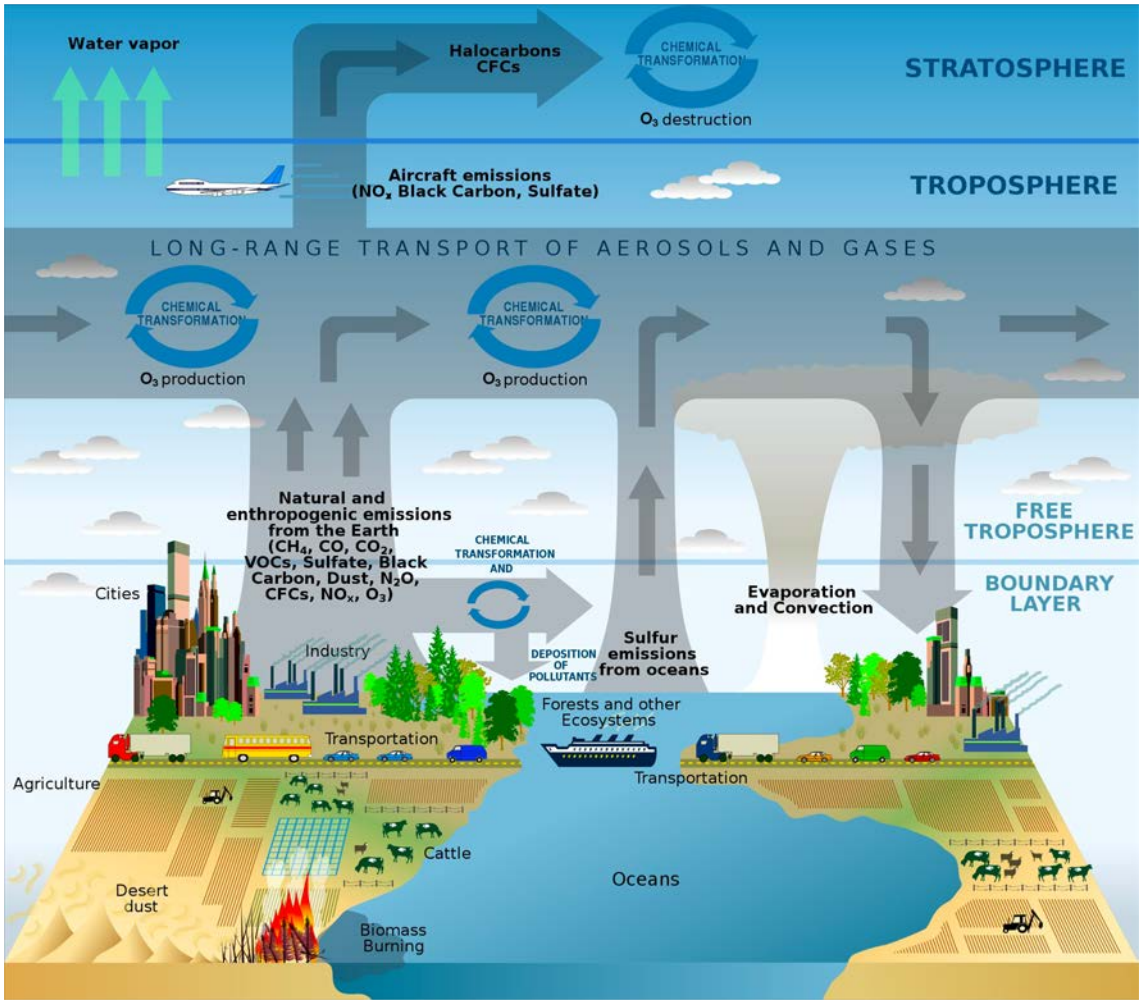
Modelling the Chemistry of the Atmosphere



Nairobi Air Quality Workshop

Eloise Marais, University of Leicester, UK (eloise.marais@le.ac.uk)

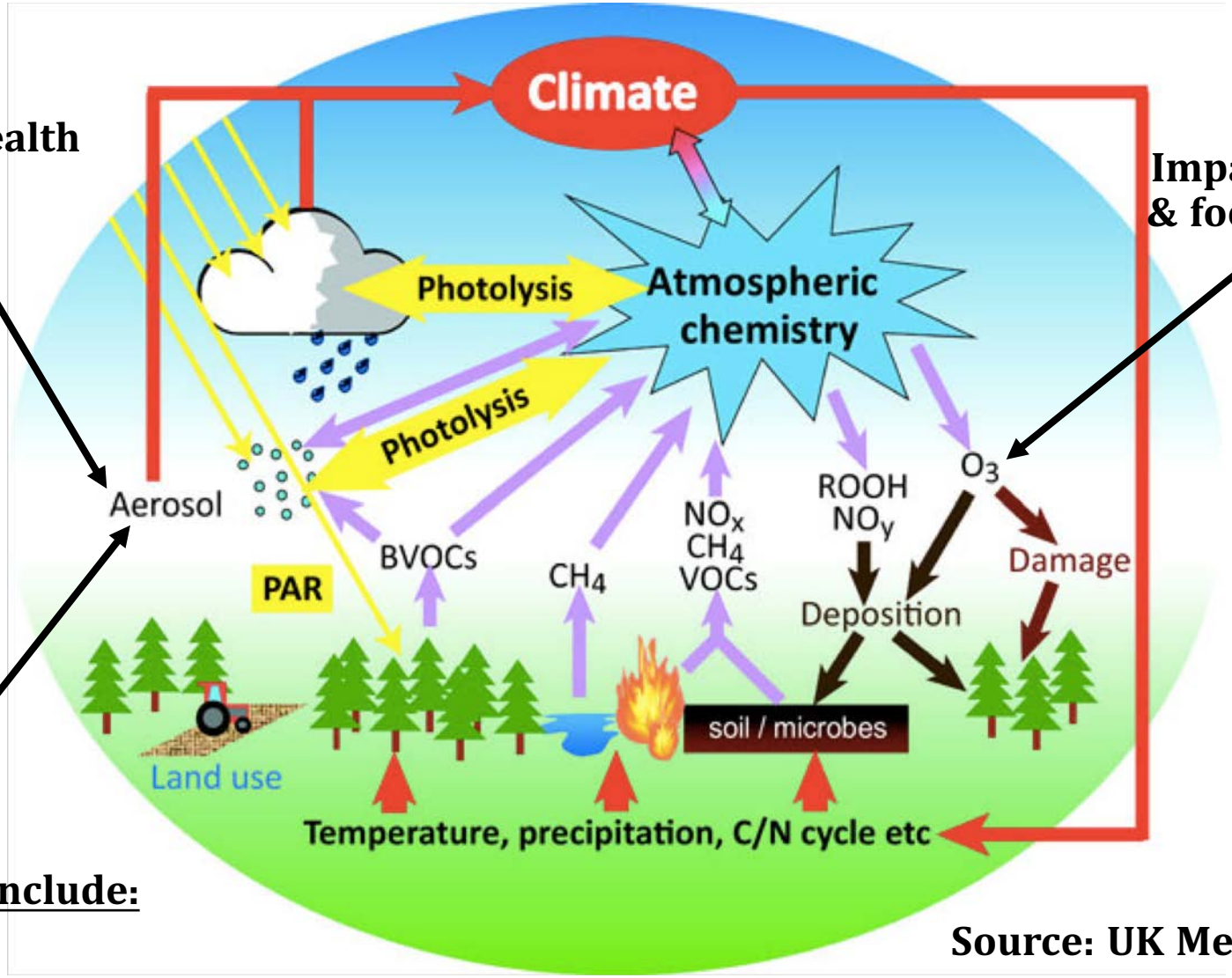
My Expectations of the Workshop

Meet new people

Help in some way to develop your research skills

Empower female scientists

Chemistry of the Atmosphere



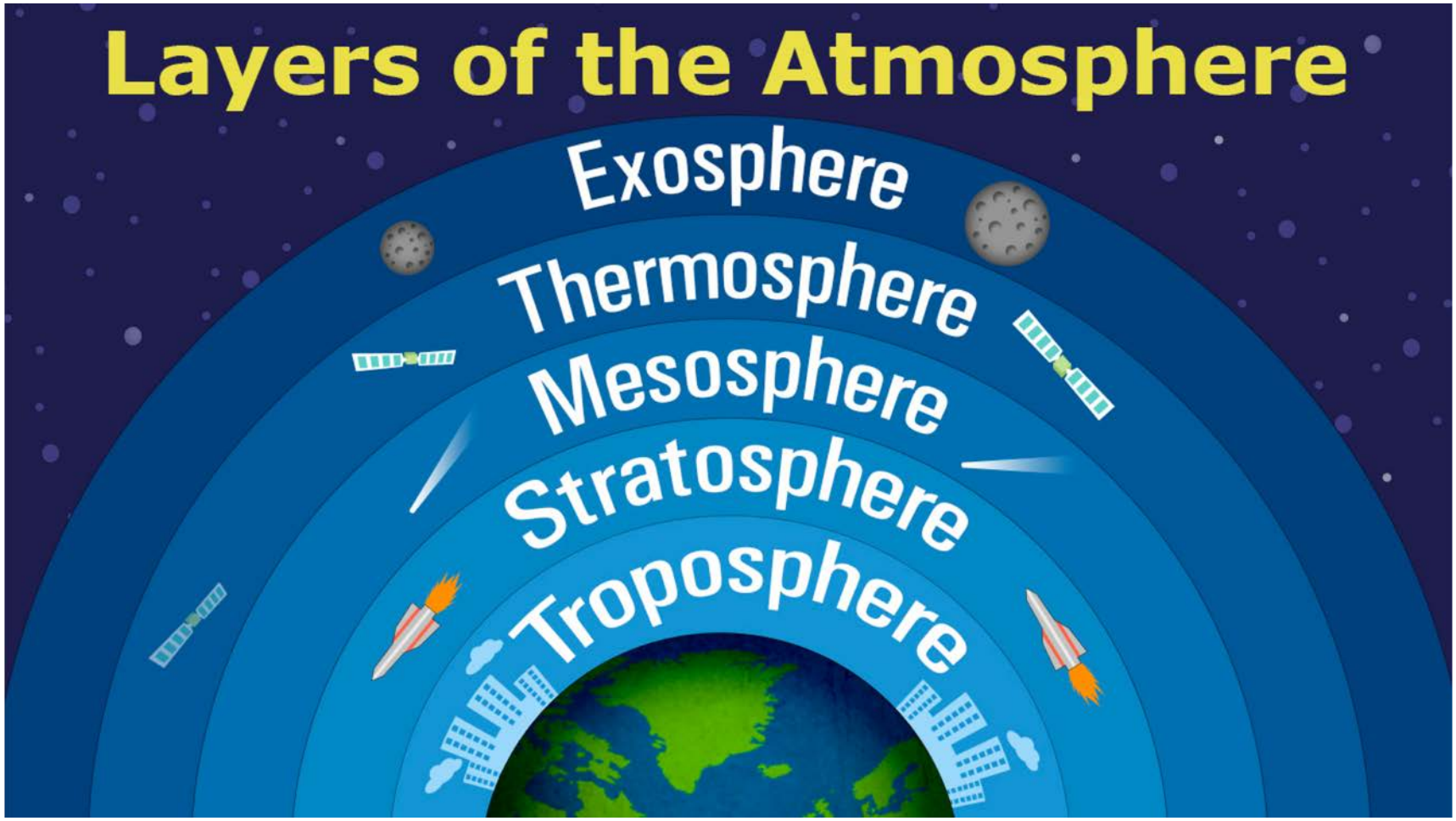
Impacts health

Impacts health & food security

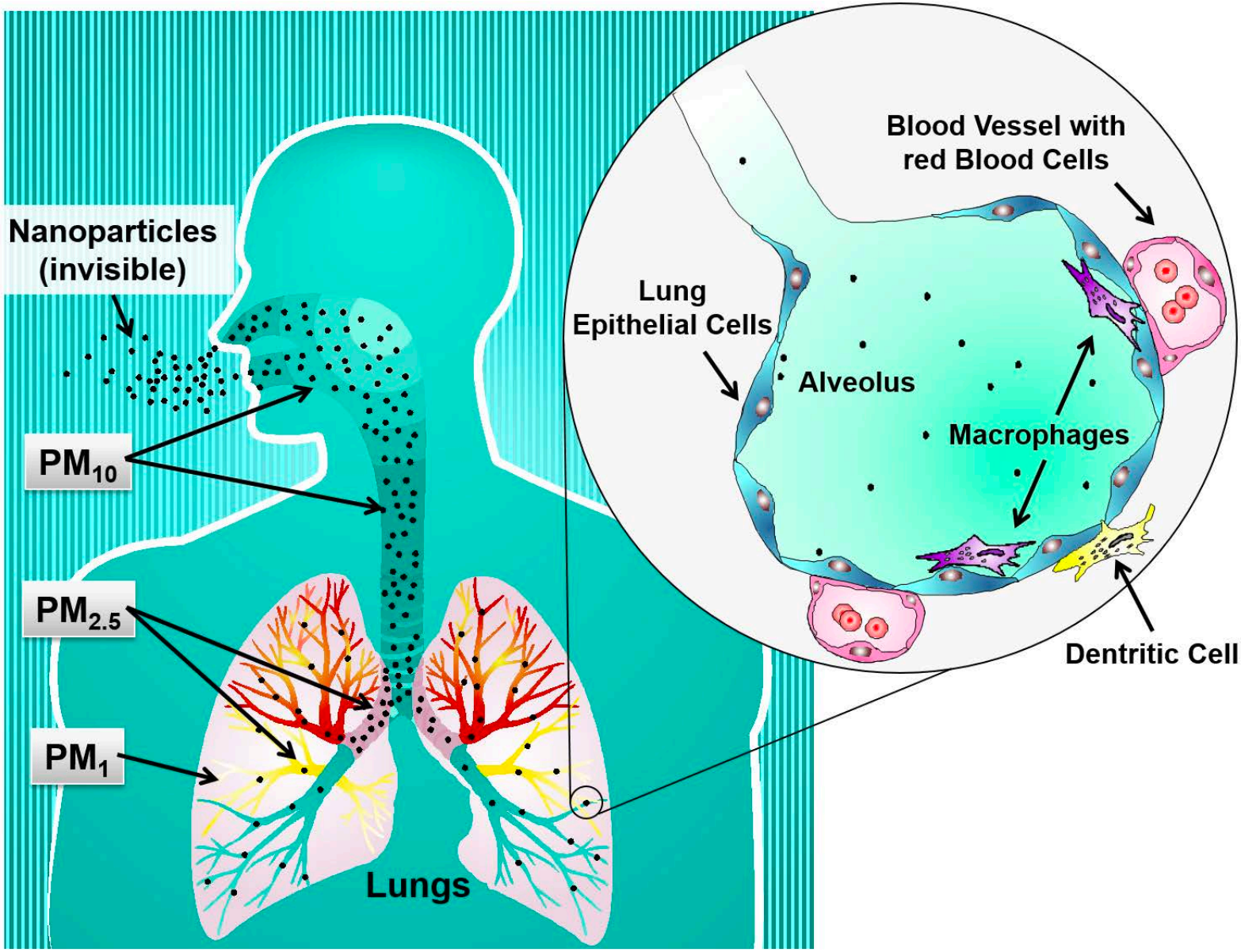
Aerosols include:
Sulfate
Nitrate
Ammonium
Organics
Black Carbon

Source: UK Met Office

Layers in the Atmosphere

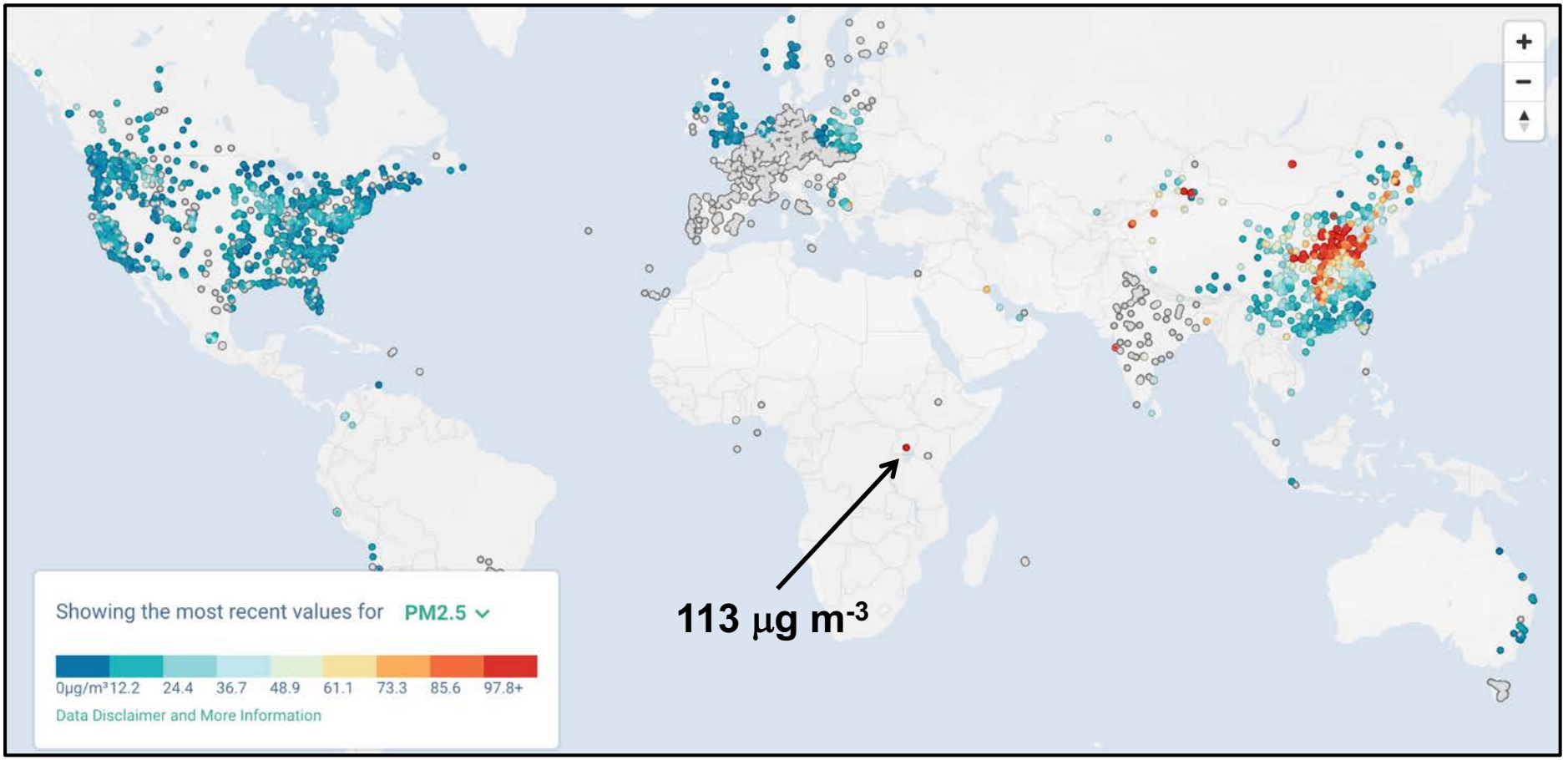


$PM_{2.5}$



[Kung and Wick, 2011]

Surface Observations of $PM_{2.5}$

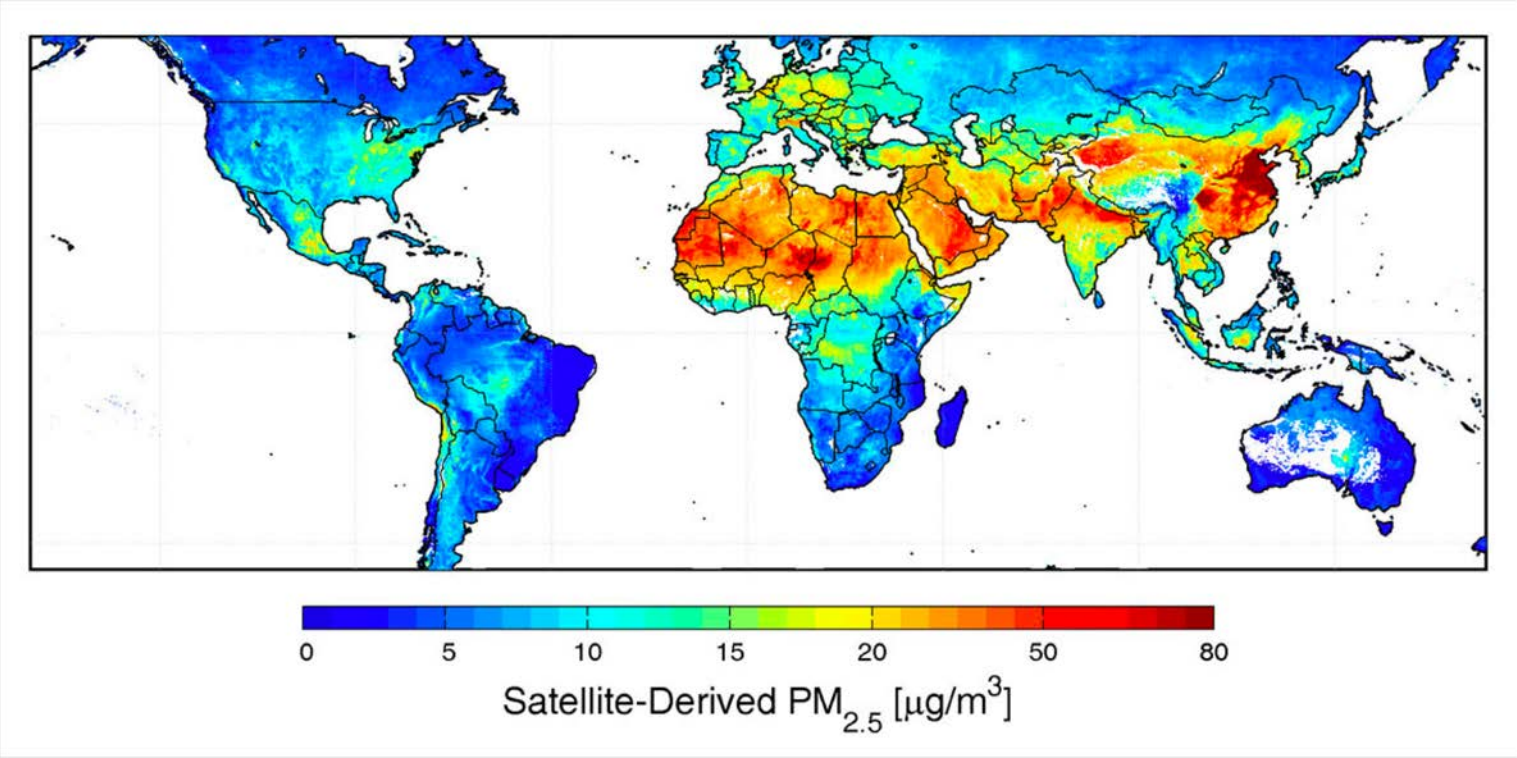


[OpenAQ, Accessed today (11 Feb 2019)]

Only a few locations have extensive coverage

Satellite Products of $PM_{2.5}$

Full global coverage



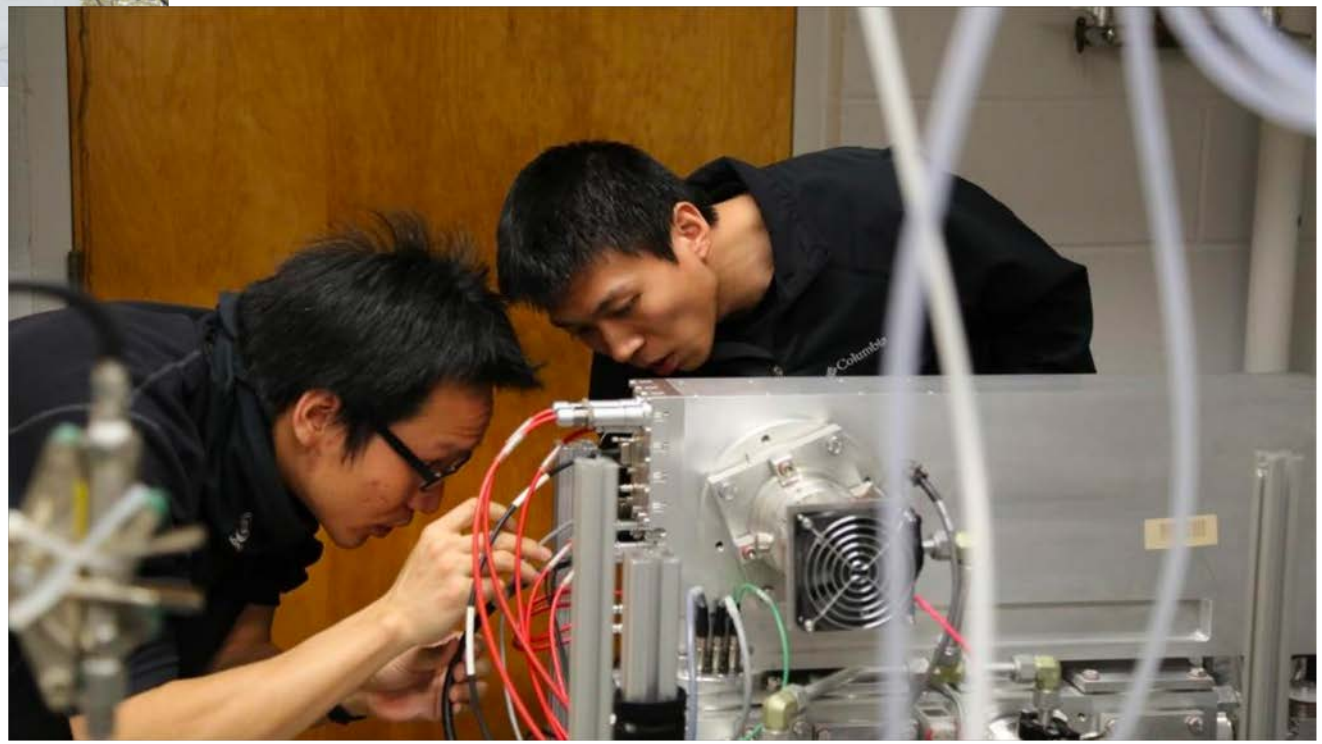
[van Donkelaar et al., 2010]

Derived. Not an actual measurement.

Only see the same location on Earth once per day (*if there are no clouds*)

Atmospheric Chemistry Transport Models

Informed by Measurements



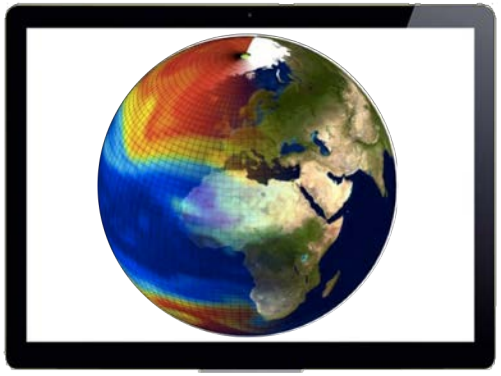
Atmospheric chemical transport models

INPUT

Emissions
(volcanoes, ocean, birds, trees, cars, industry, wood burning, fossil fuel etc.)

Meteorology
(offline, i.e. not calculated)

GEOS-Chem



Detailed chemistry
Deposition

OUTPUT

3D global concentrations of atmospheric components

Would use an atmospheric chemistry transport model (or CTM)?

What is the surface concentration of ozone in Tanzania?

Contribution of desertification to drought in Kenya.

Human health effect of cars and motorcycles in Nairobi.

Shift in the ITCZ due to desertification in the Sahel.

Climate change impact of aerosols from intense seasonal fires in Africa.

Atmospheric chemical transport model infrastructure

Code: Fortran (historical, but also efficient for solving mathematical equations)

Input/output: mix of binary punch and NetCDF files (intention is to be 100% NetCDF)

Compile: a few minutes

Run time: depends on model version. Walltime is ~10-12 hours for 1 month (1 NODE, 8 CPUs)

Not very computationally demanding, but requires lots of space for input/output

Track version history: git

Debug: Totalview

Visualization software: IDL (costly), Python (free), NCAR Common Language or NCL (free), R (free).

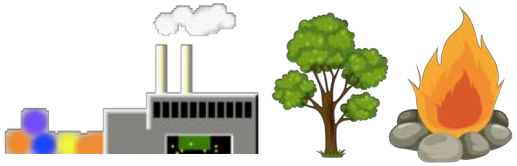
Global Access to GEOS-Chem: https://cloud-gc.readthedocs.io/en/latest/

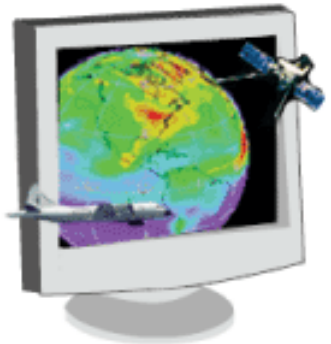
GEOS-Chem: The Model I Use

GEOS-Chem

GEOS-Chem

Emissions (natural/human)





Offline assimilated meteorology (NASA GMAO)

Chemistry
Transport
Dry/wet deposition

3D global/regional atmospheric concentrations

What the model looks like

Header of the main.F file that links everything in the model together

main.F - emacs@spectre14.cm.cluster

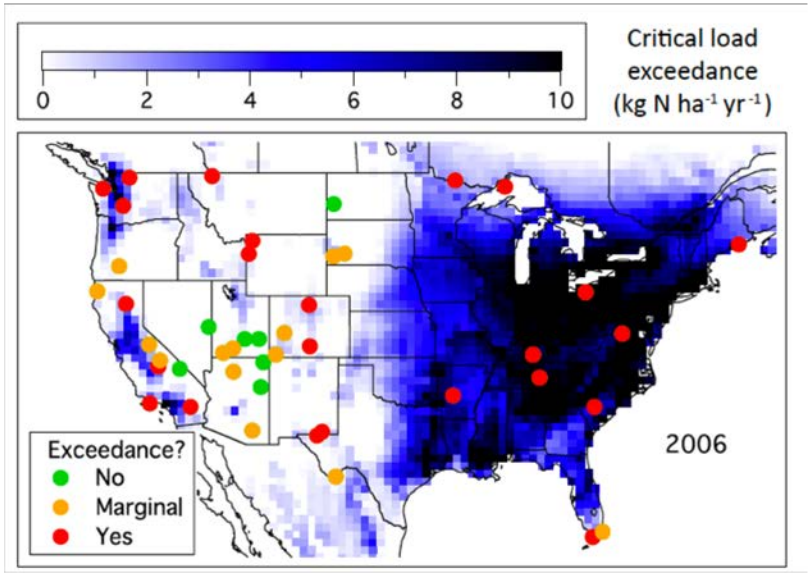
File Edit Options Buffers Tools Fortran Help

```
!EOC
!------------------------------------------------------------------------------
!                  GEOS-Chem Global Chemical Transport Model                   !
!------------------------------------------------------------------------------
!BOP
!
! !MODULE: main.F
!
! !DESCRIPTION: Program GEOS\_CHEM is the main level driver program for the
!  GEOS-Chem model of atmospheric chemistry and composition.
!\\
!\\
! !INTERFACE:
!
      PROGRAM GEOS_Chem
!
! !USES:
!
      !-----------------------------------------------------------------
      ! Parameters to define floating-point variables
      !-----------------------------------------------------------------
      USE PRECISION_MOD,    ONLY : fpp => fp  ! Flexible precision
      USE PRECISION_MOD,    ONLY : f4         ! 4-byte floating point
      USE PRECISION_MOD,    ONLY : f8         ! 8-byte floating point

      !-----------------------------------------------------------------
      ! Basic GEOS-Chem modules
      !-----------------------------------------------------------------
      USE CMN_SIZE_MOD           ! Size parameters
      USE DiagList_Mod           ! Derived type for diagnostics list
      USE Diagnostics_Mod        ! Set select netcdf diagnostics
      USE ErrCode_Mod            ! Error codes for success or failure
      USE ERROR_MOD              ! For error checking
      USE FILE_MOD               ! For file I/O
      USE GEOS_TIMERS_MOD        ! For GEOS-Chem timers (optional)
      USE GC_Environment_Mod     ! For allocating derived type objects
      USE GC_GRID_MOD            ! For defining the lons/lats/areas of the grid
      USE Input_Opt_Mod          ! Derived type for Input Options
      USE INPUT_MOD              ! For reading settings from "input.geos"
      USE MAPPING_MOD            ! For regridding MODIS LAI
```

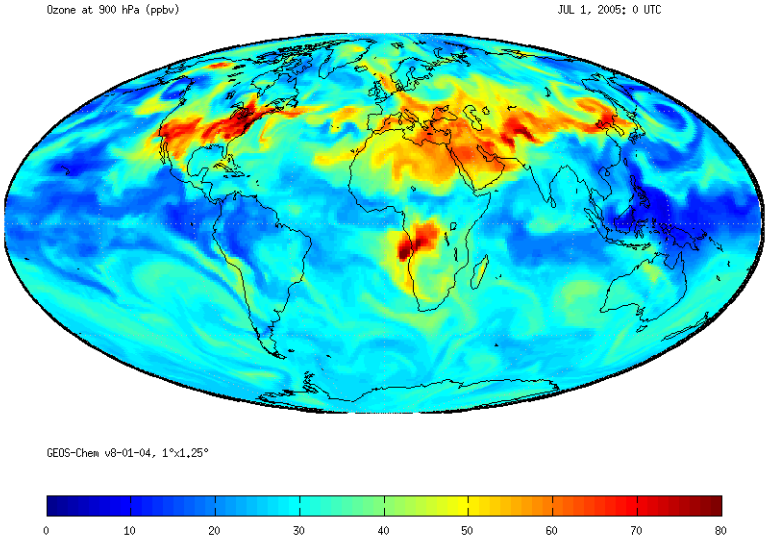
Example of Model Output

Excessive nitrogen input to the Earth's surface:



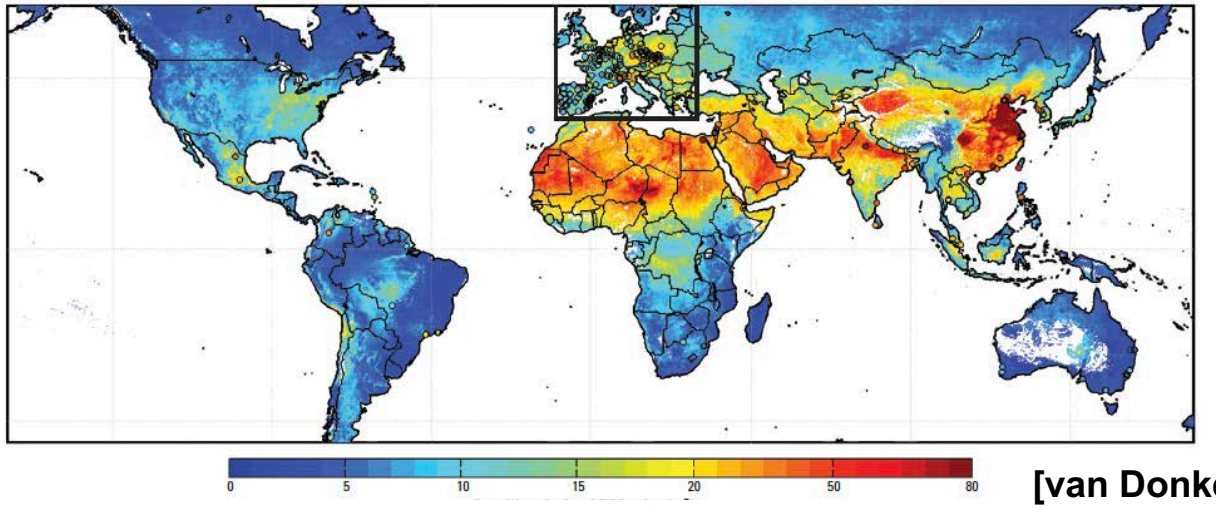
[Ellis et al., 2013]

Surface ozone concentrations:



[http://fizz.phys.dal.ca/~atmos/animation/]

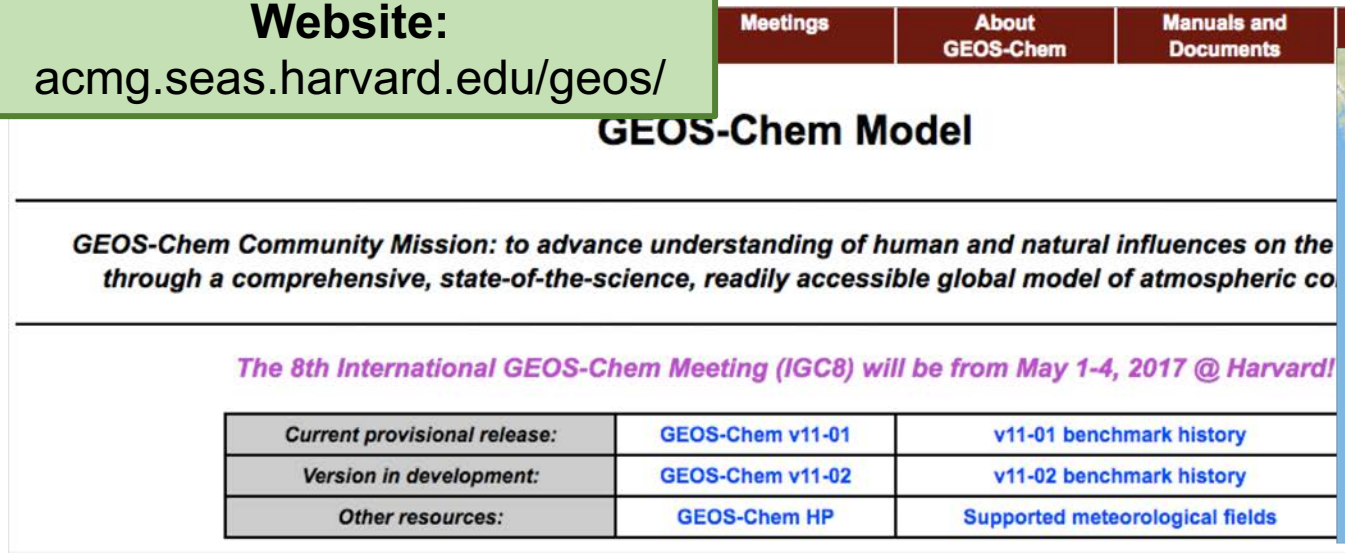
Combine with satellite observations to derive surface particulate matter concentrations



[van Donkelaar et al., 2010]

GEOS-Chem Community

Website:
acmg.seas.harvard.edu/geos/



Users throughout the world

Users Meeting every 2 years

GEOS-Chem Management

Designed for seamless incorporation of scientific updates (and bug fixes!)
Science Working Group Leaders and team leader decide on model updates.
These are incorporated by the programming team, benchmarked, scrutinized, and finally added to the official model release (now at version 11)

GEOS-Chem team leader: Daniel Jacob

GEOS-Chem subgroups led by 2 experts
(number of subgroups reflects model diversity)

Mercury/POPs

Emissions

Transport

Oxidants/Chemistry

Regional (Nested) Models

Aerosols

Chemistry-Climate

Adjoint/Data Assimilation

GEOS-Chem Models that Exist are Many

Some examples:

Standard model: global air quality model (NO_x-O_3-VOC-aerosol chemistry) at **2x2.5 degrees** (~200x250 km) or 4x5 (~400x500 km) degrees.

Other specialized options:

SOA model: Standard model with explicit treatment of secondary organic aerosols

High-performance model: Standard model at high resolution (under development)

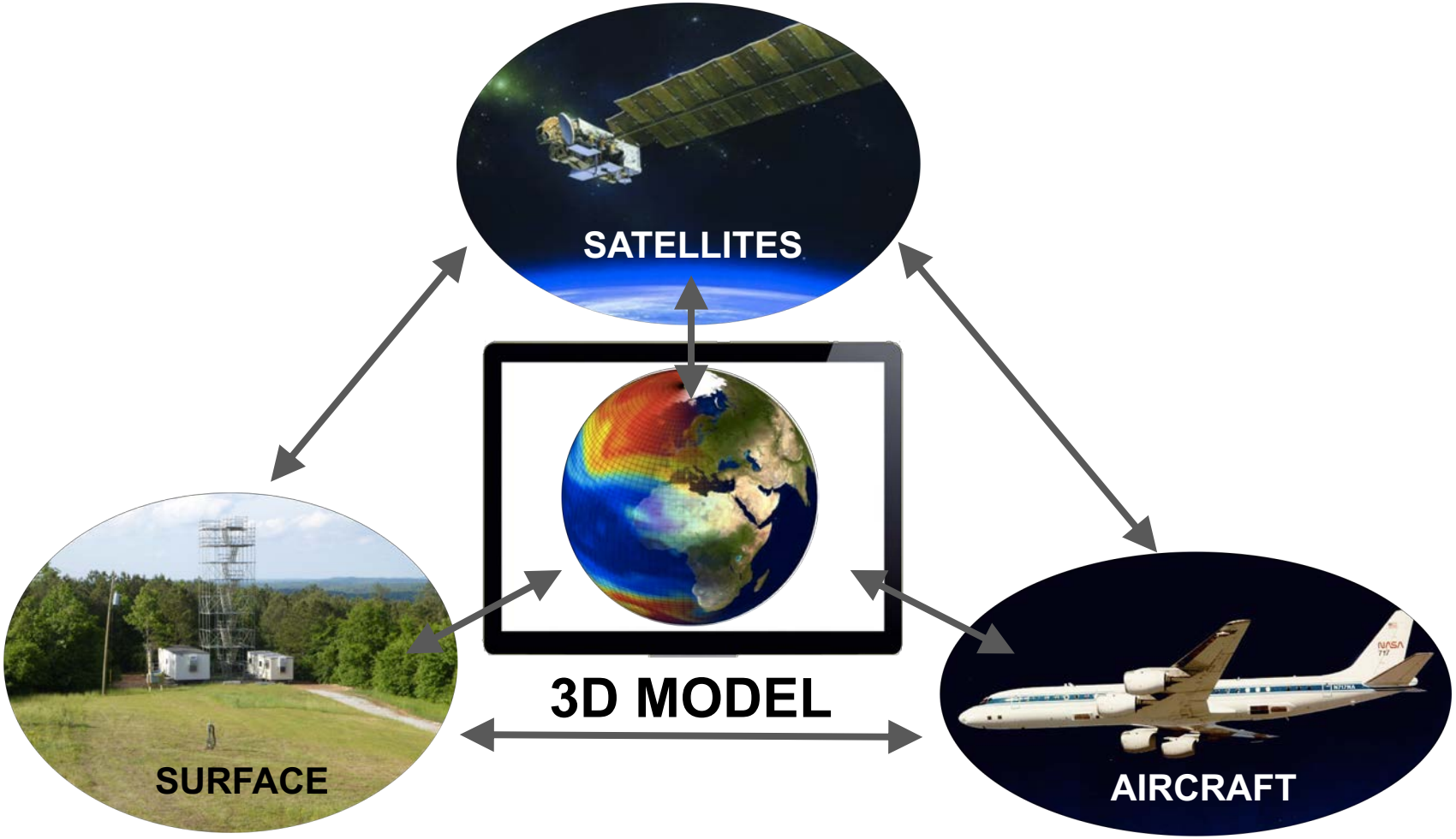
Nested models: Standard model, but at high resolution over a specific region (China, Europe, North America, **Africa**, West Africa) with boundary conditions at the coarse global resolution. High resolution dictated by resolution of meteorological fields

Others: Mercury, POPs, radon, Methane

RED: GEOS-Chem models used in my research

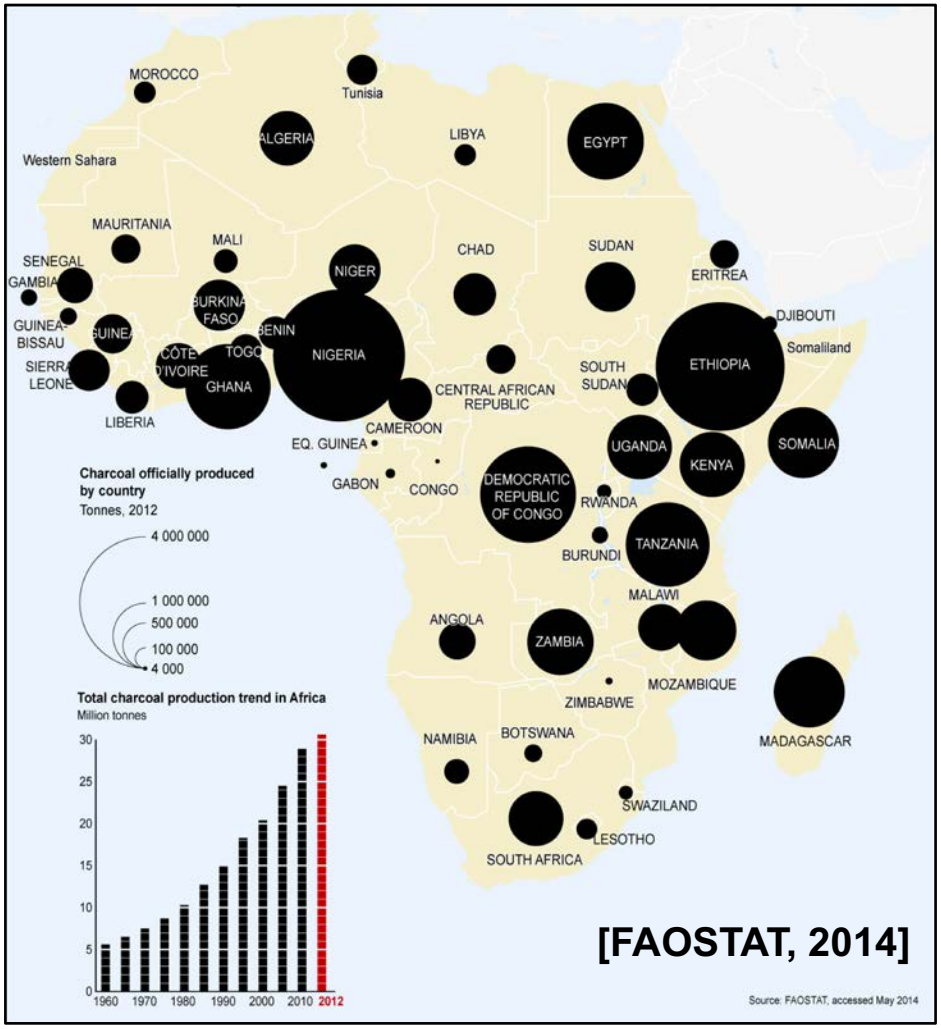
GEOS-Chem in My Research

Integrate data from multiple platforms to better understand atmospheric chemistry and inform prescient policy



A Focus on Charcoal Production

Charcoal Production in Africa

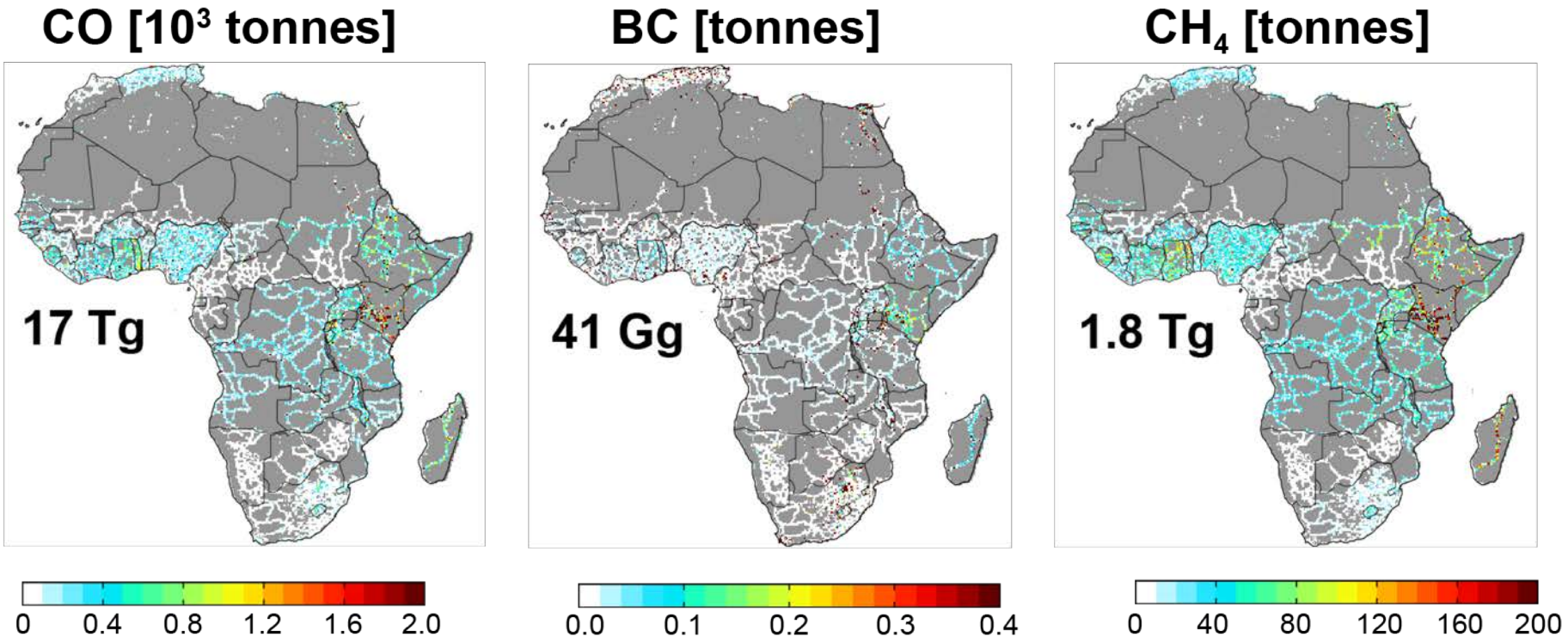


6-9% per year increase in production

Major export in Somalia fueling civil unrest there

Improved representation of charcoal emissions

Pollutant emissions from charcoal production, use and transport

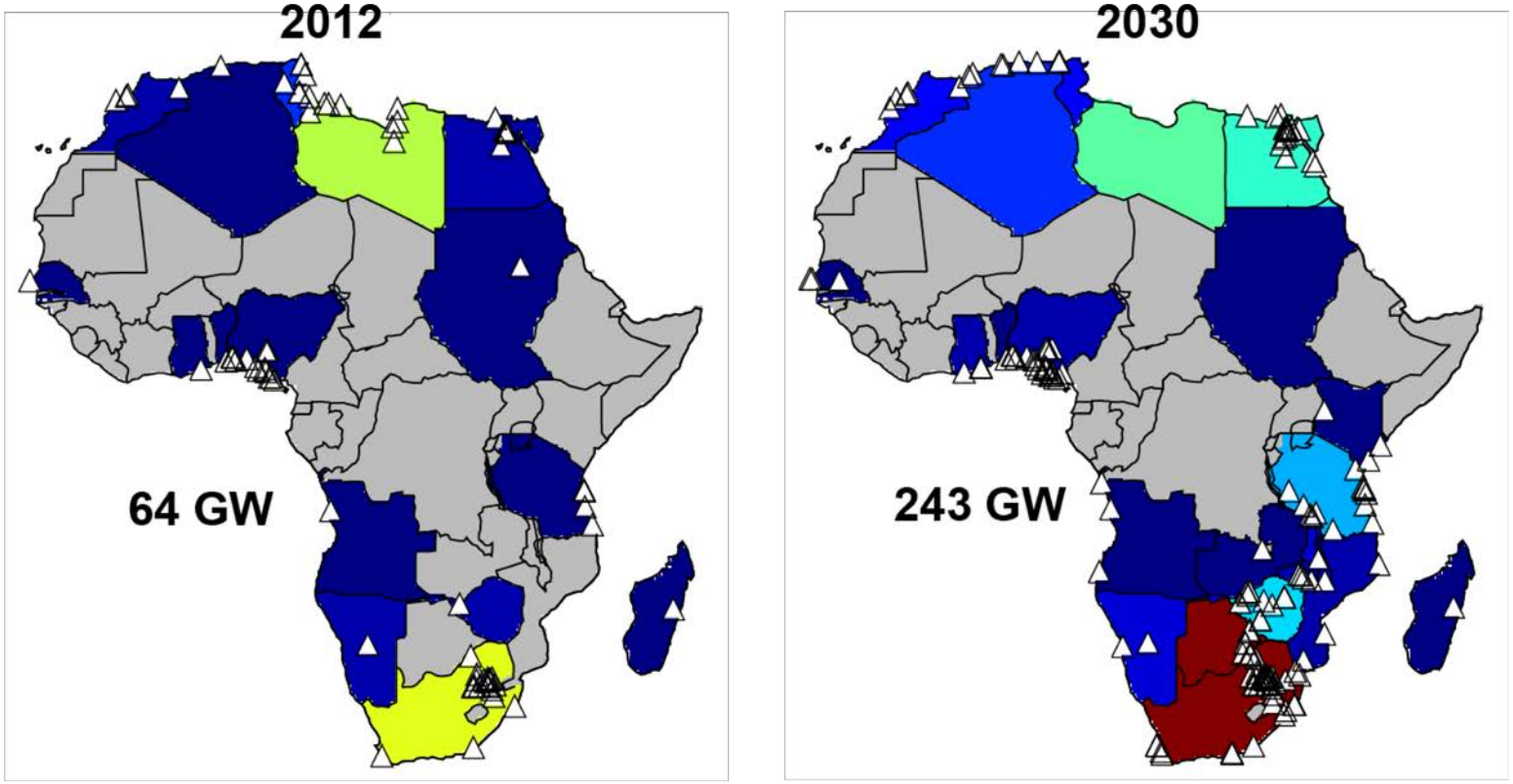


Annual biomass burning emissions in Africa:

440 Tg CO; **2.6 Tg BC**; **15 Tg CH_4** [Y. Shi et al., 2015]

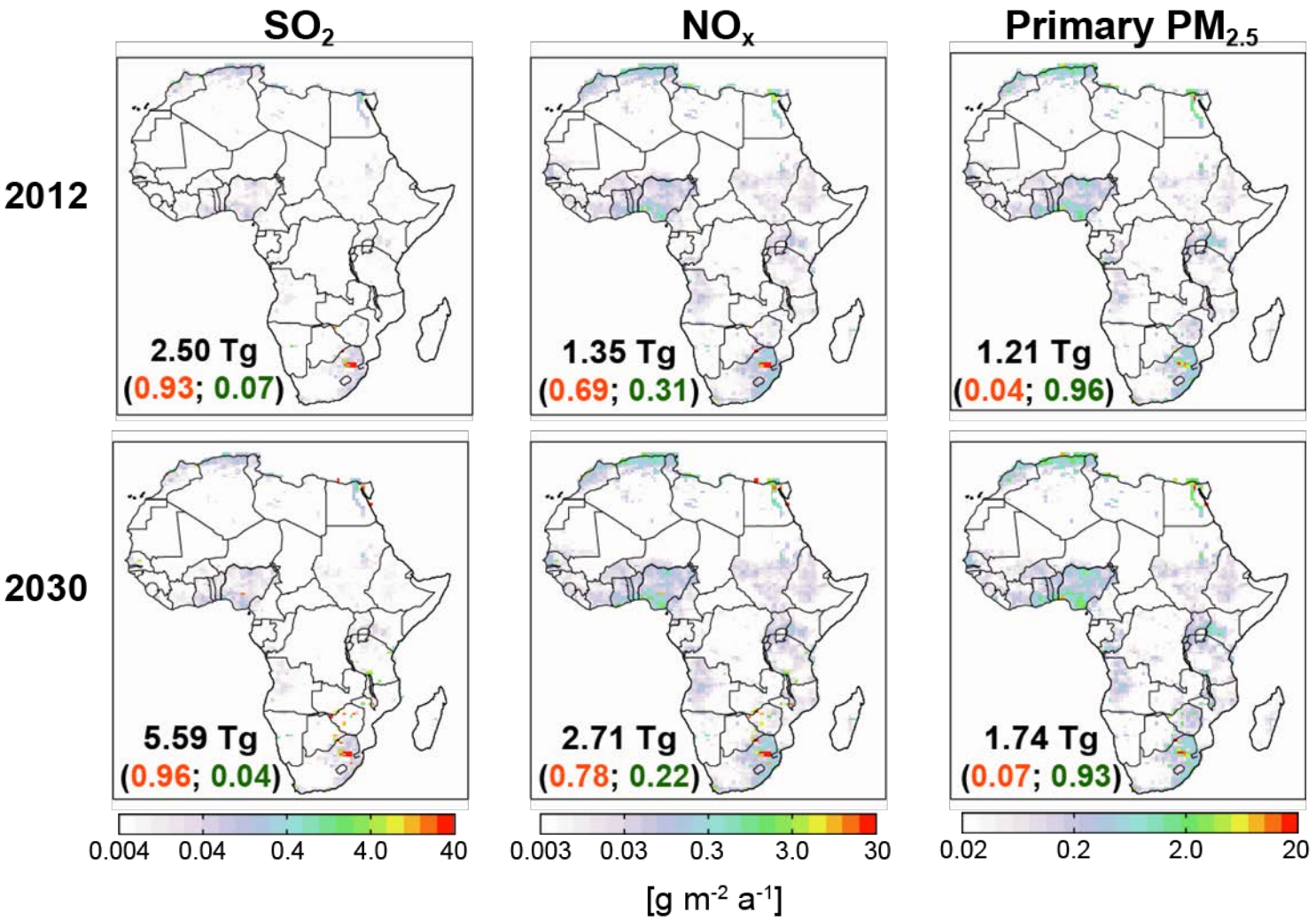
Use inventory to assess whether charcoal in Africa is sustainable.

Current and future generating capacity in Africa



Generating capacity to increase by almost 300%
(mostly North and southern Africa)

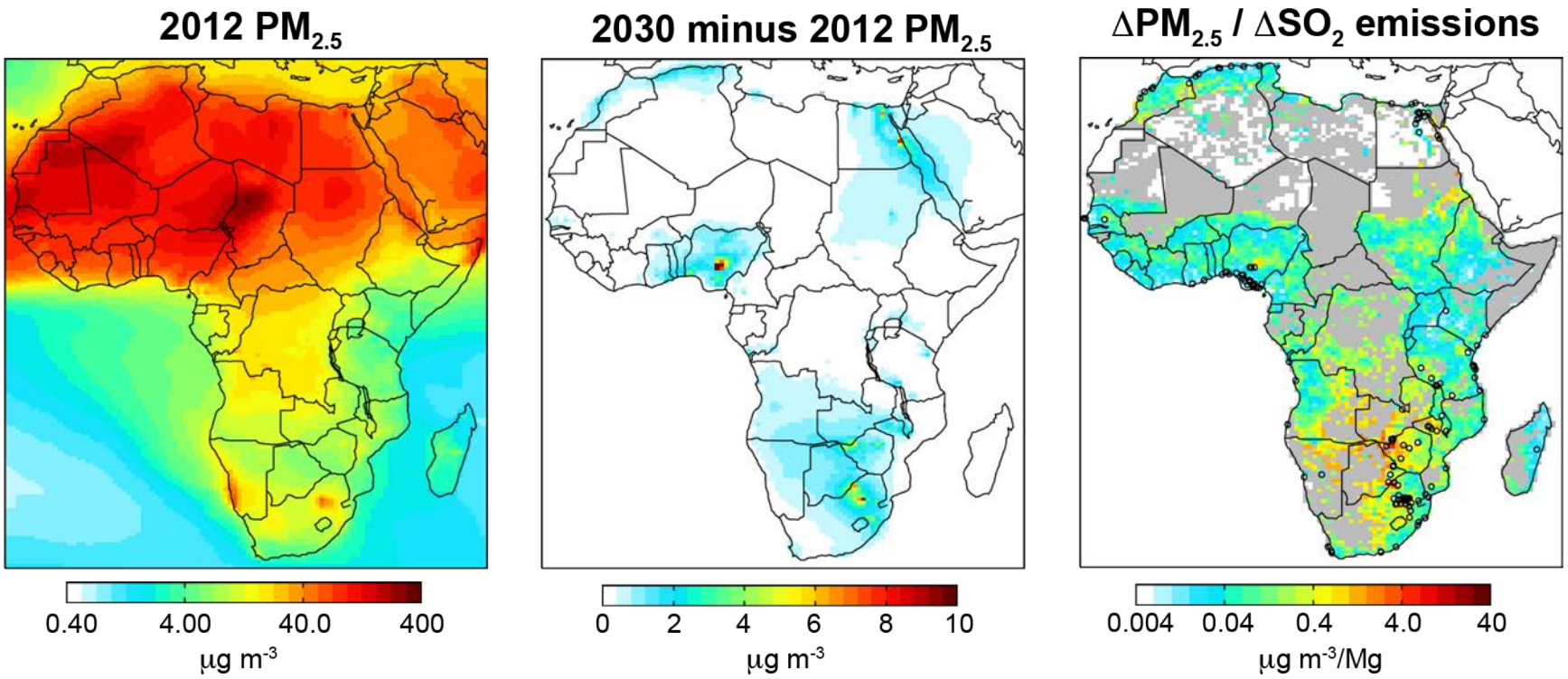
Emissions from current and future fossil fuels in Africa



Black: total continent emissions

Fractional contribution from power plants (**red**) and vehicles (**green**)

$PM_{2.5}$ from fossil fuels

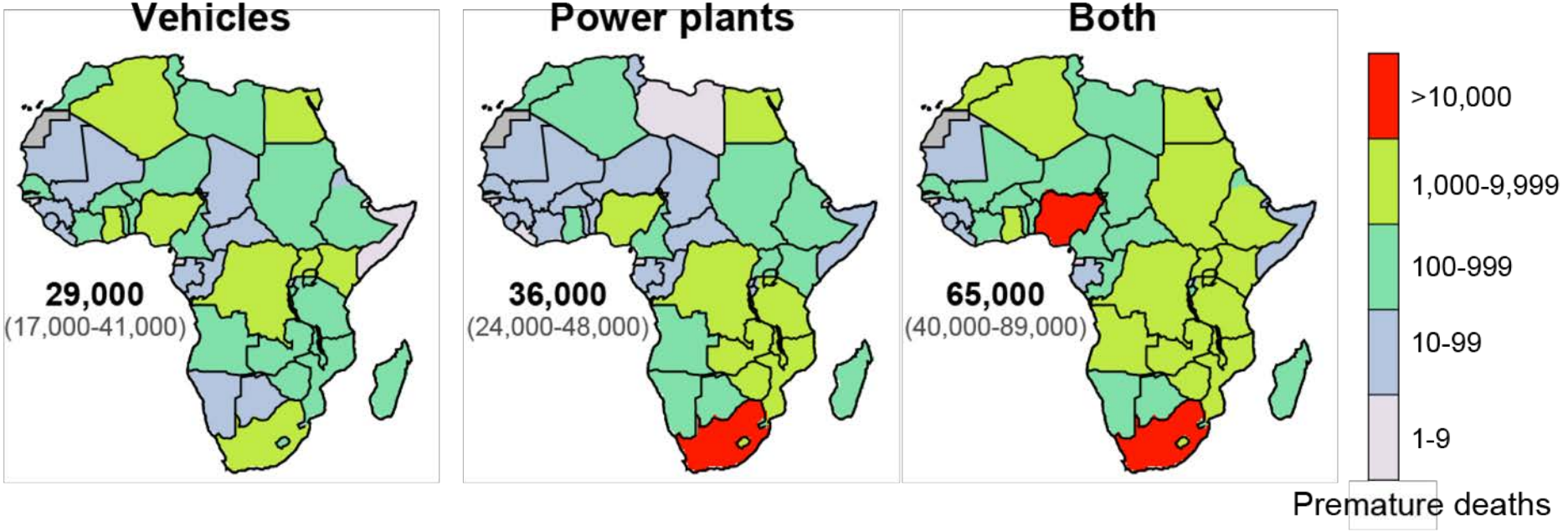


Absolute contribution dominated by dust

>10 μg m^{-3} increase in locations in Nigeria, Egypt and South Africa

Greatest sensitivity of $PM_{2.5}$ to SO_2 emissions is downwind of the source

The Impact on Health



Total premature deaths in Africa: 65,000

Equal contribution from vehicles and power plants, as increase in vehicles and population coincide (urban centres)