

Supporting information

Study of thermodynamic, transport and volumetric properties of nanofluids containing ZrO₂ nanoparticles in polypropylene glycol, polyvinyl pyrrolidone and water

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Table S1. Types of fluids including H₂O-PPG.

Base fluid types	$x_2^{\text{base fluid a}}$
4:1	0.252
3:1	0.174

^a $x_2^{\text{base fluid}}$: mole fraction of PPG in PPG-H₂O aqueous solution.

Table S2. Types of fluids including H₂O-PVP.

Base fluid types	$10^5 \cdot x_2^{\text{base fluid a}}$
H ₂ O-PVP 2%	0.776
H ₂ O-PVP5%	1.898
H ₂ O-PVP10%	4.013
H ₂ O-PVP20%	6.209
H ₂ O-PVP30%	15.533

^a $x_2^{\text{base fluid}}$: mole fraction of PVP in PVP-H₂O aqueous solution.

TableS3. Standard deviations (σ) resulting from fitting the excess molar volume (V_m^E) values in equations (3), (4) and (5) for the ZrO₂-PPG and ZrO₂-H₂O-PVP with temperature dependency at different temperatures.

	Ott et al.		Redlich-Kister		Polynomial	
	Method 1	Method 2	Method 1	Method 2	Method 1	Method 2
ZrO₂-PPG						
<i>T</i> = 293.15 K						
$10^2 \cdot \sigma(V_m^E / (\text{cm}^3 \cdot \text{mol}^{-1}))$	18.1	2.2	52.2	1.5	25.7	0.7
$10^4 \cdot \sigma(d / \text{g} \cdot \text{cm}^{-3})$	6.6	4.9	6.8	5.1	6.5	4.9
<i>T</i> = 298.15 K						
$10^2 \cdot \sigma(V_m^E / (\text{cm}^3 \cdot \text{mol}^{-1}))$	18.2	3.2	49.0	1.0	27.8	0.2
$10^4 \cdot \sigma(d / \text{g} \cdot \text{cm}^{-3})$	10.6	8.3	10.8	8.1	10.6	7.9
<i>T</i> = 308.15 K						
$10^2 \cdot \sigma(V_m^E / (\text{cm}^3 \cdot \text{mol}^{-1}))$	24.4	2.6	41.8	0.9	36.5	1.8
$10^4 \cdot \sigma(d / \text{g} \cdot \text{cm}^{-3})$	17.9	14.0	18.1	13.6	17.9	13.4
<i>T</i> = 318.15 K						
$10^2 \cdot \sigma(V_m^E / (\text{cm}^3 \cdot \text{mol}^{-1}))$	19.8	3.0	56.8	2.0	34.5	1.0
$10^4 \cdot \sigma(d / \text{g} \cdot \text{cm}^{-3})$	9.0	7.1	9.1	7.3	9.0	7.2
Overall ($10^2 \cdot \sigma(V_m^E / (\text{cm}^3 \cdot \text{mol}^{-1}))$)	20.1	2.7	49.9	1.3	31.1	0.9
Overall ($10^4 \cdot \sigma(d / \text{g} \cdot \text{cm}^{-3})$)	11.0	8.6	11.2	8.5	11.0	8.3
ZrO₂-H₂O-PVP						
<i>T</i> = 293.15 K						
$10^4 \cdot \sigma(V_m^E / (\text{cm}^3 \cdot \text{mol}^{-1}))$	4.4	1.4	17.5	1.4	15.9	1.2
$10^4 \cdot \sigma(d / \text{g} \cdot \text{cm}^{-3})$	1.0	0.8	1.0	0.9	1.0	0.8
<i>T</i> = 298.15 K						
$10^4 \cdot \sigma(V_m^E / (\text{cm}^3 \cdot \text{mol}^{-1}))$	4.4	1.5	10.0	2.6	8.5	1.2
$10^4 \cdot \sigma(d / \text{g} \cdot \text{cm}^{-3})$	1.4	1.2	1.4	1.3	1.4	1.2
<i>T</i> = 308.15 K						
$10^4 \cdot \sigma(V_m^E / (\text{cm}^3 \cdot \text{mol}^{-1}))$	1.9	1.0	13.0	2.4	11.5	0.7
$10^4 \cdot \sigma(d / \text{g} \cdot \text{cm}^{-3})$	1.9	1.6	1.9	1.6	1.9	1.6
<i>T</i> = 318.15 K						
$10^4 \cdot \sigma(V_m^E / (\text{cm}^3 \cdot \text{mol}^{-1}))$	3.5	1.2	16.4	2.2	14.9	0.8
$10^4 \cdot \sigma(d / \text{g} \cdot \text{cm}^{-3})$	2.3	1.9	2.3	2.0	2.3	1.9
Overall ($10^4 \cdot \sigma(V_m^E / (\text{cm}^3 \cdot \text{mol}^{-1}))$)	3.5	1.2	14.2	2.1	12.7	0.9
Overall ($10^4 \cdot \sigma(d / \text{g} \cdot \text{cm}^{-3})$)	1.6	1.3	1.6	1.4	1.6	1.3

TableS4. Excess molar volume (V_m^E) parameters of the polynomial equation (5) with temperature dependency using the second fitting method for ZrO₂-PPG and ZrO₂-H₂O-PVP systems.

ZrO₂-PPG						
A_0	$10^{-4}.A_1$	A_2	A_3	$10^{-4}.A_4$	$10^3.A_5$	σ
$10^6.V_m^E / (m^3.mol^{-1})$	-284.203	8.361	-176.936	0.4	-2.862	6
ZrO₂-H₂O-PVP 30%						
B_0	$10^{-3}.B_1$	$10^{-5}.B_2$	$10^{-7}.B_3$	B_4	B_5	$10^4.\sigma$
$10^6.V_m^E / (m^3.mol^{-1})$	-26.574	6.032	-1.053	3.718	558.06	0.661
						2.119

TableS5. Excess molar volume (V_m^E) parameters of the Redlich–Kister (3) temperature-dependent equation using the first fitting method for ZrO₂-PPG and ZrO₂-H₂O-PVP systems.

ZrO₂-PPG						
	$10^{-5}.A_0$	$10^{-7}.A_1$	$10^{-5}.A_2$	$10^{-6}.A_3$	$10^{-5}.A_4$	$10^{-7}.A_5$
$10^6.V_m^E / (m^3.mol^{-1})$	-1.007	-1.104	-2.774	-1.386	-1.798	1.056
ZrO₂-H₂O-PVP 30%						
	$10^{-4}.B_0$	$10^{-4}.B_1$	$10^{-5}.B_2$	$10^{-4}.B_3$	$10^{-4}.B_4$	$10^{-4}.B_5$
$10^6.V_m^E / (m^3.mol^{-1})$	3.9	2.195	100.895	-2.143	-3.917	2.09
						$10^4.\sigma$
						29.14

TableS6. Excess molar volume (V_m^E) parameters of the Ott et al equation (4) temperature-dependent equation using the first fitting method for ZrO₂-PPG and ZrO₂-H₂O-PVP systems.

ZrO₂-PPG													
A_0	A_1	A_2	A_3	A_4	A_5	$10^{-4}.A_6$	A_7	A_8	$10^{-7}.A_9$	$10^{-4}.A_{10}$	$10^{-7}.A_{11}$	σ	
$10^6.V_m^E / (m^3.mol^{-1})$	504.486	10.9	-562.522	2.995	108.856	2.715	3.269	625.36	-1.476	-2.031	-3.565	2.119	0.406
ZrO₂-H₂O-PVP 30%													
$10^{-3}.B_0$	B_1	$10^{-3}.B_2$	$10^{-3}.B_3$	$10^{-3}.B_4$	$10^{-3}.B_5$	$10^{-3}.B_6$	$10^{-4}.B_7$	B_8	$10^{-4}.B_9$	$10^{-3}.B_{10}$	$10^{-4}.B_{11}$	$10^4.\sigma$	
$10^6.V_m^E / (m^3.mol^{-1})$	6.329	81.15	2.071	3.605	-2.18	3.57	7.434	2.141	-23.492	2.125	-7.623	2.109	7.52

TableS7. Excess molar volume (V_m^E) parameters of the polynomial equation (5) temperature-dependent equation using the first fitting method for ZrO₂-PPG and ZrO₂-H₂O-PVP systems.

ZrO₂-PPG							
	$10^{-3}.A_0$	$10^{-7}.A_1$	A_2	$10^{-7}.A_3$	$10^{-5}.A_4$	A_5	σ
$10^6.V_m^E / (m^3.mol^{-1})$	-2.959	4.193	0.11	-4.107	1.383	-72.946	0.629
ZrO₂-H₂O-PVP 30%							
	$10^{-4}.B_0$	$10^{-4}.B_1$	$10^{-4}.B_2$	$10^{-4}.B_3$	$10^{-5}.B_4$	B_5	$10^4.\sigma$
$10^6.V_m^E / (m^3.mol^{-1})$	-2.619	3.179	2.592	3.245	1.303	175.638	26.157

TableS8. Excess molar volume (V_m^E) parameters of the Redlich–Kister (3) temperature-dependent equation using the second fitting method for ZrO₂-PPG and ZrO₂-H₂O-PVP systems.

ZrO₂-PPG						
	$10^{-3}.A_0$	$10^{-4}.A_1$	$10^{-4}.A_2$	$10^{-5}.A_3$	$10^{-3}.A_4$	$10^{-4}.A_5$
$10^6.V_m^E / (m^3.mol^{-1})$	-7.136	-3.656	-1.381	-1.814	-6.961	-6.01
ZrO₂-H₂O-PVP 30%						
	$10^{-3}.B_0$	$10^{-4}.B_1$	$10^{-5}.B_2$	$10^{-5}.B_3$	$10^{-3}.B_4$	$10^{-4}.B_5$
$10^6.V_m^E / (m^3.mol^{-1})$	4.186	1.371	-2.082	-1.816	-4.237	1.35
						$10^4.\sigma$
						4.44

TableS9. Excess molar volume (V_m^E) parameters of the Ott et al equation (4) temperature-dependent equation using the second fitting method for ZrO₂-PPG and ZrO₂-H₂O-PVP systems.

ZrO₂-PPG													
A_0	$10^{-3}.A_1$	A_2	A_3	A_4	A_5	A_6	A_7	A_8	A_9	$10^{-3}.A_{10}$	A_{11}	σ	
$10^6.V_m^E / (m^3.mol^{-1})$	-20.936	5.629	998.645	231.159	-291.156	210.331	998.647	231.158	-291.139	210.322	-1.617	190.106	0.056

ZrO₂-H₂O-PVP 30%													
$10^{-3}.B_0$	B_1	$10^3.B_2$	B_3	$10^3.B_4$	B_5	$10^3.B_6$	$10^{-4}.B_7$	$10^3.B_8$	B_9	$10^3.B_{10}$	B_{11}	$10^4.\sigma$	
$10^6.V_m^E / (m^3.mol^{-1})$	-16.064	0.049	-6.524	1.314	-6.057	1.316	-6.528	1.314	-6.061	1.316	-1.937	1.315	2.71

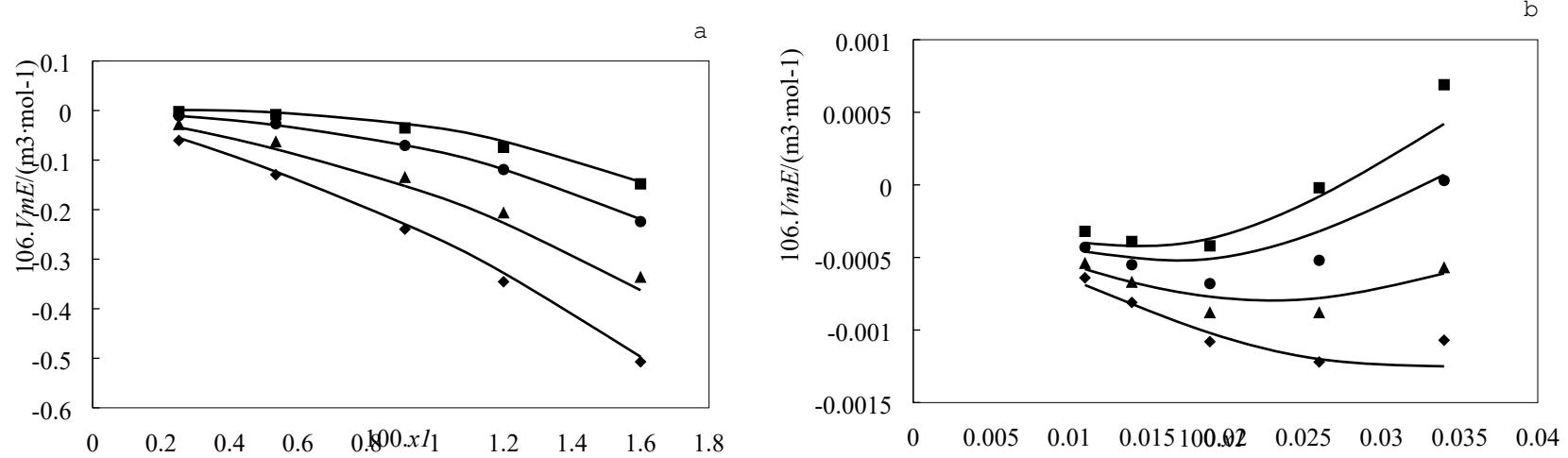


Figure (S1): The excess molar volume obtained from fitting the data in the temperature-dependent equation using the second fitting method in terms of nanoparticle molar fraction for the system (a) ZrO₂-PPG and (b) ZrO₂-H₂O-PVP at T = (293.15(■),298.15(●),308.15(▲),318.15(♦)) K compared to (—) polynomial equation with temperature dependency.