Supplemental Materials for "On the Slip Correction Factor for Simple Gas Molecules Diffusing in Air"

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Our study focuses on the diffusion of simple gas molecules in dry air given the large number of applications that involve air in both the atmospheric science and the aerospace engineering communities. However, the proposed methodology is entirely general and can be easily extended to a variety of other bath gases. The following tables compare the performance of the proposed method (C) with results obtained by the Fueller, Shetter & Giddings (F) semi-empirical method in relation to the results obtained by the Chapman-Enskog (CE) theory for the same diffusing molecules analyzed before but for the following bath gases: Ne, Ar, N_2, O_2, and CO_2. The results indicate that both C and F models are statistically equivalent, with a slightly lower bias observed for results obtained by the much simpler C model.

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Table S1 Comparison of Schmidt number (Sc) values calculated at 1 atm and 300 K using the Chapman-Enskog (CE) theory versus the proposed (C) and Fuller (F) methods for neon (Ne) as the bath (background) gas. The table below shows computed Sc_i values using the Chapman-Enskog (CE) theory, the proposed model (C) given by $Sc_{i,C} = 0.75\ \chi_i\sqrt{M_i/M_{\mathrm{Ne}}}$, and Fueller's model (F) for the 22 gas molecules used in the original study. The values of Δ_C and Δ_F are the relative deviations with respect to $Sc_{i,\mathrm{CE}}$. The mean bias deviation is of the same magnitude but slightly smaller for the simple C model. The cumulative relative standard deviation is the same at 9% for both C and F models.

Gas i	χ_i	$Sc_{i,\mathrm{CE}}$	$Sc_{i,\mathrm{C}}$	Δ_C(%)	$Sc_{i,\mathrm{F}}$	Δ_F(%)
He	1.00	0.367	0.334	− 9	0.336	− 8
Ne	1.00	0.765	0.750	− 2	0.720	− 6
Ar	1.00	1.217	1.055	−13	1.218	0
Kr	1.00	1.417	1.528	+ 8	1.543	+ 9
Xe	1.00	1.745	1.913	+10	1.984	+15
H_2	1.23	0.343	0.292	−15	0.332	− 3
OH	1.23	0.887	0.847	− 5	0.760	−14
CO	1.23	1.186	1.087	− 8	1.214	+ 2
N_2	1.23	1.205	1.087	−10	1.118	− 1
NO	1.23	1.166	1.125	− 4	1.005	−14
O_2	1.23	1.162	1.162	0	1.185	+ 2
HCl	1.23	1.330	1.240	− 7	1.346	− 1
Cl_2	1.23	1.870	1.729	− 8	1.876	0
HBr	1.23	1.583	1.847	+17	1.855	+17
Br_2	1.23	2.266	2.596	+15	2.599	+15
I_2	1.23	2.842	3.272	+15	2.511	−12
H_2O	1.39	1.008	0.985	− 2	0.937	− 7
H_2S	1.39	1.396	1.355	− 3	1.316	− 6
CO_2	1.39	1.476	1.540	+ 4	1.524	+ 3
N_2O	1.39	1.472	1.540	+ 5	1.723	+17
NO_2	1.39	1.417	1.574	+11	1.420	0
SO_2	1.39	1.808	1.857	+ 3	1.925	+ 7
			$\sum_i^n \Delta/n$	0		1
			$\overline{\sigma}$	9		9

Table S2 Comparison of Schmidt number (Sc) values calculated at 1 atm and 300 K using the Chapman-Enskog (CE) theory versus the proposed (C) and Fuller (F) methods for argon (Ar) as the bath (background) gas. The table below shows computed Sc_i values using the Chapman-Enskog (CE) theory, the proposed model (C) given by $Sc_{i,C} = 0.69\ \chi_i\sqrt{M_i/M_{\mathrm{Ar}}}$, and Fueller's model (F) for the 22 molecules used in the original study. The values of Δ_{C} and Δ_{F} are the relative deviations with respect to $Sc_{i,\mathrm{CE}}$. The mean bias deviation is smaller for the simpler C model, whereas the cumulative relative standard deviation is about the same for both models.

Gas i	χ_i	$Sc_{i,\mathrm{CE}}$	$Sc_{i,\mathrm{C}}$	Δ_{C}(%)	$Sc_{i,\mathrm{F}}$	Δ_{F}(%)
He	1.00	0.193	0.218	+13	0.194	+ 1
Ne	1.00	0.441	0.490	+11	0.441	0
Ar	1.00	0.782	0.690	−12	0.743	− 5
Kr	1.00	1.049	0.999	− 5	0.975	− 7
Xe	1.00	1.313	1.251	− 5	1.249	− 5
H_2	1.23	0.175	0.191	+ 9	0.178	+ 2
OH	1.23	0.506	0.554	+ 9	0.452	−11
CO	1.23	0.726	0.711	− 2	0.712	− 2
N_2	1.23	0.727	0.711	− 2	0.699	− 4
NO	1.23	0.728	0.736	+ 1	0.612	−16
O_2	1.23	0.725	0.760	+ 5	0.708	− 2
HCl	1.23	0.934	0.811	−13	0.801	−14
Cl_2	1.23	1.353	1.131	−16	1.139	−16
HBr	1.23	1.178	1.208	+ 3	1.140	− 3
Br_2	1.23	1.711	1.697	− 1	1.601	− 6
I_2	1.23	2.149	2.139	0	1.584	−26
H_2O	1.39	0.558	0.664	+15	0.542	− 3
H_2S	1.39	0.966	0.886	− 8	0.780	−19
CO_2	1.39	1.033	1.007	− 3	0.910	−12
N_2O	1.39	1.034	1.007	− 3	1.012	− 2
NO_2	1.39	1.002	1.029	+ 3	0.860	−14
SO_2	1.39	1.301	1.215	− 7	1.155	−11
			$\sum_i^n \Delta/n$	0		− 8
			$\overline{\sigma}$	8		7

Table S3 Comparison of Schmidt number (Sc) values calculated at 1 atm and 300 K using the Chapman-Enskog (CE) theory versus the proposed (C) and Fuller (F) methods for nitrogen (N_2) as the bath (background) gas. The table below shows computed Sc_i values using the Chapman-Enskog (CE) theory, the proposed model (C) given by $Sc_{i,C} = 0.60\ \chi_i\sqrt{M_i/M_{N_2}}$, and Fueller's model (F) for the 22 molecules used in the original study. The values of Δ_C and Δ_F are the relative deviations with respect to $Sc_{i,CE}$. The mean bias deviation is smaller for the simpler C model, whereas the cumulative relative standard deviation is the same for both models.

Gas i	χ_i	$Sc_{i,CE}$	$Sc_{i,C}$	Δ_C(%)	$Sc_{i,F}$	Δ_F(%)
He	1.00	0.221	0.227	+ 3	0.219	− 1
Ne	1.00	0.480	0.510	+ 6	0.473	− 1
Ar	1.00	0.799	0.718	−10	0.769	− 4
Kr	1.00	1.037	1.039	0	0.976	− 6
Xe	1.00	1.276	1.301	+ 2	1.229	− 4
H_2	1.23	0.201	0.198	− 1	0.202	+ 1
OH	1.23	0.537	0.576	+ 7	0.487	− 9
CO	1.23	0.752	0.739	− 2	0.748	− 1
N_2	1.23	0.752	0.739	− 2	0.734	− 2
NO	1.23	0.753	0.765	+ 2	0.642	−15
O_2	1.23	0.748	0.790	+ 6	0.740	− 1
HCl	1.23	0.958	0.843	−12	0.831	−13
Cl_2	1.23	1.341	1.176	−12	1.144	−15
HBr	1.23	1.168	1.256	+ 8	1.140	− 2
Br_2	1.23	1.649	1.766	+ 7	1.562	− 5
I_2	1.23	2.041	2.225	+ 9	1.531	−25
H_2O	1.39	0.605	0.670	+11	0.581	− 4
H_2S	1.39	0.992	0.921	− 7	0.811	−18
CO_2	1.39	1.045	1.047	0	0.934	−11
N_2O	1.39	1.046	1.047	0	1.037	− 1
NO_2	1.39	1.013	1.071	+ 6	0.882	−13
SO_2	1.39	1.295	1.263	− 2	1.165	−10
			$\sum_i^n \Delta/n$	1		− 7
			$\overline{\sigma}$	7		7

Table S4 Comparison of Schmidt number (Sc) values calculated at 1 atm and 300 K using the Chapman-Enskog (CE) theory versus the proposed (C) and Fuller (F) methods for oxygen (O_2) as the bath (background) gas. The table below shows computed Sc_i values using the Chapman-Enskog (CE) theory, the proposed model (C) given by $Sc_{i,C} = 0.65\ \chi_i\sqrt{M_i/M_{O_2}}$, and Fueller's model (F) for the 22 molecules used in the original study. The values of Δ_C and Δ_F are the relative deviations with respect to $Sc_{i,CE}$. The mean bias deviation is smaller for the simpler C model, whereas the cumulative relative standard deviation is the same for both models.

Gas i	χ_i	$Sc_{i,CE}$	$Sc_{i,C}$	Δ_C(%)	$Sc_{i,F}$	Δ_F(%)
He	1.00	0.212	0.229	+ 8	0.218	− 2
Ne	1.00	0.472	0.514	+ 9	0.481	− 2
Ar	1.00	0.813	0.723	−11	0.794	− 2
Kr	1.00	1.069	1.047	− 2	1.020	− 5
Xe	1.00	1.326	1.311	− 1	1.294	− 2
H_2	1.23	0.193	0.200	+ 3	0.201	+ 4
OH	1.23	0.538	0.580	+ 8	0.494	− 8
CO	1.23	0.762	0.745	− 2	0.768	+ 1
N_2	1.23	0.762	0.745	− 2	0.754	− 1
NO	1.23	0.762	0.771	+ 1	0.659	−14
O_2	1.23	0.758	0.796	+ 5	0.761	0
HCl	1.23	0.972	0.849	−13	0.857	−12
Cl_2	1.23	1.384	1.185	−14	1.196	−14
HBr	1.23	1.201	1.265	+ 5	1.193	− 1
Br_2	1.23	1.721	1.778	+ 3	1.652	− 4
I_2	1.23	2.148	2.241	+ 4	1.624	−24
H_2O	1.39	0.599	0.675	+13	0.592	− 1
H_2S	1.39	1.008	0.928	− 8	0.836	−17
CO_2	1.39	1.070	1.055	− 1	0.968	−10
N_2O	1.39	1.071	1.055	− 2	1.076	+ 1
NO_2	1.39	1.037	1.078	+ 4	0.914	−12
SO_2	1.39	1.335	1.273	− 5	1.216	− 9
			$\sum_i^n \Delta/n$	0		− 6
			$\overline{\sigma}$	7		7

Table S5 Comparison of Schmidt number (Sc) values calculated at 1 atm and 300 K using the Chapman-Enskog (CE) theory versus the proposed (C) and Fuller (F) methods for carbon dioxide (CO_2) as the bath (background) gas. The table below shows computed Sc_i values using the Chapman-Enskog (CE) theory, the proposed model (C) given by $Sc_{i,C} = 0.57\ \chi_i\sqrt{M_i/M_{CO_2}}$, and Fueller's model (F) for the 22 molecules used in the original study. The values of Δ_C and Δ_F are the relative deviations with respect to $Sc_{i,CE}$. The mean bias deviation is smaller for the simpler C model, whereas the cumulative relative standard deviation is slightly better for the F model as a consequence of a consistent bias.

Gas i	χ_i	$Sc_{i,CE}$	$Sc_{i,C}$	Δ_C(%)	$Sc_{i,F}$	Δ_F(%)
He	1.00	0.145	0.170	+18	0.147	+ 1
Ne	1.00	0.332	0.383	+19	0.333	+ 3
Ar	1.00	0.623	0.538	−14	0.548	−12
Kr	1.00	0.838	0.780	− 7	0.718	−14
Xe	1.00	1.047	0.976	− 7	0.911	−13
H_2	1.23	0.127	0.149	+18	0.132	+ 4
OH	1.23	0.402	0.432	+ 8	0.337	−16
CO	1.23	0.574	0.554	− 3	0.521	− 9
N_2	1.23	0.573	0.554	− 3	0.512	−11
NO	1.23	0.577	0.574	− 1	0.454	−21
O_2	1.23	0.576	0.593	+ 3	0.521	−10
HCl	1.23	0.744	0.633	−15	0.586	−21
Cl_2	1.23	1.070	0.882	−18	0.826	−23
HBr	1.23	0.946	0.942	0	0.829	−12
Br_2	1.23	1.359	1.324	− 3	1.151	−15
I_2	1.23	1.694	1.669	− 1	1.147	−32
H_2O	1.39	0.393	0.502	+28	0.399	+ 2
H_2S	1.39	0.765	0.691	−10	0.570	−25
CO_2	1.39	0.814	0.785	− 4	0.662	−19
N_2O	1.39	0.816	0.785	− 4	0.731	−10
NO_2	1.39	0.793	0.803	+ 1	0.629	−21
SO_2	1.39	1.029	0.948	− 8	0.835	−19
			$\sum_i^n \Delta/n$	0		−13
			$\overline{\sigma}$	12		10