We now present an improvement of the volumetric part of the analysis of Hofsäß et al. (17). This may be of some independent interest because volumes of the chemical components in mixtures are important, for example, in estimating electron density and neutron scattering lengths for diffraction experiments. We first define the volume per lipid $v(x)$ by

$$v(x) = \frac{V_{\text{sim}} - N_{\text{water}} v_{\text{water}}}{2(N_{\text{DPPC}} + N_{\text{chol}})}, \tag{6}$$

(keeping N_{DPPC} and N_{chol} defined per monolayer) where the volume of water has been subtracted from the volume V_{sim} of the simulation cell. Then, just as for the area $a(x)$ in Eq. 2, one requires

$$v(x) = (1 - x)v_{\text{DPPC}}(x) + xv_{\text{chol}}(x). \tag{7}$$

Fig. 2 shows that $v(x)$, unlike $a(x)$ in Fig. 1, is quite linear, so $v_{\text{DPPC}}(x)$ and $v_{\text{chol}}(x)$ are independent of x. The linear regression shown in Fig. 2 gives $v_{\text{DPPC}} = 1.220$ nm^3 and $v_{\text{chol}} = 0.541$ nm^3.