Electronic Supplementary Information (ESI)

for

New Insights into the Ideal Adsorbed Solution theory

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Number of pages 12

Number of tables 2

Number of figures 9

Table S1

Values of the best-fit parameters for simulated single-component adsorption isotherms fitted by Eq. (21).

Carbon	*MRE* [%]	$a_{m,i,1}$ [mmol/g]	$a_{m,i,2}$ [mmol/g]	$a_{m,i,3}$ [mmol/g]	$K_{i,1}$	$K_{i,2}$	$K_{i,3}$	$n_{i,1}$	$n_{i,2}$	$n_{i,3}$
$i = CO_2$										
d0.5	0.4118	124.6	0.8009	0.01617	0.1492	8.785	115.9	1.138	0.9574	0.9469
d0.9	0.4359	14.82	0.06306	0.7968	2.655	14.75	51.78	1.117	0.9193	0.9593
d1.3	0.3037	5.899	0.1244	0.5241	12.50	760.3	114.9	0.9094	1.102	1.085
d0.9_052	0.4358	13.63	1.0628	0.007729	3.510	51.87	798.2	1.156	0.9561	1.200
d0.9_104	0.4246	1.412	12.58	0.06472	46.68	4.325	273.0	0.9575	1.186	1.047
d0.9_156	0.4093	12.42	1.429	0.02606	5.385	54.83	655.6	1.114	0.9517	1.162
$i = CH_4$										
d0.5	0.3097	5.721	25.72	0.005219	0.1901	0.1947	15.57	1.886	0.9971	1.902
d0.9	0.2612	1.258	11.88	0.2845	0.05595	0.6793	9.051	0.9199	0.9872	1.040
d1.3	0.2372	1.770	3.988	0.3260	0.1951	3.006	30.34	0.9327	0.9911	1.009
d0.9_052	0.2721	11.94	0.5706	0.02157	0.6542	5.222	40.48	0.9859	1.014	1.128
d0.9_104	0.2829	0.05931	11.64	0.5692	21.4781	0.6840	5.547	1.035	0.9826	1.035
d0.9_156	0.2517	2.140	10.07	0.2639	0.1241	0.9603	12.51	0.9914	0.9949	1.008
$i = N_2$										
d0.5	0.3890	1.449	34.33	4.282×10^{-5}	0.6986	0.06031	5133	1.063	0.9942	0.9645
d0.9	0.4244	2.929	9.113	3.474	0.3263	0.04279	1.096	1.482	0.9781	1.004
d1.3	0.3411	2.929	3.330	1.145	0.02790	0.5954	3.536	0.9580	0.9798	1.016
d0.9_052	0.3338	6.900	8.118	0.5013	0.03033	0.3502	2.949	0.9580	0.9776	1.128
d0.9_104	0.4749	9.879	2.884	1.523	0.07437	1.385	0.5274	0.9538	1.018	1.684
d0.9_156	0.4149	7.951	5.731	0.05370	0.07148	0.6920	11.11	0.9909	0.9917	1.411

Table S2

The results of description of simulated data by both assumed G^{ex} expansions – Eqs. (32) and (33)

Carbon	$(a_1 + a_2)_{max}$ at 1 MPa [mmol/g]	a_{CH4} pure CH_4 at 25 MPa [mmol/g]	a_{N2} pure N_2 at 60 MPa [mmol/g]	range of a_{max} [mmol/g]	
				Eq. (32)	Eq. (33)
d0.5	13	27	29	80-100	30-180
d0.9	12	12	13	60-100	7-300
d1.3	6	5.7	6	20-50	10-250

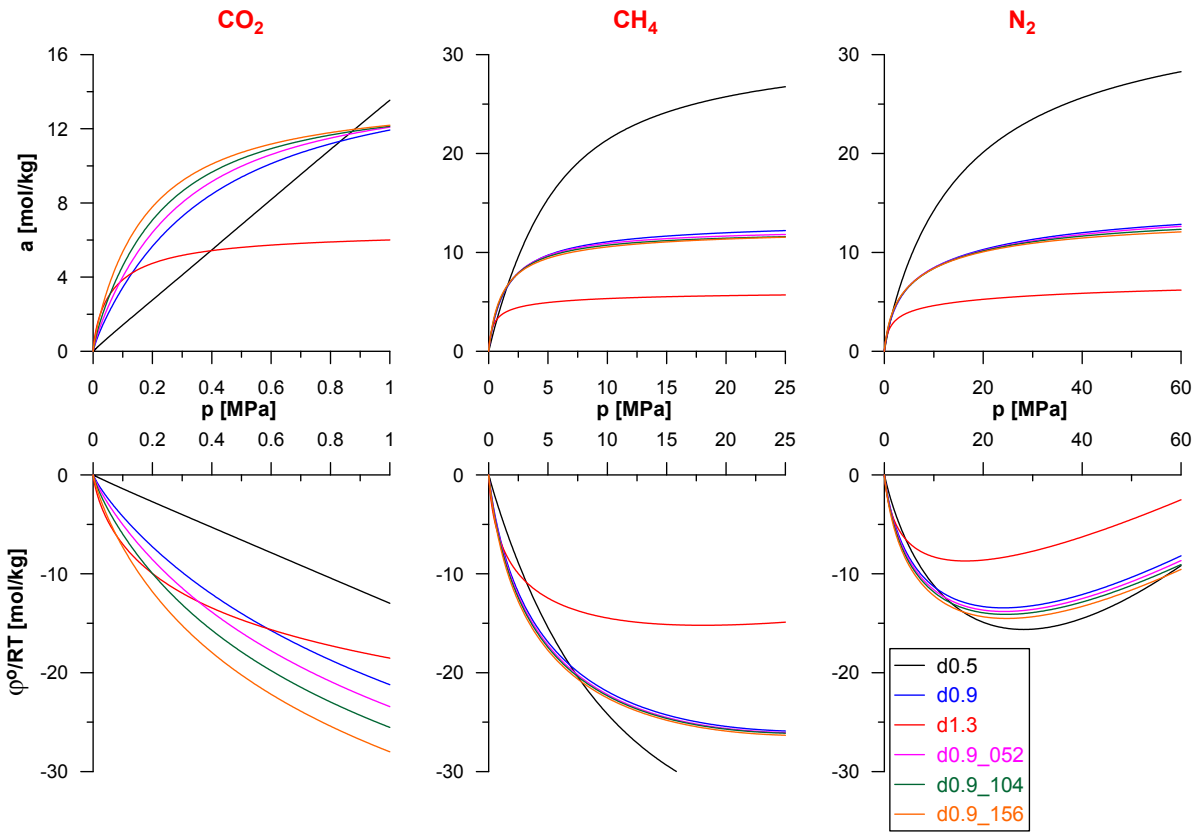

Figure S1. Comparison of single gas (CO_2, CH_4 or N_2) adsorption isotherms (approximated by Eq. (21)) for all the considered carbons and related grand potentials calculated from Eq. (8). The data are presented for the simulated pressure ranges (see section 2.2).

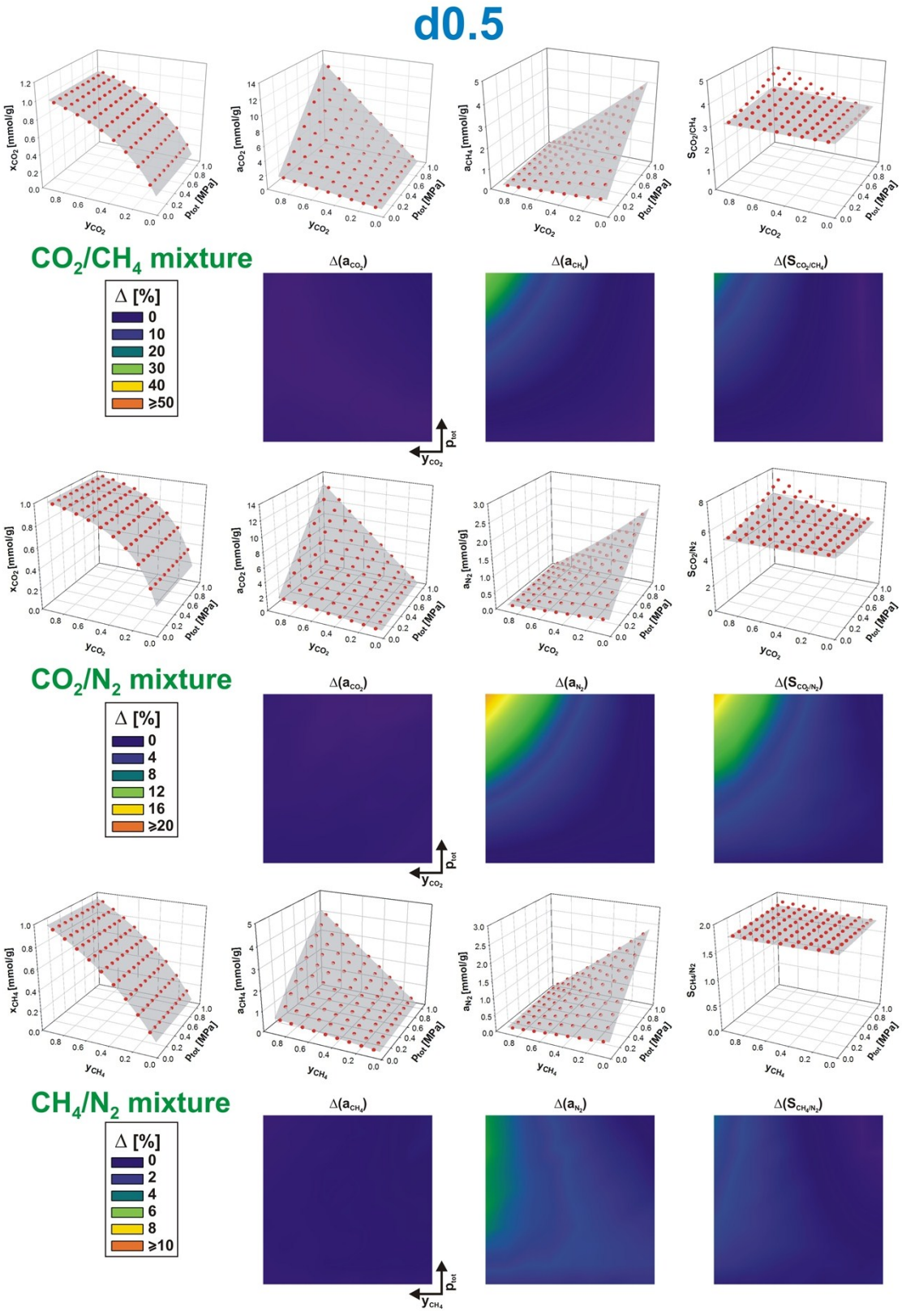

Figure S2. Comparison of the results simulated directly for ale the considered gas mixtures (points) and the predictions of IAS theory (panes) for the d0.5 carbon. The maps of the relative errors (Δ) for the values of component adsorption amounts (Δ(a_i)) and equilibrium separation factors (Δ($S_{1/2}$)) obtained from the IAS theory.

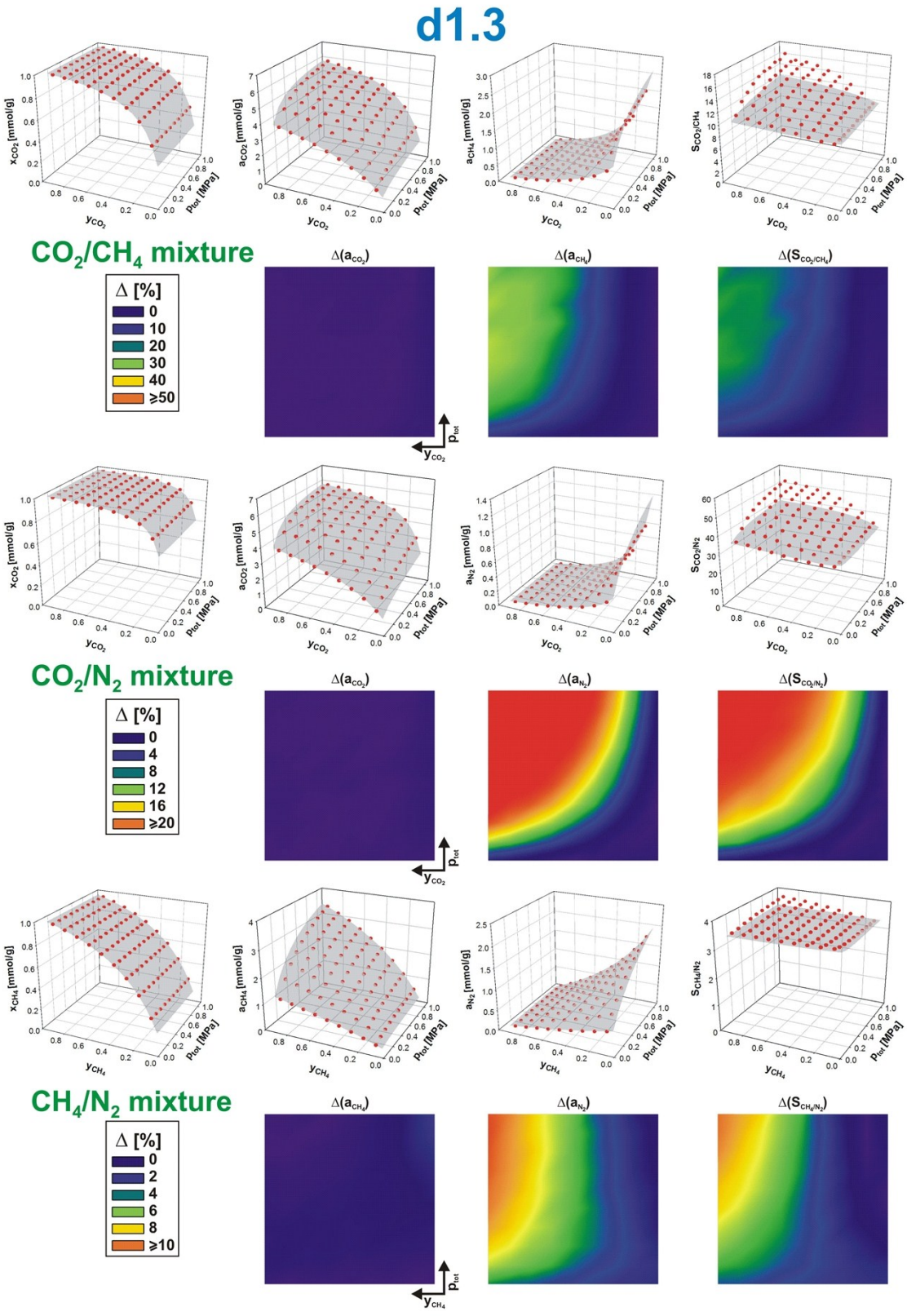

Figure S3. As in Fig. S2 but for the d1.3 carbon.

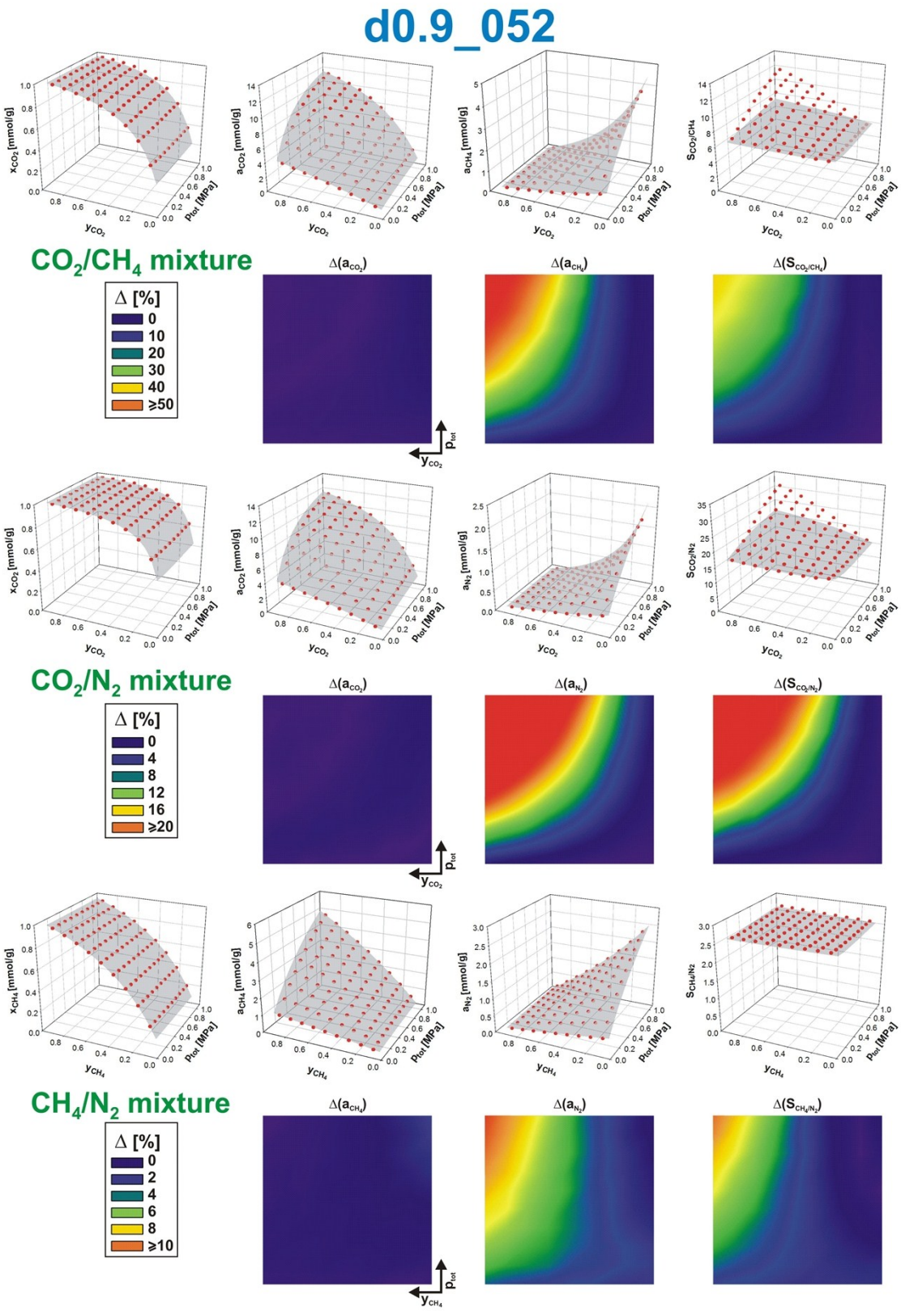

Figure S4. As in Fig. S2 but for the d0.9_052 carbon.

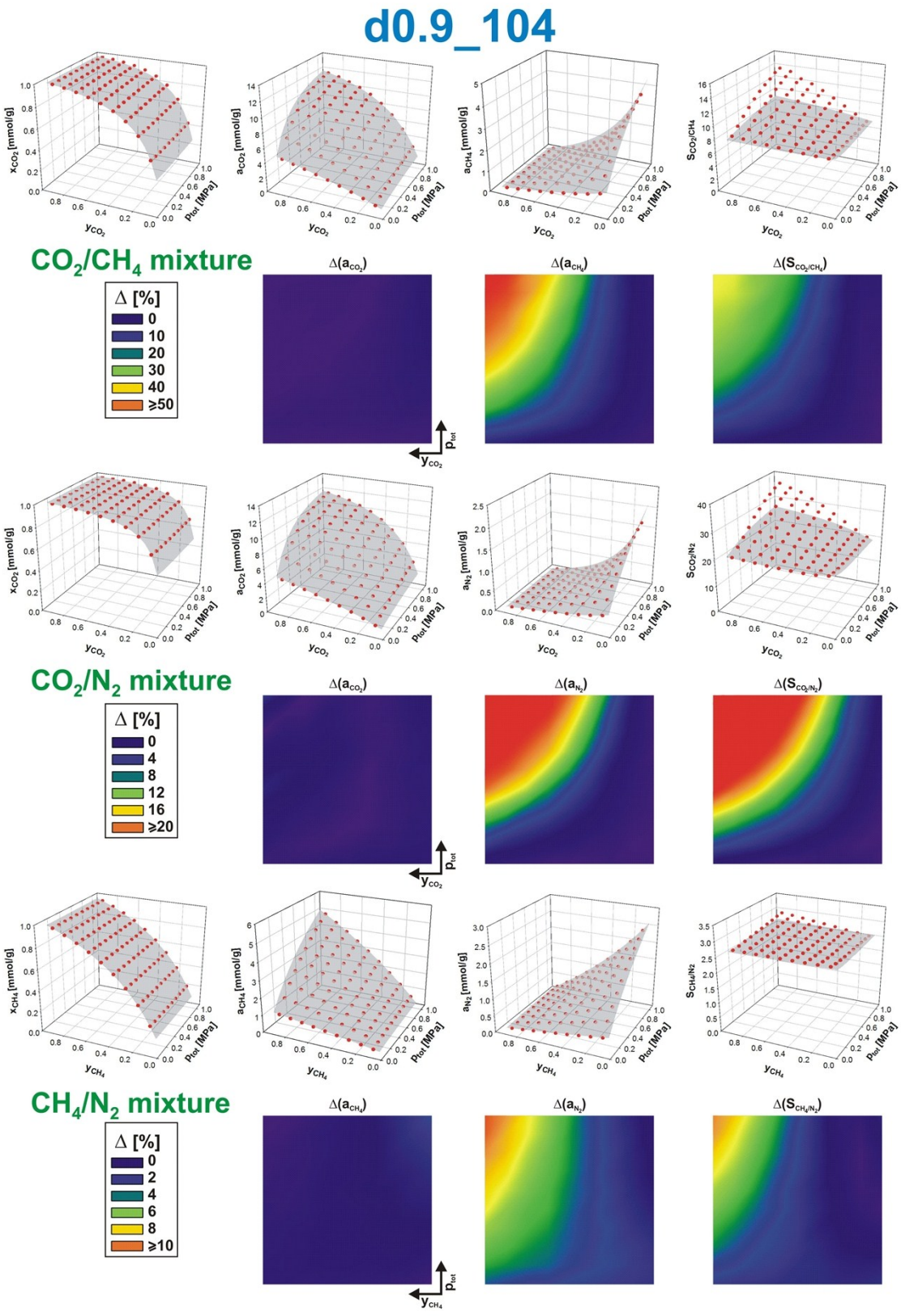

Figure S5. As in Fig. S2 but for the d0.9_104 carbon.

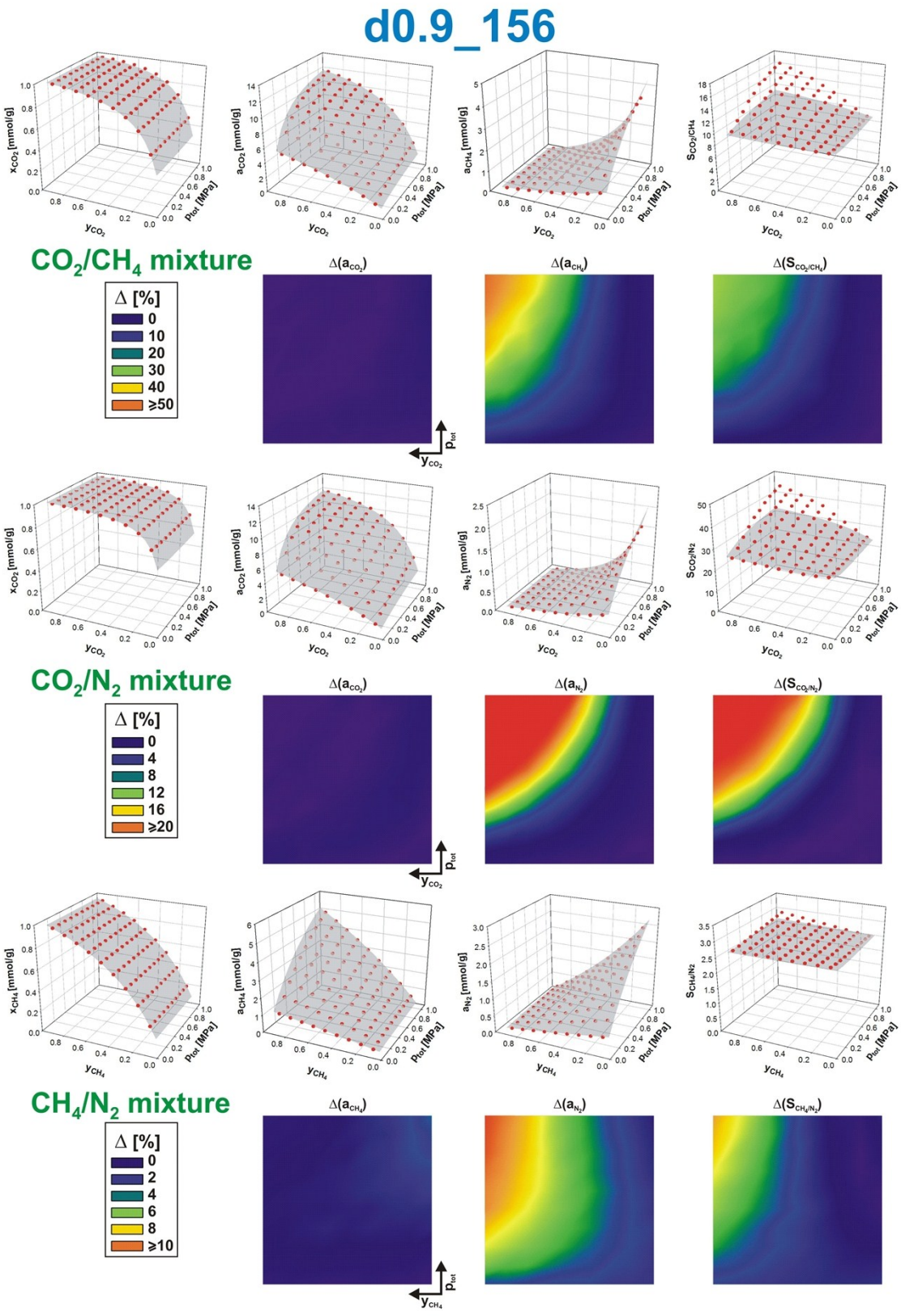

Figure S6. As in Fig. S2 but for the d0.9_156 carbon.

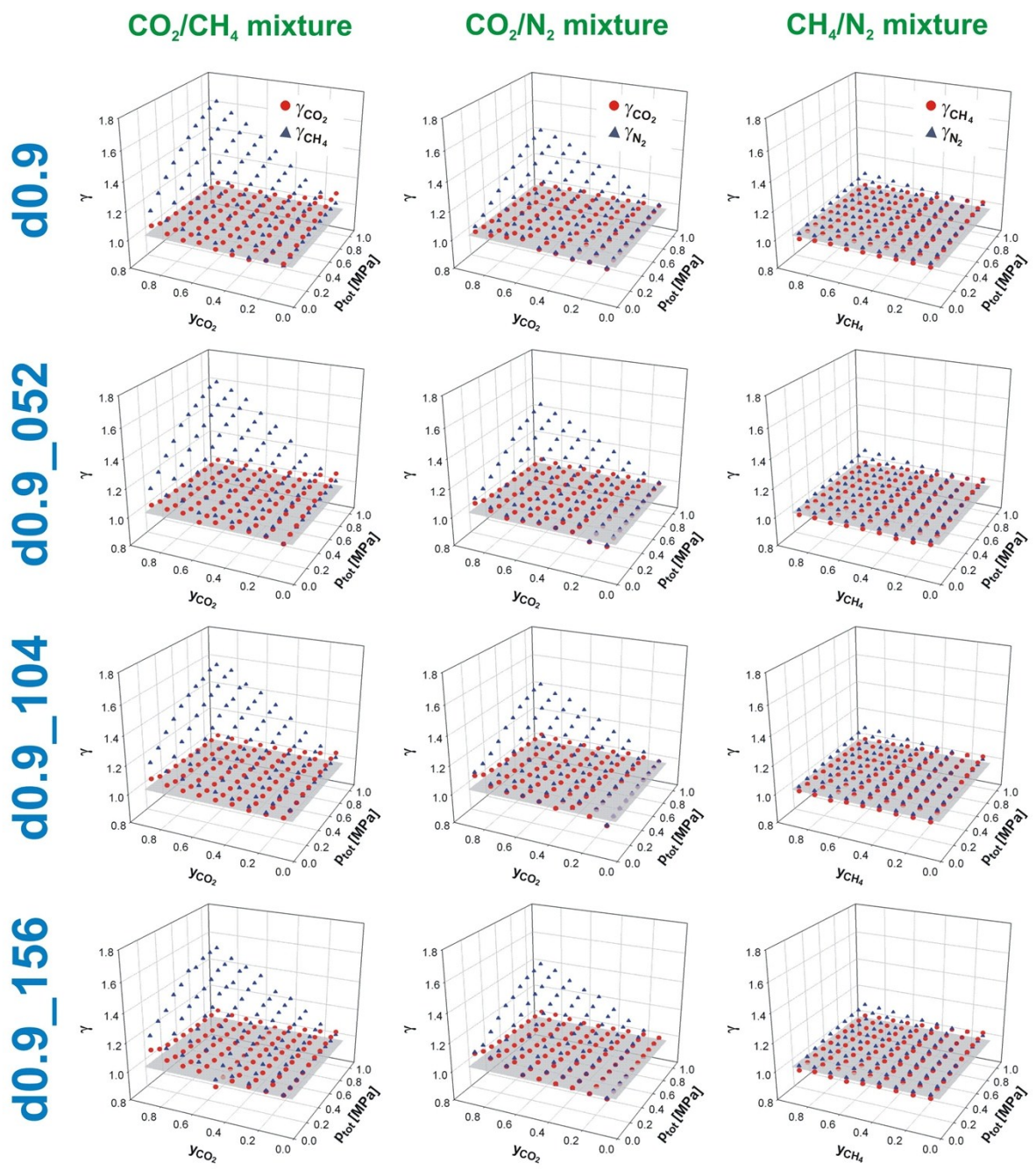

Figure S7. Comparison of calculated activity coefficients for mixture adsorption on the raw and oxidised d0.9 carbons. The grey planes represent $\gamma = 1$.

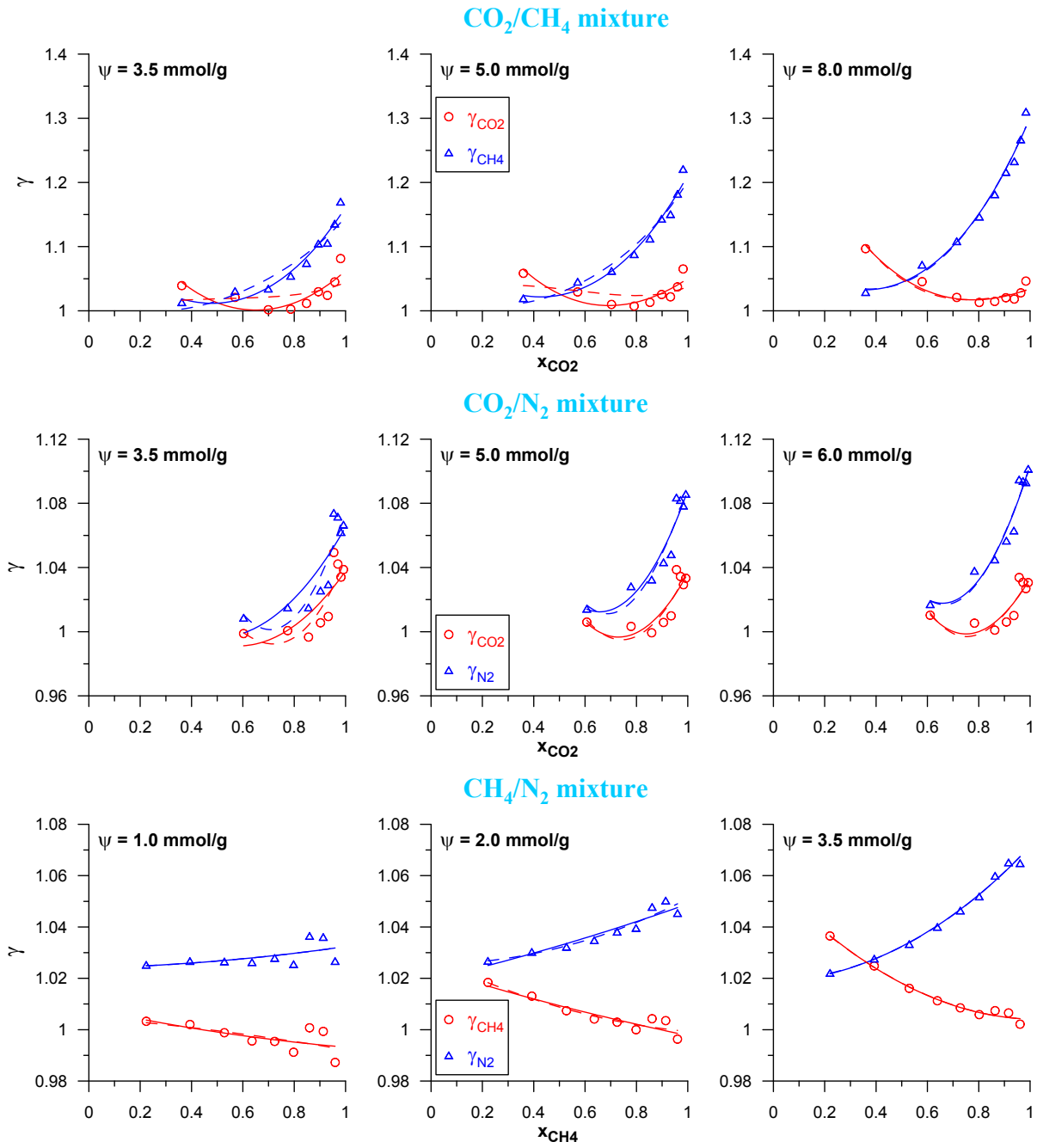

Figure S8. Comparison of the activity coefficients (plotted as the function of the mole fraction of the 1st component in the adsorbed phase) for adsorption of all the considered mixtures on the d0.9 carbon (arbitrarily chosen values of grand potential (ψ) are presented). The lines present approximation by theoretical models (solid lines – Eqs. (34) and (35), dashed lines – Eq. (36)).

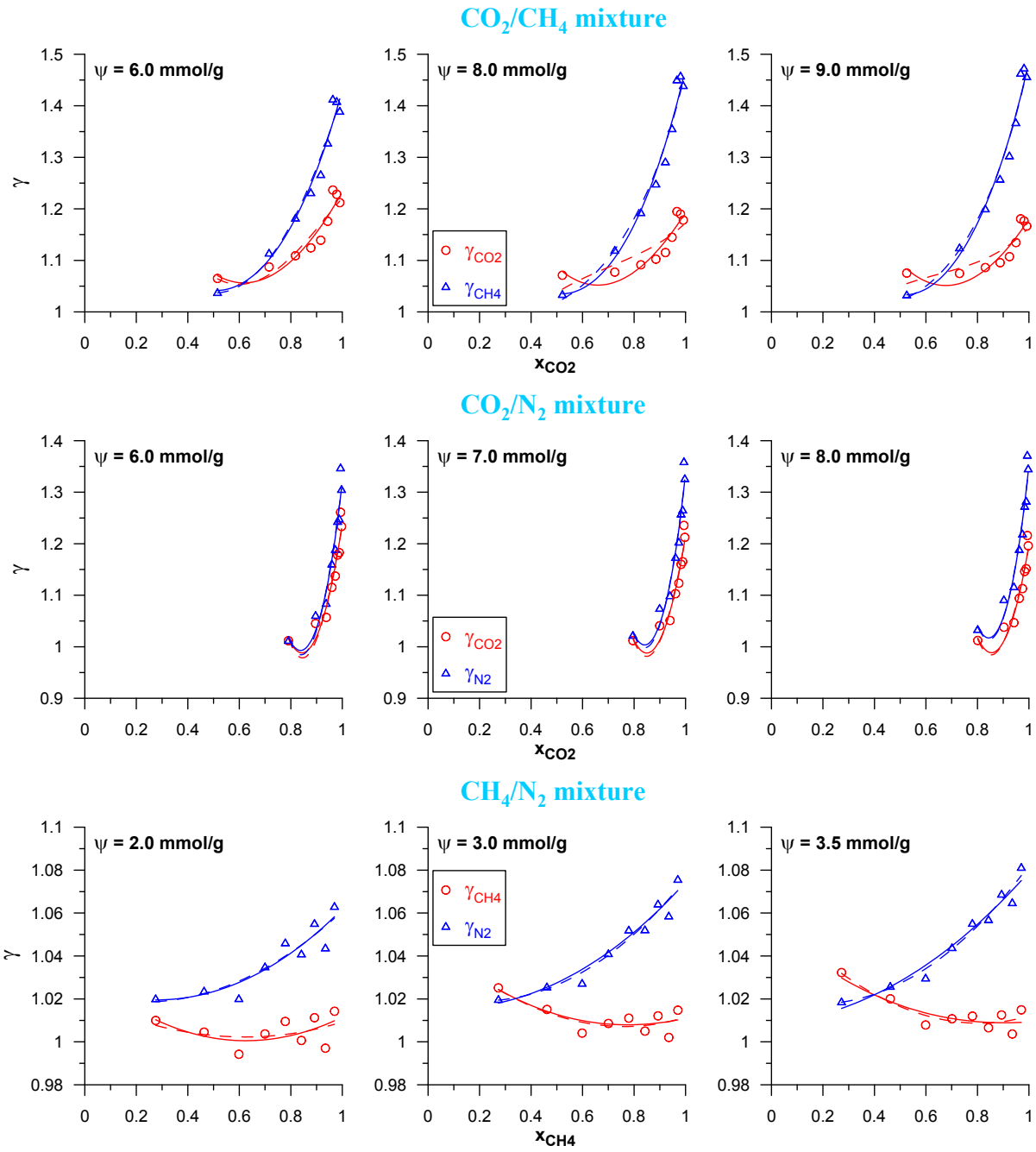

Figure S9. As in Fig. S8 but for the d1.3 carbon.