueous and organic phases decreases slightly with an increase of the total system pressure and increases significantly with an increase of the temperature. The new VLLE data of ternary system were compared with predictions of the cubic-plus-association equation of state. The model tends to under predict the concentration of CH<sub>3</sub>SH in all phases, particularly the vapor phase. However, the model underestimates the water content of the vapor phase, especially at low pressures and at the highest investigated temperature, i.e., at 365 K. Only the ethanethiol + methane + water system showed significant cross-association effects. Furthermore, no cross association (solvation) was found to be significant in 1-propanethiol + methane + water and 1-butanethiol + methane + water ternary systems.

**Highlight 1:** New vapor–liquid–liquid equilibrium (VLLE) data for methanethiol + methane + water, ethanethiol + methane + water, 1-propanethiol + methane + water, and 1-butanethiol + methane + water ternary systems have been measured at three temperatures (303, 335, and 365 K) and pressures up to 9 MPa.

**Highlight 2:** A “static-analytic” method was used for performing all the measurements. The total system pressure was maintained by CH<sub>4</sub>

**Highlight 3:** The Cubic-Plus-Association (CPA) equation of state was applied to describe the phase behavior of the investigated systems

**Keywords:** Absorption, Chromatography, Gas treatment, Separation