TD Corrélation de données

Des mesures ont été réalisées sur le glycinate de sodium. Ce sont des mesures de viscosité dynamique η en Pa·s de masse volumique ρ en kg·m^3.

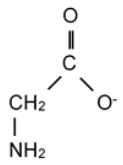


Table 5: Experimental values of dynamic viscosity η (Pa·s) vs temperature T (K) and mass fraction w for GlyK solutions[a]

		T / K							
		288.15	293.15	298.15	303.15	308.15	313.15	318.15	323.15
w	U(w)	10^3·η/Pa·s	10^3·η/Pa·s	10^3·η/Pa·s	10^3·η/Pa·s	10^3·η/Pa·s	10^3·η/Pa·s	10^3·η/Pa·s	10^3·η/Pa·s
0.04122	0.00018	1.225	1.084	0.969	0.871	0.789	0.717	0.655	0.603
0.06241	0.00023	1.272	1.122	1.001	0.900	0.818	0.742	0.676	0.620
0.07164	0.00025	1.315	1.165	1.041	0.937	0.850	0.773	0.708	0.652
0.10116	0.00033	1.371	1.214	1.085	0.978	0.889	0.810	0.743	0.685
0.11904	0.00038	1.456	1.291	1.155	1.040	0.942	0.859	0.786	0.722
0.1517	0.00047	1.575	1.394	1.247	1.124	1.018	0.927	0.850	0.783
0.19913	0.00062	1.763	1.562	1.398	1.262	1.147	1.049	0.960	0.883
0.25105	0.00077	2.045	1.807	1.613	1.448	1.311	1.193	1.091	1.002
0.29900	0.00091	2.421	2.128	1.892	1.714	1.544	1.407	1.302	1.180
0.4034	0.0012	3.714	3.242	2.856	2.538	2.270	2.047	1.854	1.689

[a] U(w) is the expanded uncertainty in mass fraction with a level of confidence of 95% (k = 2). The expanded uncertainties with a level of confidence of 95% (k = 2) are U(T) = 0.08 K and U(η) = 2.3·10^{-2} mPa·s = 2.3·10^{-5} Pa·s.

Table 6: Experimental values of dynamic viscosity η (Pa·s) vs temperature T (K) and mass fraction w for GlyNa solutions[a]

		T / K							
		288.15	293.15	298.15	303.15	308.15	313.15	318.15	323.15
w	U(w)	10^3·η/Pa·s	10^3·η/Pa·s	10^3·η/Pa·s	10^3·η/Pa·s	10^3·η/Pa·s	10^3·η/Pa·s	10^3·η/Pa·s	10^3·η/Pa·s
0.03555	0.00015	1.281	1.130	1.007	0.903	0.816	0.741	0.676	0.621
0.05881	0.00021	1.379	1.216	1.080	0.967	0.873	0.793	0.722	0.663
0.06069	0.00021	1.395	1.230	1.095	0.980	0.885	0.803	0.732	0.672
0.08657	0.00028	1.566	1.369	1.214	1.086	0.978	0.887	0.808	0.741
0.09956	0.00032	1.652	1.451	1.291	1.155	1.043	0.945	0.860	0.787
0.10506	0.00033	1.671	1.484	1.323	1.184	1.063	0.958	0.866	0.785
0.13832	0.00043	1.919	1.700	1.513	1.351	1.211	1.090	0.983	0.890
0.19743	0.00061	2.637	2.364	2.071	1.817	1.605	1.432	1.299	1.183
0.24637	0.00076	3.501	3.001	2.603	2.281	2.018	1.801	1.617	1.462
0.29332	0.0009	4.856	4.099	3.513	3.043	2.664	2.349	2.089	1.881
0.3906	0.0012	10.532	8.505	6.996	5.846	4.959	4.256	3.708	3.255

[a] U(w) is the expanded uncertainty in mass fraction with a level of confidence of 95% (k = 2). The expanded uncertainties with a level of confidence of 95% (k = 2) are U(T) = 0.08 K and U(η) = 2.3·10^{-2} mPa·s = 2.3·10^{-5} Pa·s.

Table 7: Experimental values of density ρ (kg·m^{-3}) vs temperature T (K) and mass fraction w for GlyK solutions[a]

		T / K							
		288.15	293.15	298.15	303.15	308.15	313.15	318.15	323.15
w	*U(w)*	*ρ/kg·m^{-3}*	*ρ/kg·m^{-3}*	*ρ/kg·m^{-3}*	*ρ/kg·m^{-3}*	*ρ/kg·m^{-3}*	*ρ/kg·m^{-3}*	*ρ/kg·m^{-3}*	*ρ/kg·m^{-3}*
0.04122	0.00018	1024.6	1023.5	1022.1	1020.6	1018.8	1016.9	1014.8	1012.5
0.06241	0.00023	1032.6	1031.3	1029.9	1028.2	1026.4	1024.4	1022.3	1020.0
0.07164	0.00025	1040.8	1039.5	1038.0	1036.3	1034.4	1032.4	1030.3	1027.9
0.10116	0.00033	1054.0	1052.6	1050.9	1049.2	1047.2	1045.1	1042.9	1040.6
0.11904	0.00038	1067.2	1065.7	1064.0	1062.1	1060.1	1058.0	1055.9	1053.5
0.1517	0.00047	1086.4	1084.7	1082.9	1080.9	1078.8	1076.6	1074.3	1071.8
0.19913	0.00062	1109.9	1108.0	1106.1	1104.0	1101.7	1099.4	1097.0	1094.5
0.25105	0.00077	1140.5	1138.4	1136.3	1134.0	1131.7	1129.3	1126.8	1124.2
0.299	0.00091	1169.3	1167.1	1164.8	1162.5	1160.0	1157.5	1154.9	1152.3
0.4034	0.0012	1234.7	1232.2	1229.6	1227.0	1224.3	1221.6	1218.8	1216.0

[a] U(w) is the expanded uncertainty in mass fraction with a level of confidence of 95% (k = 2). The expanded uncertainties with a level of confidence of 95% (k = 2) are U(T) = 0.08 K and U(ρ) = 0.4 kg/m^3

Table 8: Experimental values of density ρ (kg·m^{-3}) vs temperature T (K) and mass fraction w for GlyNa solutions[a]

		T / K							
		288.15	293.15	298.15	303.15	308.15	313.15	318.15	323.15
w	*U(w)*	*ρ/kg·m^{-3}*	*ρ/kg·m^{-3}*	*ρ/kg·m^{-3}*	*ρ/kg·m^{-3}*	*ρ/kg·m^{-3}*	*ρ/kg·m^{-3}*	*ρ/kg·m^{-3}*	*ρ/kg·m^{-3}*
0.03555	0.00015	1021.5	1020.3	1019.0	1017.4	1015.6	1013.6	1011.5	1009.3
0.05881	0.00021	1033.7	1032.3	1030.8	1029.1	1027.2	1025.2	1023.0	1020.7
0.06069	0.00021	1035.6	1034.3	1032.7	1031.0	1029.1	1027.1	1024.9	1022.6
0.08657	0.00028	1049.7	1048.1	1046.3	1044.4	1042.4	1040.1	1038.0	1035.7
0.09956	0.00032	1060.5	1058.9	1057.1	1055.2	1053.1	1050.9	1048.6	1045.8
0.10506	0.00033	1064.1	1062.4	1060.6	1058.7	1056.6	1054.4	1052.1	1049.7
0.13832	0.00043	1083.3	1081.5	1079.5	1077.4	1075.2	1072.9	1070.5	1068.0
0.19743	0.00061	1116.0	1113.9	1111.7	1109.4	1106.8	1104.3	1101.7	1099.1
0.24637	0.00076	1146.4	1144.0	1141.6	1139.0	1136.5	1133.8	1131.1	1128.3
0.29332	0.00090	1175.6	1173.0	1170.4	1167.7	1164.9	1162.1	1159.3	1156.4
0.3906	0.0012	1236.6	1233.6	1230.6	1227.6	1224.6	1221.5	1218.4	1215.2

[a] U(w) is the expanded uncertainty in mass fraction with a level of confidence of 95% (k = 2). The expanded uncertainties with a level of confidence of 95% (k = 2) are U(T) = 0.08 K and U(ρ) = 0.4 kg/m^3

Dans la littérature, plusieurs relations sont disponibles pour corréler ces mesures. Le tableau ci-dessous regroupe les corrélations pour estimer la viscosité :

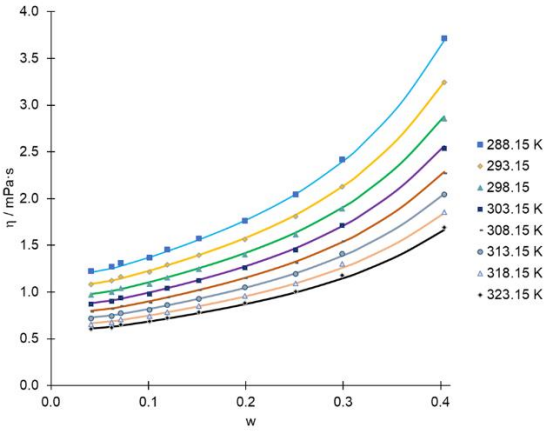
Solutions	Authors	Equation	Temperature range / K	Concentration range
Barium chloride aqueous solutions	Jones and Dole[36]	$\eta = 1 + A \cdot \sqrt{C} + B \cdot C$	298.15	0.005 – 1.0 M
GlyNa aqueous solutions	Lee et al.[29]	$\eta = exp\left(A_1 + \frac{A_2}{T + A_3}\right)$	303 – 353	10 – 50 wt% (mass fraction)
Potassium Amino-acid salts aqueous solutions	Holst et al.[28]	$\eta = A_1 \cdot exp\left(\frac{A_2 \cdot exp(A_3 \cdot C)}{R \cdot T}\right) \cdot \exp(A_4 \cdot C)$	298.15 – 333.15	0.2 – 3.5 M

GlyNa + piperazine aqueous solutions	Shaikh et al.[30]	$\eta = A_1 \cdot ln(T) + A_2$	298.15 – 343.15	GlyNa: 0.0348 – 0.0177 (mole fraction) Piperazine: 0.0348 – 0.0177 (mole fraction)
Aqueous blends of carbonic-anhydrase enzyme and L-lysine solutions	Suleman and Fosbøl[37]	$\eta = \eta_{H_2O} \cdot (k_A + k_b \cdot W_{PL} + k_c \cdot W_{CA} + k_d \cdot T + k_e \cdot W_{PL} \cdot T)$	303 – 353	W_{PL} = 0.296 – 0.489 (mass fraction) W_{PL} =0 – 3.4 g/L)

Le tableau ci-dessous regroupe les corrélations pour estimer la masse volumique :

Solutions	Authors	Equation	Temperature range / K	Concentration range
GlyNa aqueous solutions	Lee et al.[29]	$\rho = A_1 + A_2 \cdot T + A_3 \cdot T^2$	303 – 353	w = 10 – 50 wt% (mass fraction)
GlyNa aqueous solutions	Harris et al.[31]	$\rho = A_0 \cdot T + A_1$	298.15 – 353.15	w = 1 – 30 wt% (mass fraction)
Potassium Amino-acid salts aqueous solutions	Holst et al.[28]	$\rho = A_1 \cdot T + A_2 \cdot C + A_3$	298.15 – 333.15	C = 0.2 –3.5 M
GlyNa + piperazine aqueous solutions	Shaikh et al.[30]	$\rho = A_1 + A_2 \cdot T + A_3 \cdot T^2$	298.15 – 343.15	GlyNa: 0.0348 – 0.0177 (mole fraction) Piperazine: 0.0348 – 0.0177 (mole fraction)
Aqueous blends of carbonic anhydrase enzyme and L-lysine solutions	Suleman and Fosbøl[37]	$\rho = \rho_{H_2O} \cdot (k_1 + k_2 \cdot W_{PL} + k_3 \cdot W_{CA} + k_4 \cdot T)$	303 – 353	W_{PL} = 0.296 - 0.489 (mass fraction) W_{PL} =0 – 3.4 g/L)

Question 1 : Réaliser une représentation graphique de ce type (figure ci-contre).



Question 2 :

Question 2 : Tester une corrélation

Question 3 : imaginer une corrélation intégrant simultanément l'influence de la température et de la fraction massique

Question 4 :Représenter graphiquement les résultats

Question 5 : Faire un diagramme de parité

Question 6 : Tracer les deux grandeurs suivantes

root mean square error $$RMSE = \sqrt{\frac{\sum_1^N (y_{i,exp} - y_{i,model})^2}{N}}$$

average absolute relative deviation $$AARD(\%) = \frac{100}{N} \times \sum_1^N \left| \frac{y_{i,exp} - y_{i,model}}{y_{i,exp}} \right|$$