Supplementary information to "Local thermodynamic description of isothermal single-phase flow in simple porous media"

Olav Galteland, Michael T. Rauter, Mina S. Bratvold, Thuat T. Trinh, Dick Bedeaux and Signe Kjelstrup

PoreLab, Department of Chemistry, Norwegian University of Science and Technology, Trondheim, Norway.

*Corresponding author(s). E-mail(s): olav.galteland@ntnu.no; Contributing authors: michael.t.rauter@ntnu.no; minabratvold@gmail.com; thuat.trinh@ntnu.no; dick.bedeaux@ntnu.no; signe.kjelstrup@ntnu.no;

1 Surface tension

The fluid-solid surface tension was calculated from the spherical mechanical pressure tensor of a single solid sphere surrounded by a fluid of varying mass density. This was considered as the surface tension of a lattice with a large lattice constant, such that the solid surfaces were far apart. The mechanical pressure tensor can be written as a sum of an ideal gas contribution and a virial contribution. The diagonal components of the mechanical pressure tensor were calculated in spherical shells with origin at the center of the solid sphere

$$P_{\alpha\beta}(r) = \rho(r) k_{\mathrm{B}} T \delta_{\alpha\beta} + P^{v}_{\alpha\beta}(r), \tag{1}$$

where r is the distance to the origin, $\rho(r)$ is the fluid mass density of the spherical shell, $\delta_{\alpha\beta}$ is the Kroenecker delta and $P^{s,v}_{\alpha\beta}$ is the virial contribution. The subscripts α and β refer to the spherical coordinates, (r, θ, ϕ). The virial

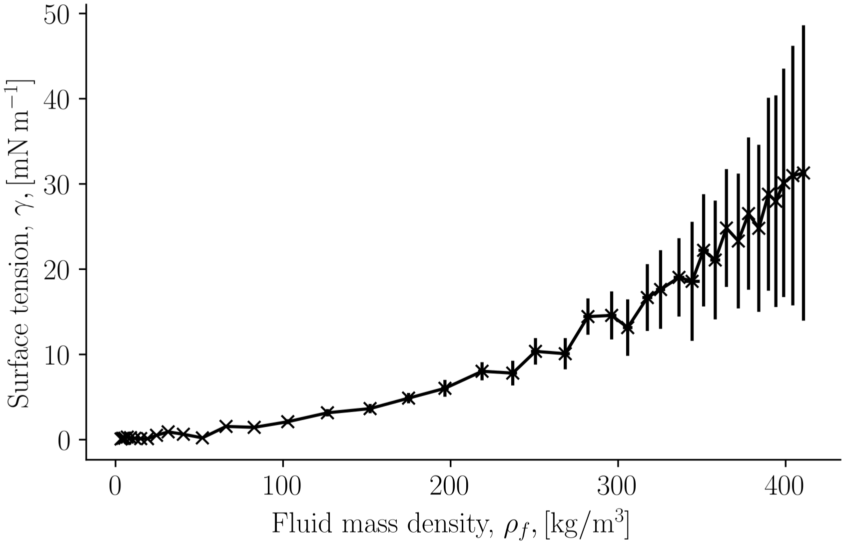

Fig. 1 Solid-fluid surface tension as a function of fluid mass density for a single solid sphere surrounded by a fluid.

contribution is

$$P^v_{\alpha\beta}(r) = -\frac{1}{V(r)} \sum_{i=1}^{N} \sum_{j>i}^{N} f_{ij,\alpha} \int_{C_{ij} \in V(r)} \mathrm{d}l_\beta. \tag{2}$$

where $V(r)$ is the volume of the spherical shell, $f_{ij,\alpha}$ is the α-component of the force acting on particle i due to particle j. The line integral is along the Irving-Kirkwood contour C_{ij} [1–3], which is the straight line between particle i and j. The line integral gives the length of the β-component of the contour C_{ij} that is contained in the spherical shell $V(r)$. The surface tension is calculated from the pressure tensor

$$\gamma = \frac{1}{R^2} \int_R^{r_0} (P_N - P_T) r^2 \mathrm{d}r, \tag{3}$$

where $P_N = P_{rr}$ is the normal to the fluid-solid surface and $P_T = (P_{\theta\theta} + P_{\phi\phi})/2$ is tangential to it. The integral limit r_0 is a position in the fluid far away from the fluid-solid surface such that $P_N = P_T$. The surface tension is shown as a function of fluid mass density in Fig. 2.

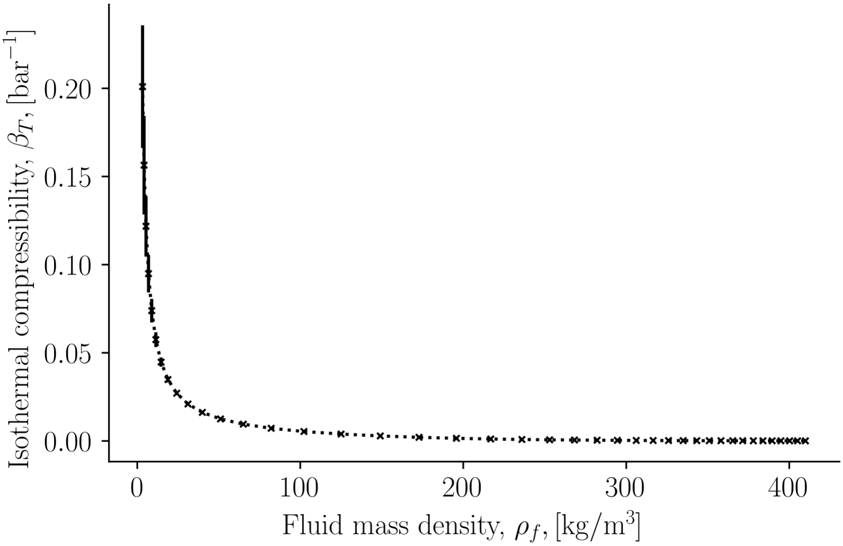

Fig. 2 Isothermal compressibility as a function of the fluid mass density of the bulk fluid.

2 Isothermal compressibility

The isothermal compressibility is

$$\beta_T = \frac{1}{\rho}\left(\frac{\partial \rho_f}{\partial p}\right)_T \tag{4}$$

where ρ_f is the fluid mass density of the bulk fluid and p is the pressure of the bulk fluid.

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