The redox-cycling of iron is responsible for many chemical interactions such as the atmosphere-vegetation-surface-water interactions (ATVSEF, 2003). The iron chemistry model was initialised with physical and chemical data from the EUROTRAC-2 project CMD (Poppe et al., 2001) and references therein. For this purpose, sensitivity studies have been performed on the importance of the water-soluble iron content for the aqueous phase oxidation capacity and the organic chemical processing of iron species in the atmosphere.

Table 1: Depiction of the modelled aqueous phase iron content fluxes for the urban scenario (Fe2).

| Iron speciation | Budget (mol m⁻² s⁻¹) | Sensitivity studies on the importance of the water-soluble iron content
|-----------------|----------------------|-------------------------------------------------
| Fe(II)          | 5.0E-09              | Sensitivity studies show significant effects of the solubility iron content on the Fe(II) partitioning.
| Fe(III)         | 1.0E-08              | Reductions in the Fe(III) content are caused by the Fe(II) oxidation reaction.
| Fe(IV)          | 1.0E-09              | Enhanced Fe(II) oxidation leads to decreased Fe(III) concentrations.
| Fe(III) oxalate | 5.0E-08              | The formation of Fe(III) oxalate is a key process in the modelled Fe(III) budget.

Figure 1: Chemical analysis of the modelled aqueous Fe(II) (top) and modelled gas phase Fe(II) (bottom) concentration profiles for the urban scenario.

Current mechanisms which include the formation and photolysis of iron-organic complexes play a crucial role in the Fe(II) oxidation reaction. Potential pathways include the Fe(II) oxidation by peroxy radical (Fe(II) + HO₂) and direct Fe(II) oxidation by HO₂ (Fe(II) + HO₂). The modelled Fe(II) oxidation rate constant is 1.0E-08 mol m⁻³ s⁻¹.

Figure 2: Modelled chemical and gas exchange fluxes of Fe(II) and Fe(III) for the urban scenario.

Iron speciation in deliquescent particles and clouds

Iron speciation in deliquescent particles and clouds is of great interest for atmospheric chemistry. Deliquescent particles are formed by the condensation of water vapor on aerosol particles (CPM, 2000). Deliquescent particles are important for the condensation of aerosol particles and cloud droplets. The modelled Fe(II) fluxes in deliquescent particles and cloud droplets are of the order of 1.0E-08 mol m⁻³ s⁻¹. The Fe(II) oxidation rate constant is 1.0E-08 mol m⁻³ s⁻¹.

Figure 3: Modeled Fe(II) fluxes in deliquescent particles and cloud droplets for the urban scenario.

Sensitivity studies on the importance of the water-soluble iron content

Sensitivity studies show significant effects of the solubility iron content on the Fe(II) partitioning.

Summary and Outlook

Simulations with the modelled SPCM/SMIC have been carried out for different atmospheric conditions to investigate the iron speciation and redox-cycling in deliquescent particles and cloud droplets. Further simulations are carried out to investigate the importance of the water-soluble iron content for the Fe(II) oxidation reaction. The modelled Fe(II) oxidation rate constant is 1.0E-08 mol m⁻³ s⁻¹.

Figure 4: Modelled chemical and gas exchange fluxes of Fe(II) and Fe(III) for the urban scenario.

Current mechanisms which include the formation and photolysis of iron-organic complexes play a crucial role in the Fe(II) oxidation reaction. Potential pathways include the Fe(II) oxidation by peroxy radical (Fe(II) + HO₂) and direct Fe(II) oxidation by HO₂ (Fe(II) + HO₂). The modelled Fe(II) oxidation rate constant is 1.0E-08 mol m⁻³ s⁻¹.

Figure 5: Modelled chemical and gas exchange fluxes of Fe(II) and Fe(III) for the urban scenario.

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