Electronic Supplementary Information

Self-assembly and friction of glycerol monooleate and its hydrolysis products in bulk and confined non-aqueous solvents

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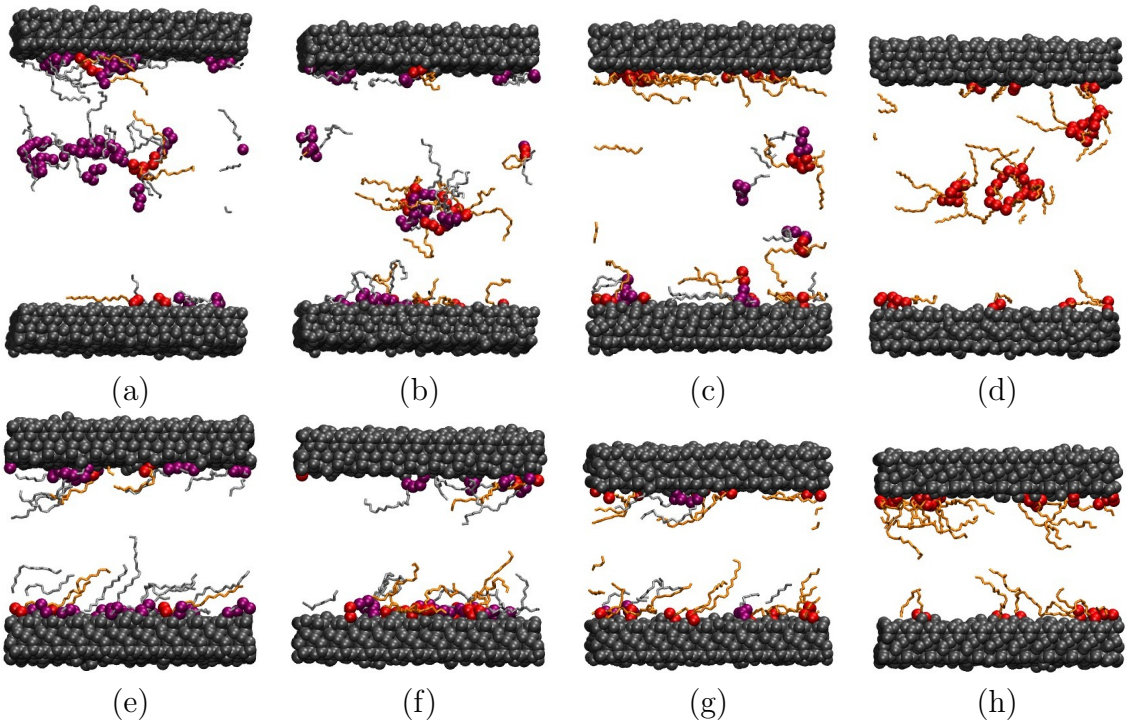
1 Snapshots from confined-fluid simulations

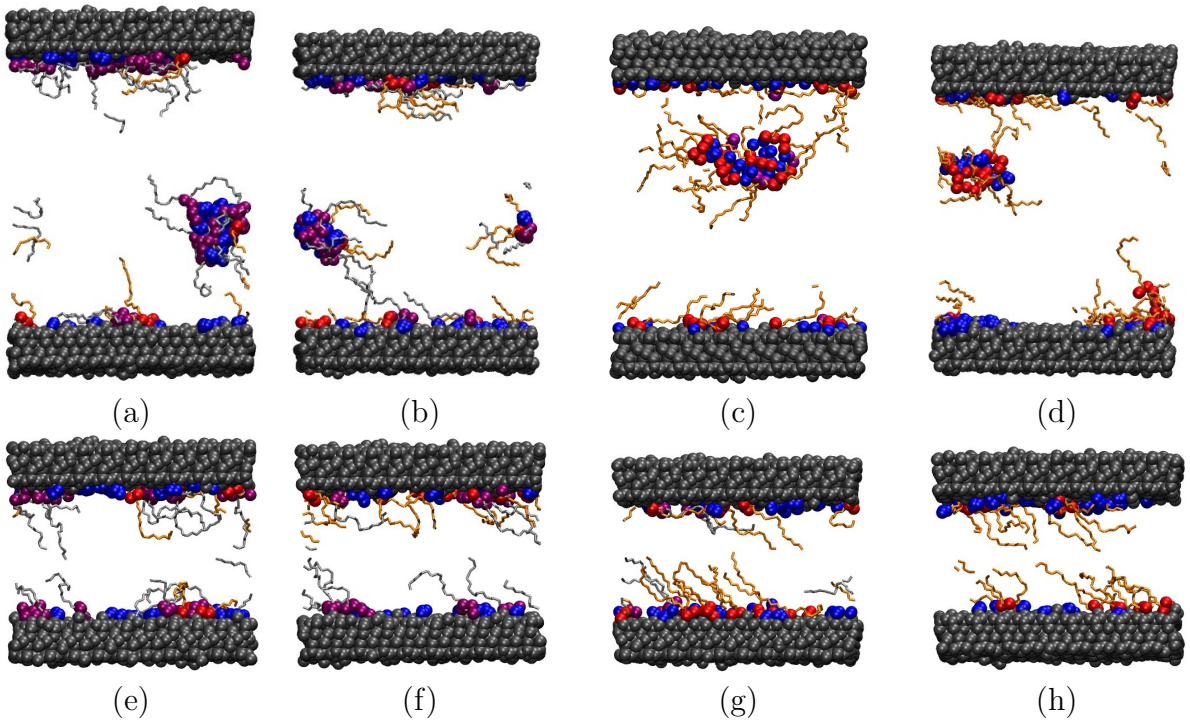
1.1 Glycerol monooleate (GMO) and oleic acid (OlH)



(a) 8.1 wt% GMO and 1.9 wt% OlH in *n*-heptane
(b) 5.6 wt% GMO and 4.4 wt% OlH in *n*-heptane
(c) 2.8 wt% GMO and 7.2 wt% OlH in *n*-heptane
(d) 10.0 wt% OlH in *n*-heptane
(e) 7.9 wt% GMO and 2.1 wt% OlH in toluene
(f) 5.6 wt% GMO and 4.4 wt% OlH in toluene
(g) 3.0 wt% GMO and 7.0 wt% OlH in toluene
(h) 10.0 wt% OlH in toluene

Figure 1: Simulation snapshots of GMO, OlH, and solvent confined between mica surfaces and sheared at $v_s = 20$ m s^{-1}: (a)–(d) in *n*-heptane; (e)–(h) in toluene. GMO is shown with purple oxygen atoms and silver tails, OlH with red oxygen atoms and orange tails, and the mica surfaces with grey atoms. The solvent is omitted.

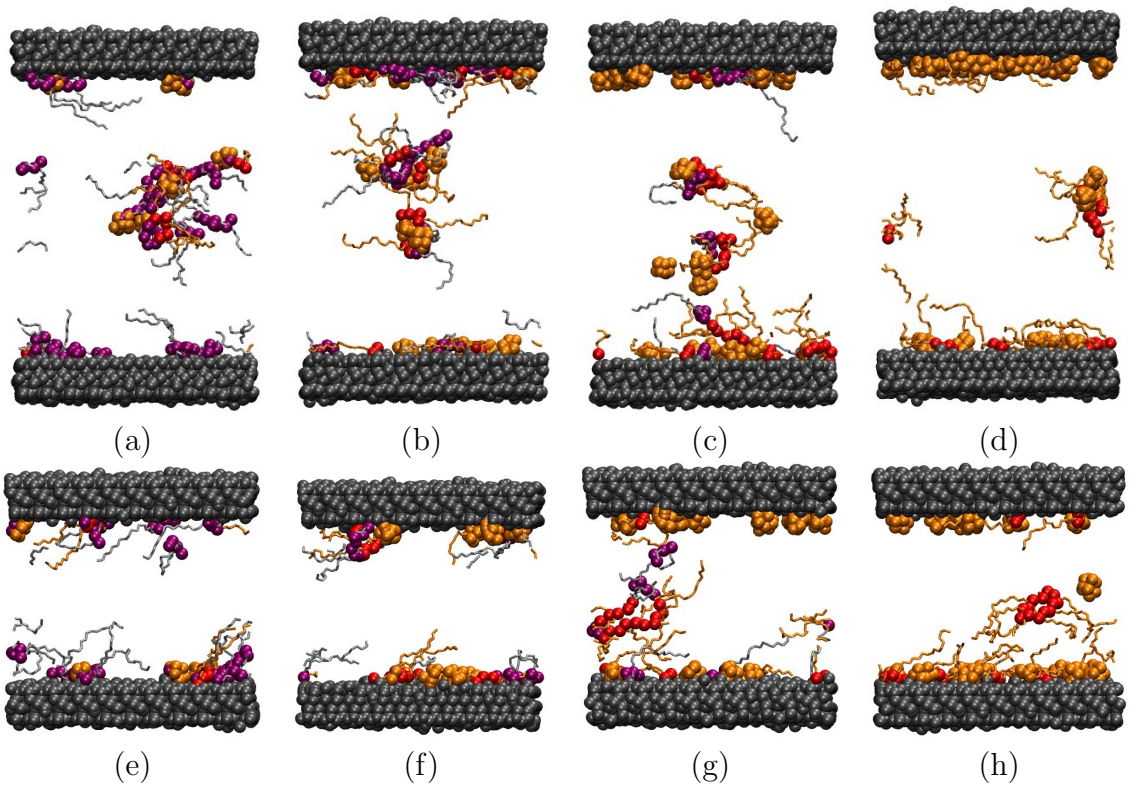
1.2 Glycerol monooleate (GMO), oleic acid (OlH), and water (H_2O)



(a) 8.0 wt% GMO, 1.9 wt% OlH, and 1.1 wt% H_2O in *n*-heptane
(b) 5.5 wt% GMO, 4.4 wt% OlH, and 1.1 wt% H_2O in *n*-heptane
(c) 2.7 wt% GMO, 7.1 wt% OlH, and 1.2 wt% H_2O in *n*-heptane
(d) 9.4 wt% OlH and 1.2 wt% H_2O in *n*-heptane
(e) 7.8 wt% GMO, 2.1 wt% OlH, and 1.1 wt% H_2O in toluene
(f) 5.5 wt% GMO, 4.4 wt% OlH, and 1.1 wt% H_2O in toluene
(g) 2.9 wt% GMO, 7.0 wt% OlH, and 1.2 wt% H_2O in toluene
(h) 9.5 wt% OlH and 1.2 wt% H_2O in toluene

Figure 2: Simulation snapshots of GMO, OlH, H_2O, and solvent confined between mica surfaces and sheared at $v_s = 20$ m s^{-1}: (a)–(d) in *n*-heptane; (e)–(h) in toluene. GMO is shown with purple oxygen atoms and silver tails, OlH with red oxygen atoms and orange tails, H_2O with blue oxygen atoms, and the mica surfaces with grey atoms. The solvent is omitted.

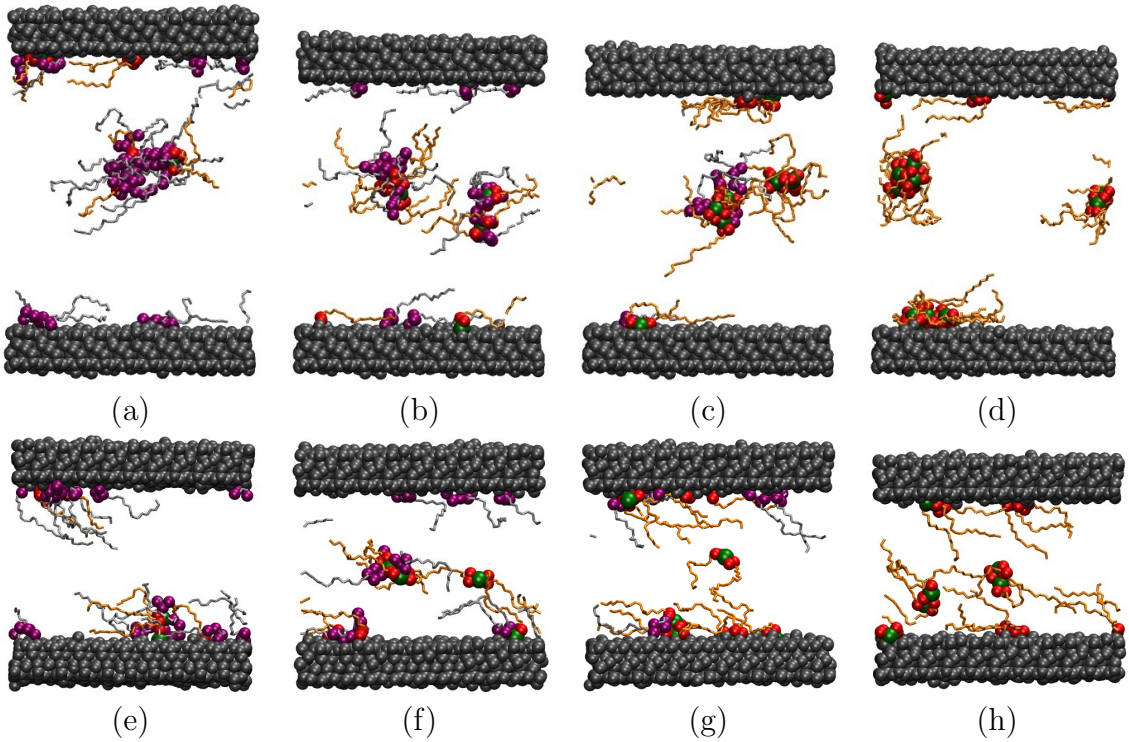
1.3 Glycerol monooleate (GMO), oleic acid (OlH), and glycerol (Gly)



(a) 7.6 wt% GMO and 2.4 wt% OlH/Gly in *n*-heptane
(b) 4.9 wt% GMO and 5.1 wt% OlH/Gly in *n*-heptane
(c) 2.2 wt% GMO and 7.8 wt% OlH/Gly in *n*-heptane
(d) 10.0 wt% OlH/Gly in *n*-heptane
(e) 7.4 wt% GMO and 2.6 wt% OlH/Gly in toluene
(f) 4.9 wt% GMO and 5.1 wt% OlH/Gly in toluene
(g) 2.4 wt% GMO and 7.6 wt% OlH/Gly in toluene
(h) 10.0 wt% OlH/Gly in toluene

Figure 3: Simulation snapshots of GMO, OlH, Gly, and solvent confined between mica surfaces and sheared at $v_s = 20$ m s^{-1}: (a)–(d) in *n*-heptane; (e)–(h) in toluene. GMO is shown with purple oxygen atoms and silver tails, OlH with red oxygen atoms and orange tails, Gly with orange atoms, and the mica surfaces with grey atoms. The solvent is omitted.

1.4 Glycerol monooleate (GMO) and calcium oleate ($CaOl_2$)



(a) 7.7 wt% GMO and 2.3 wt% $CaOl_2$ in *n*-heptane
(b) 5.4 wt% GMO and 4.3 wt% $CaOl_2$ in *n*-heptane
(c) 2.7 wt% GMO and 7.3 wt% $CaOl_2$ in *n*-heptane
(d) 10.0 wt% $CaOl_2$ in *n*-heptane
(e) 7.5 wt% GMO and 2.5 wt% $CaOl_2$ in toluene
(f) 5.4 wt% GMO and 4.6 wt% $CaOl_2$ in toluene
(g) 3.0 wt% GMO and 7.0 wt% $CaOl_2$ in toluene
(h) 10.0 wt% $CaOl_2$ in toluene

Figure 4: Simulation snapshots of GMO, $CaOl_2$, and solvent confined between mica surfaces and sheared at $v_s = 20$ m s^{-1}: (a)–(d) in *n*-heptane; (e)–(h) in toluene. GMO is shown with purple oxygen atoms and silver tails, and $CaOl_2$ with green calcium ions, red oxygen atoms, and orange tails. The solvent is omitted.

2 Velocity profiles

2.1 Glycerol monooleate (GMO) and oleic acid (OlH) in *n*-heptane

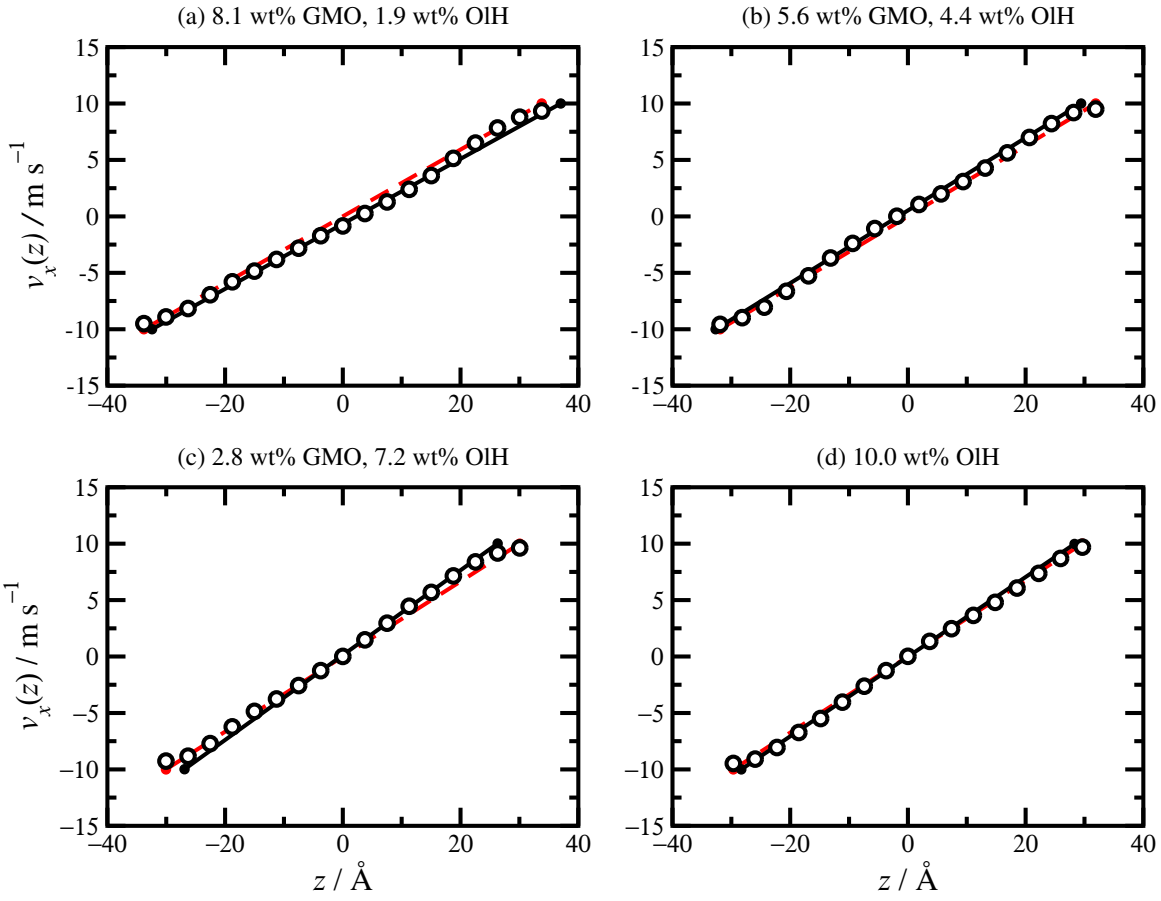


Figure 5: Velocity profiles for GMO and OlH in *n*-heptane confined between parallel mica surfaces and sheared at $v_s = 20$ m s^{-1}: (a) 8.1 wt% GMO and 1.9 wt% OlH; (b) 5.6 wt% GMO and 4.4 wt% OlH; (c) 2.8 wt% GMO and 7.2 wt% OlH; (d) 10.0 wt% OlH. The points are from simulations, the red dashed line is the ideal (no-stick) velocity profile, and the black solid line is a fit to the central, linear portion of the velocity profile.

2.2 Glycerol monooleate (GMO) and oleic acid (OlH) in toluene

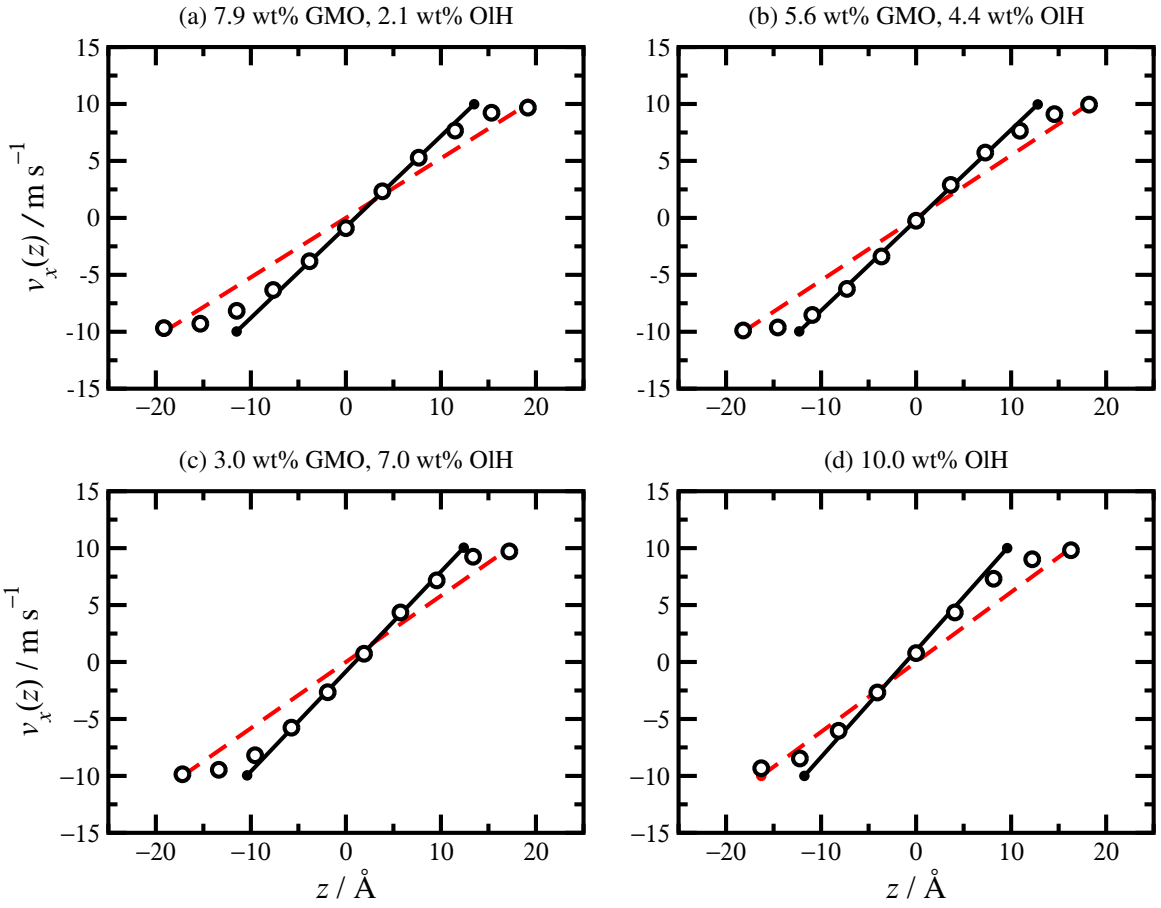


Figure 6: Velocity profiles for GMO and OlH in toluene confined between parallel mica surfaces and sheared at $v_s = 20$ m s^{-1}: (a) 7.9 wt% GMO and 2.1 wt% OlH; (b) 5.6 wt% GMO and 4.4 wt% OlH; (c) 3.0 wt% GMO and 7.0 wt% OlH; (d) 10.0 wt% OlH. The points are from simulations, the red dashed line is the ideal (no-stick) velocity profile, and the black solid line is a fit to the central, linear portion of the velocity profile.

2.3 Glycerol monooleate (GMO), oleic acid (OlH), and water (H_2O) in *n*-heptane

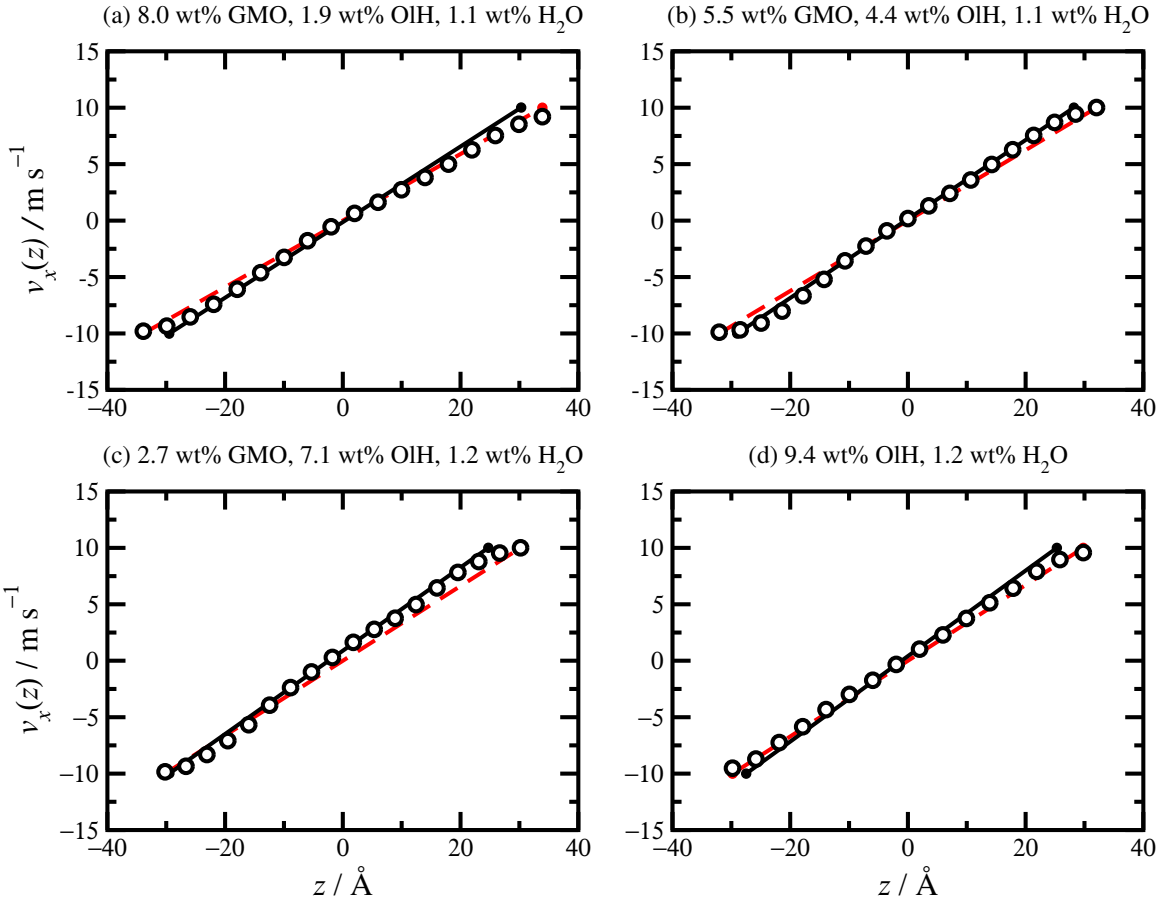


Figure 7: Velocity profiles for GMO, OlH, and H_2O in *n*-heptane confined between parallel mica surfaces and sheared at $v_s = 20$ m s^{-1}: (a) 8.0 wt% GMO, 1.9 wt% OlH, and 1.1 wt% H_2O; (b) 5.5 wt% GMO, 4.4 wt% OlH, and 1.1 wt% H_2O; (c) 2.7 wt% GMO, 7.1 wt% OlH, and 1.2 wt% H_2O; (d) 9.4 wt% OlH and 1.2 wt% H_2O. The points are from simulations, the red dashed line is the ideal (no-stick) velocity profile, and the black solid line is a fit to the central, linear portion of the velocity profile.

2.4 Glycerol monooleate (GMO), oleic acid (OlH), and water (H_2O) in toluene

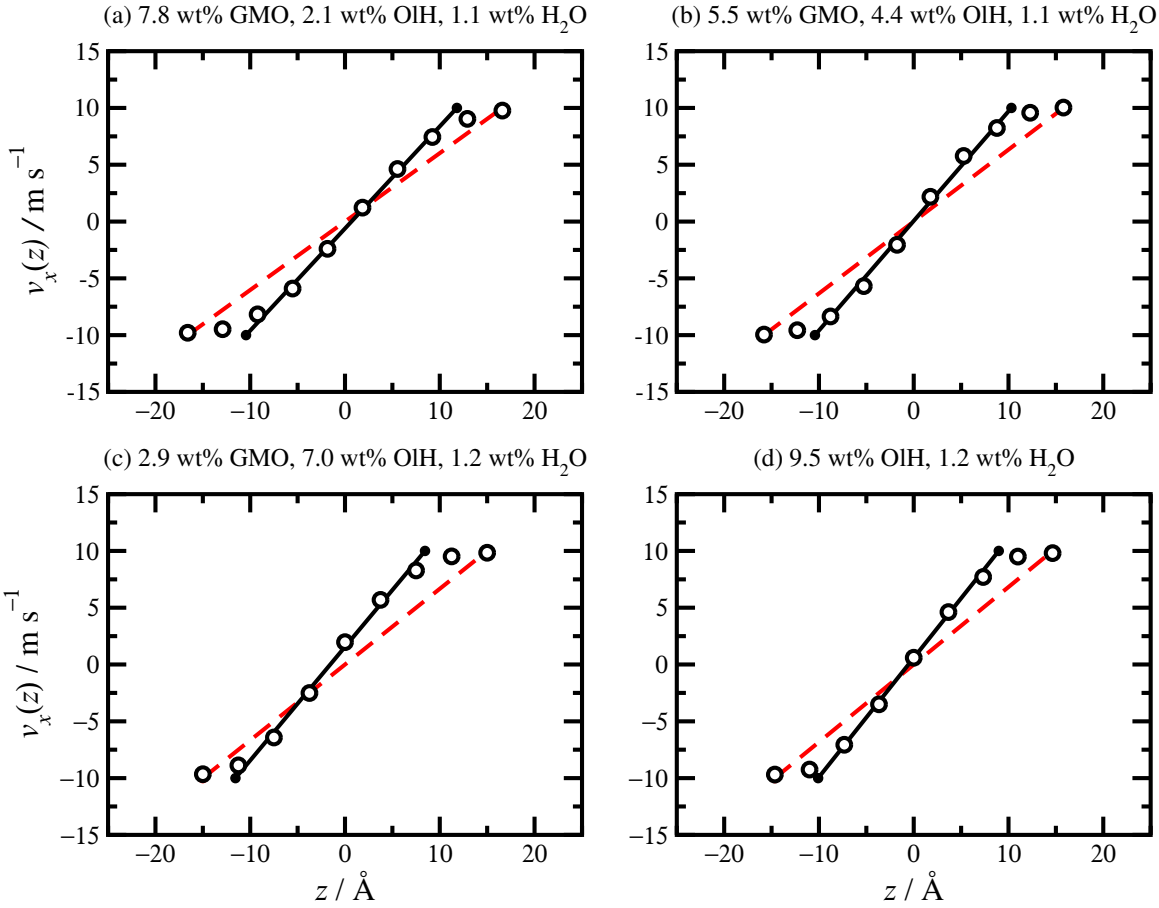


Figure 8: Velocity profiles for GMO, OlH, and H_2O in *n*-heptane confined between parallel mica surfaces and sheared at $v_s = 20$ m s^{-1}: (a) 7.8 wt% GMO, 2.1 wt% OlH, and 1.1 wt% H_2O; (b) 5.5 wt% GMO, 4.4 wt% OlH, and 1.1 wt% H_2O; (c) 2.9 wt% GMO, 7.0 wt% OlH, and 1.2 wt% H_2O; (d) 9.5 wt% OlH and 1.2 wt% H_2O. The points are from simulations, the red dashed line is the ideal (no-stick) velocity profile, and the black solid line is a fit to the central, linear portion of the velocity profile.

2.5 Glycerol monooleate (GMO), oleic acid (OlH), and glycerol (Gly) in *n*-heptane

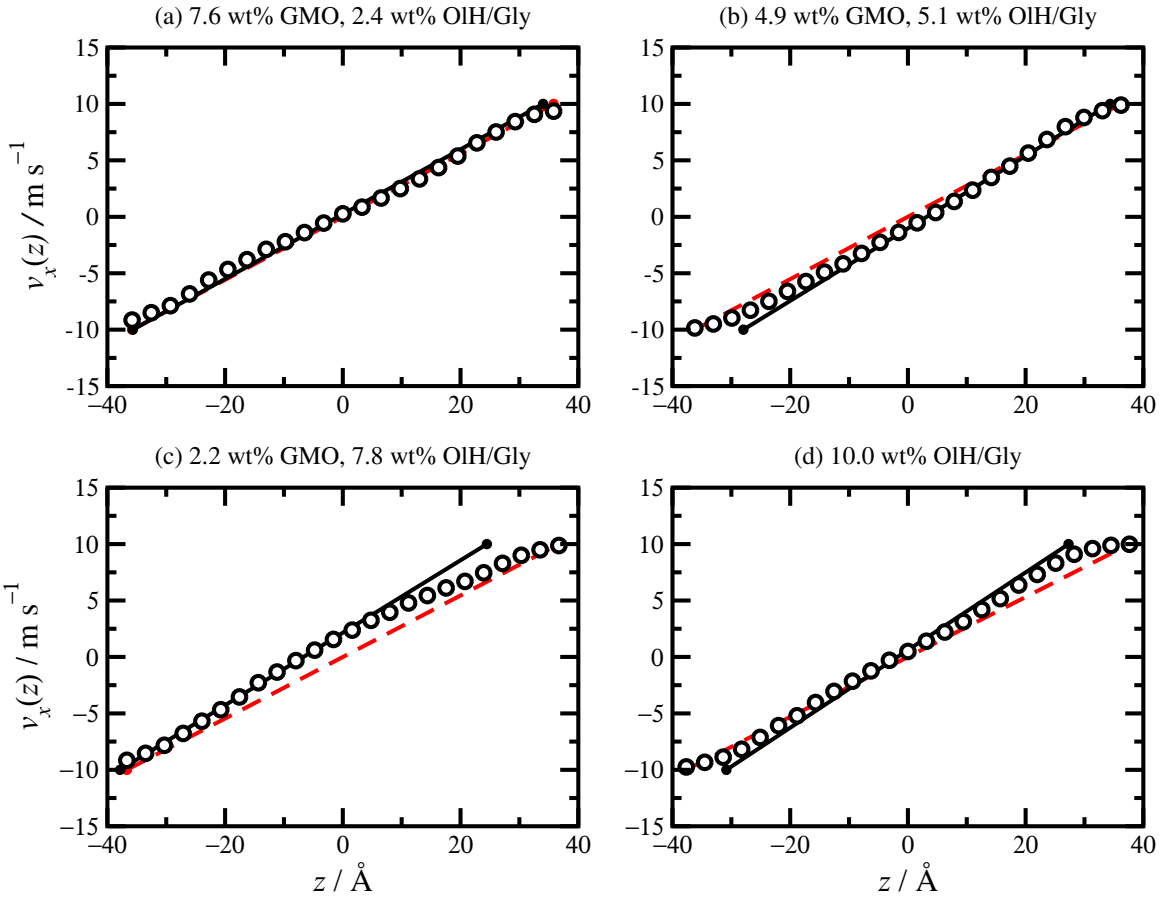


Figure 9: Velocity profiles for GMO, OlH, and Gly in *n*-heptane confined between parallel mica surfaces and sheared at $v_s = 20$ m s^{-1}: (a) 7.6 wt% GMO and 2.4 wt% OlH/Gly; (b) 4.9 wt% GMO and 5.1 wt% OlH/Gly; (c) 2.2 wt% GMO and 7.8 wt% OlH/Gly; (d) 10.0 wt% OlH/Gly. The points are from simulations, the red dashed line is the ideal (no-stick) velocity profile, and the black solid line is a fit to the central, linear portion of the velocity profile.

2.6 Glycerol monooleate (GMO), oleic acid (OlH), and glycerol (Gly) in toluene

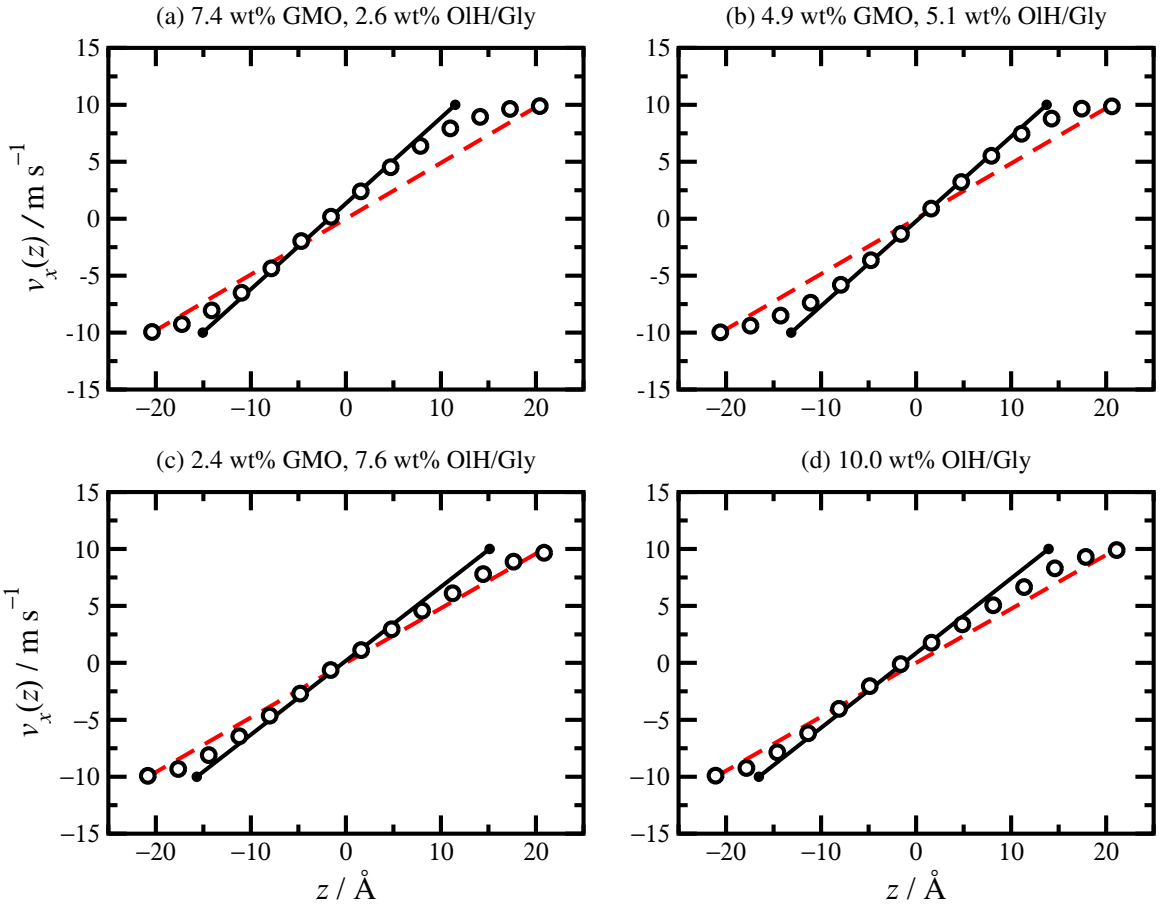


Figure 10: Velocity profiles for GMO, OlH, and Gly in toluene confined between parallel mica surfaces and sheared at $v_s = 20$ m s^{-1}: (a) 7.4 wt% GMO and 2.6 wt% OlH/Gly; (b) 4.9 wt% GMO and 5.1 wt% OlH/Gly; (c) 2.4 wt% GMO and 7.6 wt% OlH/Gly; (d) 10.0 wt% OlH/Gly. The points are from simulations, the red dashed line is the ideal (no-stick) velocity profile, and the black solid line is a fit to the central, linear portion of the velocity profile.

2.7 Glycerol monooleate (GMO) and calcium oleate ($CaOl_2$) in *n*-heptane

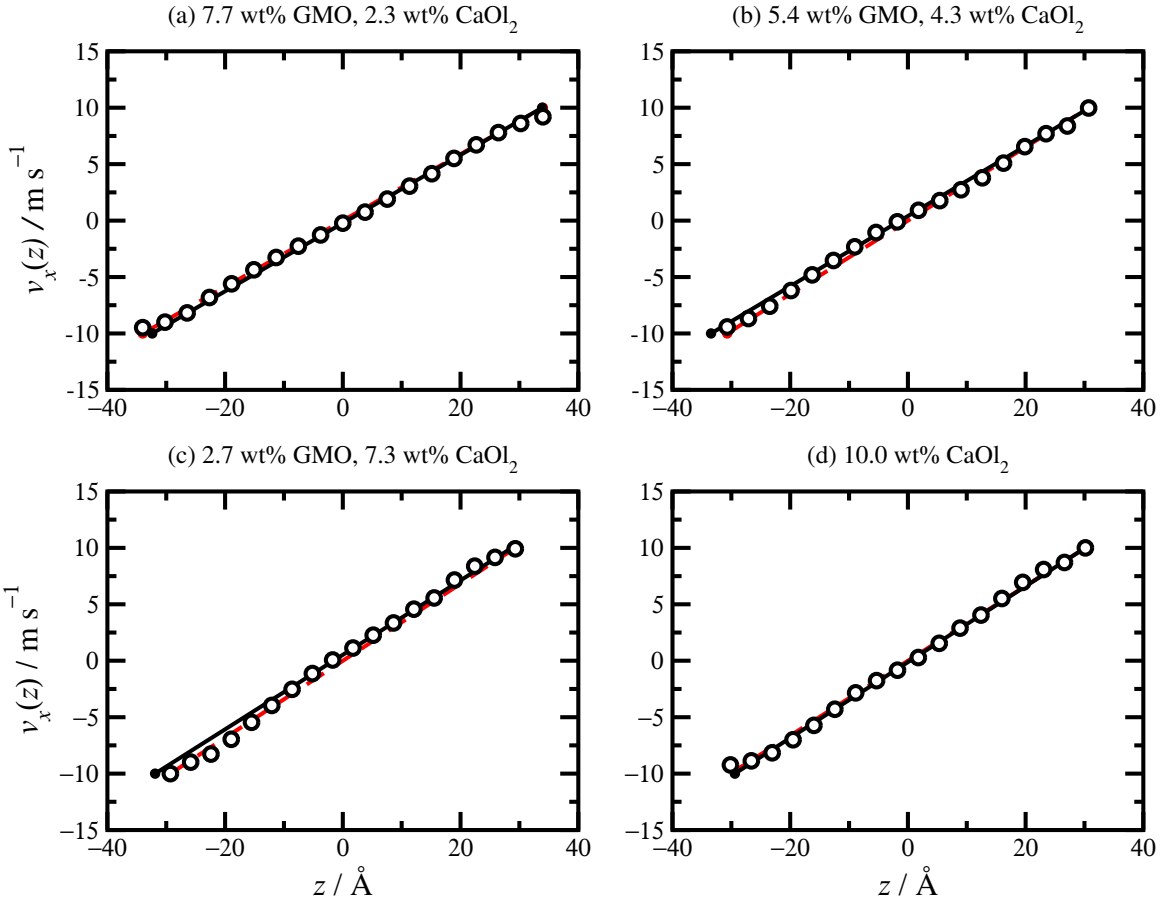


Figure 11: Velocity profiles for GMO and $CaOl_2$ *n*-heptane confined between parallel mica surfaces and sheared at $v_s = 20$ m s^{-1}: (a) 7.7 wt% GMO and 2.3 wt% $CaOl_2$; (b) 5.4 wt% GMO and 4.3 wt% $CaOl_2$; (c) 2.7 wt% GMO and 7.3 wt% $CaOl_2$; (d) 10.0 wt% $CaOl_2$. The points are from simulations, the red dashed line is the ideal (no-stick) velocity profile, and the black solid line is a fit to the central, linear portion of the velocity profile.

2.8 Glycerol monooleate (GMO) and calcium oleate ($CaOl_2$) in toluene

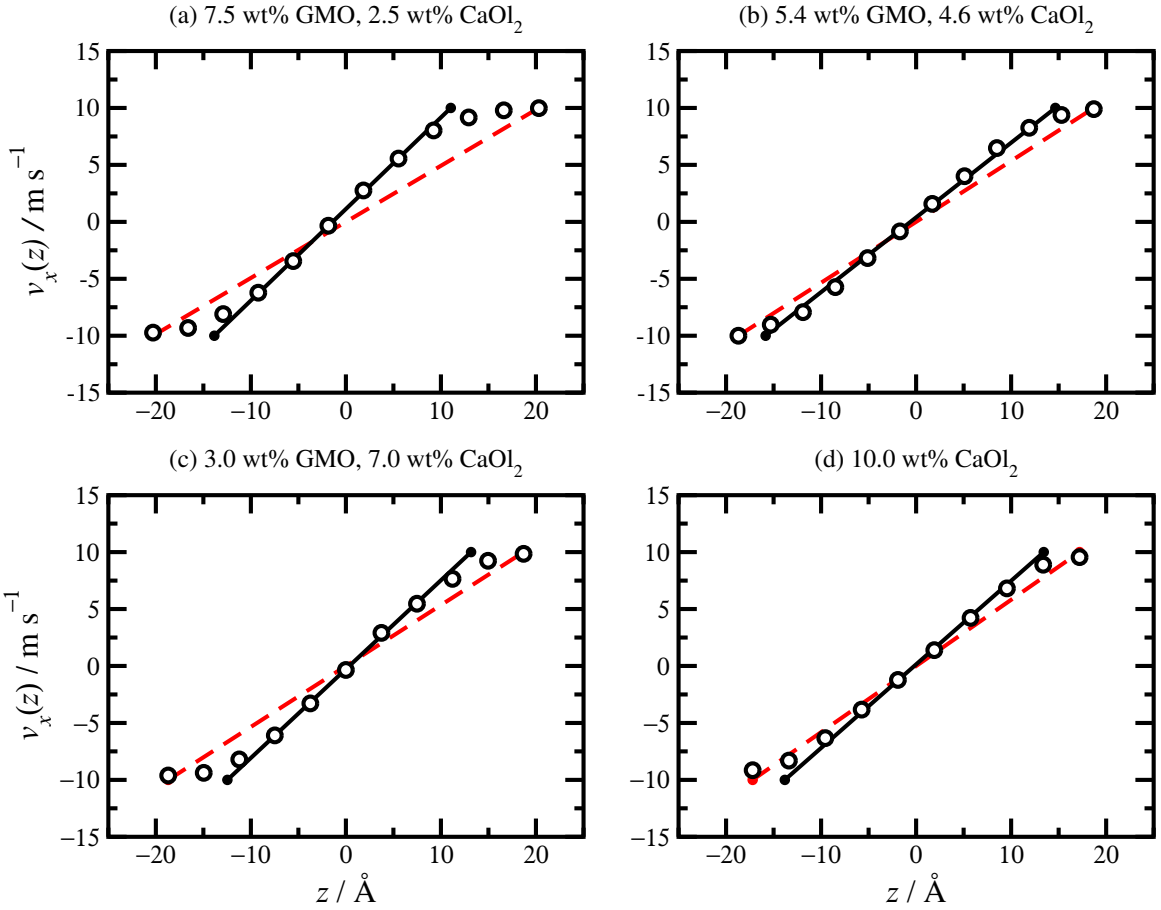


Figure 12: Velocity profiles for GMO and $CaOl_2$ *n*-heptane confined between parallel mica surfaces and sheared at $v_s = 20$ m s^{-1}: (a) 7.5 wt% GMO and 2.5 wt% $CaOl_2$; (b) 5.4 wt% GMO and 4.6 wt% $CaOl_2$; (c) 3.0 wt% GMO and 7.0 wt% $CaOl_2$; (d) 10.0 wt% $CaOl_2$. The points are from simulations, the red dashed line is the ideal (no-stick) velocity profile, and the black solid line is a fit to the central, linear portion of the velocity profile.