



Interactive comment on “A Lagrangian model of air-mass photochemistry and mixing using a trajectory ensemble: the Cambridge Tropospheric Trajectory model of Chemistry And Transport (CiTTyCAT) version 4.2” by T. A. M. Pugh et al.

Anonymous Referee #2

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General remarks

The paper by Pugh et al. (gmd-2011-54) describes a new model of photochemistry with a focus on the troposphere based on a Lagrangian description of transport.

The paper represents a contribution to modelling science within the scope of Geoscientific Model Development and the scientific approach and applied methods are valid. However, I suggest some more discussion of related Lagrangian methods (see below). The presentation in the paper is clear, concise, and well-structured and the use of
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English language is appropriate.

I recommend the paper to be published after a revision taking into account the issues raised below.

Major Points

A number of other models based on Lagrangian transport have been developed and used over the years. For example NAME (e.g., Rigby et al., 2011), Attila (e.g., Stenke et al., 2007), Atlas (e.g., Wohltmann and Rex, 2009), CIAMS (e.g., Konopka et al., 2010), Lagranto (e.g., Wernli and Davies, 1997; Cui et al., 2009), and Flexpart (e.g., Stohl et al., 2005; Cui et al., 2009). These models differ in design and are constructed for different research issues. However, there is some overlap of the CiTTyCAT model with these other Lagrangian models. Therefore I suggest including a brief discussion in the paper of other Lagrangian methodologies and how (and perhaps why) the approach adopted for CiTTyCAT model differs from the other approaches.

The vertical coordinate of the model seems to be pressure surfaces (although this is not always clear, see below). I suggest some discussion why this choice was made compared to a variety of other possible choices (Kasahara, 1974).

Finally I suggest bringing clearer across for which time scales (in my view several days but less than say a month) the model is designed. This is especially important in the abstract, conclusions and introduction.

Comments in detail

- p. 2476: I am a bit confused here: going from “Eulerian” to “Lagrangian” means changing the frame of reference so it is more than just manipulating equations.

Also: Is Eq. 2 valid for compressible flow? I suggest a bit more discussion here.

- p. 2477, eq. 3: is h a constant? If it is not state on which variables it depends on.
- p. 2476, l. 11: this is no minor point. There is a variety of vertical coordinates that could be envisaged (e.g., Kasahara, 1974). I suggest more discussion here.
- p. 2477: It is not obvious from the discussion why dry deposition is dependent on h whereas r_{wet} is not. I suggest more discussion here.
- p. 2478., l. 21: This is very hard to understand without having read the following sections of the paper. Suggest to rephrase.
- p. 2479: Chemistry schemes: there should be some discussion here of heterogeneous chemistry. It is neglected but is this assumption justified?
- p. 2479., sec 2.2.1: I do not understand: If I want to change chemical rate constants I think I should rerun DELOAD but in l. 18/19 the opposite statement is made.
- p.2480, l. 19: Perhaps it is worth mentioning also other studies suggesting problems in our understanding of organic compounds emitted by plants (e.g., Kiendler-Scharr et al., 2009).
- p. 2481, l. 2: citation for the photolysis scheme.
- p. 2481. l.18: why should the monoterpene schemes not impact say the OH chemistry of the model?
- p. 2482, l. 3: state on which measurements the ozone climatology is based on. Furthermore, I suggest adding the dataset as an electronic supplement so that others can also use the climatology.

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- p. 2482, l. 19: How realistic is the assumption of 0.1? why is the optical depth not allowed to vary?
- p. 2482: I suggest giving a bit more detail about the emissions. Are they specified as a mass flux (mass/time)? What is the time resolution (monthly, daily) of the emissions? If the emissions are part of the surface boundary condition a flux in mixing ratio is required – correct?
- p. 2488, l. 20 change “diverges” to “differs”
- p. 2490, l. 28: can a model be “informed”?
- p. 2491, l. 6: what is meant by “correction to the units”?
- p. 2492, l. 23: Mention the numerical method used in DVODE. Below the term “Jacobian Method” is used but no explanation or reference is given.
- p. 2494: Box mode: I know this is a difficult question but what is the size of the box that is assumed here. Possibly, depending on the issue in question the size of the box may vary?
- p. 2492, l. 6: “the model is in the boundary layer”?
- p. 2497, l. 27: You mean “ozone concentrations” correct?
- p. 2499, l. 26: state for how long typically the trajectory is considered, 10 days? Or longer?
- p. 2502, l. 1: Here it seems that the vertical coordinate is a hybrid-pressure coordinate, earlier in the paper pressure is mentioned as the vertical coordinate. It should be clearly stated here which vertical coordinate (and thus which vertical velocity) is used to calculate the trajectories.

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- I suggest somewhat more discussion here on the diffusivity κ . How well is this parameter known. Would a different value be deduced, if a different set of species would be used? How sensitive are the results of the model simulation to variations of κ ?
- p. 2505: There should be more discussion here on the issue of “too much divergence”. Can you quantify what is “too much”? Further, there could be interesting atmospheric situations where trajectories diverge, so isn't it a shortcoming of the model that such situations need to be excluded? Could there be a way to overcome this shortcoming.
- p. 2508, l. 9: give a reference for Fast-J.
- Fig. 10: I cannot find the orange arrow.

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