

## Supplementary Materials

**Table S1.** Twenty two-layered simulation samples with different combinations of  $\mu_{a1}$ ,  $\mu_{s1}'$ ,  $\mu_{a2}$ ,  $\mu_{s2}'$  and top-layer thickness  $d$  for investigating the effects of optical properties on reflectance prediction and comparing the estimation performance of diverse curve fitting methods.

Sample No.	$\mu_{a1}$ (mm <sup>-1</sup> )	$\mu_{s1}'$ (mm <sup>-1</sup> )	$\mu_{a2}$ (mm <sup>-1</sup> )	$\mu_{s2}'$ (mm <sup>-1</sup> )	$d$ (mm)
1	0.001	2	0.02	1	2
2	0.01	2	0.02	1	2
3	0.02	2	0.02	1	2
4	0.05	2	0.02	1	2
5	0.10	2	0.02	1	2
6	0.03	0.5	0.02	1	2
7	0.03	1	0.02	1	2
8	0.03	2	0.02	1	2
9	0.03	3	0.02	1	2
10	0.03	4	0.02	1	2
11	0.03	2	0.001	1	2
12	0.03	2	0.01	1	2
13	0.03	2	0.02	1	2
14	0.03	2	0.05	1	2
15	0.03	2	0.10	1	2
16	0.03	2	0.02	0.5	2
17	0.03	2	0.02	1	2
18	0.03	2	0.02	2	2
19	0.03	2	0.02	3	2
20	0.03	2	0.02	4	2

**Table S2.** Two-layered simulation samples with varying values of  $mfp_1'/mfp_2'$ .

Sample No.	$\mu_{a1}$ (mm <sup>-1</sup> )	$\mu_{s1}'$ (mm <sup>-1</sup> )	$\mu_{a2}$ (mm <sup>-1</sup> )	$\mu_{s2}'$ (mm <sup>-1</sup> )	$d$ (mm)	$mfp_1'/mfp_2'$	$\mu_{a1}/\mu_{a2}$	$\mu_{s1}'/\mu_{s2}'$	$\mu_{s1}'/\mu_{a1}$
21	0.025	1	0.015	0.190		0.2		5.26	
22	0.025	1	0.015	0.395		0.4		2.53	
23	0.025	1	0.015	0.600		0.6		1.67	
24	0.025	1	0.015	0.805		0.8		1.24	
25	0.025	1	0.015	1.010		1.0		0.99	
26	0.025	1	0.015	1.215	2	1.2	1.67	0.82	40
27	0.025	1	0.015	1.625		1.6		0.62	
28	0.025	1	0.015	2.035		2.0		0.49	
29	0.025	1	0.015	4.058		4.0		0.25	
30	0.025	1	0.015	5.110		5.0		0.20	

**Table S3.** Two-layered simulation samples with varying values of  $\mu_{a1}/\mu_{a2}$ .

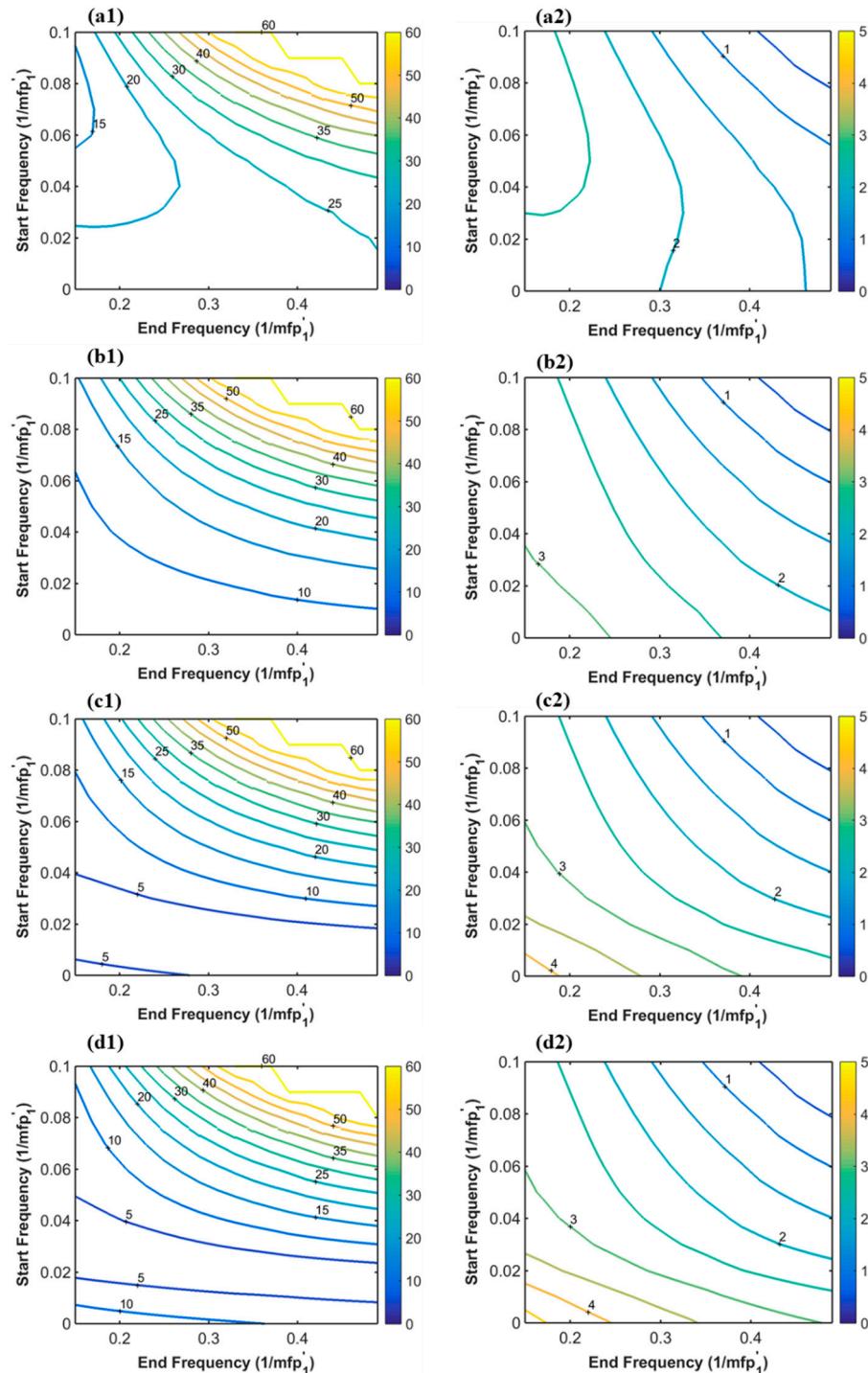
Sample No.	$\mu_{a1}$ (mm <sup>-1</sup> )	$\mu_{s1}'$ (mm <sup>-1</sup> )	$\mu_{a2}$ (mm <sup>-1</sup> )	$\mu_{s2}'$ (mm <sup>-1</sup> )	$d$ (mm)	$mfp_1'/mfp_2'$	$\mu_{a1}/\mu_{a2}$	$\mu_{s1}'/\mu_{s2}'$	$\mu_{s1}'/\mu_{a1}$
31	0.029	2	0.097	1.465			0.30	1.37	
32	0.029	2	0.065	1.497			0.45	1.34	
33	0.029	2	0.036	1.526			0.80	1.31	
34	0.029	2	0.029	1.533			1.00	1.30	
35	0.029	2	0.024	1.538	2	0.77	1.20	1.30	68.97
36	0.029	2	0.015	1.547			2.00	1.29	
37	0.029	2	0.012	1.550			2.50	1.29	
38	0.029	2	0.010	1.552			3.00	1.29	

**Table S4.** Two-layered simulation samples with varying values of  $\mu_{s1}'/\mu_{s2}'$ .

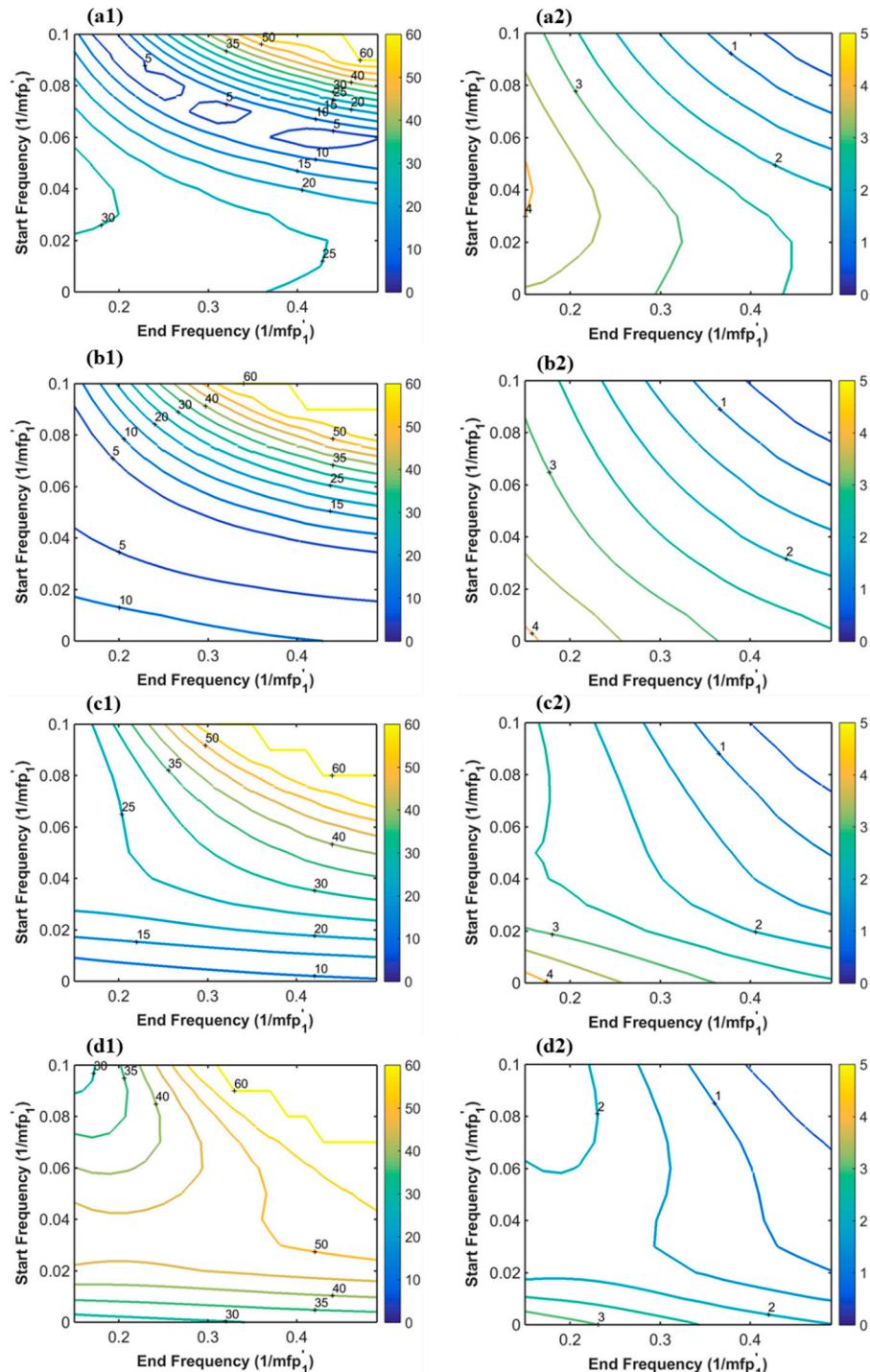
Sample No.	$\mu_{a1}$ (mm <sup>-1</sup> )	$\mu_{s1}'$ (mm <sup>-1</sup> )	$\mu_{a2}$ (mm <sup>-1</sup> )	$\mu_{s2}'$ (mm <sup>-1</sup> )	$d$ (mm)	$mfp_1'/mfp_2'$	$\mu_{a1}/\mu_{a2}$	$\mu_{s1}'/\mu_{s2}'$	$\mu_{s1}'/\mu_{a1}$
39	0.029	2	0.015	4		1.98		0.50	
40	0.029	2	0.015	3		1.49		0.67	
41	0.029	2	0.015	2		0.99		1.00	
42	0.029	2	0.015	1.6		0.80	1.93	1.25	
43	0.029	2	0.015	1	2	0.50		2.00	68.97
44	0.029	2	0.015	0.8		0.40		2.50	
45	0.029	2	0.015	0.5		0.25		4.00	
46	0.029	2	0.015	0.4		0.20		5.00	

**Table S5.** Two-layered simulation samples with varying values of  $\mu_{s1}'/\mu_{a1}$ .

Sample No.	$\mu_{a1}$ (mm <sup>-1</sup> )	$\mu_{s1}'$ (mm <sup>-1</sup> )	$\mu_{a2}$ (mm <sup>-1</sup> )	$\mu_{s2}'$ (mm <sup>-1</sup> )	$d$ (mm)	$mfp_1'/mfp_2'$	$\mu_{a1}/\mu_{a2}$	$\mu_{s1}'/\mu_{s2}'$	$\mu_{s1}'/\mu_{a1}$
47	0.010	2	0.005	1					200
48	0.015	2	0.0075	1					133
49	0.020	2	0.010	1					100
50	0.040	2	0.020	1					50
51	0.050	2	0.025	1	2	0.5	2	2	40
52	0.100	2	0.050	1					20
53	0.200	2	0.100	1					10
54	0.400	2	0.200	1					5



**Figure S1.** Absolute error contour maps for estimating  $\mu_{a1}$  (left panel) and  $\mu_{a1}'$  (right panel) of four representative two-layered simulation samples with varying values of  $\mu_{a1}/\mu_{a2}$  by using the stepwise method with different start and end frequencies. The values of  $\mu_{a1}/\mu_{a2}$  were 0.45, 1, 2 and 3 for (a), (b), (c) and (d), respectively. Different colors in the vertical bars on right of each graph denote different levels of error in percentage. Note that the absolute errors of  $\mu_{a1}$  and  $\mu_{a1}'$  larger than 60% and 20% were treated as 60% and 20% for better visual effect.



**Figure S2.** Absolute error contour maps for estimating  $\mu_{a1}$  (left panel) and  $\mu_{a1}'$  (right panel) of four representative two-layered simulation samples with varying values of  $\mu_{a1}/\mu_{a1}'$  by using the stepwise method with different start and end frequencies. The values of  $\mu_{a1}/\mu_{a1}'$  were 0.5, 1, 2 and 4 for (a), (b), (c) and (d), respectively. Different colors in the vertical bars on right of each graph denote different levels of error in percentage. Note that the absolute errors of  $\mu_{a1}$  and  $\mu_{a1}'$  larger than 60% and 20% were treated as 60% and 20% for better visual effect.