Linking Air Quality and Watershed Models

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ENVIRON

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- Trent University
- U.S. EPA

Integrated Environmental Modelling

ENVIRON

Cumulative Effects Management (CEM)

From the perspective of an air quality modeller

Air Quality Modelling

Water, Land and Biodiversity Modelling

Old Paradigm

Modellers operate in isolated spheres of expertise

New Paradigm

Two-way communication between modellers

Synergize modelling efforts and models where possible

Potential Needs Filled by Air Quality Models in an Integrated Modelling Approach

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- Supplement measurement networks that are sparse in temporal and spatial extent and chemical composition
- Provide dry and wet deposition to aquatic and terrestrial models for critical loads exceedance and other impacts
  - Acid deposition
  - Nutrient deposition
  - Mercury and other air toxics deposition
- Source attribution – Current contributions of sources and effect of changes in air emissions on ecosystems
- Ambient air concentrations for vegetation and human exposure studies
  - Ozone
  - PM
  - Hazardous air pollutants
- Data for socio-economic cost/benefit models
  - PM etc.

Air Quality Models

- **Global 3-D:** GRAHM, GEOS-Chem, MOZART etc.
- **Regional 3-D**: AURAMS, CMAQ, CAMx, RELAD etc.
- **Local puff/plume:** CALPUFF, AERMOD, SCICHEM etc.
- **Local/regional plume-in-grid:** CMAQ-APT, CAMx-PiG

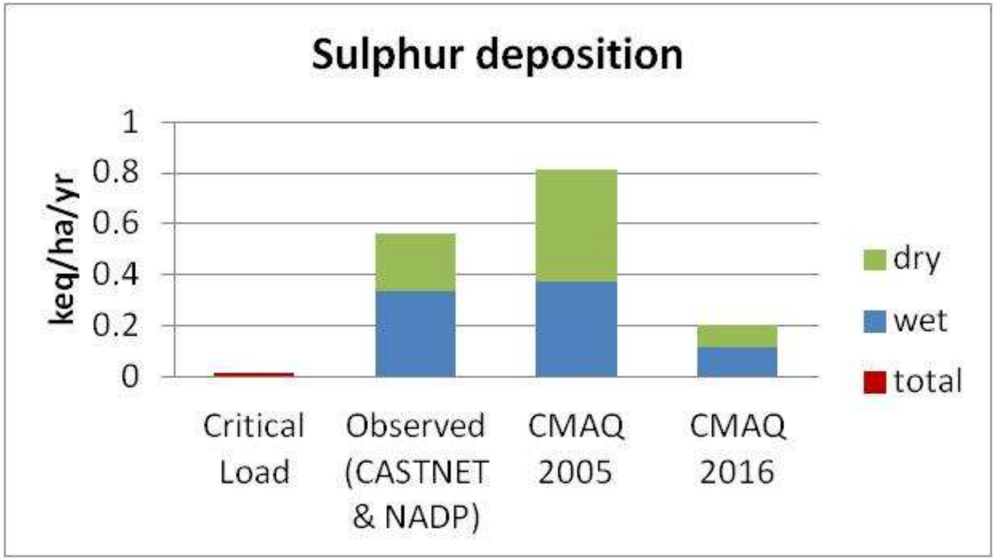
- Focus here on deposition modelled by CMAQ and its potential role in integrated modelling systems

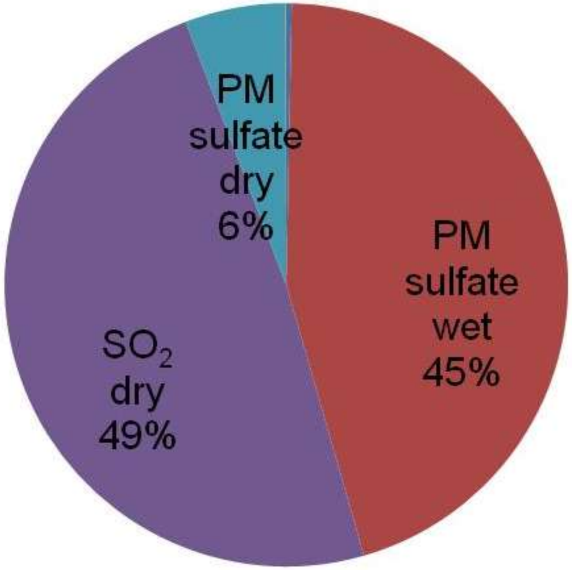
  CMAQ
  - Applied by Alberta ESRD and CEMA
  - Advanced multi-pollutant 3-D photochemical model
  - Developed by U.S. EPA with regular scientific updates from the community
  - Emissions from natural and anthropogenic sources, dispersion, chemical and physical transformations, dry and wet deposition of gases and particulate matter
  - Ozone, PM, acid deposition of N and S compounds, mercury and other air toxics
  - Base cations are modelled but emission inventories are uncertain

Sulphur Deposition in CMAQ

- Sulphur dioxide (SO_2)
- Particulate sulphate ($SO_4^{=}$)
- Sulphuric acid (gaseous H_2SO_4 quickly condenses on to PM sulphate)

Example of application to identify critical load exceedances of surface water acidity: Sulphur deposition at Shenandoah National Park in Virginia





Total = 0.8 keq/ha/yr in 2005
For comparison, levels in Alberta range approximately from 0.01 to >1 keq/ha/yr

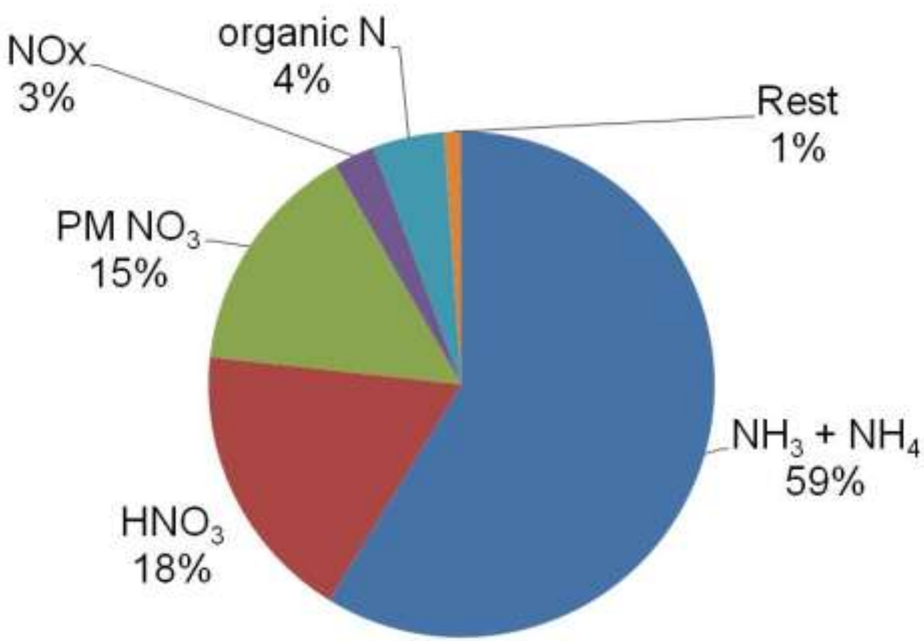
Source: Vijayaraghavan et al., 2012

Acknowledgement: U.S. EPA

Nitrogen Deposition in CMAQ

- NOx (NO, NO_2)
- Inorganic oxidized Nitrogen (HNO_3, N_2O_5, HONO, HNO_4, PM NO_3)
- Reduced Nitrogen (NH_3, PM NH_4^+)
- Organic Nitrogen (PAN, PANX, NTR)

Example: Components of nitrogen deposition at Shenandoah National Park



Total = 1.3 keq/ha/yr in 2005

Large fraction from NH_3 and NH_4

Potential in Alberta too

Source: Vijayaraghavan et al., 2012

Role of Ammonia/Ammonium Deposition

- Deposition of PM sulphate and nitrate associated with ammonium
- Reduced nitrogen itself can be a large fraction of total deposition
  - Gaseous ammonia dry deposition (wet smaller)
  - Particulate ammonium wet and dry deposition
- Eutrophication
- Acidification
  - Simpler air quality models assume constant ammonia concentrations and consider acidification due to only sulphate and nitrate
  - However, ammonia nitrification → acidification
- Alberta has one of the largest ammonia emissions inventories in Canada - large livestock population and fertilizer application
- Potential emissions from tailings, forest fires etc.
- Forest Service has measured high NH_3 (> 1 ug/m3) in remote areas in AB
- Air quality models used in integrated modelling in Alberta need to accurately characterize ammonia air concentrations and deposition

Deposition and Exceedances of Critical Loads (CL) of Surface Water Acidity

- Unlike sulphur, some of the deposited nitrogen is retained in the terrestrial system and does not contribute to acidification.
- Potential acid input = S deposited + N deposited – N retained – BC
- CL of waters already includes BC. Methods for calculating exceedance:
  - EPA: Use measurements in surface streams to estimate net N loading to water

    Exceedance = S deposition + Measured N – Critical Load

    Cannot be applied for source attribution because modelled N is not used

  - Assessments in the oil sands region assume that 25% of the nitrogen compounds are acidifying when the N deposition is < 10 kg N/ha/yr

    Exceedance = Pre-development (loading estimated from measured S and N) + Post-development (modelled S dep + modelled N dep x retention factor) – Critical Load

    Simple approach for post-development but may be applied in emissions scenarios

  - Alternative advanced approach

    Apply mechanistic watershed model to estimate terrestrial retention of deposition from air quality model. Laborious but ideal for source attribution.

    Exceedance = S dep + Modelled N calibrated using measured N – Critical Load

Mercury Deposition

- Potential for dry deposition and wet deposition in rain and snow in Alberta

- Gaseous elemental mercury (HG)
  - negligible wet but undergoes dry deposition (bidirectional like NH3)

  Gaseous oxidized mercury (HGIIGAS)

  Substantial wet and dry deposition

  Particulate-bound mercury (PHG)
  - Intermediate wet and dry deposition

- Mercury deposition → Risk due to methyl mercury in fish and wildlife ?
  - Advanced Hg watershed/biocycling model, e.g., D-MCM or WARMF
  - Simpler approach - Human health risk assessment model such as HHRAP
  - Simplest approach – assume linearity

Examples of Air-Watershed Linkages

U.S. EPA's Watershed Deposition Tool

Schwede et al., 2009

- GIS-based tool that maps gridded deposition estimates from CMAQ to 8-digit hydrologic unit codes within a watershed or region.

- Deposition components:

  Total Nitrogen – Dry and Wet; Oxidized and Reduced
  Total Sulphur – Dry and Wet
  Total Mercury – Dry and Wet

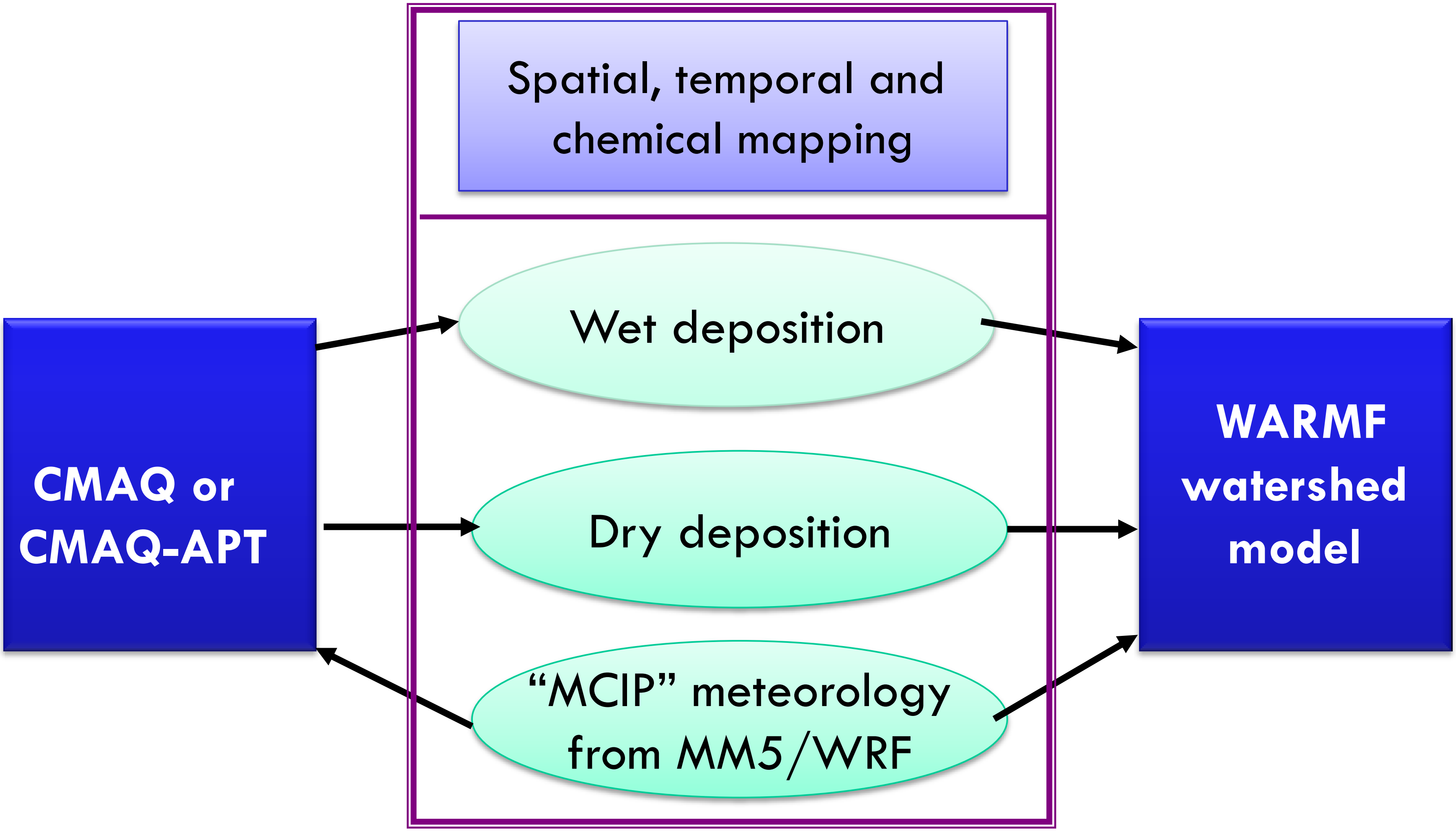
- Calculate the weighted average deposition over a HUC and the average change in a HUC between two different emission scenarios

- Advantage: Simple to use
  Disadvantage: Cannot use the deposition values to model within a watershed as values are averaged over watersheds

Examples of Air-Watershed Model Linkages

Linkage between CMAQ & WARMF and CMAQ-APT & WARMF

Herr et al., 2010; Vijayaraghavan et al., 2010



Acknowledgement: Systech Water Resources

CMAQ-WARMF Linkage
Application in Catawba River Basin, USA

Spatial Mapping

CMAQ-APT domain

Southeastern USA

Rectangular grid:

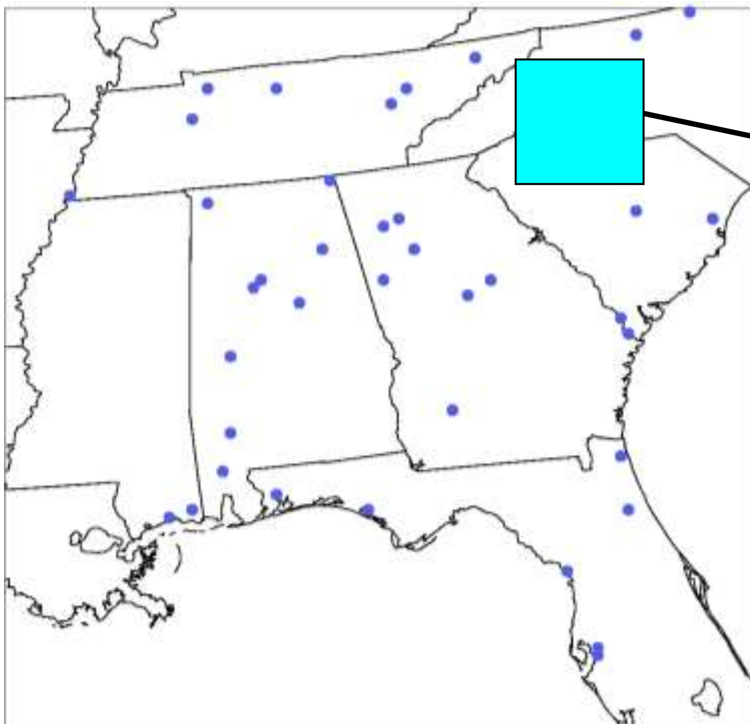
12 or 4 km resolution

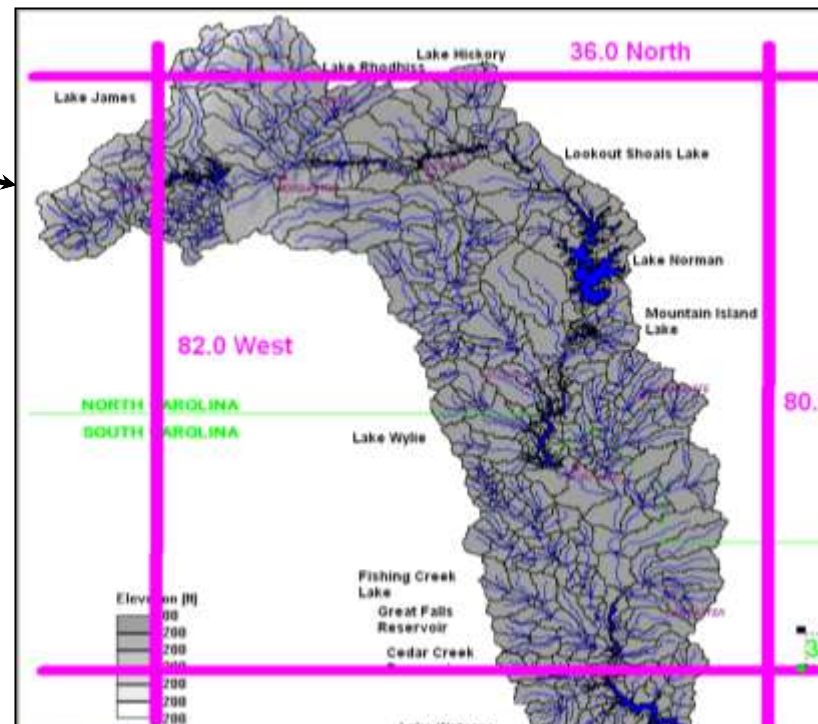
WARMF domain

Catawba watershed

Irregular catchments/ reservoirs

~ 1 km^2 and larger





CMAQ-WARMF Linkage
Temporal Resolution and Extent

- Temporal Resolution:

  CMAQ hourly temporal resolution → Daily totals for WARMF

  Match time zones
- Temporal extent:

  CMAQ 1-5 years → 50-100+ years for WARMF

  Important to model multiple years with air quality model to account for inter-annual variability in meteorology (e.g., precipitation)

  Model climatologically normal or “dry, wet and normal” years

  Communication important among modellers on extrapolating the AQ model deposition to the time period of the watershed model
- Important to identify key historical and planned future changes in emissions to get proper time record in the watershed model

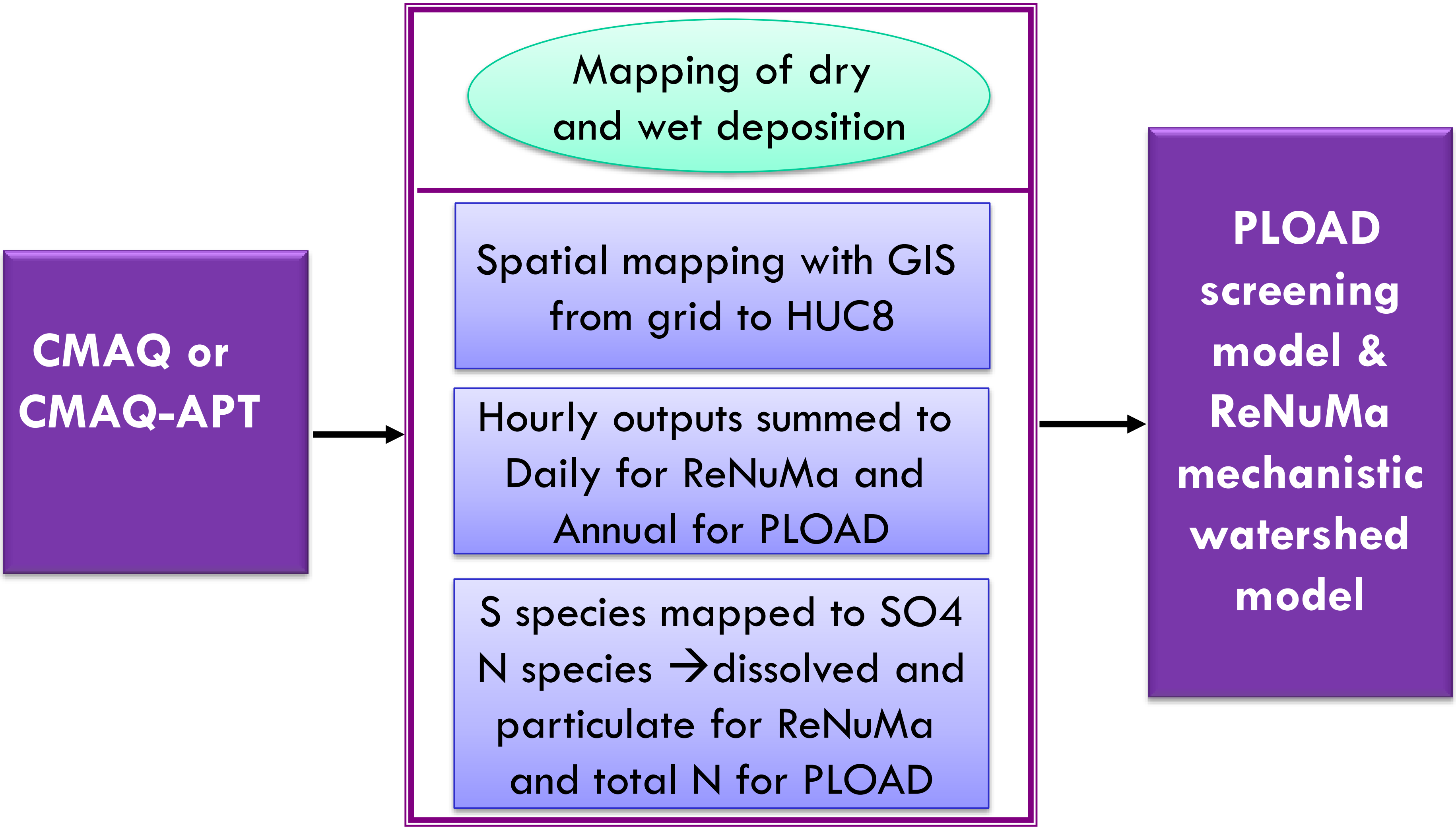
CMAQ-WARMF Linkage
Chemical Species Mapping

WARMF species	Mapping from CMAQ species	Notes
SOX	SO2	as S
SO4	PM SO4	as S
NOX	NO + NO2	as NO2
NO3	Total NOz	Oxidized N other than NOx (as N)
NH4	NH3 + PM NH4	as N
CA, MG, K	Ca, Mg, K are not commonly modelled	Interpolate from NADP data
NA, CL	Use PM Na and Cl (however concentrations uncertain)	Interpolate from NADP data
HG0, HG2	HG, HGIIGAS	
HGP	PM Hg	

Examples of Air-Watershed Model Linkages

Linkage between CMAQ & PLOAD and CMAQ & ReNuMa

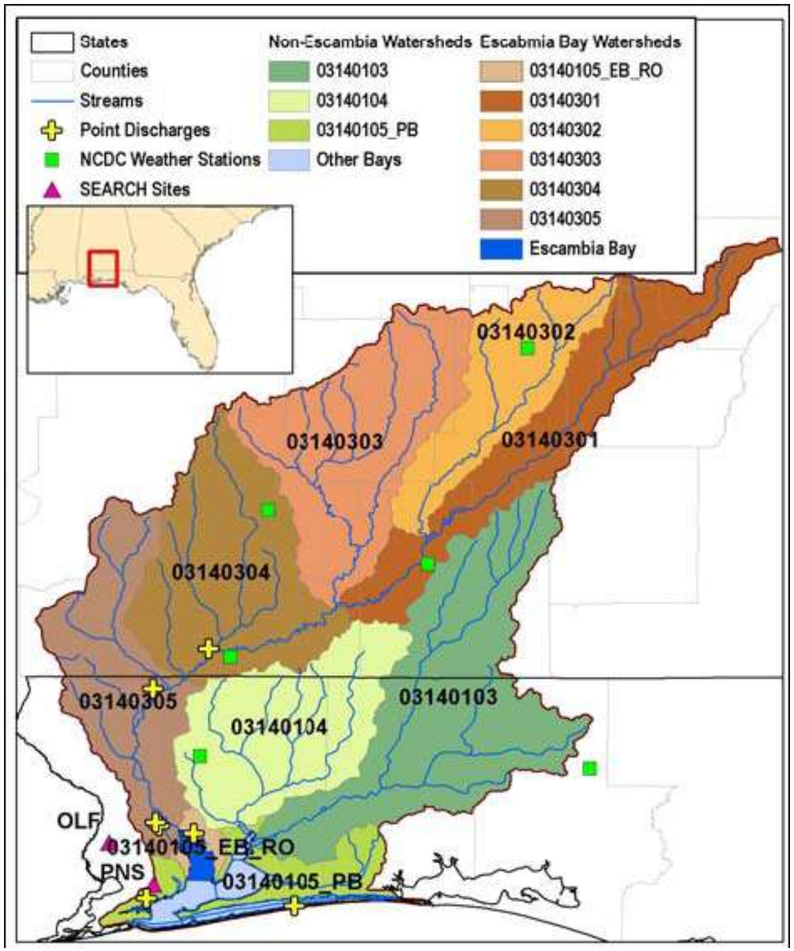
Brandmeyer et al., 2007; Vijayaraghavan et al., 2010b



Acknowledgement: RTI International

Linkage between CMAQ & PLOAD and CMAQ & ReNuMa

Escambia Bay and Watershed in Alabama/Florida



1. Increase in NH_3 dry deposition after SO_2 and NOx reductions at local power plant and regionally → Dis-benefit

Change in NOy deposition (tons/yr N)	Change in NHx deposition (tons/yr N)	Change in Total N deposition (tons/yr N)
-2571	838	-1733

2. Calculated that approximately 10-18% of N deposition to the watershed reaches the Bay after terrestrial retention

Source: Brandmeyer et al., 2007; Vijayaraghavan et al., 2010b

Example of Air-Water Model Linkage

Proposed Work

- Link CMAQ deposition outputs to MAGIC model

- MAGIC: dynamic hydrogeochemical model of water acidification

- MAGIC Inputs:
  - Precipitation
  - Wet and Dry deposition of SO4, Cl, NO3, NH4, Ca, Mg, Na, K
  - MAGIC conventionally uses measured wet deposition and scales those to estimate dry deposition

- Use CMAQ to supplement measurements by providing wet and dry deposition at selected receptor locations: average deposition over each of the catchments modelled in MAGIC

- Important to select appropriate CMAQ emissions scenarios, i.e., identify when and where deposition changes due to changes in emissions (e.g., mines coming online) to specify historical and future break-points in MAGIC

Inconsistencies in Inputs of Different Model Components of an Integrated Modelling System

- **Precipitation**

  Problem

  Hydrology in water model driven by measurements

  Wet deposition in air model driven by modelled precipitation or modelled + measured precipitation

  Partial solution

  Scale wet deposition from air model by measured precipitation before handover to water model

- **Land use**

  Problem: Land use used to simulate dry and wet deposition in the air model often different from the land use in the land/water model

  Partial solution: Keep track of deposition in air model by land use type within a grid cell and handover to land/water model

Summary

- Frequent interactions between modellers in different disciplines are important for efficient integrated modelling efforts
- Advanced air quality models such as CMAQ can serve multiple needs for cumulative effects management
- Nitrogen species have different deposition characteristics and need to be modelled separately. In particular, important to model the impact of reduced nitrogen in Alberta
- Several approaches have been reported for linking air and watershed models
- Integrated models should resolve spatial, temporal and chemical differences in model configuration and inconsistencies in model inputs