Supplement of

Treatment of non-ideality in the multiphase model SPACCIM-Part2: Impacts on the multiphase chemical processing in deliquesced aerosol particles

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Figures

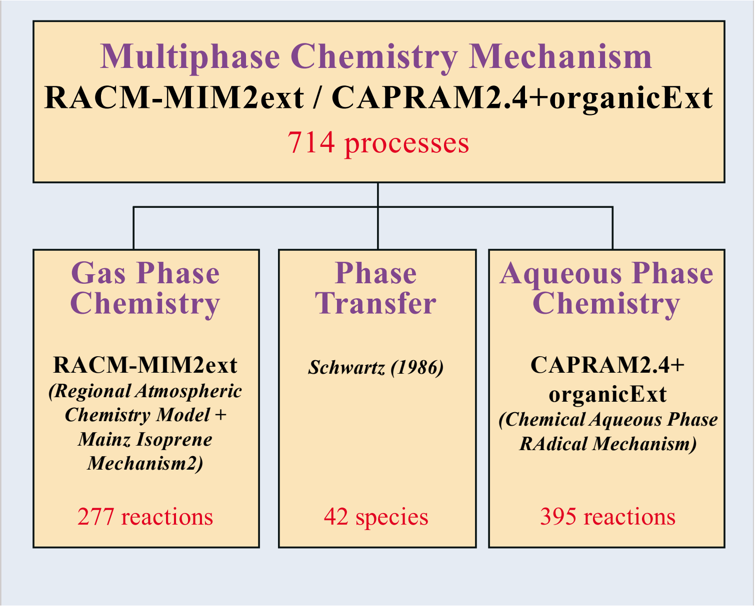

Figure S1. Schematic of multiphase mechanism employed in this study, including the number of processes, reactions, and phase transfer processes (modified from Deguillaume et al. (2009); Tilgner and Herrmann (2010)).

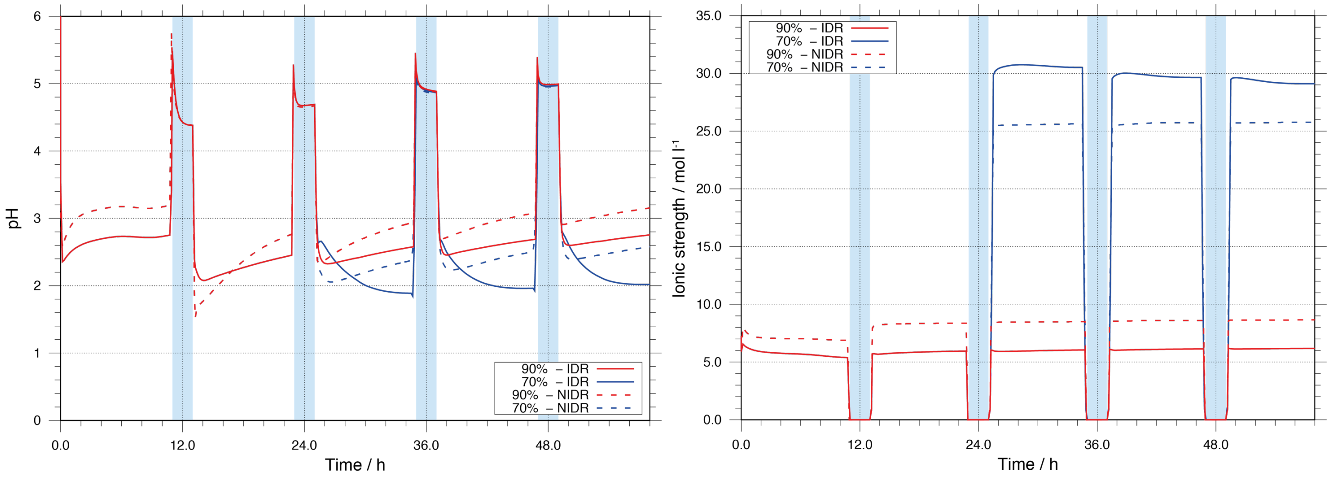

Figure S2. Modelled pH value (left) and ionic strength (I, right) as a function of simulation time for the different remote simulation cases (90 %-IDR/90 %-NIDR and 70 %-IDR/70 %-NIDR).

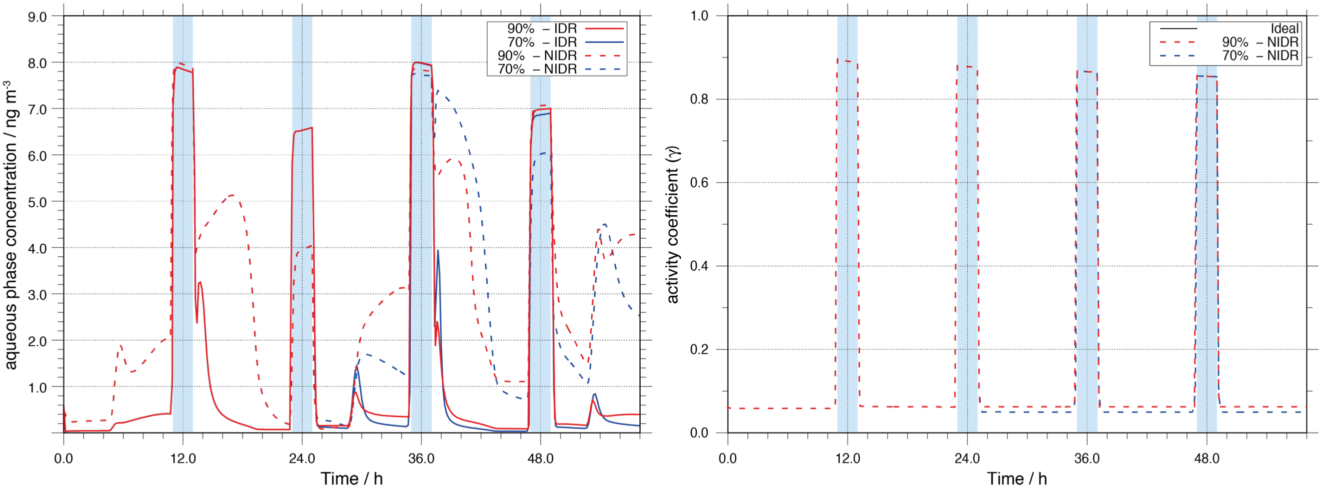

Figure S3. Modelled Fe(II) aqueous-phase concentration in ng m^{-3} throughout the modelling time (left) and corresponding time evolution of activity coefficients (right) for the different remote simulation cases (90 %-IDR/90 %-NIDR and 70 %-IDR/70 %-NIDR).

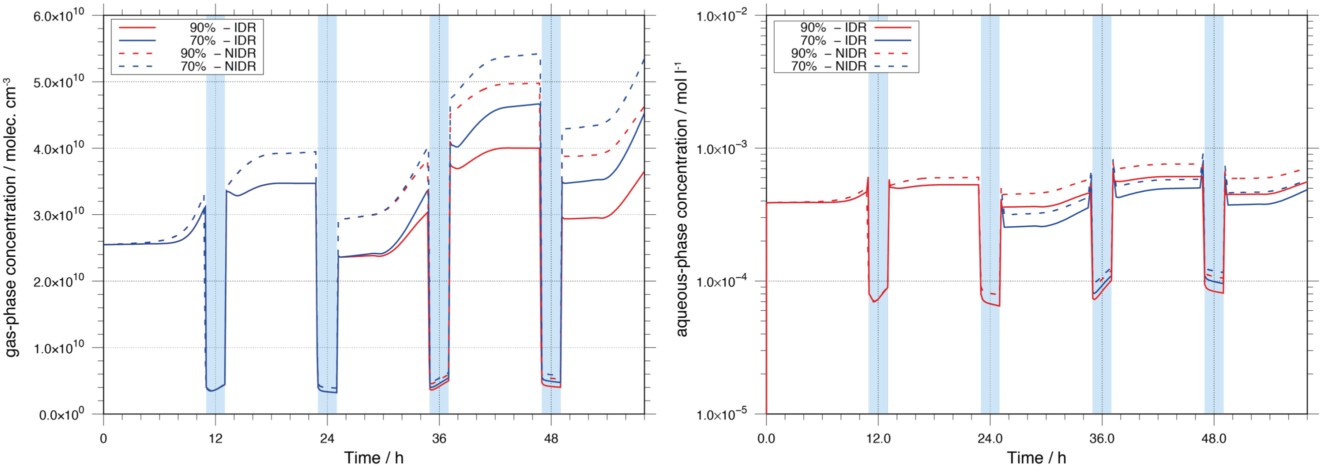

Figure S4. Modelled gas- and aqueous-phase concentration of H_2O_2 throughout the simulation time for the different remote simulation cases (90 %-IDR/90 %-NIDR and 70 %-IDR/70 %-NIDR).

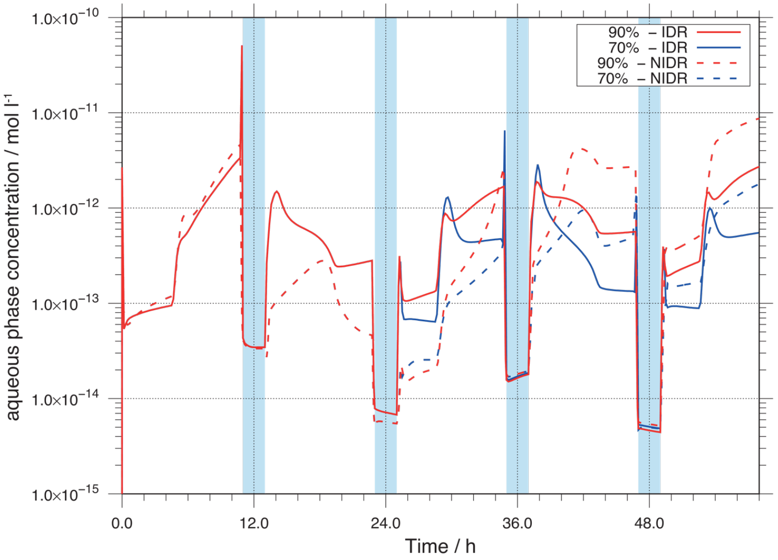

Figure S5. Modelled aqueous-phase OH concentration in mol l^{-1} throughout the simulation time for the different remote simulation cases (90 %-IDR/90 %-NIDR and 70 %-IDR/70 %-NIDR).

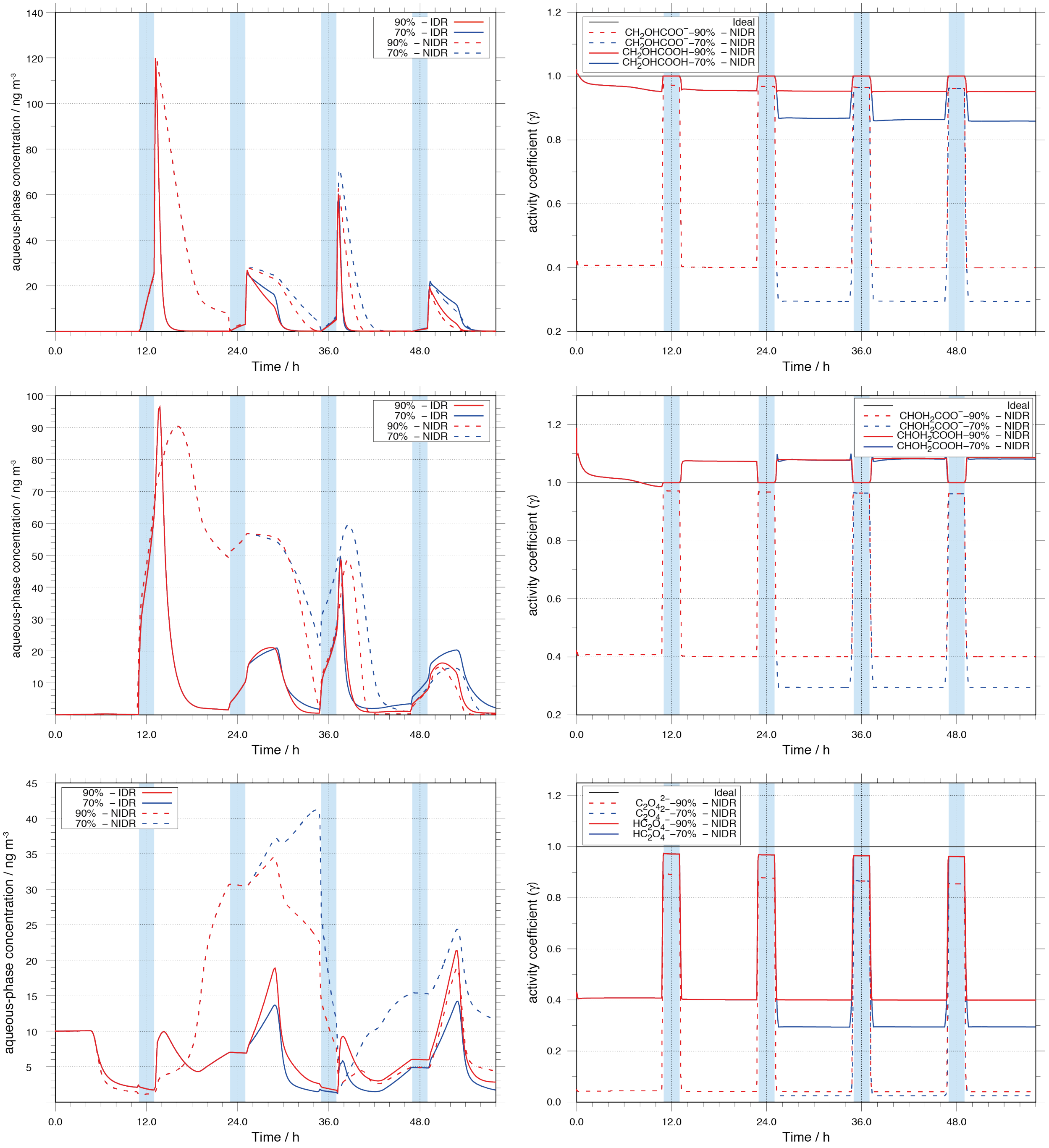

Figure S6. Modelled aqueous-phase concentrations in ng m$^{-3}{}_{(air)}$ and corresponding activity coefficients for important C_2 oxidation products, (i) glycolic acid (top), (ii) glyoxylic acid (centre), and (iii) oxalic acid (down) throughout the simulation time for the different remote simulation cases (90 %-IDR/90 %-NIDR and 70 %-IDR/70 %-NIDR). The plotted concentrations represent the sum of dissociated and undissociated forms of the carboxylic acids.

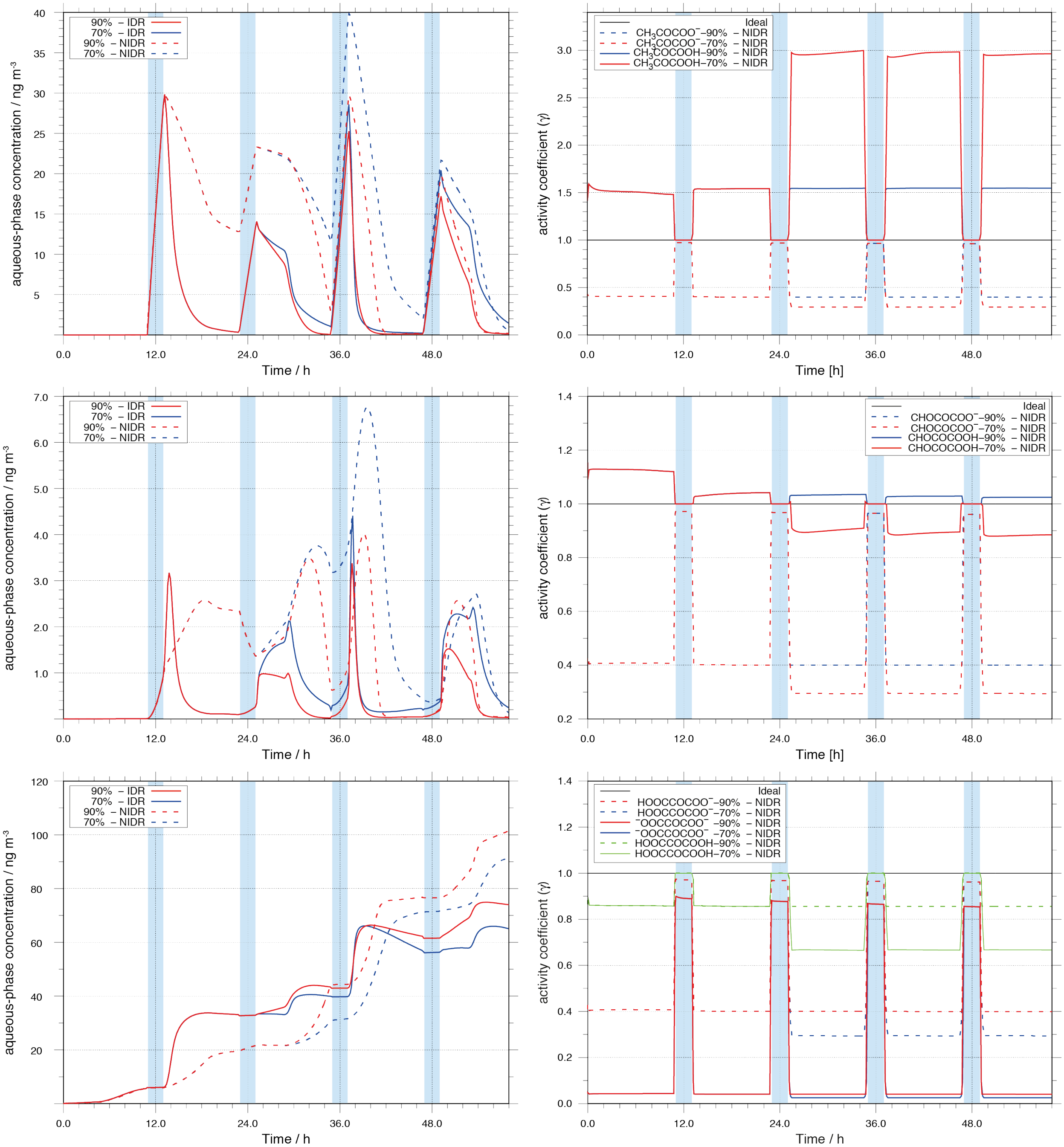

Figure S7. Modelled aqueous-phase concentrations in ng m$^{-3}{}_{\text{(air)}}$ and corresponding activity coefficients for important C_3 oxidation products, (i) pyruvic acid (top), (ii) 3-oxo-pyruvic acid (centre), and (iii) keto malonic acid (down) throughout the simulation time for the different remote simulation cases (90 %-IDR/90 %-NIDR and 70 %-IDR/70 %-NIDR). The plotted concentrations represent the sum of dissociated and undissociated forms of the carboxylic acids.

Tables

Table S1. Initial chemical aerosol particle composition (relative contributions to the total particulate non-water mass) for the urban and remote environmental model scenarios.

Compound	Urban	Remote
NH_4^+	1.00E-01	9.80E-02
NO_3^-	2.49E-02	9.27E-02
SO_4^{2-}	2.61E-01	1.91E-01
Cl^-	1.92E-02	9.70E-05
Br^-	6.53E-04	1.77E-04
I^-	1.23E-04	1.52E-07
Mn^{3+}	1.54E-04	1.15E-04
Fe^{3+}	1.46E-03	1.42E-03
Cu^{2+}	1.53E-04	1.08E-04
WSOM	1.51E-01	5.57E-02
$HC_2O_4^-$	4.38E-03	1.62E-03
$HOOCCH_2COO^-$	2.79E-03	1.03E-03
$HOOCC_2H_4COO^-$	1.59E-03	5.89E-04
WISOM	2.39E-01	8.83E-02
EC	1.56E-02	1.67E-01
Other anions	7.96E-05	1.89E-04
Cations (+)	3.26E-02	1.53E-02
Cations (2+)	1.49E-02	1.85E-02
Other metals	3.25E-02	4.05E-02
SiO2	9.53E-02	2.27E-01
P	2.87E-03	2.73E-04

Remarks: Single species and compound groups marked in italics are treated in SPACCIM as non-reactive species. The respective ions are just considered for the charge balance.

Table S2. Parameters (N: Number, ρ: Density, r: Radius) of the mono-disperse aerosol particle initialisation for the urban and remote environmental model scenarios.

Parameter	Urban	Remote
N (#/cm^3)	7.0E+08	1.0E+08
ρ (kg/m^3)	1770	1770
r (m)	2.0E+07	2.0E+07

References

Deguillaume, L., Tilgner, A., Schrödner, R., Wolke, R., Chaumerliac, N., and Herrmann, H.: Towards an operational aqueous phase chemistry mechanism for regional chemistry-transport models: CAPRAM-RED and its application to the COSMO-MUSCAT model, J. Atmos. Chem., 64, 1-35, doi:10.1007/s10874-010-9168-8, 2009.

Tilgner, A., and Herrmann, H.: Radical-driven carbonyl-to-acid conversion and acid degradation in tropospheric aqueous systems studied by CAPRAM, Atmos. Environ., 44, 5415-5422, doi:10.1016/j.atmosenv.2010.07.050, 2010.