ACCESS Documentation

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Aug 30, 2018

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Note: This is a **draft** of documentation for the BVOC version of ACCESS v3.0. Eventually it may be incorporated into the repo for the model.

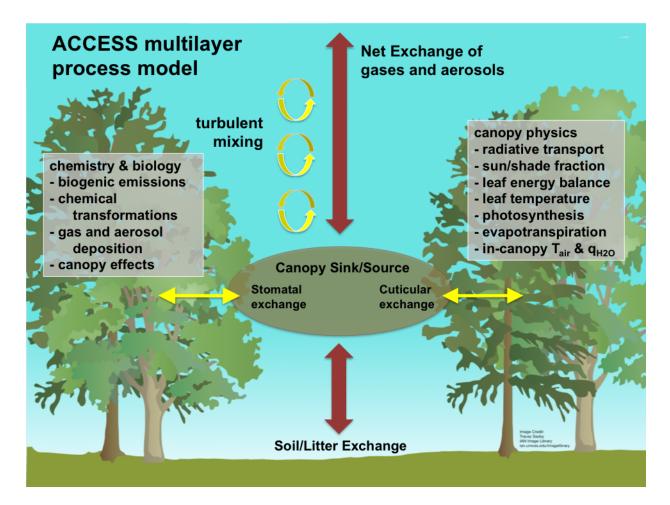
The Atmospheric Chemistry and Canopy Exchange Simulation System (ACCESS) is a 1-dimensional model for exchange of gases between the surface and the overlying atmospheric boundary layer air.

Rick Saylor has developed ACCESS since the early 2010s. ACCESS v1.0 was published in ACP¹.

¹ Saylor, R. D., 2013: The Atmospheric Chemistry and Canopy Exchange Simulation System (ACCESS): model description and application to a temperate deciduous forest canopy, Atmos. Chem. Phys., doi:10.5194/acp-13-693-2013.

Introduction

1.1 ACCESS Processes



Quickstart guide

These brief instructions should enable you to start using the model. Running with the default configuration using the provided example input files should be relatively simple.

2.1 Installation

Ideally, ACCESS should be run on a MacOS or Linux platform. It has been developed solely on the MacOS, but has been tested on Linux Ubuntu. ACCESS_2 is written in Fortran90 and is currently set up to use "gfortran" as the compiler. Other Fortran compilers will probably work without too many changes to the source, but no others have been tested so far. The only other software dependencies are for use of the quick look plotting programs in the "out" sub-directory.

Steps:

- 1. Obtain the source code from the GitHub repository.
- 2. Unzip the ACCESS_2.tgz tar bundle with tar xvf ACCESS_2.tgz into the directory where you want the code to reside.
- 3. First, to compile the ACCESS source code, cd into the "src" sub-directory and issue the command make. This will compile the code and place the executable into the "bin" sub-directory.

2.2 Analyzing your results

You can get a quick look at your results using the provided Python module.

The code "pltaccess" in this directory uses Python 2.7 and the matplotlib library, along with the wxpython library for GUI.

"pltaccess" was created only to provide a "quick look" at results of an ACCESS simulation.

The plots generated by this code are not meant to be publication quality.

Use your own favorite plotting software to create nice plots.

2.3 Running a simulation

To run an ACCESS simulation, cd to the top-level directory and issue the command ./accessx SIMNAME, where SIMNAME is the name of the simulation you want to run.

The simulations are defined by the control files located in the "ctrl" sub-directory.

So, as an example, there is a control file named "accessCTRL_ch140705d1.dat" for the simulation with SIMNAME = "ch140705d1".

To run the simulation, you would issue the command ./accessx ch140705d1.

A successful simulation will result in a new directory in the "out" sub-directory with the same name as SIMNAME.

All of the simulation results will be located in that directory.

2.3.1 Input files

For your own simulations, you will need to create 7 different input files (this is the hardest part of doing a simulation!). However, as noted elsewhere, example input files are included for testing and to help you in constructing your own.

accessCTRL_SIMNA	ME edator the simulation.
cinit.dat	initial conditions file (only ICs of simulated species that are non-zero).
envmet.dat	environmental and meteorological data file (see examples in "data" sub-directory).
canopy.dat	canopy morphological file (defines the LAI profile of the canopy you are simulating).
soil.dat	soil properties file
advect.dat	background concentrations file (only contains species for which you want to provide back-
	ground concs.)

Note: These were the required files for ACCESS v2.0. This section will need to be updated for the newer version with updated canopy physics.

The names of these files should correspond to whatever you are trying to simulate.

Examples of these files are located in the "data" sub-directory for the Chestnut Ridge canopy.

The science

3.1 Intro

ACCESS employs parameterizations to enable modeling of various physical processes that impact air chemistry. In some cases (e.g., radiative transfer and chemical reactions), these are derived analytically from physical laws. In others (e.g., deposition, turbulent mixing, vertical transport), the parameterizations are derived based on a combination of physics/theories and measurements.

3.1.1 Governing equation

$$\frac{\partial C_i(z,t)}{\partial t} = E_i(z,t) + R_i(z,t) + T_i(z,t) + D_i(z,t) + A_i(z,t)$$
(3.1)

where i identifies a certain chemical species.

Table 1: Terms in Eq. (3.1)				
$C_i(z,t)$	vertical gas-phase concentration profile			
$E_i(z,t)$	emission rate			
$R_i(z,t)$	rate of chemical transformation / reaction rate			
$T_i(z,t)$	vertical turbulent mixing rate			
$D_i(z,t)$	deposition rate			
$A_i(z,t)$	rate of mixing of species <i>i</i> with a defined background concentration			

3.2 Chemistry

Many chemical mechanisms are included with ACCESS. These include:

- others...
- GEOS-Chem ISOP 2013

- MIME
- MOZART (the original 1998 version)
- MCM 3.2
 - isoprene parent only
 - methane parent only
 - isoprene+
- RACM2
- RACM2+ ()
- simplified/toy isoprene mechanism

Todo:

- footnote references for each scheme
- in the list, links to pages about the schemes if avail

Using the chemical reaction parsing capabilities of KPP, and the tools in ACCESS gen/chmgen/ you can generate the necessary code snippets for implementing other mechanisms.

Architecture

4.1 Directory structure

4.2 Model architecture