





Global aerosol forecast and assimilation at ECCC: current status and future directions

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ECCC atmospheric models and their aerosol sub-models

GEM, Meteorology Research Division, ECCC

- **GEM** is the operational regional and global weather forecast model
 - Daily, monthly and seasonal forecasts from urban to global scale
 - Aerosol climatology for radiative transfer and cloud droplet activation

GEM-MACH, Air Quality Research Division, ECCC

- **GEM-MACH** is the operational regional (North America) air quality forecast model
 - Canadian Aerosol Model (CAM) with updates(Gong et al., 2003)
 - Single-moment sectional approach
- **GEM-MACH-Interactive** [air quality-meteorology feedbacks experimental version]
 - GEM-MACH with fully interactive meteorology with chemistry and aerosol [Makar et al, 2015(a, b)]
- **GEM-MACH-FireWorks** [April-October parallel operational forecast model]
 - GEM-MACH with real-time forest fire emissions (Chen et al. 2019)
- Daily Air Quality Surface Analysis using GEM-MACH

CanESM, Climate Research Divison, ECCC

- **CanESM** is the operational climate model; also supports ensemble seasonal forecast
 - Bulk aerosol (von Salzen et al. 2013)
 - Piecewise log-normal approximation Aerosol Model (PAM) (Von Salzen, 2006; Peng et al. 2012; Ma et al., 2008)
 - 2-moment sectional-modal hybrid approach

Global Environmental Multiscale - Modelling Air quality & Chemistry (GEM-MACH) model

- **GEM-MACH-Operational** regional grid covers much of North America
 - 10 km horizontal grid spacing
 - 80 vertical levels with top at 0.1 hPa
 - 2-bin sectional representation of PM size distribution (i.e., 0-2.5 µm and 2.5-10 µm)
 - twice-daily 48-hour operational forecasts of O₃, NO₂, PM_{2.5}, and Air Quality Health Index (AQHI)
- **GEM-MACH-FireWork** operational configuration
- GEM-MACH-Interactive 2.5 km horizontal resolution and 12 size bins for aerosol dynamics



• **GEM-MACH** is an In-line model with one-way coupling with meteorology and includes comprehensive physicochemical processes of atmospheric gases and aerosols. 8 internally-mixed species are sulfate, ammonium, nitrate, primary organic carbon, secondary organic carbon, elemental carbon, dust and sea-salt.



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GEM-MACH Chemistry

ADOM-II Tropospheric gas-phase chemistry mechanism

- 47 species, 114 reactions
- Nitrogen NO, NO2, NO3, HONO, N2O5, HNO4, HNO3, PAN, RONO2
- Oxidants O3, OH, H2O2, ROOH
- Sulfur SO2, H2SO4
- Long Lived CO, CH4, ETHA
- VOCs

 C3H8, ALKA, ETHE,
 ALKE, ISOP, TOLU,
 AROM
- OVOCs HCHO, ALD2, MEK, MGLY, DIAL, CRES

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GEM-MACH Chemistry ADOM Cloud Chemistry

Reactions 1 to 18: H_2SO_4 , SO_2 , O_3 , H_2O_2 HNO_3 , ROOH, NH_3 , CO_2 , DUST Dissolution and Acid Equilibria

Reactions 19-22: HSO₃⁻ oxidation by O₃, H₂O₂ and ROOH, metals to sulfate

Adds acidity to clouds

(1) $H_2SO_4(aq)$ $SO_4^{2-}(aq) + 2 H^+(aq)$ $SO_{2}(g) (+ H_{2}O)$ (2) $HSO_3(aq) + H^+(aq)$ $HSO_3(aq) + H^+(aq)$ $SO_{2}(aq) (+H_{2}O)$ (3) (4) $O_3(g)$ $O_3(aq)$ (5) $O_3(g)$ $O_3(aq)$ (6) $H_{2}O_{2}(g)$ $H_2O_2(aq)$ (7) $H_2O_2(aq)$ $H_2O_2(g)$ (8) $HNO_3(g)$ $NO_3(aq) + H^+(aq)$ $HNO_3(g)$ (9) $NO_3(aq) + H^+(aq)$ (10)ROOH(q) ROOH(aq) ROOH(aq) ROOH(g) (11)(12) $NH_3(g)$ $NH_4^+(aq) + OH^-(aq)$ (13) $NH_4^+(aq) + OH^-(aq)$ $NH_3(g)$ (14)"DUST" $FEMN(aq) + HCO_3^{-}(aq) + CAT1^{+}(aq)$ $HCO_3^{-}(aq) + H^+(aq)$ (15) $CO_2(g)$ $CO_2(g)$ (16) $HCO_3^{-}(aq) + H^{+}(aq)$ (17) $H^+(aq) + OH^-(aq)$ $H_2O(I)$ (18) $H_2O(I)$ $H^+(aq) + OH^-(aq)$ (19) $HSO_3(aq) + O_3(aq)$ $SO_4^{2-}(aq) + H^+(aq)$ (20) $HSO_3(aq) + H_2O_2(aq)$ $SO_4^{2-}(aq) + H^+(aq)$ (21) $HSO_3(aq) + ROOH(aq)$ $SO_4^{2-}(aq) + H^{+}(aq)$ HSO₃ (aq) $SO_4^{2-}(aq) + H^+(aq)$ (22)+ (FEMN)

+ 3 more reactions designed to approximate heterogeneous effects...

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GEM-MACH gas-aerosol partitioning Inorganic aerosol thermodynamics – HETV (based on ISORROPIA; Makar et al, *Atm. Env.*, 2015)

- Equilibrium bulk thermodynamics scheme
- HETV solves local subsystems in TA/TS to relative humidity, to determine the new particle composition.

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GEM-MACH fine particulate Sulfate forecast evaluation with surface observations in 2010



GEM-MACH PM2.5 and PM10 forecast evaluation with surface observations in 2010



GEM-MACH Operational forest fire air quality forecast system - FireWork

- Official operational system since April 2016 <u>https://weather.gc.ca/firework</u>
- System runs twice daily (00/12 UTC) during Canadian fire season from April to October
- Near-real-time fire data from Canadian Wildland Fire Information System (CWFIS) bottom-up approach
- Hourly fire emissions (PM, VOC, NOx, NH₃, CO, SO₂) are input by FireWork, a clone of the ECCC Regional Air Quality Deterministic Prediction System (Pavlovic et al. JA&WMA, 2016)
- New forest fire emissions system, Canadian Forest Fire Emissions Prediction System (CFFEPS) (also bottom-up), will replace CWFIS in near term (Chen et al. GMD 2019)

FireWork products

- 1) *PM*_{2.5}/*PM*₁₀ maps and animations from fire sources
- 2) AQHI based on FireWork forecasts
- 3) Accumulated PM_{2.5} impacts over 24h
- 4) Total column PM_{2.5}/PM₁₀
- 5) Other specialized products upon request (e.g., special fire activity near urban areas) http://collaboration.cmc.ec.gc.ca/cmc/air/firework



Hourly surface fire-PM_{2.5} concentrations for 23 Aug. 2018



GEM-MACH Experimental FIREX-AQ Forecast - July 20th, 12 UT, 2019



Canadian Earth System Model (CanESM) - Piecewise lognormalapproximation Aerosol Model (PAM) (von Salzen ACP, 2006; von Salzen et al. Atmos. Ocean 2013)

- CanESM is an entirely separate model developed at Canadian Center for Climate modeling and analysis (CCCma), Climate Research Division, ECCC, with its own dynamics core and physicochemical processes representations.
- CanESM supports IPCC and AMAP Assessments and Canadian Seasonal to Interannual Prediction System (CanSIPS)

Aerosol Chemical Species and mixing state in PAM

Piecewise Lognormal Approximation (PLA) method Aerosol Model (PAM)

- 2-moment numerical scheme for simulation of aerosol size distributions based on combination of bin and modal schemes
- External and internal mixing of aerosol chemical species
- Sulfur chemistry including DMS
- Aerosol optical properties and radiative forcings depend on particle size and aerosol mixing state
- Includes model for cloud droplet nucleation and aerosol indirect effects

Piecewise Log-normal Approximation (PLA)

Aerosol number size distribution

$$n(\varphi) = \sum_{i} n_{i}(\varphi) \quad \text{, with } \varphi = \ln(R/R_{0})$$
$$n_{i}(\varphi) = n_{0,i} \exp\left[-\psi_{i}(\varphi - \varphi_{0,i})^{2}\right] H(\varphi - \varphi_{i-1/2}) H(\varphi_{i+1/2} - \varphi)$$

(section boundaries at $\varphi_{i\pm 1/2} = \ln(R_{i\pm 1/2}/R_0)$)

- Series of truncated, non-overlapping log-normal distributions within fixed particle size sections
- 2 independent PLA parameters (mode size $\varphi_{0,i}$, mode number $n_{0,i}$)

PAM Sea-salt source parameterization Near-Surface Sea Salt Aerosol Size Distribution

PAM Mineral Dust Emission

Physically-based emission scheme (Peng et al., 2012)

Parameterized emission flux depends upon:

- Friction velocity (U_{*}³) above friction velocity threshold
- Emission particle size distributions for 17 different soil types
- Soil properties (roughness length, soil moisture content)

Size distributions of emitted aerosol

PAM Aerosol Nucleation representation

CERN CLOUD (Cosmics Leaving Outdoor Droplets) chamber data

Dunne et al. (2016); Hamish Gordon (Leeds University)

$$\begin{split} J_{b,n} &= k_{b,n}(T) [\mathrm{H}_2 \mathrm{SO}_4]^{p_{b,n}} \\ J_{t,n} &= k_{t,n}(T) f_n \left([\mathrm{NH}_3], [\mathrm{H}_2 \mathrm{SO}_4] \right) \\ J_{b,i} &= k_{b,i}(T) n_- [\mathrm{H}_2 \mathrm{SO}_4]^{p_{b,i}} \\ J_{t,i} &= k_{t,i}(T) n_- f_i \left([\mathrm{NH}_3], [\mathrm{H}_2 \mathrm{SO}_4] \right) \\ J_{org} &= k_{t,org} [\mathrm{BioOxOrg}] [\mathrm{H}_2 \mathrm{SO}_4]^2 \end{split}$$

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PAM Aerosol-Cloud Interactions

- Novel adiabatic cloud parcel model for calculation of cloud droplet number concentration in stratiform (layer) clouds
 - Input: PLA Aerosol size distribution at cloud base and effective updraft velocity above cloud base
 - Model simulates activation of aerosol and condensation of water vapour on cloud droplets
 - Numerically efficient iterative approach
- Cloud droplet number concentration affects optical properties of clouds and conversion of cloud water to precipitation
- Integrated with parameterization of aerosol wet scavenging

PAM Aerosol-radiation interaction

Direct, semi-direct, BC snow-albedo, 1st and 2nd indirect effects included

- New parameterization with size-dependent aerosol optical properties for internally (Maxwell-Garnett mixing rule) and externally mixed types of aerosols. Look-up table generated by Mie code
- Calculates wet size optical properties for aerosols
- Enhancements in absorption of solar radiation by BC when BC is coated (internal mixing with sulphate, organic carbon, liquid water)
- Updated BC refractive index and BC density

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Microscopic image of a tropospheric aerosol particle (Adachi et al., 2010)

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PAM Evaluation Near-Surface Sulfate Concentration

PAM Evaluation Aerosol Optical Depth (550 nm) 2004-2008

- Good overall agreement of CanESM with observations
- Regional biases: Emissions of mineral dust from South America and African biomass burning

Circles: AERONET

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PAM Evaluation: Cloud Droplets Concentration in Low Clouds 2004-2008

PAM Evaluation Mineral Dust Deposition Flux

Secondary Organic Aerosol

• CanESM:

 Condensation of terpene to account for formation of SOA using AEROCOM fields (15% yield = 19 Tg POM/year)

• GEM-MACH:

- SOA yield calculated within model as a function of temperature and existing organic aerosol mass based on a 2-product fit to smog chamber data (Odum et al. 1996). Different emitted precursors considered, based on their function groups, such as aromatics, alkenes and alkanes. Once formed, the SOA is considered non-volatile. The SOA yields are also NOx-dependent.
- Advanced VBS version of SOA model is in progress

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ECCC Aerosol Modeling Systems: Major Gaps

- Two separate dynamics core models and their aerosol sub-models
- No operational global aerosol forecast system
- No regional or global aerosol assimilation system
- No routine GEM-MACH aerosol forecast evaluation with remote sensing data
- No operational interactive prognostic aerosol weather prediction model

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ECCC Aerosol Modeling Coordination: In progress (better focused since January 2018)

- Consolidation of models across ECCC (Unified modeling approach) is ongoing
 - Common dynamical core is expected to be GEM dynamics
 - Common library of physicochemical processes representations

ECCC Working Group on Cooperative AerosoL Modeling (ECCC WG-CALM) Objective: Coordinate aerosol (and its interactions) modeling between weather, air quality and climate groups. Coordinator: Ashu Dastoor

- Aerosol model development for climate simulation (PI: Knut von Salzen)
- Global and regional aerosol model development for air quality simulation (PI: Ashu Dastoor)
- GEM-MACH organic and cloud-phase aerosol chemistry representations (PI: Craig Stroud)
- GEM-MACH Interactive chemistry-aerosol-meteorology simulation (PI: Paul Makar)
- GEM-MACH Fire emissions system (PI: Jack Chen)
- GEM Cloud microphysics representation (PI: Jason Milbrandt)
- GEM-MACH emissions (PI: Mike Moran)
- Radiative transfer (PI: Howard Barker)
- Regional and global aerosol assimilation system (PI: Richard Ménard)
- Remote sensing of atmospheric composition (PI: Chris McLinden)
- and others

Global GEM-MACH aerosol forecasting development in progress

- Implementation of PAM in GEM-MACH for global aerosol forecast (First version expected by Fall 2020)
 - Relatively efficient and accurate 2-moment aerosol dynamics
 - A well-tested aerosol model on global scale and fully coupled with meteorology
 - Nitrate and ammonium species need to be added
 - Comprehensive in-line gas-phase chemistry need to be added
- Model for Simulating Aerosol Interactions and Chemistry(MOSAIC) aerosol model developed at PNNL, Zeveri et al. 2008, JGR, has been implemented in GEM-MACH
 - Two-moment aerosol dynamics
 - Advanced aerosol thermodynamics (i.e., gas-aerosol partitioning)
 - A good test-bed for improving aerosol modeling at various scales
 - Regional and global configurations are being tested
- ECCC seasonal forecast system produces global aerosol forecast with CanESM (bulk aerosol scheme) but needs updating and testing
- Implementation of SAPRC-CS07A gas-phase chemistry (47 species and 140 reactions) (being tested)
 - Advanced organic chemistry
 - More photolysis reactions (HNO₄, PAN, NO₃)
 - Will support improved SOA and heterogeneous chemistry

MOSAIC aerosol model in **GEM-MACH**

Model for Simulating Aerosol Interactions and Chemistry(MOSAIC) - Zaveri et al. JGR 2008

- Sectional two-moment dynamic gas-aerosol mass transfer including Kelvin effect using an efficient Adaptive Step Timesplit Euler Method (ASTEM; Zeveri et al., 2008).
- Size-segregated thermodynamics
 - Activity coefficients are computed by Multicomponent Tyler Expansion Method, shown to be more accurate than widely used Bromley mixing rules and improves estimation of particle pH (MTEM; Zaveri et al. 2005a).
 - The intraparticle solid-liquid phase equilibrium is calculated using a computationally efficient Multicomponent Equilibrium Solver for Aerosols (MESA; Zaveri et al. 2005b).
 - Explicit treatment of Na, Cl, Ca, CO₃, MSA in aerosol thermodynamics. More realistic over oceans and in coastal regions.
 - Better treatment of aerosol water and water hysteresis

New Cloud Microphysics Parameterization -Improved Ice-Phase Microphysics (Milbrandt et al.)

Traditional bulk approach:

Partition Ice phase into representative categories

with prescribed bulk physical properties

• bulk density

mass-diameter (m-D) relations

- shape
- fall speed-diameter (V-D) relations
- etc.

New Cloud Microphysics Scheme: Predicted Particle Properties (P3)

- Freely evolving hydrometeor types and prediction of particle properties (e.g mass-Diameter relations; $m(D) = \alpha D^{\beta}$) for process rate calculations based on conceptual model of particle growth (Heymsfield 1982); 2-moment bulk scheme
- Operational since Sept. 2018
- Supports better treatment of cloud radiative effects
- Implementation of prognostic aerosols for droplet nucleation is in progress

Morrison and Milbrandt (2015), Morrison et al. (2015), Milbrandt and Morrison (2016)

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P3 Evaluation: Example

Full resolution version (3400x1700 pixels - 220k

Model Reflectivity (P3 – 1 ice category)

da

Radar Observations (1 km CAPPI)

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ECCC Operational Air Quality Analysis O₃, NO₂, SO₂, PM_{2.5}, PM₁₀ and Air Quality Health Index (AQHI) each hour

Experimental since 2002, operational since Feb 2013

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Environme Robichaud et al. 2016, Robichaud and Ménard 2014

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ECCC Regional Air Quality Assimilation System (based on GEM-MACH)

- Issues with current ECCC operational air quality analysis
 - Only surface observations
 - Isotropic correlation model
 - Variances in observation space
 - Independent PM2.5 and PM10 analysis
 - No assimilation cycle
- ECCC new air quality analysis (operational implementation in fall 2019)
 - Climatological correlations
 - Model error variances in model space
 - Joint PM2.5 and PM10 aerosol analysis
 - New validation process
- Regional chemical assimilation cycle (first version in 2020)
 - likely using (a variant of) the 4DEnVar scheme used for meteorology assimilation cycle
- Global/Regional assimilation of satellite observations is expected in 2020-2021

New air quality analysis The Gain K containscorrelations and variances (Ménard and Deshaies-Jacques 2018a &b)

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 $\mathbf{K} \sim \frac{\langle \varepsilon_b \varepsilon_b \rangle}{\langle \varepsilon_b \varepsilon_b \rangle + \langle \varepsilon_o \varepsilon_o \rangle}$ $\mathbf{K} = \mathbf{B} \mathbf{H}^{\mathrm{T}} (\mathbf{H} \mathbf{B} \mathbf{H}^{\mathrm{T}} + \mathbf{R})^{-1}$

From information on

- Model error in model space ε_b , and observation space ε_b
- Observation error, ε_ο

We estimate or model

- Variances σ_b^2 , σ_b^2 , σ_o^2
 - Statistical weight
- Correlation
 - Propagates information

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Aerosol Speciation

Building a 3D IC for GEM-MACH

- Speciated increment for both exclusive bins (Txx1, Txx2)
- Increment vertical projection or sequential analysis

-4

-6

0.8

0.4

0.1

Evaluation of analysis by cross-validation

3 sets of spatially random distributed observations O_1 , O_2 and O_3 are used (Ménard and Deshaies-Jacques 2018a &b)

Thank you for inviting!

- ICAP team experience is valuable to ECCC aerosol prediction system development!
- We hope to contribute to ICAP-MME in near future!

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