Geosci. Model Dev. Discuss.,
https://doi.org/10.5194/gmd-2019-192-RC1, 2019

Geoscientific Model Development Discussions

Interactive comment on "AtChem, an open source box-model for the Master Chemical Mechanism" *by* Roberto Sommariva et al.

Anonymous Referee #1

Received and published: 10 October 2019

This paper documents a boxmodeling system for the Master Chemical Mechanism (MCM). The MCM is a very large, near explicit mechanism describing the degradation of 143 primary compounds into CO2 and H2O. As such, the MCM is too computationally expensive to be run in global chemistry models or even air quality models. However the MCM is often used to benchmark smaller 'lumped' chemistry schemes by comparison using a zero-dimensional boxmodel, or by comparison with results from controlled chamber experiments. Much of the boxmodeling work in the past used expensive commercial software, and this new open source system was developed in part to avoid these costs, but also to provide potential additional capability beyond commercial 'black-box' systems.

The paper is generally well written, with examples provided on how the model works

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Discussion paper

and performs. However, AtChem is presented as being a new and novel free system (line 52) without acknowledging any of the recent efforts to produce similar open source boxmodels, some if not all are also designed to run the MCM. These models are missing from the literature review. The literature cited between lines 23-29 are studies using boxmodels, some were commercial like FACSIMILE, some not. The review does not cover the models themselves. I have scored 'fair' for scientific significance (substantial new concepts, ideas, or methods) and scientific quality (consideration of related work, including appropriate references) based on this and the decision not to upgrade the representation of photolysis, which many of the other open source boxmodels have done (see major questions).

If the paper is to be published, acknowledgement of previous work towards production of open source boxmodels should be included in the literature review. I also would suggest the authors look into (at least comparing) other photolysis schemes.

Major questions

More than 10 years ago, the MCM website moved to output the entire mechanism (or a chosen subset) in a variety of formats. One of those formats was KPP (kinetic PreProcessor software) which is the basis for some of these recent open source codes – Knote et al's (2015) boxmodel extensions to KPP (BOXMOX, https://www2.acom.ucar.edu/modeling/boxmox-box-model-extensions-kpp), Sander et al's (2011) Chemistry As A Box Model Application (CAABA), and the Dynamically Simple Model of Atmospheric Chemical Complexity (DSMACC, http://wiki.seas.harvard.edu/geos-chem/index.php/DSMACC_chemical_box_model) (Emmerson and Evans, 2009). There is a wiki page listing 10 of these models: https://en.wikipedia.org/wiki/Kinetic_PreProcessor I am also aware of boxmodels which do not use these KPP format codes – F0AM (Wolfe et al., 2016) uses Matlab. So I'm missing why the authors developed their own model from scratch rather than building on another system which is freely available?

The method for calculating photolysis rates in AtChem is a shortcoming. AtChem uses (quite an old) 2-stream method for calculating photolysis rates, and looking at figure 4, consistently underpredicts the measured rates. This photolysis scheme has been used with MCM modeling for ∼20 years or so. Yes, it is important to adjust for cloudy conditions using measured photolysis rates. However not all investigators (and particularly students using AtChem in the classroom) have the luxury of being able to measure photolysis rates to perform the correction in equation 4, or to use directly as a constraint. If equation 3 can only be relied upon to produce good results at 500 m altitude, 45 degrees N on July 1st, then why was the photolysis method not updated given the opportunity for designing this new system? If AtChem had used one of the other open source systems as a basis, photolysis could be calculated on-line, where such parameters can be changed. CAABA gives users a range of options for calculating photolysis - JVAL, RADJIMT, DISSOC, (Sander et al., 2019). There's also FAST-JX (Wild et al., 2000) which users of GEOSChem and the UK chemistry and aerosol (UKCA) community prefer (https://www.ess.uci.edu/researchgrp/prather/scholar_software/fast-jx). BOXMOX and DSMACC use the Tropospheric Ultraviolet and Visible radiation (TUV, (Madronich and Flocke, 1997)), now at version 5.3.2 https://www2.acom.ucar.edu/modeling/tuv-download. i.e., there are plenty of other systems available. Given that photolysis is so important to OH production, correcting the underestimation produced by the 2-steam method is crucial for AtChem to be of use to other researchers, and should be considered.

As this is a model description paper, please explain how the dilution factor is calculated. In a number of places in the text constraining the boundary layer height is mentioned which would impact the chemical concentrations, but it is not explained. This also applies to the chamber open roof experiments. Please also mention whether the model has a capability for entrainment of stratospheric air into the troposphere (which is a feature of BOXMOX), or exchange of air with air masses outside the box (a feature of CAABA).

The choice of examples shown to demonstrate the AtChem system are at odds with the description of why it was developed. For example line 345 “AtChem2 was developed specifically for the long and complex simulations need for field studies”. AtChem2 is then demonstrated using only 2 days from a ∼40 day TEXAQs campaign. Were these two days chosen because they provided the best model-observation comparison? Why not show the whole TEXAQs time series, which would show that AtChem has been rigorously tested?

Editorial comments:

Title. I think GMD prefers a version number to be assigned to the model being described.

line 174 represents the start of a new paragraph but mentions ‘this’ modeling technique, which is not defined, or must relate to the paragraph above. I assume the latter, in which case it isn’t a new paragraph.

Line 204. ‘study’ not studies

Line 268. “since the model. . ..’ This and the following sentence are both very long, and could be broken up.

Line 350. Why is the latest version of the MCM not being used here?

Line 371. The reader needs to know what compounds were being constrained here – for example I’m assuming NO was constrained because of the statement about NO being the main destruction term. Earlier in this section reference is given to the model set-up in Sommariva et al (Sommariva et al., 2011), but as the results here rely upon the constraints they should be stated.

Figure 2. the plots are too small to be seen properly.

Figure 6, top right panel. A legend is missing for the three colors.

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