

Supplementary Information

Brownian Dynamics Simulations of AUC SV Experiments Exhibiting Hydrodynamic and Thermodynamic Non-ideality Phenomena

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Simulation of hydrodynamic non-ideality in SV

Table 1: Non-ideality parameters retrieved by the non-ideal sedimentation model in SEDFIT for BD simulation of hydrodynamic non-ideality in SV data. Deviations from input values are given in parentheses.

Series	Input to BD simulation			Retrieved by non-ideality model in SEDFIT			
	s_0 / S	$D_0 / 10^{-7} \text{ cm}^2 \text{ s}^{-1}$	$k_{s,BD} / \text{mL} \cdot \text{g}^{-1}$	$c / \text{g L}^{-1}$	s_0 / S	$D_0 / 10^{-7} \text{ cm}^2 \text{ s}^{-1}$	$k_s / \text{mL} \cdot \text{g}^{-1}$
1	44.76	8.56	-150	0.25	44.79 (0.06 %)	8.73 (1.91 %)	-144.4 (3.74 %)
				0.5	44.73 (0.07 %)	8.59 (0.27 %)	-150.1 (0.03 %)
				0.75	44.74 (0.04 %)	8.66 (1.13 %)	-149.9 (0.10 %)
				1.0	44.78 (0.04 %)	8.77 (2.37 %)	-149.1 (0.63 %)
				1.25	44.71 (0.11 %)	8.60 (0.41 %)	-150.4 (0.28 %)
				1.5	44.71 (0.11 %)	8.59 (0.35 %)	-150.4 (0.23 %)
				2.5	44.72 (0.09 %)	8.57 (0.10 %)	-150.1 (0.09 %)
				3.0	44.74 (0.04 %)	8.71 (1.73 %)	-150.0 (0.02 %)
				4.0	44.75 (0.02 %)	8.74 (2.05 %)	-150.0 (0.02 %)
				5.0	*	*	*
2	44.76	8.56	100	0.25	44.83 (0.16 %)	8.76 (2.35 %)	110.5 (10.5 %)
				0.5	44.85 (0.19 %)	8.75 (2.15 %)	105.5 (5.47 %)
				0.75	44.85 (0.20 %)	8.75 (2.22 %)	104.3 (4.27 %)
				1.0	44.79 (0.08 %)	8.64 (0.92 %)	101.8 (1.83 %)
				1.25	44.86 (0.22 %)	8.74 (2.08 %)	102.9 (2.92 %)
				1.5	44.81 (0.11 %)	8.66 (1.08 %)	101.6 (1.55 %)
				2.5	44.85 (0.19 %)	8.67 (1.22 %)	101.4 (1.38 %)
				3.0	44.83 (0.15 %)	8.64 (0.95 %)	100.7 (0.70 %)
				4.0	44.78 (0.04 %)	8.59 (0.31 %)	100.5 (0.45 %)
				5.0	44.78 (0.05 %)	8.60 (0.38 %)	100.4 (0.42 %)
3	44.76	8.56	200	0.25	44.85 (0.19 %)	8.77 (2.38 %)	212.1 (6.07 %)
				0.5	44.90 (0.32 %)	8.73 (1.99 %)	209.5 (4.72 %)
				0.75	44.86 (0.23 %)	8.73 (1.97 %)	205.1 (2.56 %)
				1.0	44.79 (0.06 %)	8.65 (1.06 %)	201.8 (0.89 %)
				1.25	44.85 (0.20 %)	8.67 (1.30 %)	203.0 (1.47 %)
				1.5	44.79 (0.08 %)	8.56 (0.02 %)	201.4 (0.71 %)
				2.5	44.77 (0.02 %)	8.59 (0.27 %)	200.6 (0.32 %)
				3.0	44.78 (0.05 %)	8.61 (0.56 %)	200.9 (0.38 %)
				4.0	44.84 (0.17 %)	8.61 (0.53 %)	201.2 (0.61 %)
				5.0	44.91 (0.33 %)	8.61 (0.51 %)	201.9 (0.90 %)
4	44.76	8.56	500	0.25	44.86 (0.06 %)	8.74 (1.91 %)	514.7 (2.93 %)
				0.5	44.86 (0.07 %)	8.61 (0.27 %)	508.3 (1.65 %)
				0.75	44.81 (0.04 %)	8.62 (1.13 %)	503.6 (0.72 %)
				1.0	44.70 (0.04 %)	8.51 (2.37 %)	498.8 (0.24 %)
				1.25	44.82 (0.11 %)	8.61 (0.41 %)	502.9 (0.59 %)
				1.5	44.65 (0.11 %)	8.50 (0.35 %)	498.1 (0.39 %)
				2.5	44.90 (0.09 %)	8.59 (0.10 %)	503.8 (0.77 %)
				3.0	44.89 (0.04 %)	8.60 (1.73 %)	503.1 (0.62 %)
				4.0	44.75 (0.02 %)	8.53 (2.05 %)	500.9 (0.18 %)
				5.0	44.73 (0.18 %)	8.53 (0.37 %)	500.7 (0.14 %)

* Data could not be evaluated as SEDFIT crashed when datasets were evaluated.

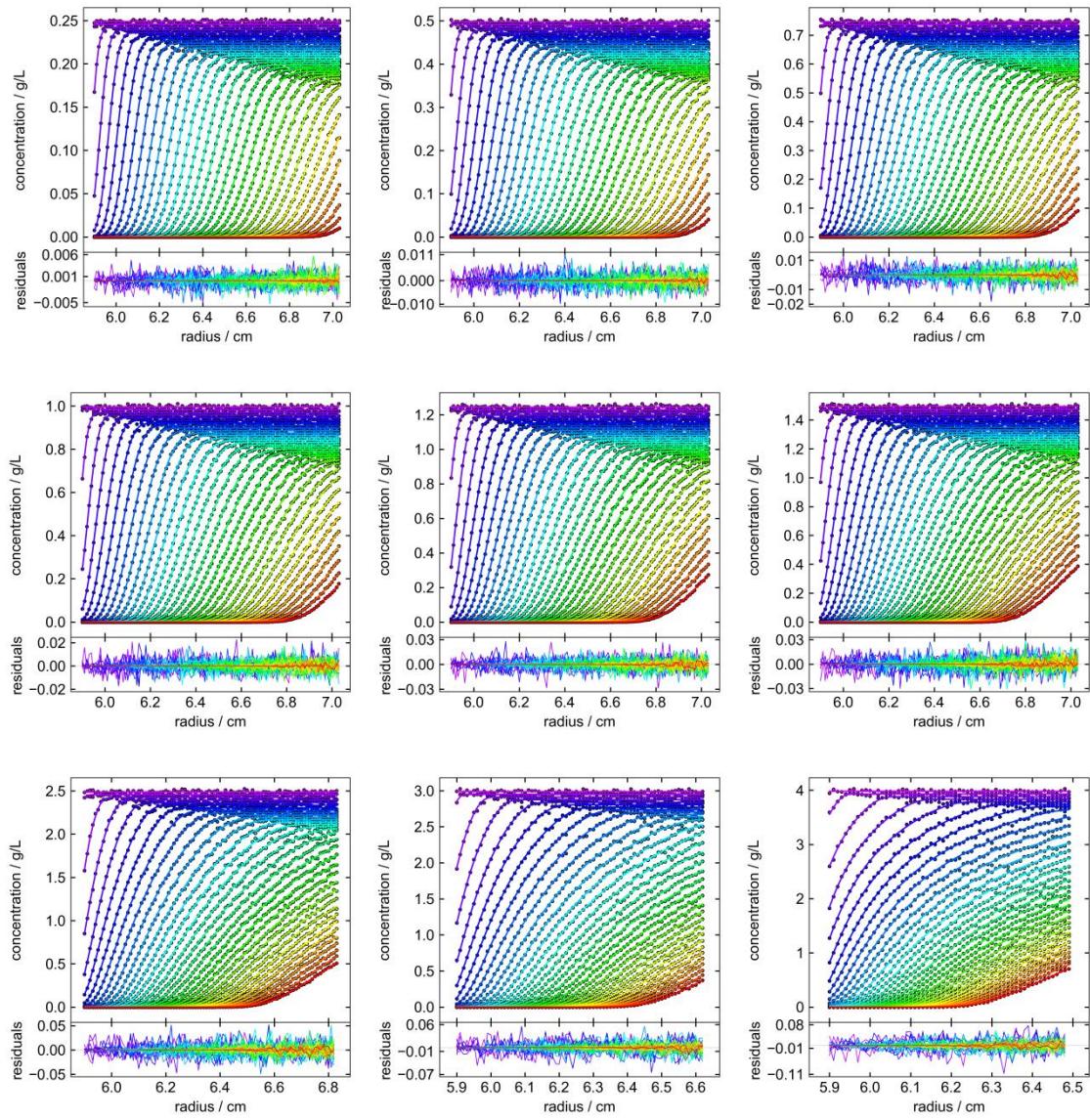


Figure 1: Sedimentation profiles, fitted profiles and residuals of the non-ideal sedimentation model in SEDFIT. Simulation parameters were $s_0 = 44.76 \text{ S}$, $D_0 = 8.56 \cdot 10^{-7} \text{ cm}^2 \cdot \text{s}^{-1}$, $c = 0.25\text{-}4 \text{ g} \cdot \text{L}^{-1}$, $k_s = -150 \text{ mL} \cdot \text{g}^{-1}$ and $k_d = 0 \text{ mL} \cdot \text{g}^{-1}$. Every third profile and every second data point is shown.

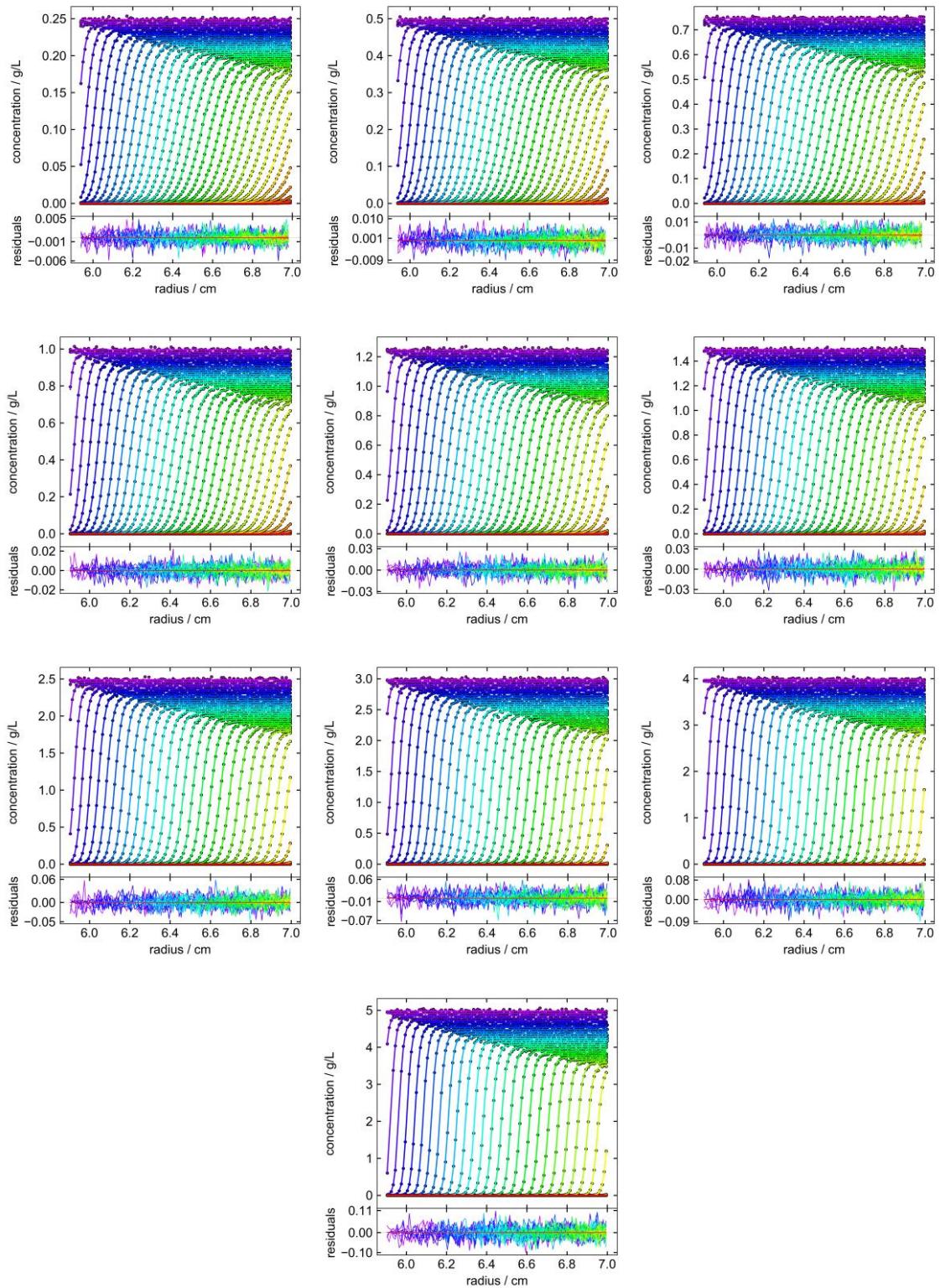


Figure 2: Sedimentation profiles, fitted profiles and residuals of the non-ideal sedimentation model in SEDFIT. Simulation parameters were $s_0 = 44.76 \text{ S}$, $D_0 = 8.56 \cdot 10^{-7} \text{ cm}^2 \cdot \text{s}^{-1}$, $c = 0.25\text{--}5 \text{ g} \cdot \text{L}^{-1}$, $k_s = 100 \text{ mL} \cdot \text{g}^{-1}$ and $k_d = 0 \text{ mL} \cdot \text{g}^{-1}$. Every third profile and every second data point is shown.

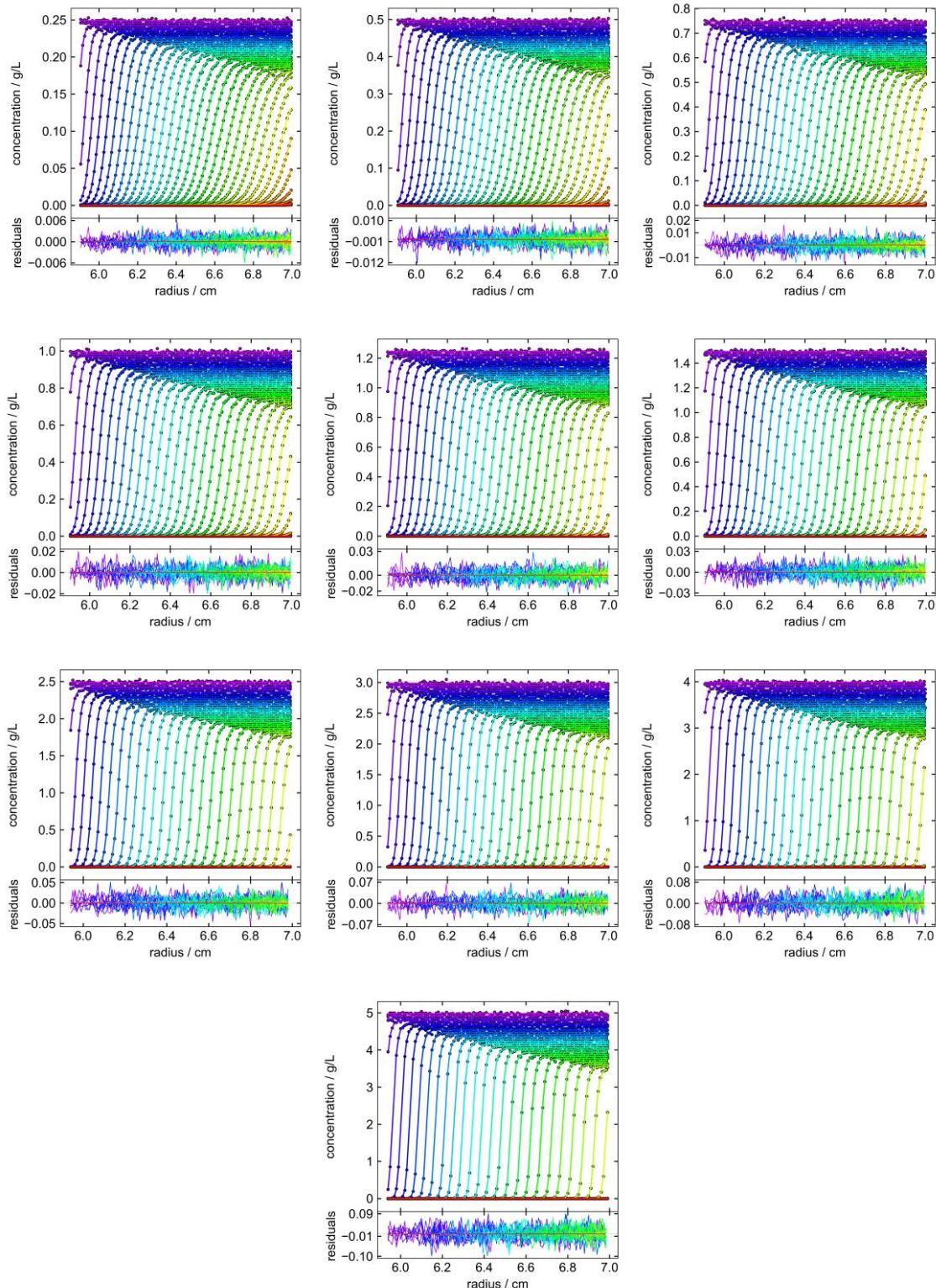


Figure 3: Sedimentation profiles, fitted profiles and residuals of the non-ideal sedimentation model in SEDFIT. Simulation parameters were $s_0 = 44.76 \text{ S}$, $D_0 = 8.56 \cdot 10^{-7} \text{ cm}^2 \cdot \text{s}^{-1}$, $c = 0.25\text{--}5 \text{ g} \cdot \text{L}^{-1}$, $k_s = 200 \text{ mL} \cdot \text{g}^{-1}$ and $k_d = 0 \text{ mL} \cdot \text{g}^{-1}$. Every third profile and every second data point is shown.

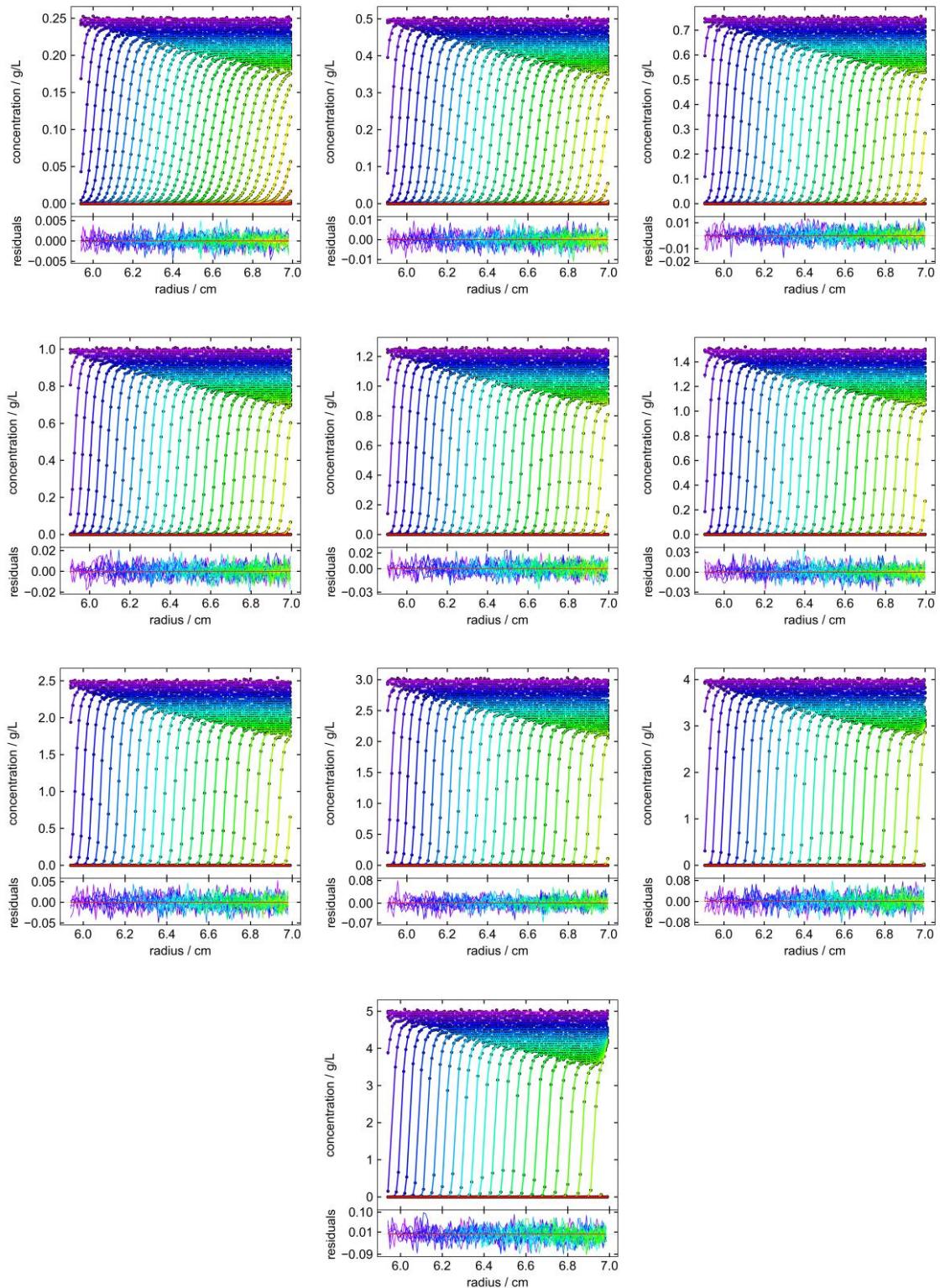


Figure 4: Sedimentation profiles, fitted profiles and residuals of the non-ideal sedimentation model in SEDFIT. Simulation parameters were $s_0 = 44.76 \text{ S}$, $D_0 = 8.56 \cdot 10^{-7} \text{ cm}^2 \cdot \text{s}^{-1}$, $c = 0.25 \text{ g} \cdot \text{L}^{-1}$, $k_s = 500 \text{ mL} \cdot \text{g}^{-1}$ and $k_d = 0 \text{ mL} \cdot \text{g}^{-1}$. Every third profile and every second data point is shown.

Simulation of thermodynamic non-ideality in SV

Table 2: Non-ideality parameters retrieved by the non-ideal sedimentation model in SEDFIT for BD simulation of thermodynamic non-ideality in SV data. Deviations from input values are given in parentheses.

Input to BD simulation				Retrieved by non-ideality model in SEDFIT			
Series	s_0 / S	$D_0 / 10^{-7} \text{ cm}^2 \text{s}^{-1}$	$2BM / \text{mL}\cdot\text{g}^{-1}$	$c / \text{g L}^{-1}$	s_0 / S	$D_0 / 10^{-7} \text{ cm}^2 \text{s}^{-1}$	$2BM / \text{mL}\cdot\text{g}^{-1}$
5	44.76	8.56	-150	0.25	44.74 (0.05 %)	8.51 (0.66 %)	185.6 (23.1 %)
				0.5	44.72 (0.09 %)	8.51 (0.64 %)	229.0 (52.69 %)
				0.75	*	*	*
				1.0	*	*	*
				1.25	*	*	*
				1.5	*	*	*
				2.5	*	*	*
				3.0	*	*	*
				4.0	*	*	*
				5.0	*	*	*
6	44.76	8.56	100	0.25	44.74 (0.05 %)	8.49 (0.82 %)	333.3 (233.3 %)
				0.5	44.74 (0.05 %)	8.51 (0.65 %)	258.2 (158.2 %)
				0.75	44.74 (0.05 %)	8.51 (0.60 %)	236.8 (136.8 %)
				1.0	44.74 (0.06 %)	8.50 (0.69 %)	230.3 (130.3 %)
				1.25	44.73 (0.06 %)	8.51 (0.64 %)	223.4 (123.4 %)
				1.5	44.73 (0.06 %)	8.51 (0.62 %)	219.1 (119.1 %)
				2.5	44.73 (0.05 %)	8.50 (0.70 %)	212.5 (112.5 %)
				3.0	44.73 (0.06 %)	8.50 (0.72 %)	210.7 (110.7 %)
				4.0	44.73 (0.07 %)	8.51 (0.66 %)	207.7 (107.7 %)
				5.0	44.73 (0.08 %)	8.49 (0.81 %)	207.2 (107.2 %)
7	44.76	8.56	200	0.25	44.74 (0.05 %)	8.50 (0.68 %)	519.2 (159.6 %)
				0.5	44.74 (0.06 %)	8.51 (0.66 %)	459.1 (129.5 %)
				0.75	44.73 (0.06 %)	8.50 (0.75 %)	442.6 (121.3 %)
				1.0	44.73 (0.06 %)	8.51 (0.64 %)	429.4 (114.7 %)
				1.25	44.73 (0.06 %)	8.51 (0.62 %)	423.5 (111.7 %)
				1.5	44.73 (0.07 %)	8.50 (0.69 %)	420.7 (110.3 %)
				2.5	44.73 (0.08 %)	8.50 (0.70 %)	412.8 (106.4 %)
				3.0	44.72 (0.08 %)	8.50 (0.76 %)	411.4 (105.7 %)
				4.0	44.72 (0.09 %)	8.49 (0.81 %)	409.2 (104.6 %)
				5.0	44.72 (0.10 %)	8.48 (0.93 %)	408.6 (104.3 %)
8	44.76	8.56	500	0.25	44.73 (0.06 %)	8.50 (0.73 %)	1126 (125.2 %)
				0.5	44.73 (0.06 %)	8.50 (0.73 %)	1064 (112.7 %)
				0.75	44.73 (0.07 %)	8.51 (0.59 %)	1038 (107.6 %)
				1.0	44.73 (0.07 %)	8.51 (0.67 %)	1031 (106.3 %)
				1.25	44.72 (0.08 %)	8.49 (0.87 %)	1031 (106.2 %)
				1.5	44.72 (0.09 %)	8.49 (0.86 %)	1026 (105.2 %)
				2.5	44.71 (0.12 %)	8.62 (0.63 %)	987 (97.30 %)
				3.0	44.70 (0.13 %)	8.44 (1.47 %)	1007 (101.3 %)
				4.0	44.69 (0.16 %)	8.41 (1.81 %)	1007 (101.3 %)
				5.0	44.68 (0.18 %)	8.58 (0.19 %)	987 (97.42 %)

*data could not be evaluated as SEDFIT crashed when these datasets were evaluated.

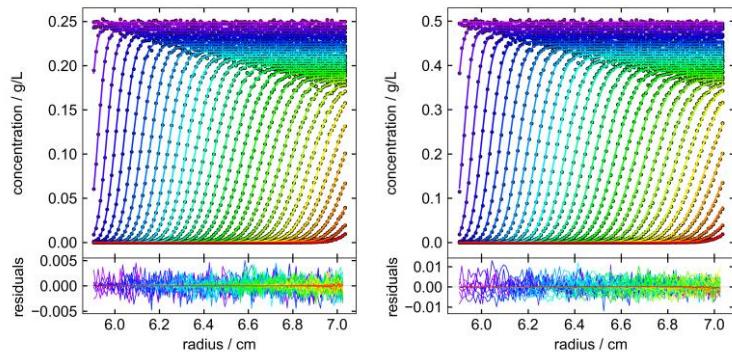


Figure 5: Sedimentation profiles, fitted profiles and residuals of the non-ideal sedimentation model in SEDFIT. Simulation parameters were $s_0 = 44.76 \text{ S}$, $D_0 = 8.56 \cdot 10^{-7} \text{ cm}^2 \cdot \text{s}^{-1}$, $c = 0.25\text{--}0.5 \text{ g} \cdot \text{L}^{-1}$, $k_s = 0 \text{ mL} \cdot \text{g}^{-1}$ and $2BM = -150 \text{ mL} \cdot \text{g}^{-1}$. Every third profile and every second data point is shown.

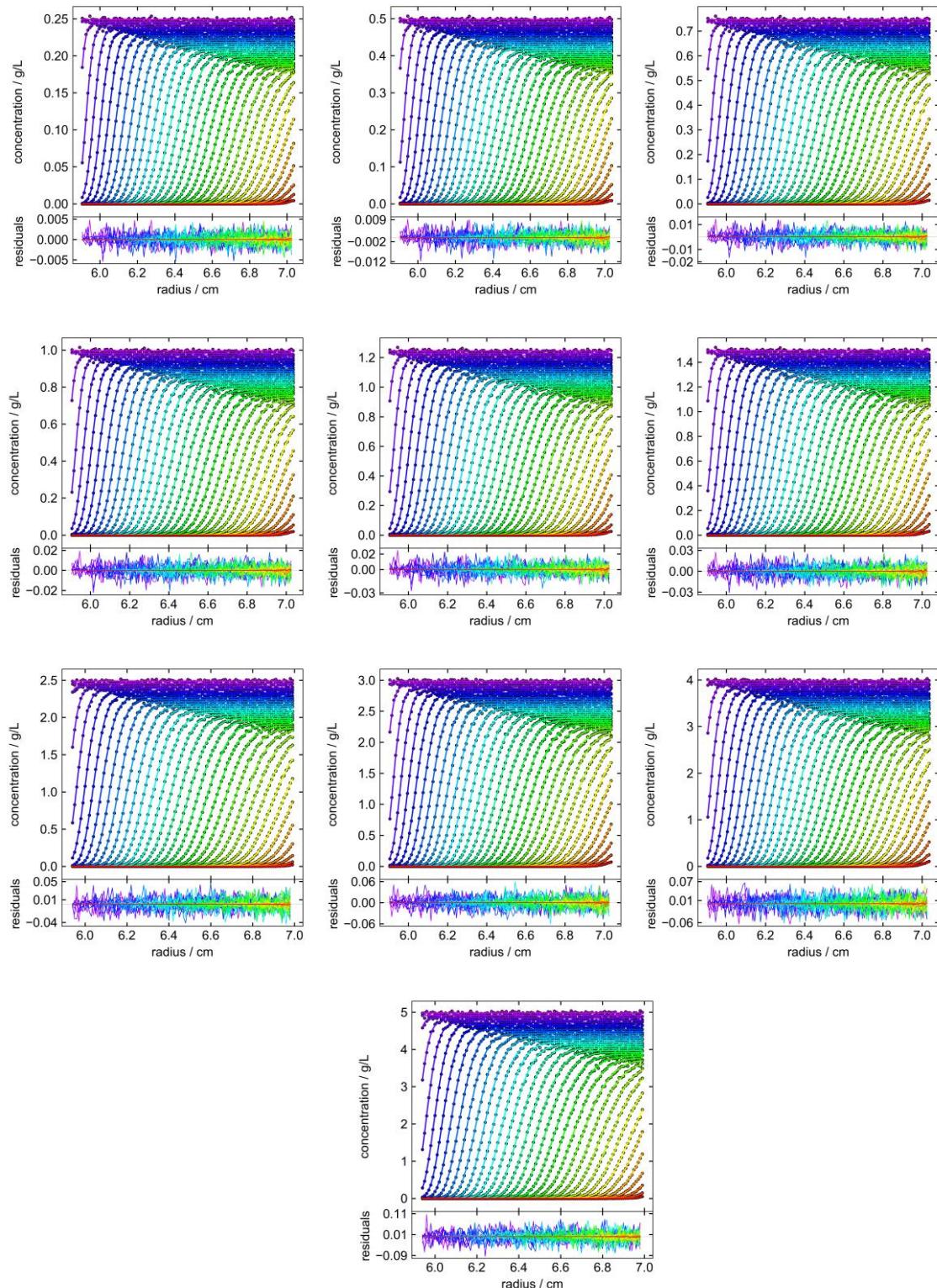


Figure 6: Sedimentation profiles, fitted profiles and residuals of the non-ideal sedimentation model in SEDFIT. Simulation parameters were $s_0 = 44.76 \text{ S}$, $D_0 = 8.56 \cdot 10^{-7} \text{ cm}^2 \cdot \text{s}^{-1}$, $c = 0.25\text{-}5 \text{ g} \cdot \text{L}^{-1}$, $k_s = 0 \text{ mL} \cdot \text{g}^{-1}$ and $2BM = 100 \text{ mL} \cdot \text{g}^{-1}$. Every third profile and every second data point is shown.

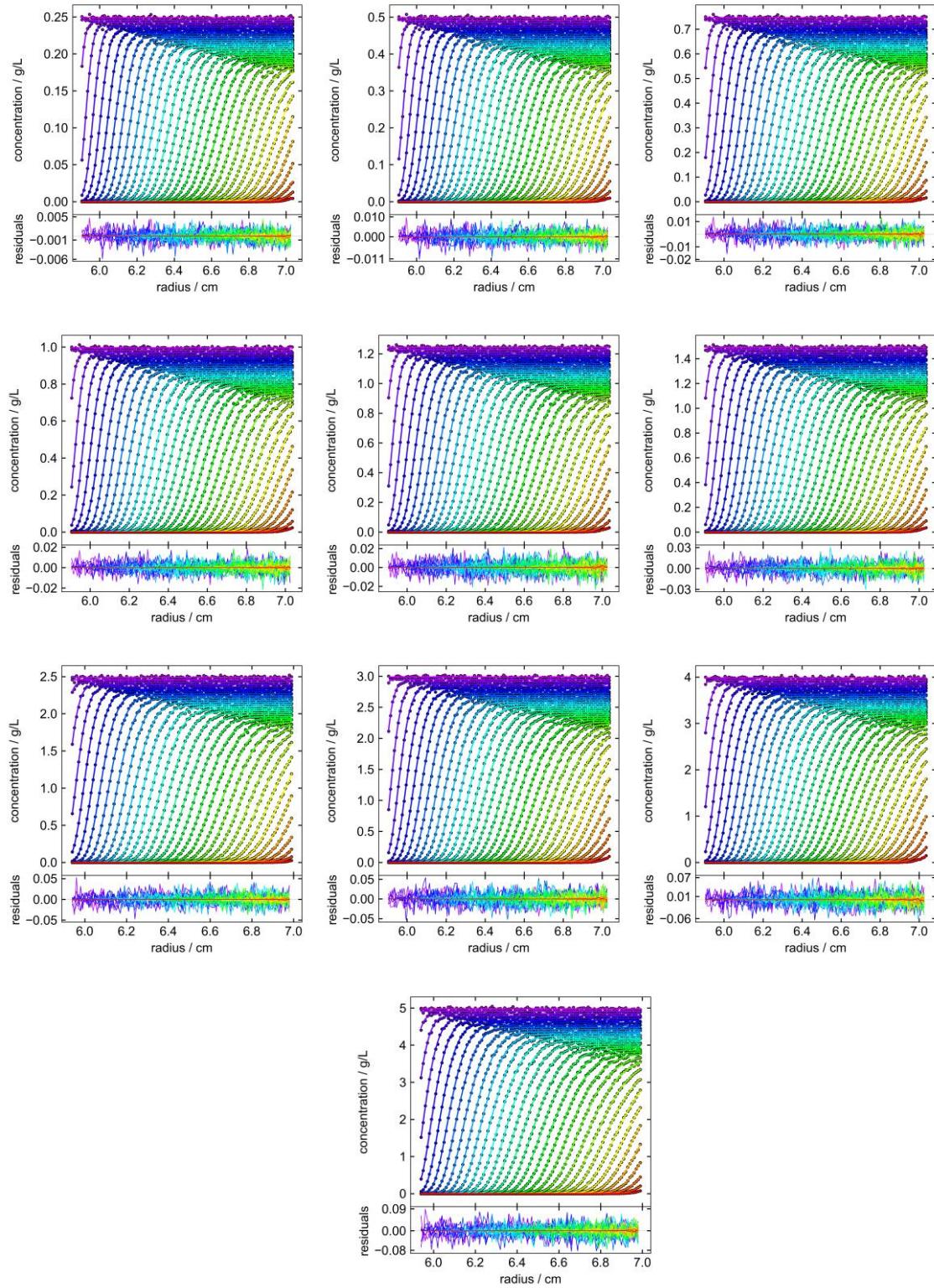


Figure 7: Sedimentation profiles, fitted profiles and residuals of the non-ideal sedimentation model in SEDFIT. Simulation parameters were $s_0 = 44.76 \text{ S}$, $D_0 = 8.56 \cdot 10^{-7} \text{ cm}^2 \cdot \text{s}^{-1}$, $c = 0.25\text{--}5 \text{ g} \cdot \text{L}^{-1}$, $k_s = 0 \text{ mL} \cdot \text{g}^{-1}$ and $2BM = 200 \text{ mL} \cdot \text{g}^{-1}$. Every third profile and every second data point is shown.

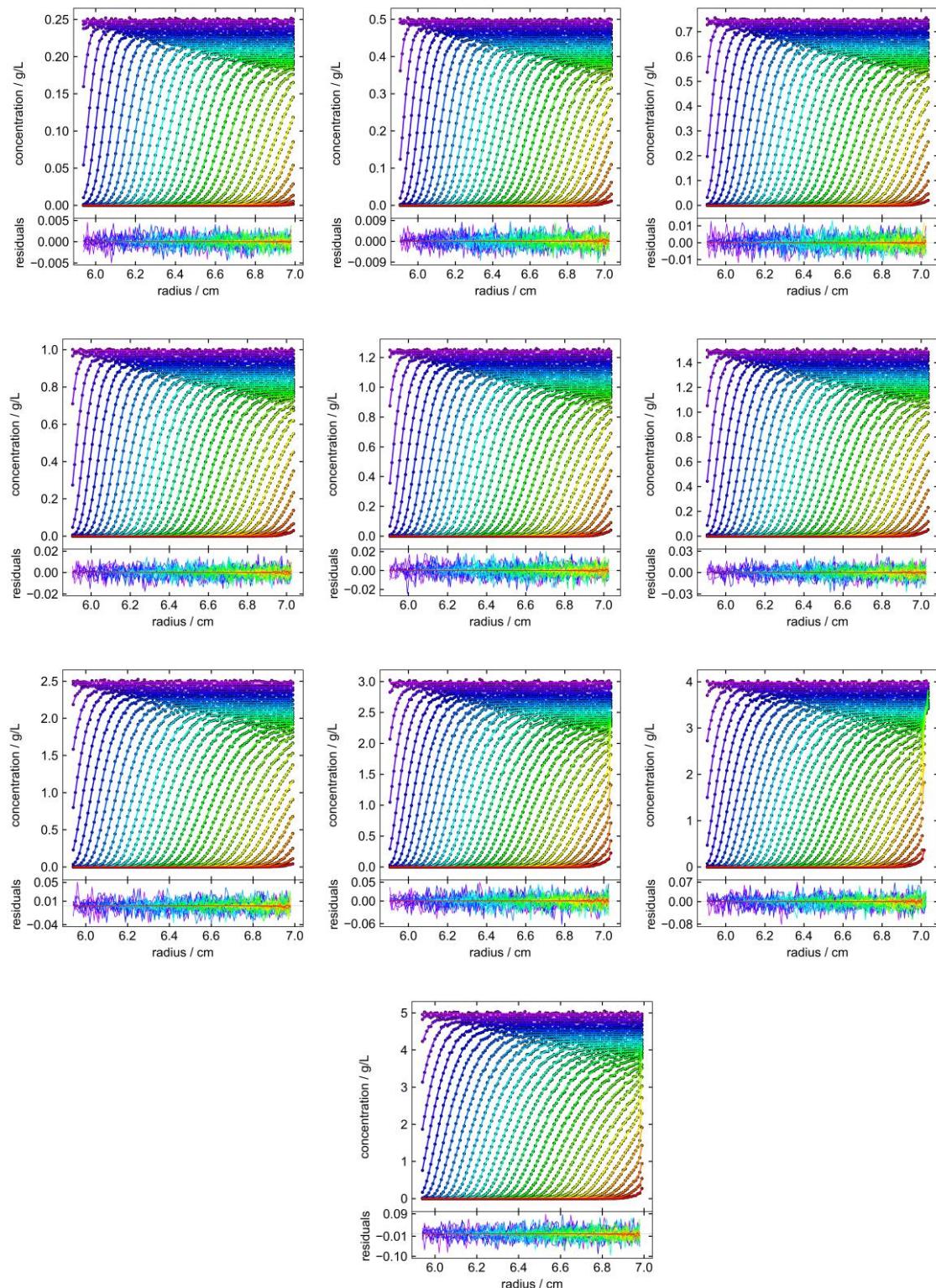


Figure 8: Sedimentation profiles, fitted profiles and residuals of the non-ideal sedimentation model in SEDFIT. Simulation parameters were $s_0 = 44.76 \text{ S}$, $D_0 = 8.56 \cdot 10^{-7} \text{ cm}^2 \cdot \text{s}^{-1}$, $c = 0.25\text{-}5 \text{ g} \cdot \text{L}^{-1}$, $k_s = 0 \text{ mL} \cdot \text{g}^{-1}$ and $2BM = 500 \text{ mL} \cdot \text{g}^{-1}$. Every third profile and every second data point is shown.

Determining k_d from SEDFIT forward simulations

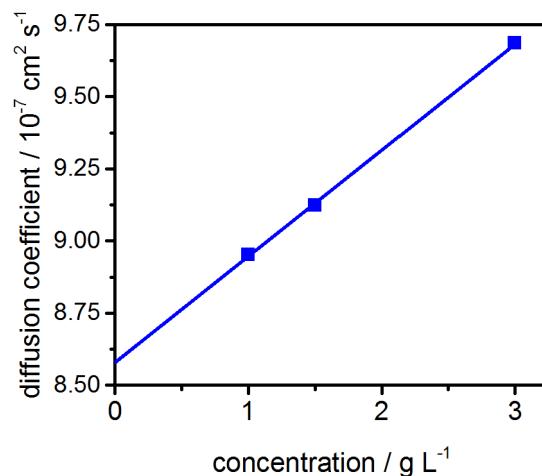


Figure 9: Apparent diffusion coefficient versus concentration. The apparent diffusion coefficient was extracted from data analysis using the ideal sedimentation model of SEDFIT. Sedimentation data was simulated by SEDFIT forward simulations

Table 3: Results from the evaluation of SEDFIT forward simulations with respect to thermodynamic non-ideality. Evaluation is carried out by fitting a straight line to the plot of the apparent diffusion coefficient versus concentration. Deviations from input values are given in parentheses.

Simulation	Input to SEDFIT simulation				Retrieved by ideal model in SEDFIT		
	s_0 / S	$D_0 / 10^{-7} \text{ cm}^2 \cdot \text{s}^{-1}$	$k_d / \text{mL} \cdot \text{g}^{-1}$	$c / \text{g L}^{-1}$	$D_{app} / 10^{-7} \text{ cm}^2 \cdot \text{s}^{-1}$	$D_0 / 10^{-7} \text{ cm}^2 \cdot \text{s}^{-1}$	$k_d / \text{mL} \cdot \text{g}^{-1}$
1				1.0	8.95		
2	44.76	8.56	100	1.5	9.12	8.58 (0.18 %)	42.88 (57.12 %)
3				3.0	9.68		

Dilution error estimation

k_s can be determined by extraction from a plot of the reciprocal sedimentation coefficient vs. the concentration. Instead of using the initial concentration, the mean concentration with regard to the plateau concentrations during the sedimentation from r_m to the right boundary of fitting interval r_f can be used.

The concentration within the plateau region is given by the position of the boundary r_{bnd} at time t :

$$c(t) = c(r_{bnd}(t)) = c_0 \cdot \left(\frac{r_m}{r_{bnd}} \right)^2 = c_0 \cdot \left(\frac{r_m}{r_m \cdot \exp(s\omega^2 t)} \right)^2 = c_0 \cdot \exp(-2s\omega^2 t)$$

The time Δt for the boundary to reach r_f can be determined according to:

$$r_f = r_m \cdot \exp(s\omega^2 \Delta t)$$

$$\Delta t = \frac{1}{s\omega^2} \ln \frac{r_f}{r_m}$$

The mean value of concentration within the plateau region can be calculated according to:

$$c_{mean} = \frac{1}{\Delta t} \int_0^{\Delta t} c(t) dt = \frac{1}{\Delta t} \int_0^{\Delta t} c_0 \cdot \exp(-2s\omega^2 t) dt = \frac{c_0}{\Delta t 2s\omega^2} (1 - \exp(-2s\omega^2 \Delta t))$$

This finally gives:

$$c_{mean} = c_0 \cdot \frac{\left(1 - \frac{r_m^2}{r_f^2}\right)}{2 \cdot \ln \frac{r_f}{r_m}} = c_0 \cdot A$$

Extracting k_s from two experimental apparent sedimentation coefficient values s_1, s_2 with concentrations c_1, c_2 provides:

$$k_s = \frac{1}{c_1 - c_2} \cdot s_0 \cdot \left(\frac{1}{s_1} - \frac{1}{s_2} \right)$$

Using this equation to derive the ratio of the non ideality parameter given by the initial c_{01}, c_{02} and the mean concentrations c_{mean1}, c_{mean2} with similar s_0 gives:

$$\frac{k_{s0}}{k_{smean}} = \frac{c_{1mean} - c_{2mean}}{c_{01} - c_{02}} = \frac{c_{01} \cdot A - c_{02} \cdot A}{c_{01} - c_{02}} = \frac{A(c_{01} - c_{02})}{(c_{01} - c_{02})} = A$$

Using $r_f = 7.0 \text{ cm}$ and $r_m = 5.8 \text{ cm}$ as typical fitting limits results in:

$$\frac{k_{s0}}{k_{smean}} = 0.83$$

This result indicates that there is a deviation of 17 % between the values derived from the initial concentration and the mean concentration.

Error estimation of non-ideality approximation

The diffusion coefficient at infinite dilution is set to be 8.56E-07 cm²/s. The density of the particles is taken to be 4230 kg/m³. The concentration is taken to be 1 g/L and the non-ideality parameters are $k_s = 100 \text{ mL/g}$ and $BM = 100 \text{ mL/g}$. The respective apparent diffusion coefficient calculated using Equation 6 in the main manuscript is 9.33E-07 cm²/s. The particular k_d value can be determined to be 90.6 mL/g using Equation 7. Calculating BM from this k_d value gives 95.22 mL/g. This value deviates from the input parameter by 4.77 %. At a concentration of 5 g/L, this deviation is 16.86 %.

A graphical representation of the numerical deviations is shown in the following figure. Evidently, the deviations are dependent upon the magnitude of k_s as well as $2BM$. For certain combinations of k_s and $2BM$, the deviations are dependent on the concentration.

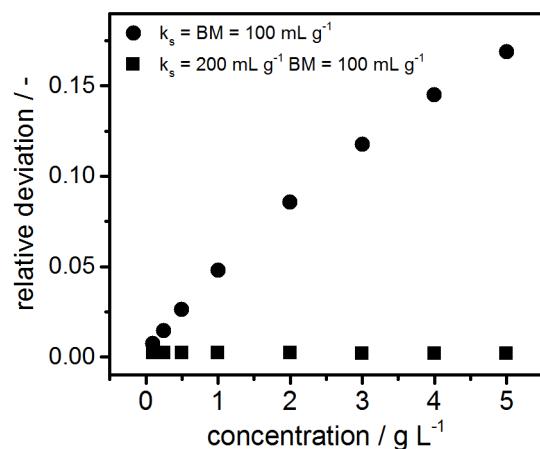


Figure 10: Numerical inaccuracies from the approximation made in equation 7 are illustrated for values for k_s and BM of 100 mL g^{-1} and k_s and BM of 200 mL g^{-1} and 100 mL g^{-1} .

Simulation of hydrodynamic and thermodynamic non-ideality in SV experiments

Table 4: Individual and combined analysis of hydrodynamic and thermodynamic non-ideality from BD simulations *via* the non-ideal sedimentation model of SEDFIT.

Simulation	Input to BD simulation				Retrieved by non-ideality model in SEDFIT				
	s_0 / S	$D_0 / 10^{-7} \text{ cm}^2 \text{ s}^{-1}$	$k_{s,BD} / \text{mL}\cdot\text{g}^{-1}$	$k_d / \text{mL}\cdot\text{g}^{-1}$	$c / \text{g L}^{-1}$	s_0 / S	$D_0 / 10^{-7} \text{ cm}^2 \text{ s}^{-1}$	$k_s / \text{mL}\cdot\text{g}^{-1}$	
1	44.76	8.56	200	200	0.25	44.81 (0.11 %)	8.62 (0.68 %)	207.9 (3.94 %)	490.6 (145.3 %)
					0.5	44.91 (0.33 %)	8.81 (2.86 %)	210.2 (5.11 %)	400.8 (100.4 %)
					0.75	44.84 (0.19 %)	8.68 (1.31 %)	204.4 (2.22 %)	410.6 (105.31 %)
					1.0	44.85 (0.19 %)	8.66 (1.15 %)	204.0 (1.98 %)	417.4 (108.7 %)
					1.25	44.84 (0.17 %)	8.65 (0.99 %)	202.8 (1.39 %)	402.7 (101.3 %)
					1.5	44.82 (0.14 %)	8.62 (0.66 %)	202.2 (1.10 %)	404.1 (102.1 %)
					2.5	44.84 (0.17 %)	8.64 (0.85 %)	201.8 (0.87 %)	397.3 (98.63 %)
					3.0	44.80 (0.10 %)	8.70 (1.60 %)	202.6 (1.30 %)	394.2 (97.07 %)
					4.0	44.92 (0.35 %)	8.73 (1.98 %)	202.4 (1.21 %)	387.8 (93.90 %)
					5.0	44.93 (0.38 %)	8.74 (2.03 %)	202.4 (1.20 %)	388.1 (94.04 %)
2	44.76	8.56	100	200	0.25	44.68 (0.19 %)	8.01 (6.43 %)	92.00 (8.04 %)	984.8 (392.4 %)
					0.5	44.81 (0.11 %)	8.62 (0.66 %)	104.0 (4.19 %)	448.9 (124.5 %)
					0.75	44.77 (0.02 %)	8.48 (0.93 %)	101.2 (1.24 %)	448.7 (124.3 %)
					1.0	44.72 (0.09 %)	8.49 (0.83 %)	99.90 (0.18 %)	427.3 (113.6 %)
					1.25	44.87 (0.24 %)	8.68 (1.38 %)	103.2 (3.16 %)	410.4 (105.2 %)
					1.5	44.88 (0.26 %)	8.69 (1.51 %)	102.9 (2.93 %)	405.5 (102.8 %)
					2.5	44.76 (0.01 %)	8.52 (0.49 %)	100.5 (0.50 %)	409.2 (104.6 %)
					3.0	44.87 (0.24 %)	8.67 (1.25 %)	101.7 (1.66 %)	398.9 (99.47 %)
					4.0	44.88 (0.27 %)	8.66 (1.09 %)	101.5 (1.51 %)	398.6 (99.31 %)
					5.0	44.89 (0.30 %)	8.70 (1.51 %)	101.5 (1.45 %)	394.4 (97.22 %)
3	44.76	8.56	200	100	0.25	44.73 (0.07 %)	8.47 (1.07 %)	199.6 (0.21 %)	346.8 (246.8 %)
					0.5	44.81 (0.12 %)	8.64 (0.88 %)	204.5 (2.27 %)	228.2 (128.2 %)
					0.75	44.83 (0.16 %)	8.65 (1.07 %)	203.9 (1.96 %)	213.9 (113.9 %)
					1.0	44.83 (0.15 %)	8.67 (1.21 %)	203.0 (1.47 %)	199.8 (99.75 %)
					1.25	44.84 (0.19 %)	8.71 (1.70 %)	202.9 (1.47 %)	189.9 (89.94 %)
					1.5	44.83 (0.15 %)	8.70 (1.61 %)	202.7 (1.13 %)	190.2 (90.22 %)
					2.5	44.87 (0.24 %)	8.68 (1.39 %)	202.2 (1.11 %)	193.8 (93.85 %)
					3.0	44.86 (0.22 %)	8.66 (1.17 %)	201.9 (0.93 %)	195.5 (95.49 %)
					4.0	44.87 (0.25 %)	8.69 (1.49 %)	201.8 (0.90 %)	192.8 (92.77 %)
					5.0	45.01 (0.57 %)	8.77 (2.48 %)	203.0 (1.51 %)	189.7 (89.66 %)

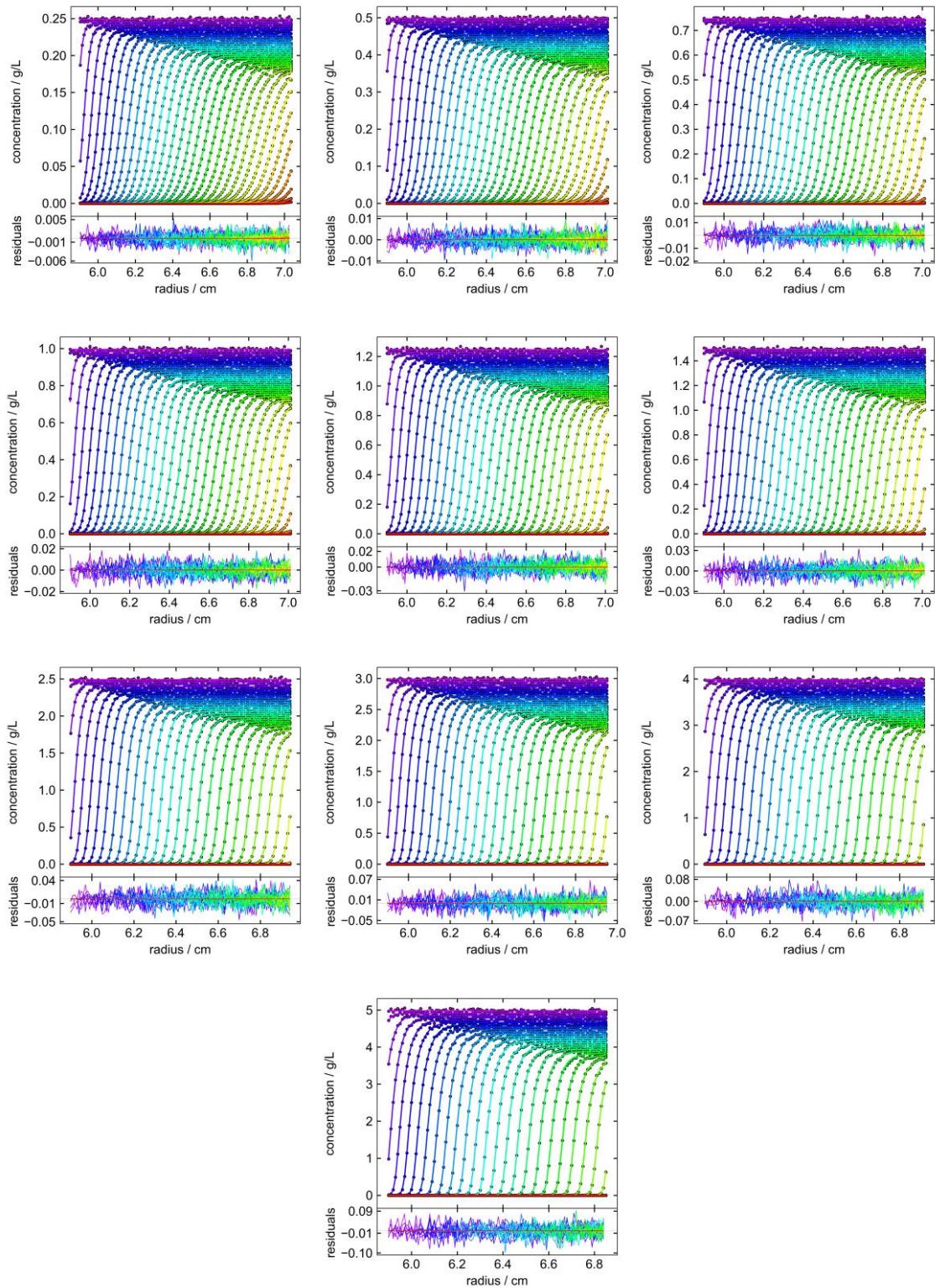


Figure 11: Sedimentation profiles, fitted profiles and residuals of the non-ideal sedimentation model in SEDFIT. Simulation parameters were $s_0 = 44.76 \text{ S}$, $D_0 = 8.56 \cdot 10^{-7} \text{ cm}^2 \cdot \text{s}^{-1}$, $c = 0.25\text{--}5 \text{ g L}^{-1}$, $k_s = 200 \text{ mL g}^{-1}$ and $2BM = 200 \text{ mL g}^{-1}$. Every third profile and every second data point is shown.

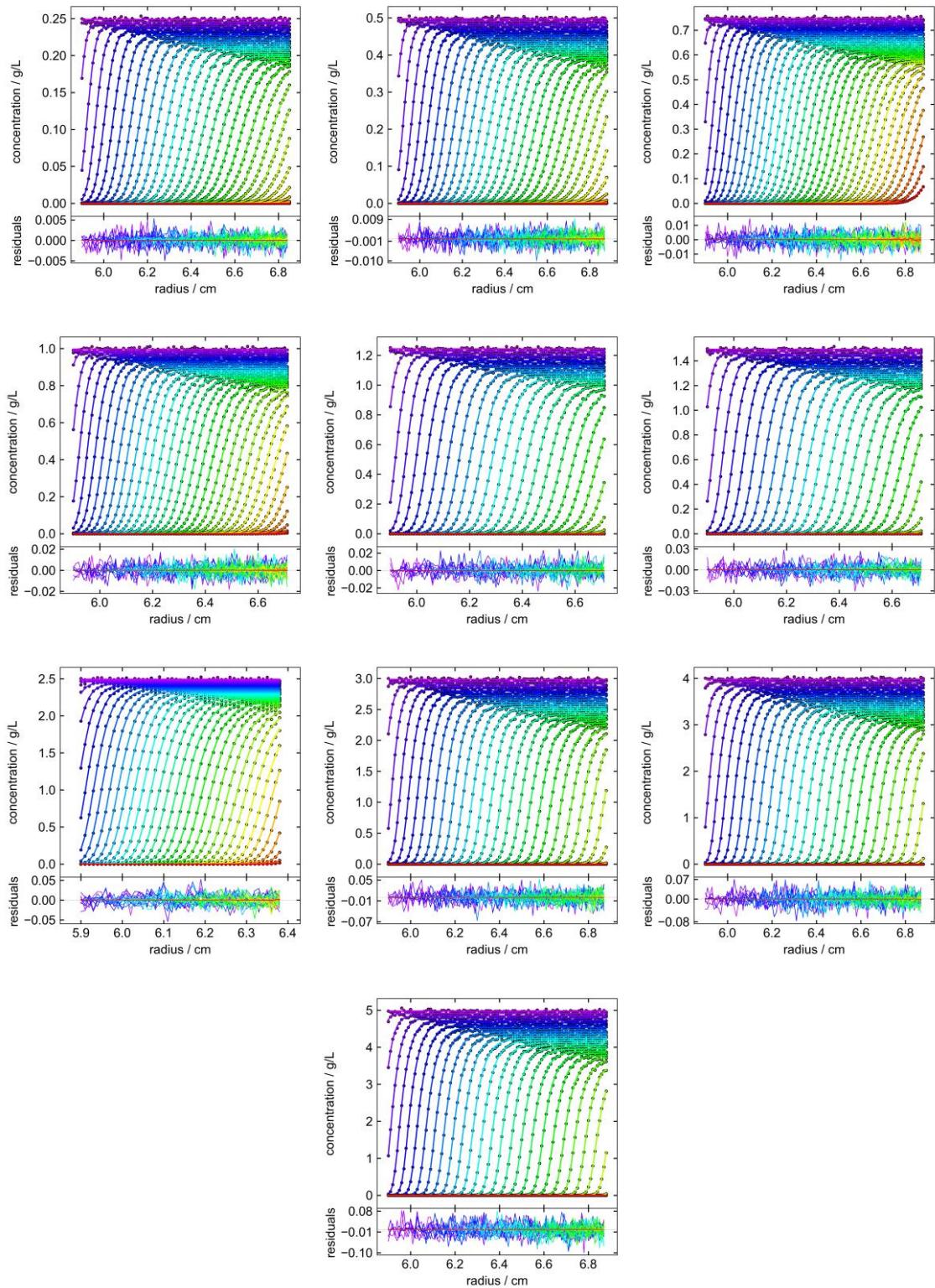


Figure 12: Sedimentation profiles, fitted profiles and residuals of the non-ideal sedimentation model in SEDFIT. Simulation parameters were $s_0 = 44.76 \text{ S}$, $D_0 = 8.56 \cdot 10^{-7} \text{ cm}^2 \cdot \text{s}^{-1}$, $c = 0.25\text{--}5 \text{ g L}^{-1}$, $k_s = 100 \text{ mL g}^{-1}$ and $2BM = 200 \text{ mL g}^{-1}$. Every third profile and every second data point is shown.

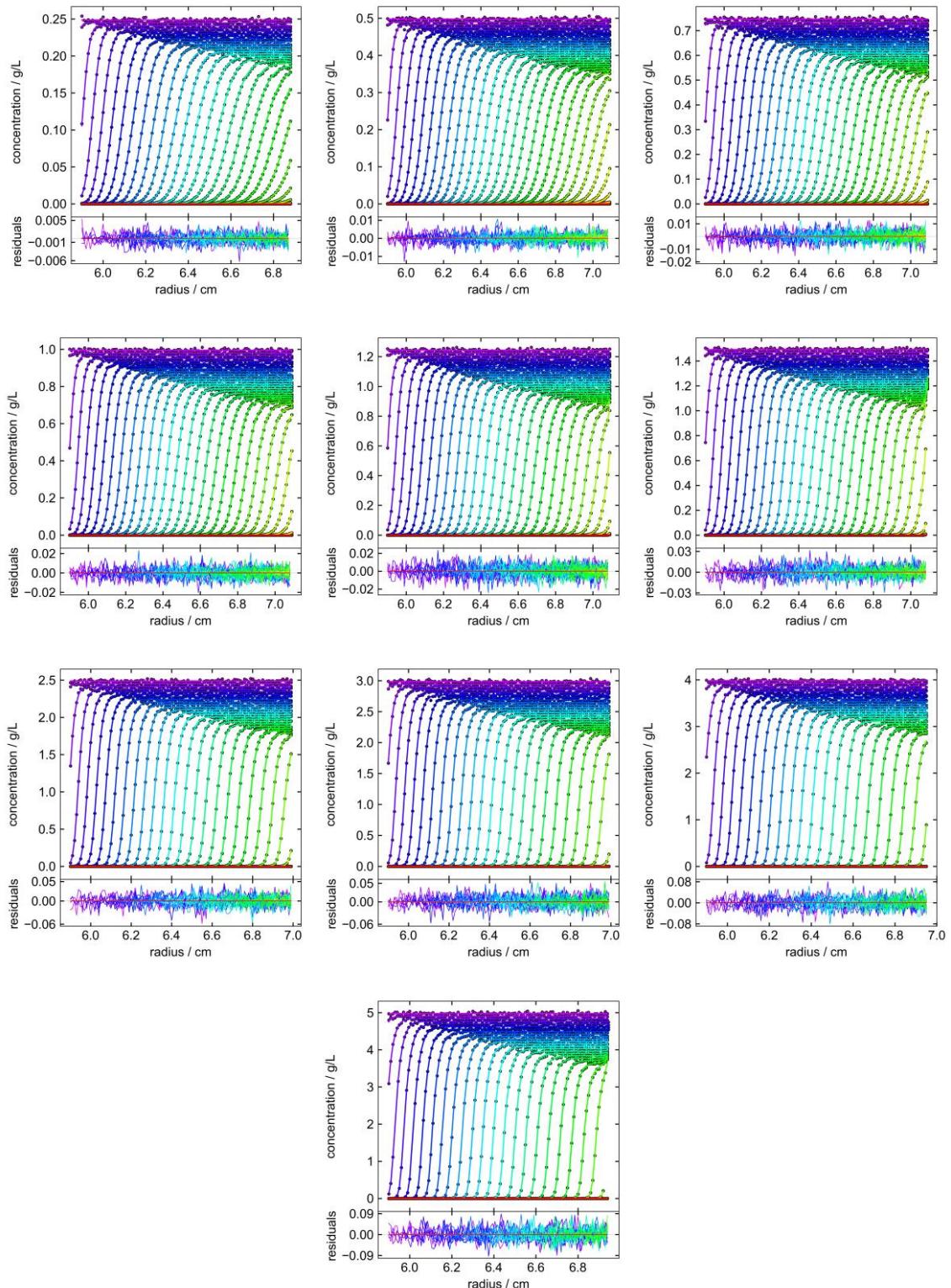


Figure 13: Sedimentation profiles, fitted profiles and residuals of the non-ideal sedimentation model in SEDFIT. Simulation parameters were $s_0 = 44.76 \text{ S}$, $D_0 = 8.56 \cdot 10^{-7} \text{ cm}^2 \cdot \text{s}^{-1}$, $c = 0.25\text{-}5 \text{ g} \cdot \text{L}^{-1}$, $k_s = 200 \text{ mL} \cdot \text{g}^{-1}$ and $2BM = 100 \text{ mL} \cdot \text{g}^{-1}$. Every third profile and every second data point is shown.

Simulation of hydrodynamic and thermodynamic non-ideality in SV experiments of polydisperse PSDs

In the following figure, the analysis of the sedimentation data from figure 9 has been evaluated via the $c(s)$ -method in SEDFIT. As it does not account for non-ideality, one cannot reproduce the sedimentation coefficient distribution. Clearly, the sedimentation coefficient distribution cannot be reproduced from the analysis methods, as non-ideality is not taken into account. Without analyzing different concentrations, there is no information on the non-ideality parameters k_s or $2BM$.

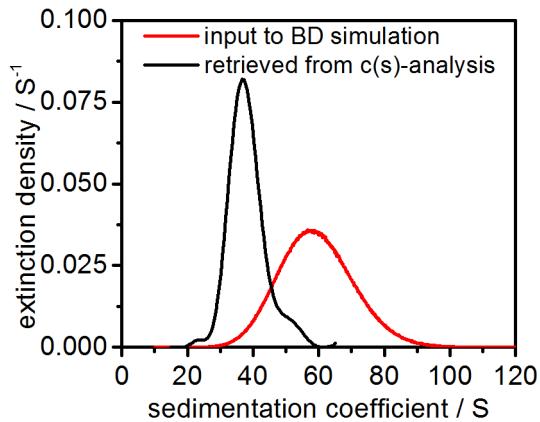


Figure 14: Sedimentation coefficient distribution for hydrodynamic and thermodynamic non-ideality in SV experiments of polydisperse PSDs as input to BD simulations (red) and as analysed by the $c(s)$ -method of SEDFIT (black).

Different approaches to incorporate non-ideality phenomena

In order to describe the concentration dependency of the Diffusion coefficient by one parameter (analogously to the sedimentation coefficient in equation (5), an approximation is necessary, which is only valid at low concentrations. The following figure illustrates that very approximation and shows that the two solutions are congruent at low concentrations.

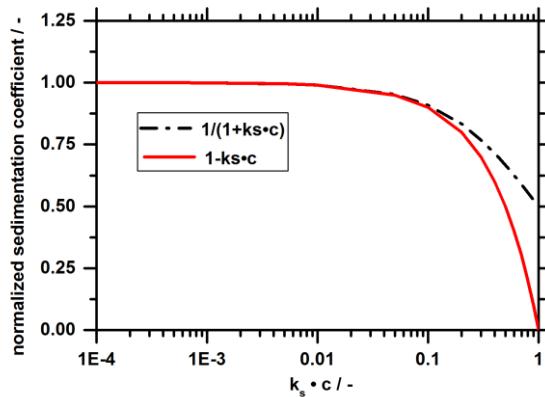


Figure 15: Normalized sedimentation coefficient vs the product of ks and the concentration using different approximations. For low values of the product of ks and the concentration, the concentration dependency is described equivalently. At larger products ($ks \cdot c > 0.1$), the two approximations no longer equally describe the concentration dependency