An Approach to an Unified Process-Based Regional Emission Flux Modeling Platform

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Unified Process-Based Regional Emission Flux Model

- Background – how we arrived at the current status
- Need for a unified process-based emission model
- Description of an unified emission model approach

Background – the Current Status

- Originally, emission inventories contained annual estimates of all known emission types
- The need to reflect episodic events brought air quality modeling with hourly time steps
- The first approach was to disaggregate or “temporally allocate” annual data to hourly intervals using source-category specific profiles
- Realization came that emissions dependent on environmental variables can be modeled more realistically with process-based algorithms
- Limited by knowledge of processes and availability of input data

Background – Process-based emission models

- Initial process-based emission models focused on the larger sources – mobile sources and biogenic emissions
- These “one-directional” emission models use:
  - Meteorological data from a regional model (MM5), e.g. temperature, radiation, humidity
  - Emission factors approximating processes (e. g. species-specific factors for biogenics, classes of vehicles for mobile sources)
  - “Activity data” – e.g. vegetation land cover for biogenics, miles traveled for mobile sources

Current Needs for Process-Based Emission Models

- Current air quality modeling results indicate inaccuracies in emission inventory estimates for environmentally-influenced emission sources. This highlights the need for process-based models, e.g.,
  - Blowing dust (from land surfaces, unpaved roads, construction, and agricultural tilling)
  - Fires (wild fires and prescribed burning)
  - Ammonia (initially by modulating inventory values with meteorology data – later by bi-directional flux modeling
  - Pesticides (uses soils, meteorology, and vegetation data)

Current Needs for Process-Based Emission Models (2)

- Sea salt and chlorides (important to particulate matter chemistry – being addressed in a developmental version of CMAQ)
- Mercury (currently addressed in a developmental version of CMAQ)

Merging of Emission Data

- Merging of process-based emission data and inventory-based data accomplished by emission processor, e.g. SMOKE
  - Annual inventory data allocated to hourly intervals
  - Emission data assigned to a modeling grid by coordinate or by using spatial surrogate data representing location of the emission sources
  - Emission species “speciated” or assigned to the lumped species used by the chemical mechanism being used in CMAQ

Unified Approach

Current biogenic and mobile source emission models are coupled to SMOKE for operational efficiency. Adding several other parallel models may:

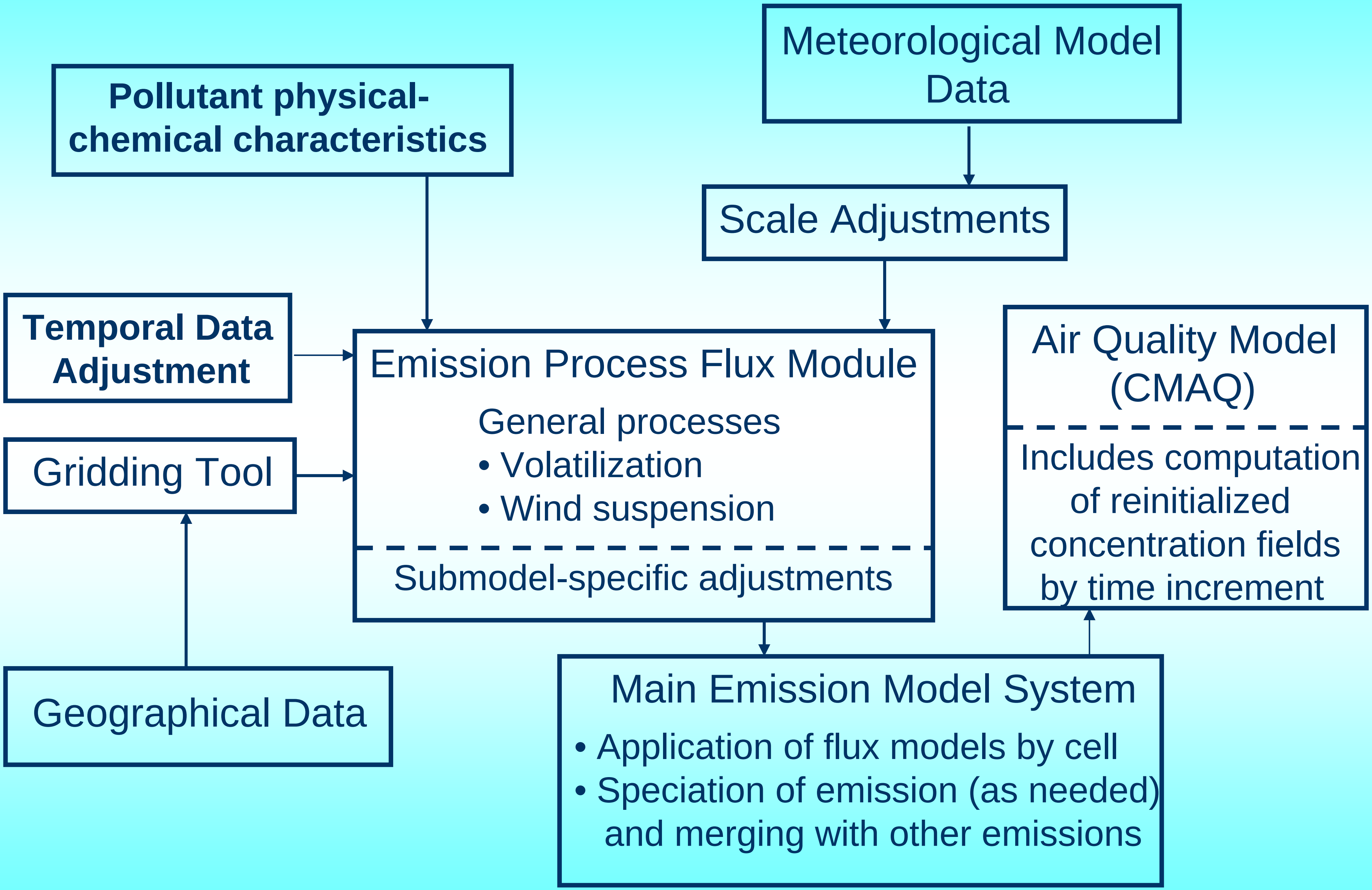
- impede computational efficiency
- permit inconsistencies in like data, grid definitions and computations between emission models
- Complicates consistent of data input for models using similar data
- Complicates maintaining consistency between emission models needed reinitialization of modeled emission fields at time intervals

Unified Approach (2)

The proposed unified structure consists of:

- A suite of tools for spatial gridding and temporal adjustments of input data
- A general emission flux model module computing processes held in common by several models, e.g. volatilization and wind suspension
- An extensible suite of compound or source-specific sub-models for processes not held in common
- Additional sub-modules or algorithms could be added to each general component as knowledge is gained
- Modeling results go to SMOKE for speciation and merging with other (inventory-based) emissions before being supplied to CMAQ

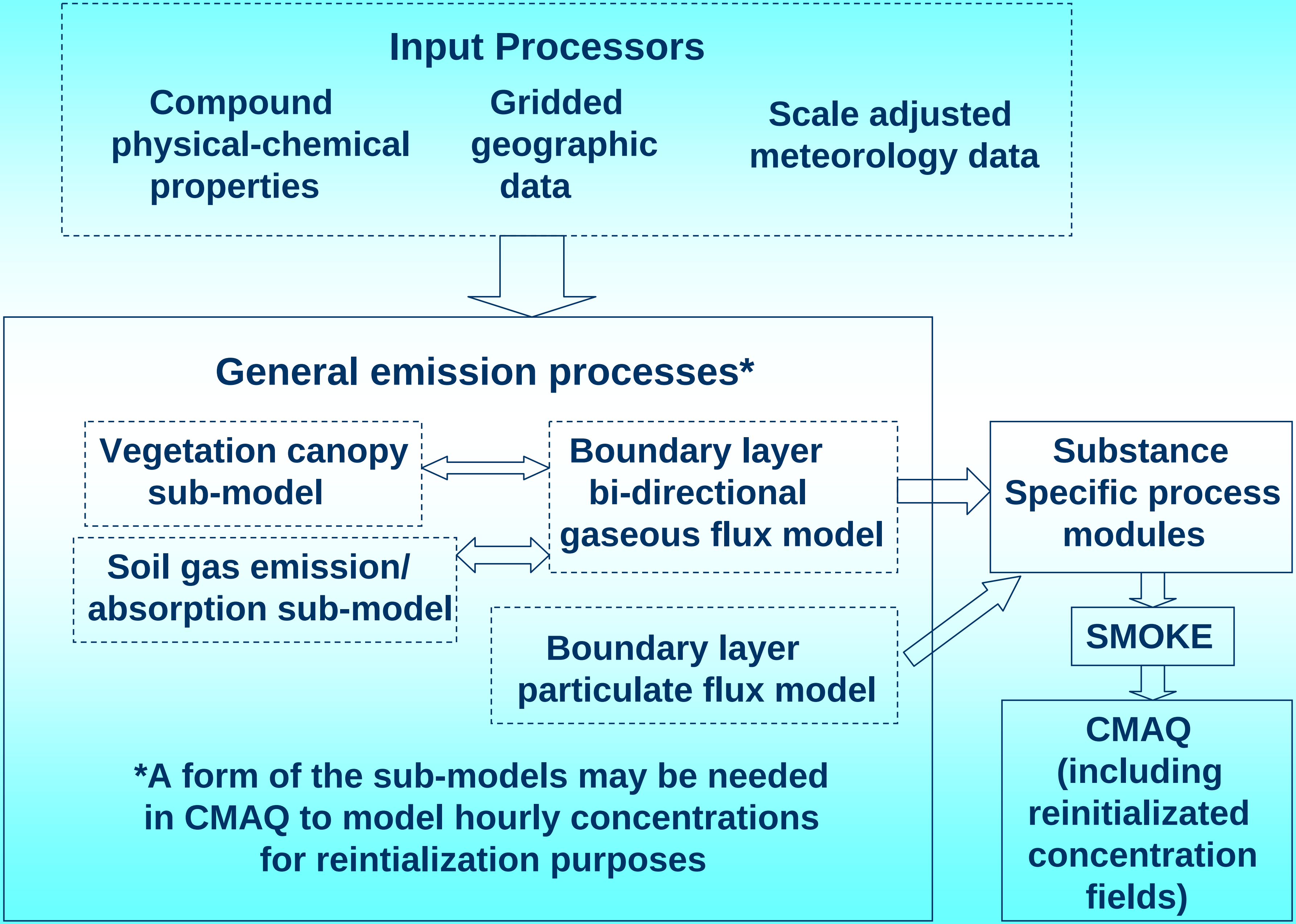
Unified Emission Modeling Functional Schematic



Unified Approach (3)

- Computations of volatilization in the common model requires sub-models for, at a minimum:
  - Vegetation canopy effect on emission flux
  - Soil-air and water interface, including water vapor flux
- For some emission models (e.g., ammonia, pesticides) sub-models will link to boundary layer models to compute initial bi-directional fluxes. The time interval updates of bi-directional fluxes may best be done in CMAQ.

Emission process module



Substance-Specific Process Examples (Sub-modules by Substance or Source)

Several algorithms are under development to address substance or source-specific processes and adjustments. These may be placed in the emission model module and/or CMAQ as computationally most efficient.

Examples include:

- Emission tools and one-way fluxes
  - Biogenic plant species-specific modeling
  - Computations for fuel loading, tree species, and prior fires for wild fire emission modeling
  - Adjustments for application, seasonality, and crop type for emissions from pesticides and nitrogen fertilizer use

Substance Specific Process Examples (2) (Sub-modules by substance)

- **Bi-directional flux related computations, such as:**
  - **Ammonia compensation points**
  - **Semi-volatile phase changes**
  - **Chlorine and sea salt chemistry**

What is Needed to Implement?

- Collaboration between process model developers in design of a common emission process module
- A design suited for easy modification and/or addition of supplemental process modules over time
- Collaboration in design of unified model support tools – many may be adapted from existing tools
- Bi-directional aspects will require close collaboration with air quality model developments