representing in-cloud oxidation of sulfur in a particle-based cloud-microphysics scheme

Anna Jaruga, Hanna Pawłowska, Sylwester Arabas

Institute of Geophysics
Faculty of Physics, University of Warsaw

18th Conference on Atmospheric Chemistry
AMS, New Orleans, January 2016
Eulerian microphysics

- available liquid water is divided into histogram bins
Eulerian microphysics

- available liquid water is divided into histogram bins
- for aerosol - cloud interaction studies 2D histogram is created with ”wet” and ”dry” radius
Eulerian microphysics

- available liquid water is divided into histogram bins
- for aerosol - cloud interaction studies 2D histogram is created with "wet" and "dry" radius
- parametrisations of source and sink terms are applied to each bin
Eulerian microphysics

- available liquid water is divided into histogram bins
- for aerosol - cloud interaction studies 2D histogram is created with "wet" and "dry" radius
- parametrisations of source and sink terms are applied to each bin
- new histogram dimensions needed for chemical compounds...
Lagrangian microphysics

super-droplets in the domain
Lagrangian microphysics

super-droplets in the domain attributes:
Lagrangian microphysics

super-droplets in the domain attributes:
  ▶ location
Lagrangian microphysics

super-droplets in the domain
attributes:
  ▶ location
  ▶ wet radius
Lagrangian microphysics

super-droplets in the domain
attributes:
  ▶ location
  ▶ wet radius
  ▶ dry radius
Lagrangian microphysics

super-droplets in the domain

attributes:
  ▶ location
  ▶ wet radius
  ▶ dry radius
  ▶ multiplicity
Lagrangian microphysics

super-droplets in the domain

attributes:
  ▶ location
  ▶ wet radius
  ▶ dry radius
  ▶ multiplicity
  ▶ . . .
Cloud microphysics

- Maxwell-Mason equation of condensational growth for each super-droplet using $\kappa$-Koehler parametrisation of higroscopicity (Petters & Kreidenweis, 2007)

- CCN activation
- Condensational growth
Cloud microphysics

- Maxwell-Mason equation of condensational growth for each super-droplet using $\kappa$-Koehler parametrisation of higroscopicity (Petters & Kreidenweis, 2007)
- collisions for each super-droplet by a Monte-Carlo coalescence scheme (Shima et al. 2009)

- CCN activation
- condensational growth
- collision - coalescence
Cloud microphysics

- Maxwell-Mason equation of condensational growth for each super-droplet using $\kappa$-Koehler parametrisation of higroscopicity (Petters & Kreidenweis, 2007)
- collisions for each super-droplet by a Monte-Carlo coalescence scheme (Shima et al. 2009)
- sedimentation of each super-droplet (Khvorostyanov & Curry, 2002)

- CCN activation
- condensational growth
- collision - coalescence
- precipitation
- wet deposition
- droplet deactivation
Example results with collisions (2D kinematic set-up)

- **set-up:** Grabowski & Lebo (ICMW 2012)
- **2D prescribed flow**
- **advection:** libmpdata++ (2-pass FCT)
- **µ-physics:** libcloudph++
Example results with collisions (2D kinematic set-up)
Example results with collisions (2D kinematic set-up)
Example results with collisions (2D kinematic set-up)

cloud water mixing ratio [g/kg]

rain drop spec. conc. [mg⁻¹]

aerosol concentration [mg⁻¹]
Example results with collisions (2D kinematic set-up)
Example results with collisions (2D kinematic set-up)
Figure 9: Plots of dry and wet size spectra for ten locations within the simulation domain. The locations and their labels (a–j) are overlaid on plots in Figure 8. The vertical bars at 0.5 \( \mu \text{m} \) and 25 \( \mu \text{m} \) indicate the range of particle wet radii which is associated with cloud droplets. See section 5.4 for discussion.
representing in-cloud oxidation of sulfur in a particle-based cloud-microphysics scheme

- CCN activation
- condensational growth
- collisional growth
- precipitation
- wet deposition
- droplet deactivation
representing in-cloud oxidation of sulfur in a particle-based cloud-microphysics scheme
Lagrangian microphysics + aqueous chemistry

super-droplets in the domain

with attributes:

- location
- wet radius
- dry radius
- multiplicity

mass of chemical compounds within droplets:

- $\text{H}_2\text{O}$
- $\text{SO}_2$
- $\text{O}_3$
- $2\text{H}_2\text{O}$
- $\text{H}_2\text{O} \cdot \text{CO}_2$
- $\text{H}_2\text{O} \cdot \text{NH}_3$
- $\text{HNO}_3$
- $\text{HSO}_3^-$
- $\text{SO}_3^{2-}$
- $\text{HCO}_3^-$
- $\text{CO}_3^{2-}$
- $\text{NO}_3^-$
- $\text{NH}_4^+$
- $\text{H}^+$
- $\text{OH}^-$
- $\text{HSO}_4^-$
- $\text{SO}_4^{2-}$
Lagrangian microphysics + aqueous chemistry

super-droplets in the domain with attributes:

- location
- wet radius
- dry radius
- multiplicity
- mass of chemical compounds within droplets:
  - $\text{H}_2\text{O} \cdot \text{SO}_2$, $\text{O}_3$, $\text{H}_2\text{O}_2$,
  - $\text{H}_2\text{O} \cdot \text{CO}_2$, $\text{H}_2\text{O} \cdot \text{NH}_3$,
  - $\text{HNO}_3$, $\text{HSO}_3^-$, $\text{SO}_3^{2-}$,
  - $\text{HCO}_3^-$, $\text{CO}_3^{2-}$, $\text{NO}_3^-$, $\text{NH}_4^+$,
  - $\text{H}^+$, $\text{OH}^-$, $\text{HSO}_4^-$, $\text{SO}_4^{2-}$
Aqueous chemistry

- dissolving of trace gases
Aqueous chemistry

- dissolving of trace gases
- dissociation

- gas uptake is treated as nonequilibrum process
- gas-liquid and liquid-liquid equilibra are computed for all super-droplets
- oxidation of sulfur is computed only for cloud droplets
- no adjustment for high-ionic strength of some droplets
- impacts condensation via dry radii, but no impact on $\kappa$ (yet)
Aqueous chemistry

- dissolving of trace gases
- dissociation
- oxidation

- gas uptake is treated as nonequilibrium process
- gas-liquid and liquid-liquid equilibria are computed for all super-droplets
- oxidation of sulfur is computed only for cloud droplets
- no adjustment for high-ionic strength of some droplets
- impacts condensation via dry radii, but no impact on $\kappa$ (yet)
Aqueous chemistry

- dissolving of trace gases
- dissociation
- oxidation

- gas uptake is treated as nonequilibrium process
Aqueous chemistry

- dissolving of trace gases
- dissociation
- oxidation

- gas uptake is treated as nonequilibrium process
- gas-liquid and liquid-liquid equilibra are computed for all super-droplets
Aqueous chemistry

- dissolving of trace gases
- dissociation
- oxidation

- gas uptake is treated as nonequilibrium process
- gas-liquid and liquid-liquid equilibria are computed for all super-droplets
- oxidation of sulfur is computed only for cloud droplets
Aqueous chemistry

- dissolving of trace gases
- dissociation
- oxidation

- gas uptake is treated as nonequilibrium process
- gas-liquid and liquid-liquid equilibria are computed for all super-droplets
- oxidation of sulfur is computed only for cloud droplets
- no adjustment for high-ionic strength of some droplets
Aqueous chemistry

- dissolving of trace gases
- dissociation
- oxidation

- gas uptake is treated as nonequilibrium process
- gas-liquid and liquid-liquid equilibria are computed for all super-droplets
- oxidation of sulfur is computed only for cloud droplets
- no adjustment for high-ionic strength of some droplets
- impacts condensation via dry radii, but no impact on $\kappa$ (yet)
Validation of the chemistry module

- adiabatic parcel simulations from model comparison study by Kreidenweis et al 2003
Validation of the chemistry module

- adiabatic parcel simulations from model comparison study by Kreidenweis et al 2003
- initial lognormal monomodal dry aerosol size distribution
Validation of the chemistry module

- adiabatic parcel simulations from model comparison study by Kreidenweis et al 2003
- initial lognormal monomodal dry aerosol size distribution
Example results with chemistry (2D kinematic set-up)

- set-up: Grabowski & Lebo (ICMW 2012)
- 2D prescribed flow
- advection: *libmpdata++* (2-pass FCT)
- $\mu$-physics: *libcloudph++*
Example results with chemistry (2D kinematic set-up)
Example results with chemistry (2D kinematic set-up)
Example results with chemistry (2D kinematic set-up)

- Cloud droplet effective radius [μm]
- Dry radius [μm]
- Aerosol concentration [mg$^{-1}$]
Example results with chemistry (2D kinematic set-up)

Cloud droplet effective radius [μm]

Dry radius [μm]

Aerosol concentration [mg⁻¹]
Example results with chemistry (2D kinematic set-up)
2×2 cell particle-derived spectra

(a) [mg⋅m⁻¹] particle radius [μm] (i)
wet radius
dry radius

(b) [mg⋅m⁻¹] particle radius [μm] (j)
wet radius
dry radius

(c) [mg⋅m⁻¹] particle radius [μm] (e)
wet radius
dry radius

(d) [mg⋅m⁻¹] particle radius [μm] (h)
wet radius
dry radius

(e) [mg⋅m⁻¹] particle radius [μm] (f)
wet radius
dry radius

(f) [mg⋅m⁻¹] particle radius [μm] (g)
wet radius
dry radius

(g) [mg⋅m⁻¹] particle radius [μm] (h)
wet radius
dry radius

(h) [mg⋅m⁻¹] particle radius [μm] (j)
wet radius
dry radius

(i) [mg⋅m⁻¹] particle radius [μm] (i)
wet radius
dry radius

(j) [mg⋅m⁻¹] particle radius [μm] (j)
wet radius
dry radius

(aerosol concentration [mg⁻¹])

Rule 1: The Effective Radius

Rule 2: The Rainfall Rate

Rule 3: The Evaporation Rate

Rule 4: The Aerosol Concentration
Final remarks

- available online as a part of libcloudph++ library of cloud microphysics schemes
  http://libcloudphxx.igf.fuw.edu.pl/
Final remarks

- available online as a part of **libcloudph++** library of cloud microphysics schemes

- reusable:
  - design: no assumptions on dimensionality or dyn-core type
  - documentation: API described in the paper/manual
  - legal/practical matters: open source, GPL, hosted on github

Thank you for your attention!
Final remarks

- available online as a part of `libcloudph++` library of cloud microphysics schemes

- reusable:
  - design: no assumptions on dimensionality or dyn-core type
  - documentation: API described in the paper/manual
  - legal/practical matters: open source, GPL, hosted on github

- Lagrangian scheme optionally GPU-resident (via Thrust)
Final remarks

- available online as a part of *libcloudph++* library of cloud microphysics schemes

- reusable:
  - design: no assumptions on dimensionality or dyn-core type
  - documentation: API described in the paper/manual
  - legal/practical matters: open source, GPL, hosted on github

- Lagrangian scheme optionally GPU-resident (via Thrust)

- compact code (5000 lines of code)
Final remarks

- available online as a part of **libcloudph++** library of cloud microphysics schemes

- reusable:
  - design: no assumptions on dimensionality or dyn-core type
  - documentation: API described in the paper/manual
  - legal/practical matters: open source, GPL, hosted on github

- Lagrangian scheme optionally GPU-resident (via Thrust)

- compact code (5000 lines of code)

- equipped with Python bindings

Thank you for your attention!
Final remarks

- available online as a part of **libcloudph++** library of cloud microphysics schemes
  

- reusable:
  - design: no assumptions on dimensionality or dyn-core type
  - documentation: API described in the paper/manual
  - legal/practical matters: open source, GPL, hosted on github

- Lagrangian scheme optionally GPU-resident (via Thrust)

- compact code (5000 lines of code)

- equipped with Python bindings

- **Thank you for your attention!**