Selection and Tuning of Fluid Models with a Liquid Volume Sensor


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Background and Aim

Selecting a suitable fluid property model is the first decision engineers make when building a process simulation.

Many equations of state (EOS) are available to predict fluid properties and phase behaviour, but not all are suitable for the fluid or simulation methodology.

- Cubic EOS, such as the Peng-Robinson (PR), are widely used for their broad range of application and low computational intensity.
- Multiparameter EOS, like GERG2008, are useful for their high accuracy, if a cubic EOS is insufficient.

The challenge is how to select the most suitable EOS.

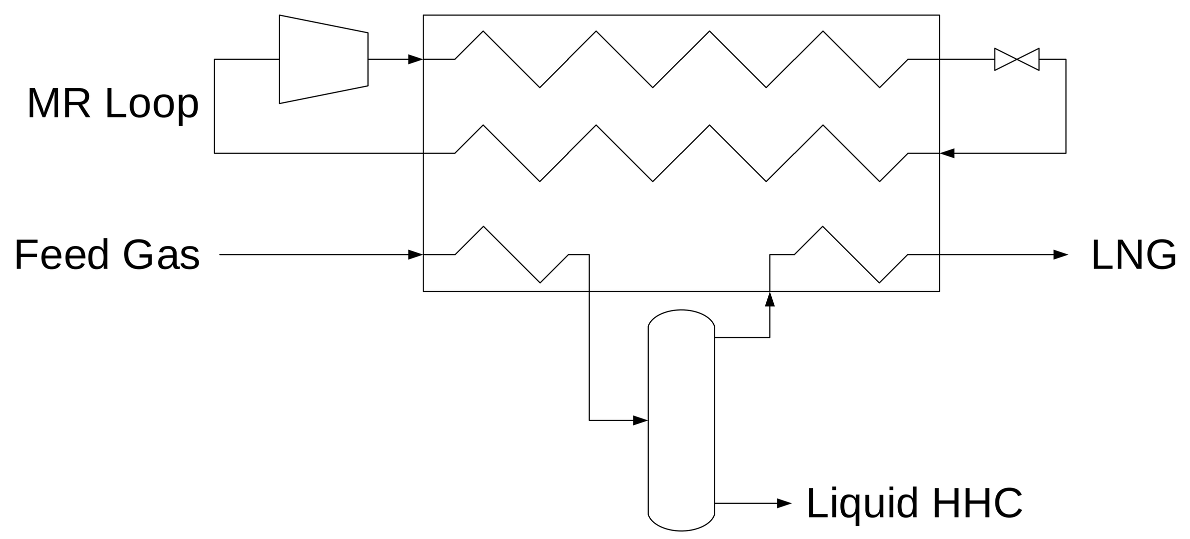

Figure 1. Example mixed refrigerant (MR) cycle to liquify natural gas (LNG). Sizing the separation vessel, which removes the liquid heavy hydrocarbons (HHC) before the final liquefaction step, requires accurate predictions of liquid volume fraction.

In this example, a gas condensate undergoes constant-temperature volume expansion. As the pressure reduces across the phase boundary, volume increases and a liquid phase forms.

- GERG2008 predicts liquid phase where the measurement was vapour only.
- Cubic EOS (PR, SRK) have the right shape but don't scale well.

In this case, a cubic EOS would be selected, and the model regressed to the liquid volume fraction data.

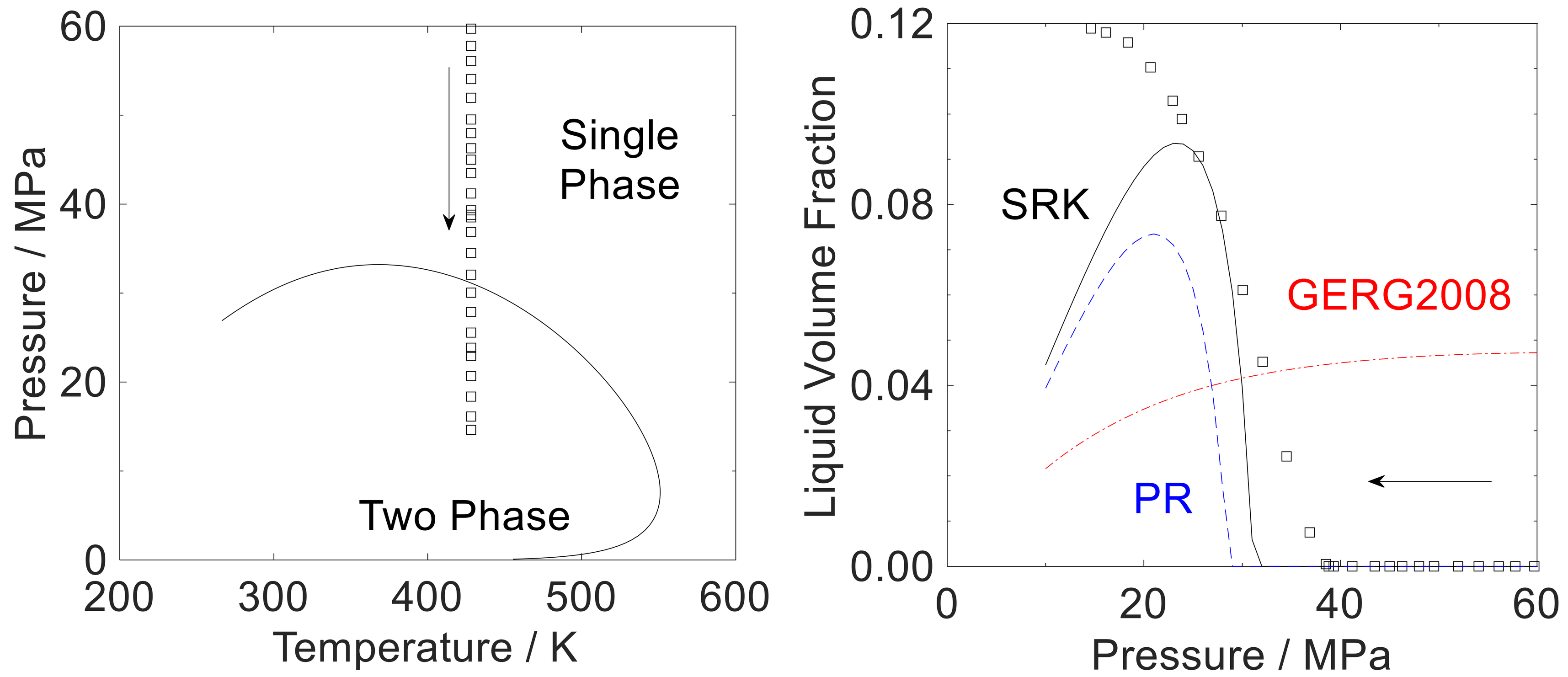

Figure 2. Model selection for a gas condensate experiment where liquid volume fraction is measured as the gas is expanded. Peng-Robinson (PR), Soave-Redlich-Kwong (SRK), and the GERG2008 EOS are plotted to compare models.

Conventional liquid volume fraction apparatus use visual techniques which require large volumes for accuracy, and this leads to long equilibration times.

This work develops a new sensor for rapid liquid volume fraction measurement to quickly inform model selection for industrially relevant fluids.

New Liquid Volume Fraction Sensor

A new sensor has been developed to non-invasively characterise fluid phase behaviour.

Three microwave resonators measure the refractive index of the liquid and vapour phases and the liquid volume fraction.

Benefits of the new sensor design include:

- Automated measurement
- Automated data analysis
- 2 hours per measurement
- 2 mL sample volume
- In situ mixing

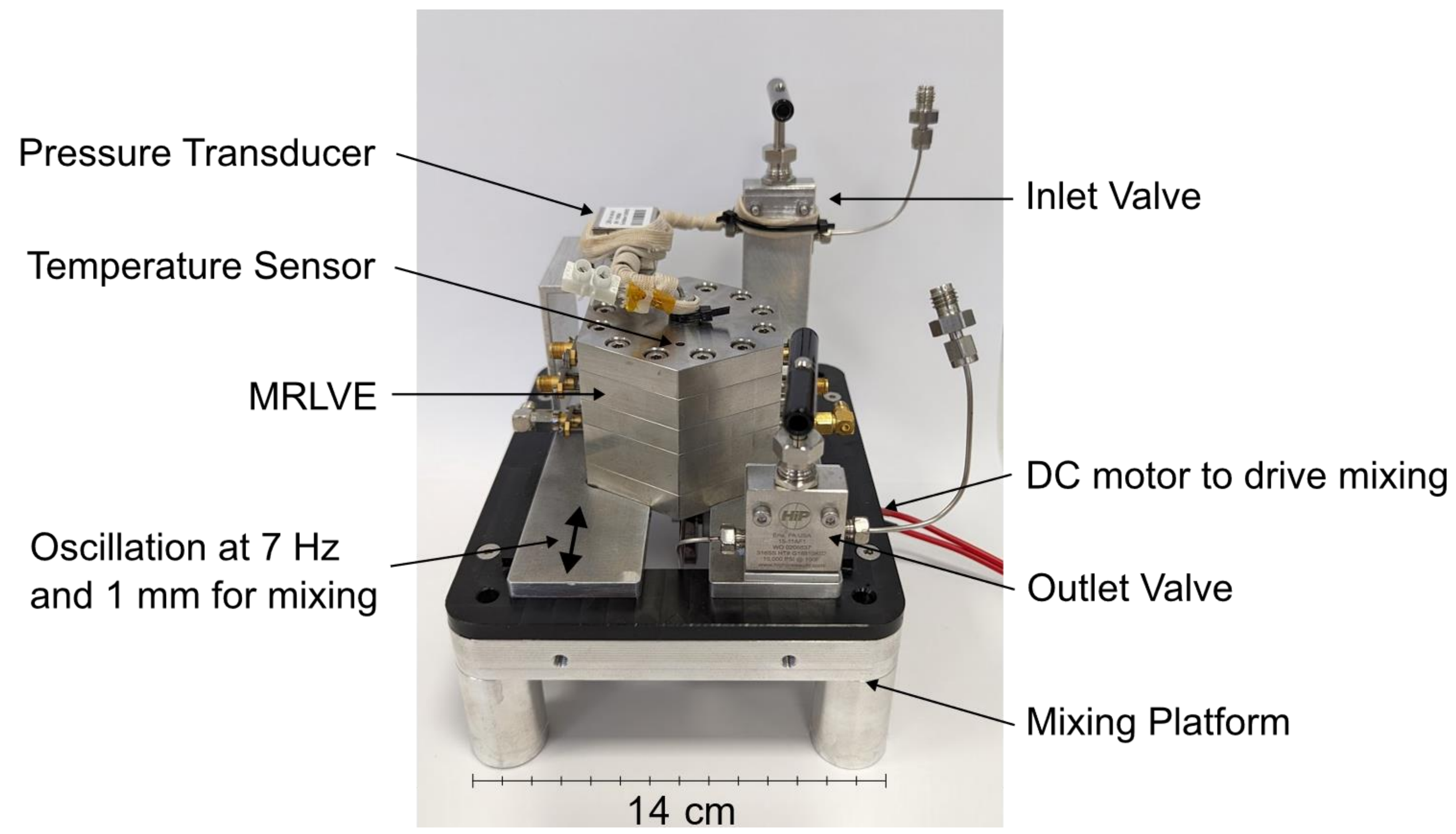

Figure 3. The Microwave Resonator for Vapour Liquid Equilibrium (MRVLE) apparatus for measurements of liquid volume fraction, mounted on a custom mixing platform.

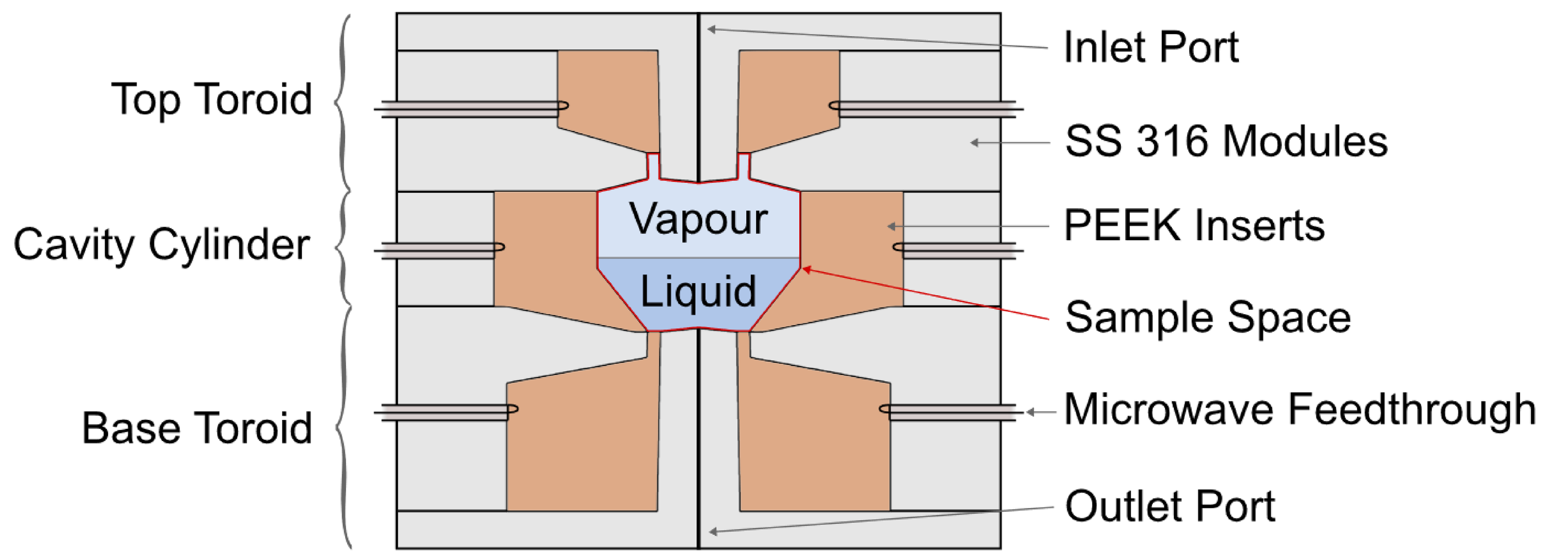

Figure 4. Cross-section of the MRVLE resonator showing the three sensors bounding the sample space containing a two-phase fluid.

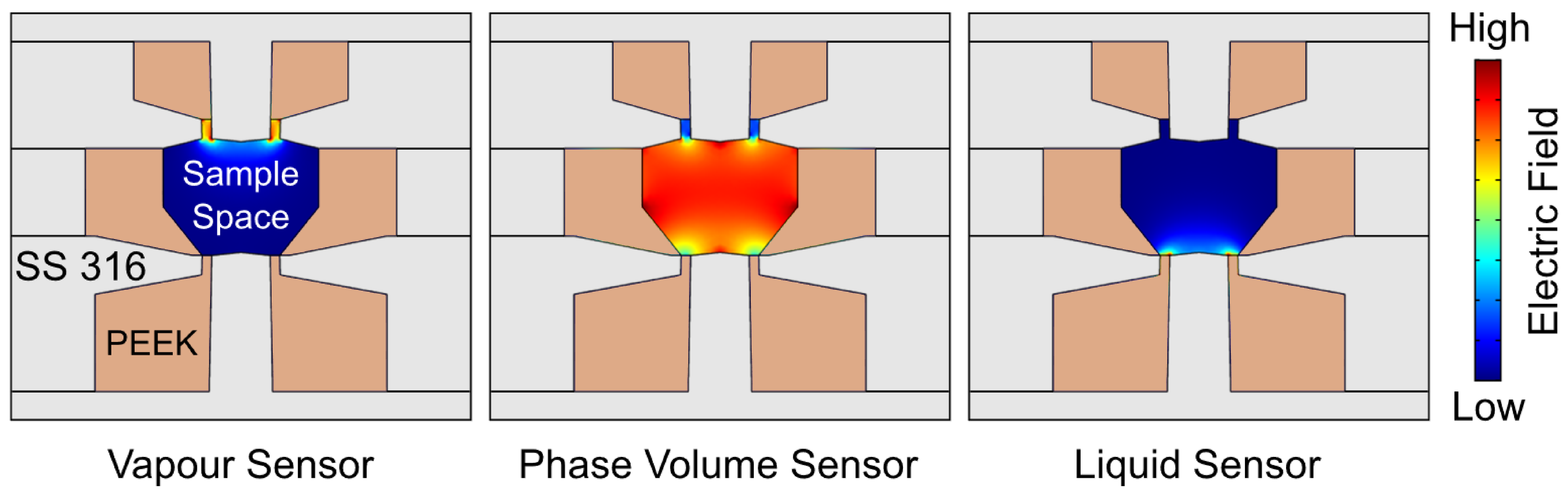

Figure 5. Finite element simulation of the three resonators and their electric field distribution in the sample space. The intense electric field regions (red) are most sensitive to the refractive index and thus density of the fluid in the same region.

Demonstration: (CO_2 + R32) Mixed Refrigerant

Carbon dioxide (CO_2) and difluoromethane (R32) mixtures are currently being assessed for domestic and industrial refrigeration applications, to replace less environmentally friendly refrigerants like R134a.

The MRVLE sensor was used to characterise the liquid volume fraction of this mixture. The sensor was loaded with the mixed refrigerant in the supercritical region, and cooled along an isochor while liquid volume fraction was measured.

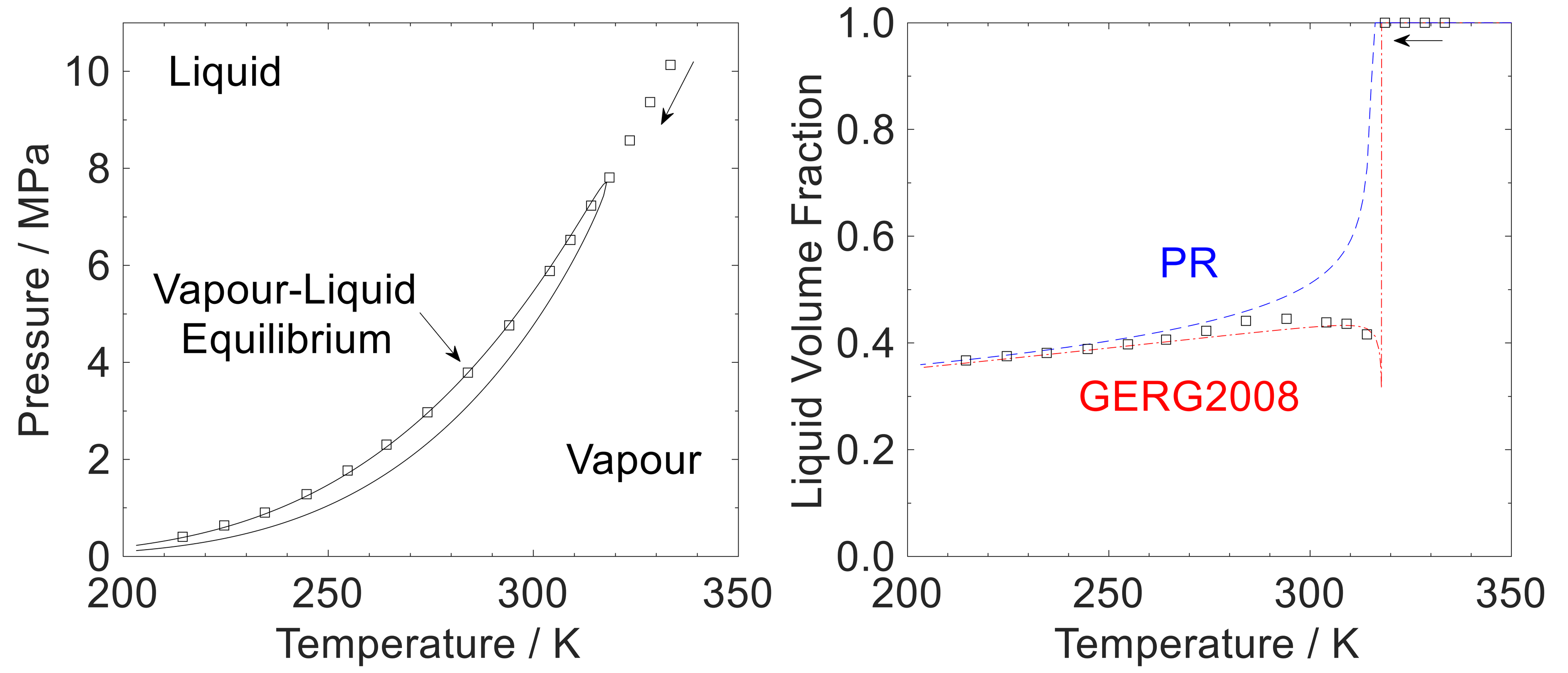

Figure 6. Liquid volume fraction measurements with the MRVLE demonstrate that the GERG2008 EOS is best to represent mixtures of CO_2 and R32.

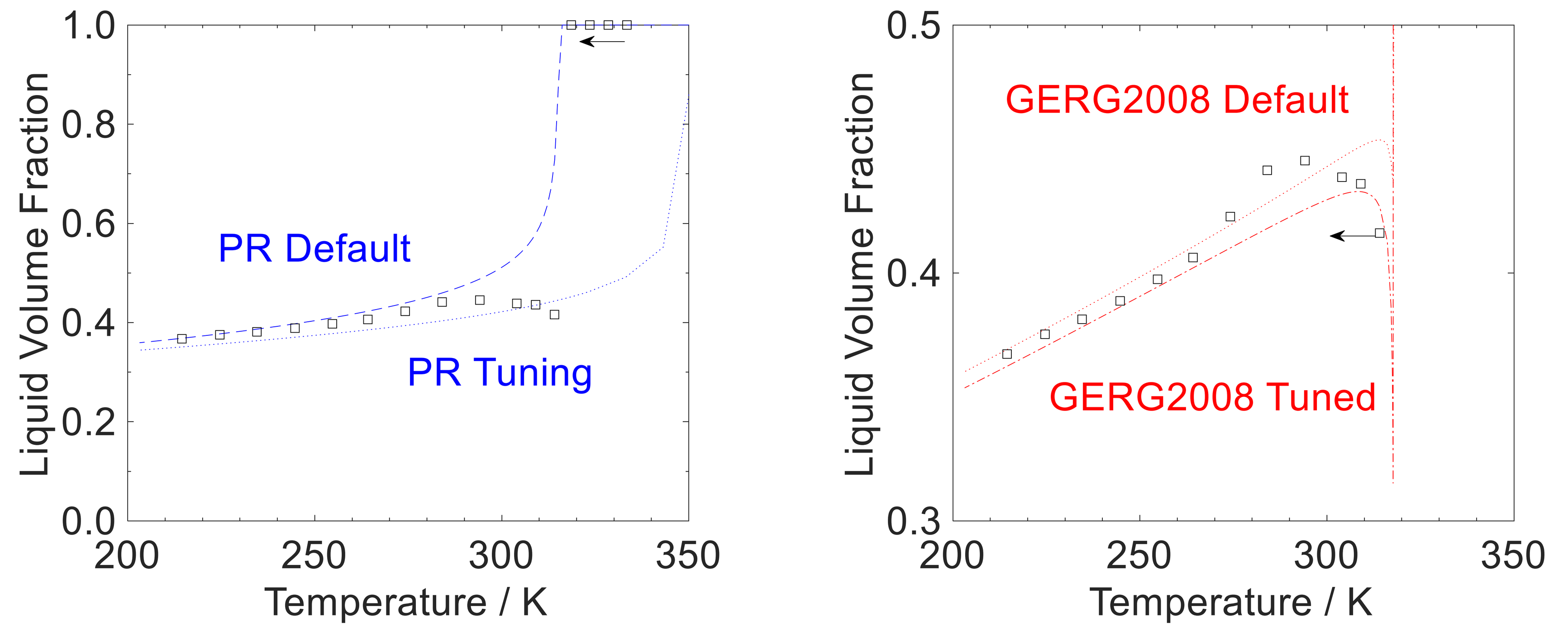

Figure 7. Tuning the binary interaction parameter (BIP) in the PR EOS does not affect the shape of the line, just the location of the dew point. Therefore, it cannot be used to accurately represent the mixture. GERG2008 on the other hand, when tuned, agreed better with the liquid volume fraction measurements.

Outcomes and Impact

This work designed, characterised, and tested a new sensor using microwave resonator technology to rapidly measure liquid volume fraction.

The MRVLE sensor provides a unique opportunity for rapid laboratory measurements to quickly inform industrial model selection and tuning. It is applicable to the phase behaviour of natural gas, carbon dioxide, hydrogen and their refrigerant processes.

Although it was not demonstrated here, when combined with polarization mixing equations, complete phase behaviour can be measured in binary mixtures:

- Saturated densities
- Saturated compositions
- Vapour/liquid mole fractions
- Dew points
- Bubble points