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## Gas/liquid interfaces at high pressure: Neutron Imaging, Molecular Dynamics

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The exposure of liquids to pressurized gases induces gas adsorption at the interface, its diffusion into the bulk, and liquid swelling. Neutron imaging of systems from deuterated liquids (hydrocarbons, water) and protium-containing gases ( $H_2$ ,  $CH_4$ ,  $C_2H_6$ ) at up to 100 bar and near-ambient temperatures provides interface shape, liquid level, and concentration distribution over time. Interfacial tension, apparent molar volume, diffusivity, and solubility of the gas in the liquid are thus used to calibrate the molecular dynamics model. The contributions are summarized as: *i*) the technical improvements that led us to the 2<sup>nd</sup> generation of the neutron imaging process [1-3], *ii*) lessons learned for the neutron imaging and molecular interpretation of three-phase systems (gas, two liquids) [4], and *iii*) simulation-based predictions of physico-chemical properties at industrially relevant temperatures and pressures [5] beyond the reach of the neutron imaging setup.

### REFERENCES

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