

***Interactive comment on* “Technical Note: Simulating chemical systems in Fortran90 and Matlab with the Kinetic PreProcessor KPP-2.1” by A. Sandu and R. Sander**

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We thank the reviewer for his/her suggestions. Specific replies are embedded in the text below.

> Generally, I think that the paper has a little bit too
> much the character of a software manual. The authors might
> consider reducing the detailed description of the software
> details and describe the features of the new
> implementation in a more general way.

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We have changed the text as suggested by the reviewer. Details of our changes are listed below.

> 1. Implementation of the software. The possibility for
> different platforms for implementation should be
> discussed. As far as I can see, the code download from the
> internet page given, is suited for UNIX/LINUX based
> environment. Is there a windows version? Can cygwin be
> used as platform?

Installation of KPP under Windows is not officially supported by us. However, one KPP user has reported a successful installation of KPP (as part of the MECCA model) under windows using the cygwin tools. He compiled the KPP-generated code using the g95 compiler. We have made his information available on our web page at <http://www.mpch-mainz.mpg.de/~sander/messy/mecca/cygwin.html>.

Although not officially supported by us either, we also expect that KPP runs under the operating system “MAC OS X” which is based on UNIX.

> 2. The spelling of the links should be rechecked, there
> are problems with capital letters.

We could not find any dead links in the published ACPD article. However, we did have to correct spelling errors in the galley proofs of this paper. Therefore, we suspect that the reviewer refers to a preliminary version.

> 3. Section 2.1, end. The SUN command should either be
> omitted, or explained: What is day and night for the
> integration routine?

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At the end of section 2.1, we have already defined: “SUN is the normalized sunlight intensity, equal to one at noon and zero at night”. To clarify how SUN is obtained, we have now added another sentence here: “The value of SUN can either be calculated with the KPP-generated subroutine `Update_SUN` or provided by the user.”

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> 4. Section 2.3: The authors claim: All methods in the KPP
> library have excellent stability properties for stiff
> problems . If all methods are excellent, I wonder why
> there are different methods implemented. Thus, this
> statement needs quantification. What degree of stiffness
> can be solved? Where are the limits? What can be said
> about the accuracy of the different methods? How do they
> compare? Here I would suggest to add an additional section
> which discusses these issues.
```

The reviewer is right: Even though the numerical integrators have excellent stability properties, this does not mean that all methods are equally suited for all purposes. Other properties, like accuracy and efficiency need to be considered as well. To address these questions, we have added more text at the end of section 2.3.

```
> It might also be of interest to compare with the
> frequently used FACSIMILE software.
```

Such a comparison between KPP and FACSIMILE has already been done in a previous paper (Sander et al., ACP, 5, 445-450, 2005) for the MECCA model. The results showed good agreement between these programs.

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> 5. section 2.4: The authors refer to the 3D-code. This
> reference needs an explanation. Can 3-D problem be solved
> using predefined tools? What is implemented in KPP?
```

In our current implementation of KPP into a 3D model (Sander et al., ACP, 5, 445-450, 2005), the chemical mechanism is integrated separately for each grid cell. The interaction between the grid cells (advection, diffusion, convection ...) is calculated outside of KPP, i.e. the operator splitting approach is used. This information has been added to Section 2.4.

> 6. Section 3.7 - 3.10: These sections have very much the
> character of a Software handbook. In a paper it might be
> sufficient to refer to the software manual, which comes
> with KPP. The authors may consider to shorten and to
> clarify this section without describing technical details,
> such as the directory structure of KPP, and the explicit
> definition of commands, such as #STOCIOMAT. It might be
> enough to briefly describe the new features of the new KPP
> version in general terms.

We have changed the text as suggested by the reviewer. Details of our changes are listed below.

> Section 3.1: Do the explicit values (e.g. NH₂SS = 10)
> refer to the example in section 2.1?

Yes. We have added this information now to the text.

> Section 3.3: The subroutine FUN, can be understood by
> someone who has programming experience. I suggest that all
> parameters should be defined either in the text of in a
> table in the appendix.

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The explanation in the current text is: “KPP computes the vector A of reaction rates and the vector Vdot of variable species time derivatives. The input arguments V and F are the concentrations of variable and fixed species, respectively. RCT contains the rate coefficients.” This includes all variables used in the subroutine FUN. We are not sure which additional information the reviewer requests.

```
> Section 3.5: This section can be understood by someone who
> has some knowledge about differential equations. As the
> paper addresses the atmospheric science community, I would
> at least introduce the differential equation explicitly,
> and based on this explain how equation (1) is related to
> the differential equation.
```

To illustrate our example better, we now show its ODE system and its Jacobian explicitly.

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> Section 3.6: It should be explained where the Hess Matrix
> is used in the numerical solver.
```

The Hessian is used for sensitivity analysis calculations. This information has been added to Section 3.6.

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> Section 3.7: I do not understand this section. It should
> be omitted, or the command #STOICMAT should be explained
> explicitly using and example of equations. Section 3.8.
> Here I also have problems to understand. What do the
> authors mean by the formulation in the first sentence
> (allows a direct computation with respect to rate
> coefficients)? This section might be omitted as well.
```

We have removed these sections. The information that was contained in them is still available in similar form in the KPP-manual in the electronic supplement.

> Section 3.9 and 3.10: These sections should be omitted as
> well, as they contain technical information, which should
> be provided in the KPP manual.

We have reduced and rewritten Section 3.9 to make it less technical. We have removed section 3.10. The information that was contained there is still available in similar form in the KPP-manual in the electronic supplement.

> Chapter 5: Applications. The authors performed benchmark
> tests of the different types of integration routine. For
> all systems, integration times are short (0.5 - 2
> minutes). It would be of interest how the numerical
> accuracy of the different methods compares.

So far, we have only made a few such tests. However, we are planning to perform systematic benchmark tests with KPP and the complex MECCA chemistry mechanism under a variety of atmospheric conditions and with different numerical solvers. The aim is to define more precisely which numerical solvers are most useful in atmospheric chemistry calculations. These will be published in a separate paper.

Interactive comment on Atmos. Chem. Phys. Discuss., 5, 8689, 2005.

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