Implementation of nitrate in NorESM

Dirk Olivié, Alf Kirkevåg, Øyvind Seland, Michael Schulz, Trond Iversen

Boulder, 22 June 2017
Overview

- Motivation/introduction
- The aerosol scheme in NorESM
- Extending the aerosol scheme with nitrate
- Results – validation
- Conclusions
What is nitrate?

Diagram showing the cycle of nitrate formation and consumption in the atmosphere, involving reactions with NO, NO₂, N₂O₅, HNO₃, NH₃, (NH₄)₂SO₄, and SO₂.
Why modelling nitrate?

**Expected increased relative importance of nitrate aerosol in 21st century**

**Hauglustaine et al. [2014] (only direct radiative forcing)**

<table>
<thead>
<tr>
<th></th>
<th>2000</th>
<th>2030</th>
<th>2050</th>
<th>2100</th>
</tr>
</thead>
<tbody>
<tr>
<td>SO$_4$ [W m$^{-2}$]</td>
<td>-0.315</td>
<td>-0.118</td>
<td>-0.094</td>
<td>-0.033</td>
</tr>
<tr>
<td>NO$_3$ [W m$^{-2}$]</td>
<td>-0.056</td>
<td>-0.095</td>
<td>-0.102</td>
<td>-0.096</td>
</tr>
</tbody>
</table>

**Air-quality models**

**Nitrate in climate models**: Feng and Penner [2007], Bauer et al. [2007], Bellouin et al. [2011], Xu and Penner [2012], Hauglustaine et al. [2014]

**Aerocom inter-comparison study**: Bian et al. [2017, ACPD]
What is NorESM?

NorESM - Norwegian Earth System Model

Before 2007
- Atmosphere: development of aerosol module and study of indirect aerosol effect in various versions of CAM (CAM-Oslo)
- Ocean: development of BCC (Bergen Climate Model) including MICOM, with marine bio-geochemistry (HAMOCC) (ARPEGE as atmosphere model in BCC)

Since 2007 Working on development of NorESM – resulted in NorESM-1 based on CCSM-4

Current development of aerosol-scheme in CAM-Oslo
explicit SOA formation, aerosol nucleation, interactive emissions of DMS and OM from the ocean, new sea-salt emission parameterisation, nitrate aerosol
The CAM-Oslo aerosol scheme

Gas-phase species (8): DMS, SO₂, H₂SO₄, H₂O₂, isoprene, mono-terpenes, semi-volatile SOA precursors, low-volatile SOA precursor

Oxidant climatologies (4): OH, HO₂, NO₃, O₃ (+ daily cycle)

Aerosol species (12 modes – 20 tracers)

Remarks: Explicit nucleation / Aging of particles / No evaporation of SOA / NH₄ implicit
Comparison with MAM7 aerosol scheme

Liu et al. [2012]

Remarks Aerosol number, variable mode radius
Some issues with CAM-Oslo

BC [HIPPO, 2009–2011]

SO₂ [Aerocom]
New gas-phase species: $\text{HNO}_3$, $\text{NH}_3$, NO, NO$_2$, NO$_3$, N$_2$O$_5$, PAN

NH$_3$ and HNO$_3$ can condensate on existing aerosol:

1. NH$_4$: ammonium (bi)sulfate: (NH$_4$)$_2$SO$_4$, (NH$_4$)HSO$_4$
2. NH$_4$ and NO$_3$: equilibrium of $\text{NH}_3(g) + \text{HNO}_3(g) \leftrightarrow \text{NH}_4\text{NO}_3$ (aerosol) [Ackermann et al., 1995; Hauglustaine et al., 2014; Bellouin et al., 2011]
3. NO$_3$(dst): irreversible condensation of HNO$_3$ on dust
4. NO$_3$(ss): irreversible condensation of HNO$_3$ on sea-salt

Aerosol tracers

| SO$_4$ / SOA | SO$_4$ / SOA / NH$_4$ / NO$_3$ |
| BC | SO$_4$ / SOA / NH$_4$ / NO$_3$ |
| OC / BC | SO$_4$ / SOA / BC / OM / NH$_4$ / NO$_3$ |
| SEA SALT | SO$_4$ / SOA / BC / OM / NH$_4$ / NO$_3$ / NO$_3$(dst) |
| DUST | SO$_4$ / SOA / BC / OM / NH$_4$ / NO$_3$ / NO$_3$(ss) |
How to validate?

Two issues

1. How well is nitrate represented?
2. Impact of the simplified NO$_x$ chemistry?

Possible validation

1. Comparison with a full-chemistry version
2. Comparison with observations (aerocom-tool)
3. Comparison with other models

Simulations

- Simplified chemistry and full chemistry (both nudged to same meteorology)
- 5 years: averages over year 2–5 are shown
- Resolution: 1.9° $\times$ 2.5°, 30 levels
- Year 2000 conditions (emissions, GHG, ...)

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Implementation of nitrate in NorESM
Comparison with observations: SO$_2$ and SO$_4$

Surface observations

**Simplified chemistry with nitrate**

**SO$_2$**

- SCONC$_{SO2}$ #:1594 #st:136
- Obs: 0.987
- Mod: 2.363
- NMB: 139.5%
- MNMB: 87.6%
- R: 0.338
- RMS: 2.259
- Fact2: 12.7%

**Full-chemistry with nitrate**

- SCONC$_{SO2}$ #:2856 #st:248
- Obs: 0.753
- Mod: 0.790
- NMB: 4.8%
- MNMB: 0.3%
- R: 0.857
- RMS: 0.537
- Fact2: 56.0%

**SO$_4$**

- SCONC$_{SO4}$ #:1594 #st:136
- Obs: 0.753
- Mod: 0.790
- NMB: 4.8%
- MNMB: 0.3%
- R: 0.857
- RMS: 0.537
- Fact2: 56.0%

**Full-chemistry with nitrate**

- SCONC$_{SO4}$ #:2856 #st:248
- Obs: 0.753
- Mod: 0.852
- NMB: 13.1%
- MNMB: 0.1%
- R: 0.650
- RMS: 0.594
- Fact2: 50.7%

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Implementation of nitrate in NorESM
Comparison with observations: NH$_3$ and NH$_4$

Surface observations

Simplified chemistry with nitrate

NH$_3$

Full-chemistry with nitrate

NH$_4$

Simplified chemistry with nitrate

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Implementation of nitrate in NorESM
Comparison with observations: HNO$_3$ and NO$_3$

Surface observations

**Simplified chemistry with nitrate**

**HNO$_3$**

- SCONC$_{HNO3}$ #:824 st:71
- Obs: 0.181 Mod: 0.464
- NMB: 156.6% MNMB: 62.5%
- R: 0.235 RMS: 0.564
- Fact2: 20.0%

**Full-chemistry with nitrate**

**NO$_3$**

- SCONC$_{NO3}$ #:2438 st:212
- Obs: 0.284 Mod: 0.541
- NMB: 90.6% MNMB: 47.3%
- R: 0.560 RMS: 0.547
- Fact2: 28.1%

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Implementation of nitrate in NorESM
NH$_4$ mixing ratio

April 2008

NH$_4$ mixing ratio

Observations
full chem
fixed oxid

July 2008

NH$_4$ mixing ratio

Observations
full chem
fixed oxid

NO$_3$ mixing ratio

SO$_4$ mixing ratio

Observations
full chem
fixed oxid

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Implementation of nitrate in NorESM
Nitrate column burden
Aerosol-only – annual mean

Nitrate (in NH$_4$NO$_3$) (0.12 Tg)

NO$_3$ burden (fine mode) [mg m$^{-2}$]

Nitrate on dust (0.44 Tg)

NO$_3$ burden (on dust) [mg m$^{-2}$]

Nitrate on seasalt (0.13 Tg)

NO$_3$ burden (on sea-salt) [mg m$^{-2}$]
### Global burden

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<tbody>
<tr>
<td></td>
<td>aerosol-only</td>
<td></td>
<td></td>
</tr>
<tr>
<td>NH$_4$</td>
<td>[Tg] 0.35</td>
<td>0.28 (0.39)</td>
<td>0.32</td>
</tr>
<tr>
<td>NO$_3$</td>
<td>[Tg] 0.59</td>
<td>0.80 (0.79)</td>
<td>0.63</td>
</tr>
<tr>
<td>NO$_3$(a1)</td>
<td>[Tg] 0.10</td>
<td>0.22</td>
<td></td>
</tr>
<tr>
<td>NO$_3$(dst)</td>
<td>[Tg] 0.38</td>
<td>0.31</td>
<td></td>
</tr>
<tr>
<td>NO$_3$(ss)</td>
<td>[Tg] 0.10</td>
<td>0.27</td>
<td></td>
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</tbody>
</table>

### Neutralization

<table>
<thead>
<tr>
<th></th>
<th>full-chemistry</th>
<th>aerosol-only</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\frac{[\text{NH}<em>4]</em>{\text{vmr}}}{[\text{SO}<em>4]</em>{\text{vmr}}}$</td>
<td>1.25</td>
<td>1.30</td>
</tr>
</tbody>
</table>
Effective radiative forcing

**Total**: \(-1.145 \text{ W m}^{-2}\)

<table>
<thead>
<tr>
<th></th>
<th>Longwave [W m(^{-2})]</th>
<th>Shortwave [W m(^{-2})]</th>
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<tbody>
<tr>
<td>Direct</td>
<td>0.032</td>
<td>-0.184</td>
</tr>
<tr>
<td>Indirect</td>
<td>0.076</td>
<td>-1.132</td>
</tr>
<tr>
<td>Surface albedo</td>
<td>0.057</td>
<td>0.006</td>
</tr>
</tbody>
</table>

Geographical distribution (annual mean)

Net downward SW+LW flux (TOA) [W m\(^2\)]

![Map showing geographical distribution of net downward SW+LW flux (TOA)](image-url)
Simplified chemistry: \( \text{NH}_4\text{NO}_3 \)

Full chemistry: \( \text{NH}_4\text{NO}_3 \)

Boundary layer height
Simplified NO\(_x\) chemistry ... Gridpoint in western Europe – June – lowest layer

\[\text{NH}_4\text{NO}_3\]

\[\text{HNO}_3\]

\[\text{HNO}_3 + \text{NO}_3\]

**Full-chemistry with nitrate**

**Aerosol-only with nitrate**
Comparison with observations: NO₂

Aerosol-only

Full-chemistry

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Conclusions

**Aerosol module now contains nitrate and ammonium**
- 4 extra aerosol tracers: NH$_4$, NO$_3$, NO$_3$(dst), NO$_3$(ss)
- 7 extra gas-phase species
- Aerosol-only version: 29 → 40 tracers.
- Implemented both in aerosol-only as well as in full-chemistry version of NorESM.

**Remaining issues**
- Possibly too fast aerosol aging?
- Optimization of the simplified NO$_x$ chemistry

**Future**
- Look at AOD
- Look at nitrogen deposition measurements
- Extend to more global observations
- (Daily cycle of emissions?)
Thank you!