Response to comments from Referees #1 and #2.

We thank the two referees for their constructive and useful comments. We begin (Section 0) by addressing some queries and comments which were made by both referees, then provide a point by point answer to each referee's comments.

The original referee comments are given in black, and our comments given in blue.

0. Common Issues

0.1 Responses to comments

Both referees commented that the manuscript could be hard to read.

Reply: In order to make the paper easier to read we have:

1. *Modified the headings as suggested by the referee #1*
2. *Harmonised the model naming system, with the more explicit CTM of EMEP MSC-W CTM on first mention, then simply EMEP CTM model.*
3. *Merged some sections to improve the flow:*

   a) moved and simplified some of the previous TWOSTEP text (old Sect. 1.1) to be part of the main introduction.

   b) Merged the boxChem setup texts (start of old Sect. 3 and Sect.4) into one Sect. 3: 'Getting started - GenChem and boxChem basics'.

   c) Moved the old Sect.3 text on EMEP CTM preparation into the more explicit new Sect. 4: 'Generating Fortran code for the EMEP CTM model'
4. *Added a short paragraph at the end of the introduction which describes the structure of the manuscript, and hopefully makes it easier for the reader to focus on the relevant sections, be it overview, installation and usage or mechanistic detail:*

   This paper is mainly intended as a compliment to the user-guide and code provided with GenChem, but we aim to provide here some more discussion of the background and benefits for the approaches chosen. Section 2 focuses on the installation and code structure of the GenChem system. Section 3 illustrates the steps needed to set up and run the boxChem simulations, including plotting commands. This allow users to get a quick-start on the GenChem system, ie to actually run and compare chemical schemes. Section 4 explains how to create and transfer files to the EMEP CTM system. Section 5 explains the many possible options associated with the 'base' and 'extra' chemical mechanisms. Sections 6 explains how to define the chemical mechanisms: detailing the input files which contain chemical species information and reaction mechanisms. Section 7 documents the output files of GenChem, which consist mainly of Fortran code needed for boxChem and EMEP

CTM runs. Finally, Section 8 (Conclusions) discusses some ideas for future development of the GenChem system.

5. *Added some more introductory text at the beginning of some sections*

6. *Greatly shortened the section about the GenIn_Species.csv file (Sect.6.1), since this information was rather too technical, and is available on the readthedocs web-site.*

7. *Generally added some smaller explanatory sentences to improve the flow of the manuscript.*

0.2 CPU requirements

The original manuscript stated that 'we believe the EMEP model is among the fastest CTMs', and both referees asked more about this.

Reply: The statement was mainly based upon experiences and comments made by others over many years about their CPU requirements. For this reply we have tried to investigate this in a more quantative manner, but find mixed results:

- *In the EuroDelta multi-model exercise (Bessagnet et al., 2016; Colette et al., 2017), several chemical transport models were run using common meteorology and domains, and a CAMx model was also run with similar but not identical setups. We have been able to compare run times with three of these models, CAMx, CHIMERE, and MATCH (see Bessagnet et al. 2016; Colette et al. 2017; Jiang et al. 2020 for details of models and setup). We found that the EMEP model was several times faster than CHIMERE, somewhat faster than MATCH and slower than CAMx (times from pers. comm. CAMx: Sebnem Aksoyoglu, CHIMERE: Augustin Colette, MATCH: Robert Bergström). However, the CAMx version used a very simple 2-product SOA scheme and 15 vertical layers, CHIMERE used 9 layers, EMEP 20 layers, and MATCH 39 layers, so the CPU times are not straightforward to intepret.*

- *The CAMx webside (www.camx.com/about/speed-scalability.aspx) gives an example of CAMx (v6.40) model performance for a 225×225×25 grid at 12km resolution, using CB6r2 gas-phase chemistry and also various advanced features (e.g plume-in-grid and source apportionment for 9 regions). With 64 cores a walltime of about 20 mins/day is achieved.*

  For a similar domain (225×225×20) at 0.1 deg resolution, 64 processors, and with CB6r2Em chemistry, the EMEP model uses 2.15 mins/per day. Of course, the CAMx model given in this example uses advanced features such as plume-in-grid modelling, and has more vertical levels, so again it is hard to make a consistent comparison.

- *Delic (2018) investigated the MPI performace of the CMAQ model, using a 24h test-case, for a grid of* 100×80 *California domain of 12 km resolution, with 35 vertical layers. They used a chemical mechanism of 149 active species and 329 reactions. Their test case required 16.7 mins per day using 32 processors (with an MPI efficiency of 0.63), or 10.8 mins/day with 64 processors (efficiency of 0.49). Although we cannot perform identical tests with the EMEP system, we have set up a simulation which should be reasonably comparable: a* 100×82 *European domain of* 0.1×0.1 *lat./lon. (ca. 10 km) resolution, with 35 vertical layers. As the EMEP model does a lot of pre-processing to interpolate e.g. emissions and landcover to the in-use grid on the first time step, the CPU times of a 1-day simulation are not representative of the typical time needed. We therefore tested a 31-day simulation to get average run-times for 24h also. With EmChem19a the EMEP model requires 0.74 mins/day from a 1-day run, or 0.48 mins/day from a 31-day run, using 64 processors. With CB6r2Em these runs take 0.85 mins/day and 0.6 mins/day.*

In summary, it is difficult to ensure comparability of many factors, including model setup, computing platforms and usage (number of processors, etc), so we are reluctant to publish CPU numbers from these different comparisons. We have also simplified the text surrounding TWOSTEP in the introduction, and found it best to simply omit any attempt to compare with other models. We do however add explicit CPU time for EMEP CTM runs in Table 3 (new numbering).

0.3 NPAS

Line 227 explain what is NPAS

Reply: We have added text to explain that NPAS means no-partitioning of primary organic matter, and with aging of secondary organics. Further details can be found in the cited reference of Simpson et al. 2012.

0.4 Other changes

A number of changes have been made in the GenChem system since publication of the original manuscript as a Discussions paper:

- The file 'GenIn_Shorthands.txt' which used to reside the chem/scripts directory, and which serves as the initial default set of shorthands, has now been moved and renamed as chem/generic_Shorthands.txt, in order to make it more visible to users.

- The logarithms used for CB6 in the Shorthands file should have been log10 rather than natural logarithms. This bug has been fixed.

- The emissions speciation file for CRIv2R5Em has been modified to bring it into line with the version used in the Bergström et al. (2020a) paper.
- The boxChem script box/scripts/getboxconcs.py has been updated so that its arguments are more similar to boxplots.py; with -v and -i, following the comment of Ref.#2.
- The boxChem script do.testChems now uses the default output directory OUTPUTS, see the new Table 2.

As a final comment on the code, we can note that the github code is currently tagged as 1.0.0-beta. If the resubmitted manuscript is accepted this code will be re-tagged as 1.0 when the manuscript is published.

1 Referee #1

1.1 General comments

The authors emphasize that the GenChem system can be used as a solver enabling testing of different chemical mechanisms. Several mechanism which are in the system are described in the paper. It is not clear if the system includes mechanisms that are currently the most popular in chemical transport models. The authors should provide information which mechanisms are the most frequently used in CTMs, recently. Which of these mechanisms are included in GenChem?

Reply: The intention of this paper is to focus on GenChem as a tool and not too much on the actual chemical mechanisms, but we have added some words to the conclusions of the manuscript:

The mechanisms included now reflect those used or made available for the EMEP CTM, as well as the MCM scheme which works in the boxChem mode. The EmChem19a scheme is only used in the EMEP CTM, but we include slightly adapted versions of CB6 which is used in the widely used CAMx model (`http://www.camx.com`) or CMAQ (Luecken et al., 2019), and CRIv2-R5 scheme which is used in STOCHEM (Archibald et al., 2010; Khan et al., 2015). It is hoped that some of the other widely-used mechanisms can be added in future, for example the MOZART scheme (Emmons et al., 2010; Surendran et al., 2015), the RACM scheme (Stockwell et al. (1997); Goliff et al. (2013)), or SAPRC-07 (Carter, 2010) which is also used in CMAQ (`https://www.airqualitymodeling.org/index.php/CMAQv5.1_Mechanisms`).

The system can be a valuable tool for converting chemical equations to EMEP, which is an open-source model, used by a wider community. It is not clear how about the ESX model. It should be clarified if you can share the code of ESX. Provide the recent applications of this model.

Reply: The ESX model should indeed be released as an open-source model, but we decided we had to finish and release the GenChem and updated EMEP CTM systems first. The only published information on ESX is the EMEP chapter which was cited, and the final report (which seems unaccessible now) of the EU ECLAIRE project which initiated the work. Since then a lot of work has been done with the ESX model, and a proper documentation is needed. Looking over the GenChem manuscript now we see that ESX is indeed mentioned many times. In view of its in-preparation status, we have reduced the number of references to the ESX model in the revised manuscript. (We hope to release ESX as open-source on github in the next months, but some preparatory work and final-checks are needed prior to this.)

The paper is quite difficult to read, e.g. chapters/subchapters names are taken from the names of files (e.g. 6.1. GenIn_Shorthands.txt). The names should be more descriptive/should tell what the chapter is about. There are also inconsistencies in use of the models names, e.g. the same model is called with different names EMEP MSC-W, EMEP, EMEP CTM, EMEP 3-D CTM, which can make difficult to understand the text for people not familiar with the EMEP model.

Reply: Please see comments given in Section 0.1 above.

1.2 Other comments

- The number of examples of the system application is very limited. The authors often refer to two papers which are in preparation (Bergstrom et al. 2020a and b). I would suggest to add an example of application of e.g. two different chemical mechanisms in EMEP and show the differences in the modelling results.

Reply: As noted above, the intention of this paper is to focus on GenChem as a tool and not too much on the actual chemical mechanisms. The Bergström et al 2020a paper compares the mechanisms in detail, and presents both boxChem and EMEP CTM results for the different mechanisms. This paper is in its final stages of preparation and will shortly be submitted to GMD. We think it would confuse the intention of the current GenChem paper if we start comparisons of the actual mechanisms.

- In the introduction: include information which are the most popular chemical mechanisms recently used in CTMs and which of these mechanism are in the GenChem system.

Reply: As noted in the reply to the referee given above, we have now mentioned other popular schemes (MOZART, CAM-4, RADM, SAPRC) in the conclusions section, and identified these as candidates for future inclusion in the GenChem system.

- Do not use EMEP/ESX system it should be ”EMEP or ESX or ”EMEP and ESX

Reply: We have changed the text as requested, and indeed removed many mentions of ESX

- Add information how much time it takes to run the system for different chemical mechanisms and how much time it takes to run the EMEP model with these mechanisms. Precise which of the chemical mechanisms can be used with the EMEP model.

Reply: We have extended Table 2 (now Table 3) with times for boxChem and EMEP model runs, and made it clear that all mechanisms except MCMv3.3Em can be used in the EMEP model. Further examples will be presented in Bergström et al. (2020a)

1.3 Technical comments

Line 47 explain what is TWOSTEP, you have not mentioned it before.

Reply: We have added the simple '(see below)' on first mention in the bullet points, but then brought forward a short explanation of TWOSTEP. As noted in Sect. 0.1 above, the original subsection on TWOSTEP has now been shortened and brought into the main introduction text.

Line 70 - "We believe the EMEP model is among the fastest CTMs" how do you believe that?

Reply: Please see comments given in Section 0.2 above.

Line 128 options of what?

Reply: We have changed 'list of available options' to be more explicit. These options are a usage message, a debug flag, and a list of available chemical mechanisms, and a debug option.

Line 146 "if emissions are wanted" explain what is the difference in using the model with and without emissions included

Reply: We have modified the text as follows:

By default, boxChem uses the set of emission rates as specified by variables set in config_box.nml, currently set with the lines beginning:

```
emis_kgm2day = 'nox', 18.3 !  NOx, kg/m2/day,
```

with 'voc' emissions set on the next line as 15.4 kg/m2/day. These emissions are converted by boxChem to instantaneous production rates in molecules cm^{-3} s^{-1}, accounting for molecular masses, emissions speciation (e.g. nox as NO and NO_2) and the mixing height, Hmix (also set in config_box.nml). Such emission rates can be modified by the user, or indeed all emissions set to zero if the variable use_emis is set to 'F' (False).

Line 215 correct “in ?”

Reply: This should have been Bergström et al. 2020b

Line 225 explain what is remPPM

Reply: We have added text to explain that this is the remaining PPM component.

Line 227 explain what is NPAS

Reply: Please see reply above, in Sect.0.3

2 Referee #2

2.1 General comments

This manuscript documents the software package GenChem used to generate the code for calculation of chemical reactions in atmospheric chemical transport models (CTMs). Although in principle being a standalone pre-processor, GenChem is in practice strongly tied to the EMEP CTM. The naming convention, structure etc are closely linked to that model and users without knowledge of the EMEP model could presumably have difficulties getting into the nomenclature. This is not meant as a negative comment. The EMEP CTM is a key model in atmospheric science and European abatement policies and the documentation of GenChem is an important issue in that respect.

Reply: Yes, these are fair comments.

Additionally, the possibility of using GenChem for testing and comparing various chemical mechanisms in a box model setup is a very valuable facility. The manuscript is a technical documentation that appears somewhat like an extended user manual and is somewhat hard to read without actually sitting down and trying out the various parts of the pre-processor. That said, the manuscript seems very well worked through without any major shortcomings and could be accepted with a few minor or technical corrections.

Reply: Yes, this is also a fair summary. As noted in the reply to Ref.#1 we have tried to make the manuscript easier to read in some respects, but it remains quite technical due to the nature of the system description.

2.2 Specific comments

The authors use various names for the EMEP model. It would help the clarity if they stick to one name (e.g. EMEP CTM).

Reply: We have simplified this, referring to the EMEP MSC-W CTM on first use, and thereafter just EMEP CTM.

Line 70. It is probably true (as the authors believe) that the EMEP model is among the fastest CTMs, but it would be of to interest to know if there actually has been any comparison of the speed of some of todays main CTMs.

Reply: Please see comments given in Section 0.2 above.

Table 1: The authors might consider to add the output files generated by boxChem either in this table or in a separate table. Now, Table 1 contains the files generated by the GenChem only and not the boxChem.

Reply: We have modified the caption and column headers for Table 1 to make it clear what that table refers to. We have added a new table (Table 3, new numbering) with the output files from do.testChem runs. We also modified the do.testChems script so that the log file (eg RES.EmChem19a) is also written into this directory.

2.3 Technical corrections

Line 105. Replace box-model code with boxChem.

Reply: We have made this change.

Line 150: Species M should be explained here (it is explained later in the doc).

Reply: We have added a reference to the Sect. 6.2 where this is explained.

Line 168: Should there be a -v in the command similarly to the command at Line 163?

Reply: The script getboxconcs.py had different arguments, so the line as given was correct. However, as noted in Sect. 0.4 above, we have now modified the script so that its arguments are more similar to boxplots.py; with -v and -i.

Line 215. Missing chapter info (?)

Reply: This should have been the in-preparation manuscript of Bergström et al. 2020b

Line 227: What does NPAS stand for?

Reply: Please see reply above, in Sect.0.3

Line 304: OXN- indicates that this species that belong to a group. Rephrase.

Reply: Done.

Table 4 (caption). Mentions EMEPs default PNAS scheme. Presumably misspelling of NPAS?

Reply: Corrected. Yes, this should have been NPAS.

Suppl. Info (p S6): Even with dt of 120 s RRMSk values dont exceed 1

Reply: Done.

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GenChem v1.0 – a chemical pre-processing and testing system for atmospheric modelling

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Abstract. This paper outlines the structure and usage of the GenChem system, which includes a chemical pre-processor (GenChem.py), and a simple box-model (boxChem). GenChem provides scripts and input files for converting chemical equations into differential form for use in atmospheric chemical transport models (CTMs) and/or the boxChem system. Although GenChem is primarily intended for users of the EMEP MSC-W CTM and related systems, boxChem can be run as a standalone chemical solver, enabling for example easy testing of chemical mechanisms against each other. This paper presents an outline of the usage of the GenChem system, explaining input and output files, and presents some examples of usage.

The code needed to run GenChem is released as open-source code under the GNU license.

1 Introduction

Atmospheric chemical transport models (CTMs), which simulate the emissions, transport, chemistry and loss processes of pollutants are essential tools for understanding air quality, and for assisting governments in setting environmental goals and emissions targets. Such CTMs are typically advanced 3-dimensional models with perhaps a million grid-cells. The models account for transport (advection, dispersion) between the cells, and within each cell the chemistry of the atmosphere is simulated, usually with a 'condensed' chemical mechanism (see below), and time-steps ranging from seconds to minutes.

An important CTM in terms of policy is that used by the Meteorological Synthesising Centre-West of the European Monitoring and Evaluation Programme (EMEP MSC-W). The EMEP MSC-W CTM (hereafter EMEP CTM), described in detail in Simpson et al. (2012) and subsequent articles and EMEP reports (e.g. Stadtler et al. 2018; Simpson et al. 2020 and references therein), is a 3-dimensional Eulerian model whose main aim is to support governments in their efforts to design effective emissions control strategies. The EMEP CTM has been available as open-source code (www.emep.int) since 2008, and it has since been run by several institutes across Europe (e.g. Solberg et al. 2008; Jeričevič et al. 2010; Karl et al. 2014; Omstedt et al. 2015; Vieno et al. 2016; Ots et al. 2018).

As with most CTM systems, the EMEP CTM code does not directly read chemical equations, but rather requires the production and loss terms of each species to be specified, in a differential form suitable for numerical integration. In order to convert between chemical equations and the numerical form, a chemical pre-processor is used, together with support software, which together comprise the 'GenChem' system.

In addition to the 3-dimensional EMEP CTM, a 1-D model system, the Ecosystem Surface Exchange model (ESX, Simpson and Tuovinen 2014) is being developed as a complementary system. ESX allows for the investigation of for example chemistry and deposition processes within the lowest tens of meters of the atmosphere (similar in concept to e.g. Makar et al. 1999; Ashworth et al. 2015). The most recent version of the ESX model also allows for Lagrangian trajectory simulations, which will enable the exploration of detailed chemical analysis as air masses traverse perhaps 100s of km (similar to e.g. Hertel et al. 1995; Vieno et al. 2010; Lowe et al. 2011; Murphy et al. 2011). ESX makes use of many components of the EMEP CTM, including many routines for e.g. radiation, emissions, and the GenChem system.

The most well known chemical pre-processor is probably KPP (Kinetic PreProcessor, Damian et al. 2002; Sandu and Sander 2006), which is used in a number of CTMs (e.g. Ashworth et al. 2015; Eller et al. 2009; Lowe et al. 2009; Langner et al. 1998; Squire et al. 2015; Stroud et al. 2016). KPP is more flexible than GenChem, with for example a range of different chemical solvers available, and with the capability to output as Fortran, C or MATLAB code. GenChem does not aim to compete with KPP in these regards, and in future KPP (or some descendent) may well replace GenChem in the EMEP CTM system also, but for the purposes of the EMEP CTM, GenChem does have a number of useful features:

1. The GenChem code is tailor-made to produce Fortran which can be directly included in the EMEP CTM and ESX systems.

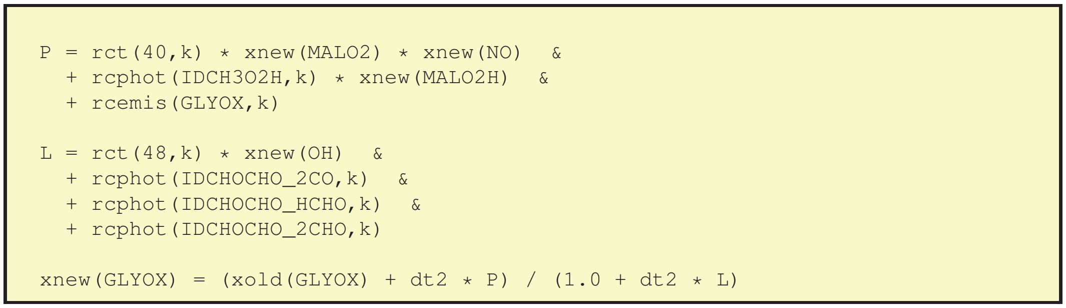
2. The integrated boxChem system allows both direct testing of code prepared for the EMEP CTM and ESX model, and side-by-side comparison of chemical schemes.

3. The Fortran code produced is more human-readable than with other processors such as KPP, with for example the gas HNO_3 being represented by the Fortran integer named 'HNO3' instead of by some numeric or abstract variable representation. Similarly, equations in the code produced by GenChem are readily understood, as illustrated in Fig. 1.

4. The code also establishes dry and wet deposition mapping of the chemical species, as well as a number of other characteristics (which can be readibly extended through the 'Groups' system, see Sect. 6), such as volatility of organic aerosols or extinction coefficients for aerosol species.

5. The numerical solver, TWOSTEP (described below), is extremely efficient for 3-D chemical transport models, and is thus very apt for the EMEP CTM or for running complex chemical mechanisms such as the Master Chemical Mechanism in boxChem or ESX (Sect. 5).

6. GenChem has a flexible system that can either calculate molecular weights from chemical formulas, or can use user-provided values.



```
P = rct(40,k) * xnew(MALO2) * xnew(NO)  &
  + rcphot(IDCH3O2H,k) * xnew(MALO2H)  &
  + rcemis(GLYOX,k)

L = rct(48,k) * xnew(OH)  &
  + rcphot(IDCHOCHO_2CO,k)  &
  + rcphot(IDCHOCHO_HCHO,k)  &
  + rcphot(IDCHOCHO_2CHO,k)

xnew(GLYOX) = (xold(GLYOX) + dt2 * P) / (1.0 + dt2 * L)
```

Figure 1. Example equations from the output file, ***CM_Reactions1.inc***, for the model species GLYOX (glyoxal). ‘P’ gives the production terms, and ‘L’ gives the loss terms, with the last line giving the TWOSTEP solution for this species. See Sect. 7.5

The original GenChem system was written in perl in the 1990s for earlier EMEP CTM versions (e.g., Simpson 1995; Simpson et al. 2012), but was converted to a python (2.7) script in 2014. The current structure of the GenChem system, now based entirely on python3, including boxChem, improvements in GenChem.py, and various scripts, was developed between 2016 and 2020.

The numerical solver used for the chemical equations in the EMEP CTM is the so-called TWOSTEP scheme (Verwer, 1994; Verwer et al., 1996; Verwer and Simpson, 1995). Sandu et al. (1997) commented that TWOSTEP was an excellent candidate for very large tropospheric gas-phase problems with very small operator split steps. The main limitation noted by Sandu et al. (1997) was that TWOSTEP is not suitable for aqueous-phase problems, but those are not explicitly treated within the gas-phase mechanisms considered here. It is not the purpose of this article to give details of the TWOSTEP scheme, except to note the simple formulation which results from its use. For example, Fig. 1 illustrates one of the major outputs of GenChem: example code (for the species glyoxal) from the GenChem output file ***CM_Reactions1.inc***. This code is very easy to read, with first the production term (P) which includes time-varying rate cofficients (rct terms), photolysis rates (rcphot) and emissions (rcemis), then the chemical loss terms (L), and finally the Gauss-Seidel TWOSTEP solution for the change in concentrations over time-step dt2. These terms are discussed further in Sects. 6.3 and 7.5.

Although primarily intended for users of the EMEP CTM, the GenChem system can also be run as a stand-alone chemical solver using the provided "boxChem" driver, enabling for example easy testing of chemical mechanisms against each other. boxChem also provides a useful learning tool for general GenChem usage. This paper outlines the structure of the GenChem system, including boxChem usage and preparation of EMEP-ready model files.

This paper is mainly intended as a compliment to the user-guide and code provided with GenChem, but we aim to provide here some more discussion of the background and benefits for the approaches chosen. Section 2 focuses on the installation and code structure of the GenChem system. Section 3 illustrates the steps needed to set up and run the boxChem simulations, including plotting commands. This allow users to get a quick-start on the GenChem system, ie to actually run and compare chemical schemes. Section 4 explains how to create and transfer files to the EMEP CTM system. Section 5 explains the many possible options associated with the ‘base’ and ‘extra’ chemical mechanisms. Sections 6 explains how to define the

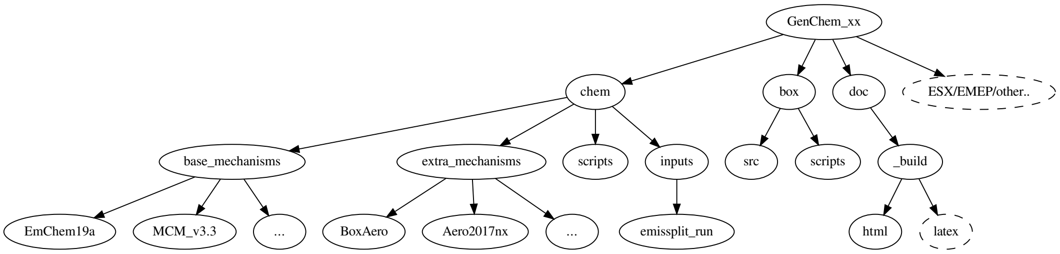


Figure 2. Directory structure of GenChem's chem and box directories. The dashed 'ESX/EMEP/other' directory indicates the possible placement of future EMEP, ESX or other model directories in this system.

chemical mechanisms: detailing the input files which contain chemical species information and reaction mechanisms. Section 7 documents the output files of GenChem, which consist mainly of Fortran code needed for boxChem and EMEP CTM runs. Finally, Section 8 (Conclusions) discusses some ideas for future development of the GenChem system.

2 Installation and code

The code needed to run the GenChem system is released as open-source code under the GNU license, (https://github.com/metno/genchem), with the user-guide provided at https://genchem.readthedocs.io. GenChem has been developed and tested in a Linux environment, mainly XUbuntu 16.04–19.10, but has also been tested on Windows systems via a virtual environment. For those familiar with the Docker system (https://www.docker.com/products/docker-desktop), a Dockerfile and Dockerfile_README are provided to enable consistent installation on Windows PCs. See the user-guide for further details.

GenChem is designed to work with modern Fortran compilers (tested with gfortran and intel f95), together with python3 ($\geq$3.5). As in the EMEP CTM, double-precision is enforced by compiler options (e.g. -r8 for ifort) rather than through explicit Fortran 'double precision' or 'selected_real_kind' coding. This is partly for aesthetic reasons (we prefer numbers typed as 1.2 rather than 1.2_wp), and partly for simplicity. Use of these flags ensures that all variables and constants are automatically elevated to the required precision. Failure to compile with these options will result in an error message. The testing for this release has mainly been done with the freely available GNU gfortran version 5.

After unpacking the GenChem directory structure should look like Fig. 2. The **chem/base** directory contains the main gas-phase mechanisms which we will use (e.g. EmChem19a). These are almost always supplemented by additional smaller mechanisms (e.g. for aerosol formation or biogenic emissions) which are contained in the **chem/extras** directory; see Sect. 5 for more details. The scripts ***GenChem.py*** and ***do.GenChem*** reside within the **chem/scripts** directory, but we will usually make use of these from the **box** directory as explained in Sect. 3. The main technical documentation of this system is provided at https://genchem.readthedocs.io as noted above, but various markdown-format README.md files are also located throughout this structure. For example each chemical mechanism should have a README.md file to summarise the mechanism and any comments.

Table 1. Input files to the GenChem system and output Fortran files.

Inputs		Outputs: Fortran files	
File	Section	File	Section
GenIn_Species.csv$^{(a)}$	6.1	CM_ChemSpecs.f90	7.2
GenIn_Shorthands.txt$^{(a)}$	6.2	CM_ChemGroups.f90	7.2
GenIn_Reactions.txt$^{(a)}$	6.3	CM_Reactions1.inc	7.5
BASE_emissplit_defaults_voc.csv$^{(b)}$	6.4	CM_Reactions2.inc	7.5
		CM_Reactions.log	7.5
		CM_ChemRates.f90	7.6
		CM_DryDep.inc	7.4
		CM_WetDep.inc	7.4
		CM_EmisFile.inc	6.3.2
		CM_emislist.csv	6.3.2
		CM_EmisSpecs.inc	6.3.2
emep_extras$^{(b,c)}$/			
BASE_BiomassBurningMapping_FINNv1p5.txt		CMX_BiomassBurningMapping_FINNv1.5.txt	
BASE_BiomassBurningMapping_GFASv1.txt		CMX_BiomassBurningMapping_GFASv1.txt	
BASE_BoundaryConditions.txt		CMX_BoundaryConditions.txt	

Notes: (a) These GenIn files are generated from one or more equivalent files, see Sects.6.1–6.3 (b) For the input emissplit_defaults_voc.csv file and emep_extras the 'BASE' string is replaced by the name of the base chemical mechanism, e.g. EmChem19a. (c) The files in emep_extras are for the EMEP CTM rather than boxChem usage. If intended for the EMEP CTM then appropriate Fortran code is required. If for boxChem, only dummy files are provided. These files are essential only for the base mechanisms. See the README_emep_extras.md files in the sub-directory.

3 Getting started - GenChem and boxChem basics

The boxChem system is an integral part of the GenChem system. boxChem provides a way of testing GenChem implementations and is indeed strongly recommended as the main method of preparing ~~ESX and/or~~ EMEP CTM codes. As a stand-alone model, boxChem is also a valuable way to compare results from different chemical mechanisms.

3.1 Initial setup of boxChem

boxChem, and indeed all GenChem work is usually done from a temporary 'work' directory of the box system, e.g. from **tmp_work**. This is created from the box location with:

Example 3.1.

```
./scripts/box_setup.sh tmp_work
```

This will create the working directory, and copy all the files needed for boxChem into it. Once setup, the user is ready to build and run some chemical schemes. With the example of EmChem19a, and now from our **tmp_work** directory, the simplest next step is in principle to run:

Example 3.2. `./do.GenChem -b EmChem19a`

This will run the ***GenChem.py*** script on the base-mechanism (-b flag) EmChem19a, and generate CM and CMX files, but it will not attempt to compile or run boxChem. However, a far more useful approach is to run do.testChems, e.g.:

Example 3.3. `./do.testChems EmChem19a`

Running do.testChems will run ***GenChem.py*** on the EmChem19a scheme (also adding a few extra_mechanism files as discussed in Sect. 5), copy all necessary CM-files and the configuration file config_box.nml to the user's work directory. The script compiles boxChem, and then runs the resulting box-model code. Input variables needed by boxChem (e.g. meteorology, emissions, boundary conditions) are set in config_box.nml (also copied by ***do.testChems***).

Table 2. Outputs$^{(a)}$ for a boxChem run achieved via 'do.testChems EmChem19a'

File	Comment
boxEmChem19a.csv	hourly outputs as comma-separated values for all pollutants
RES.EmChem19a	log file, with streamed output of boxChem run
config_box.EmChem19a	copy of config file used for run

(a) Files are produced in OUTPUTS directory by default. Can modify in do.testChems script

Results of the boxChem run will appear as three files in the outputs directory as given in Table 2. The main result file uses a simple comma-separated format, and is is readable with e.g. libreoffice. Plot scripts are also available for easy visualisation and comparison of these csv results (Sect. 3.3).

The 'CM_' and 'CMX_' Fortran files produced by this process are saved in directories, e.g. here in 'ZCMBOX_EmChem19a'. Now, if one wants to compare several schemes, one can do e.g.:

Example 3.4. `./do.testChems EmChem19a CB6r2Em CRIv2R5Em`

This would produce 3 output .csv files, which again are easily plotted against each other (see Sect. 3.3).

3.2 Controlling boxChem inputs and outputs: config_box.nml

The namelist input file config_box.nml allows the user to control many aspects of the boxChem model run. This file specifies the start and end time as well as the time step (dt) to be used. The concentration of the fixed species M and H2O (concentrations of air and water molecules, see see Sect. 6.2), and initial concentrations of all species, are set in config_box.nml. M and H2O can either be set directly in molecules cm^{-3} or by defining the pressure and relative humidity, respectively. Variables such as temperature, relative humidity or anthropogenic emissions are also set in config_box.nml and stay constant over the simulation time. Photolysis rates, however, change every time-step according to the sun's zenith angle. Biogenic emissions may also be modified by zenith-angle, if the simple SUN variable is used (see Sect. 6.3.2).

By default, boxChem uses the set of emission rates as specified by variables set in config_box.nml, currently set with the lines beginning:

```
emis_kgm2day = 'nox', 18.3 ! NOx, kg/m2/day,
```

with 'voc' emissions set on the next line as 15.4 kg m^{-2} day^{-1}. These emissions are converted by boxChem to instantaneous production rates in molecules cm^{-3} s^{-1}, accounting for molecular masses, emissions speciation (e.g. nox as NO and NO2) and the mixing height, Hmix (also set in config_box.nml). Such emission rates can be modified by the user, or indeed all emissions set to zero if the variable use_emis is set to 'F' (False). boxChem makes use of default speciations of compound emissions such as NOx or VOC — see Sect. 6.4 and Sect. S2.3 in Supplementary Information for more information on these splits and how they can be changed.

The OutSpecs_list variable in config_box.nml specifies which pollutants are required in the output file, though by default it is set to 'all'. This output file, e.g. box_dt30s.csv (where 30s is the 'external' timestep used), is generated in the outputs directory (e.g **box/tmp_work/OUTPUTS**), and gives hourly values for each species specified in OutSpecs_list, along with appropriate units. For gaseous species we use ppb or molecules cm^{-3}, and for particulate matter μg m^{-3}.

The choice of time-step is discussed in the Supplementary Information. See the comments in config_box.nml for further details about boxChem and config_box.nml setup and usage.

3.3 Plotting boxChem outputs

The python/matplotlib script boxplots.py (found in the **box/scripts** directory) can plot either individual or multiple species produced by boxChem, and for one or several output files. For example, if one has run do.testChems on say two chemical schemes, the results are easily plotted from the **box/tmp_work/OUTPUTS** directory:

Example 3.5. *`../../scripts/boxplots.py -h for help!`*

Example 3.6. *`../../scripts/boxplots.py -v O3 -i boxEmChem19a.csv boxChemX.csv -p`*

where -v gives compound to be plotted, and -p produces a png graphics file as well as screen output. Using 'ALL' or 'DEF' with -v results in all or many common species being plotted at once (-p is assumed in this case). For example, Fig. 3 shows a comparison of three schemes produced with this script.

Another helpful script just grabs the concentrations:

Example 3.7. *`../../scripts/getboxconcs.py O3 boxEmChem19a.csv`*

which results in ResConcs_boxEmChem19a_O3_ppb.txt

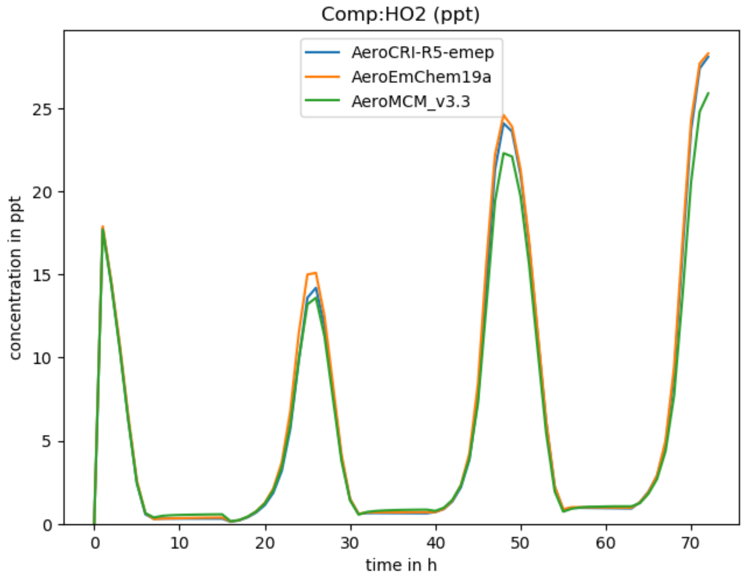


Figure 3. Example of comparison of three chemical schemes, produced for HO2 with the boxplots.py script

4 Generating Fortran code for the EMEP CTM model

The ***do.testChems*** script described above is best for quickly testing and comparing different mechanisms. Usually these comparisons only involve gas-phase mechanisms such as EmChem19a or MCMv3.3Em. However, the EMEP CTM usually requires a host of extra species and reactions to accommodate secondary inorganic aerosol, sea-salt, dust, organic aerosols, and pollen, as discussed in Sect. 5. The EMEP CTM also requires files to specify how emissions and boundary conditions should be distributed among specific species, e.g. how a VOC emission should be split into C2H6, C2H4, nC4H10 etc.

In fact, GenChem produces many Fortran files which need to be copied into the appropriate ZCM_ directories, e.g. ZCM_EmChem19a-vb for the scheme EmChem19a-vbs, as indicated in Table 1. The recommended way to get this directory is to use the script ***emep_setup.py*** from your temporary work directory within the box system. So, from e.g. **box/tmp_work**, do:

Example 4.1. ***`./emep_setup.py EmChem19a-vbs`***

or just run without arguments:

Example 4.2. ***`./emep_setup.py`***

and this will provide ~~a list of available options~~ a usage message, a debug flag, and a list of the available chemical mechanisms. Users can easily edit the ***emep_setup.py*** scripts to modify the extra_mechanisms used – see Sect. S2 in the Supplementary Information.

After ***emep_setup.py*** has successfully run, the ZCM_ directory produced contains all the files needed to run the EMEP CTM. The CM_ and CMX_ files can be copied directly to the CTM's source directory, and the EMEP CTM compiled as normal (make clean, make). The emissplit_run files need to be sent to a location specified by the user (via the EMEP CTM's emep_config.nml namelist).

5 Chemical mechanisms in GenChem

We provide a number of chemical mechanisms which have been formatted for GenChem usage. These mechanisms are organised into two types, with separate directory trees:

- ***base_mechanisms***

  These schemes are typically fairly complete sets of gas-phase photochemical mechanisms, and are designed to be the core for any boxChem, ESX or EMEP CTM runs. Apart from the EMEP-developed EmChem19a, the other base-schemes have been adapted from other sources for EMEP CTM usage, hence the 'Em' postfix. Details of these schemes and adaptations can be found in Bergström et al. (2020a). The schemes provided with GenChem currently comprise (see also Table 3):

  - EmChem19a — the base EMEP chemical scheme, which has 158 gas-phase reactions in the core mechanism, and in addition to these a number of heterogeneous reactions are also included, bring the total to 171 reactions for simple boxChem usage (c.f. Table 3). This scheme is a surrogate-species scheme that has evolved over many years (Eliassen et al., 1982; Simpson et al., 1993, 2012; Bergström et al., 2020a), and has over the years been shown to compare well against other and more extensive chemical mechanisms (Kuhn et al., 1998; Andersson-Sköld and Simpson, 1999; Bergström et al., 2020a). The most recent changes have included a revised isoprene chemistry based on the CheT2 mechanism of Squire et al. (2015), and the addition of toluene and benzene as well as o-xylene to represent aromatics. A new feature of EmChem19a compared to earlier EMEP schemes is the addition of an RO2POOL species, representing the total concentration of all peroxy radicals; RO2POOL is used for setting the rates of peroxy + peroxy radical reactions. A set of new nitrate radical reactions has also been added, and reaction rates have been revised to be in line recent IUPAC recommendations. For details see Bergström et al. (2020a).
  - MCMv3.3Em — based on the 'Master Chemical Mechanism' v3.3.1, with a few updated reactions (mainly updates of some reaction rates to be in agreement with IUPAC recommendations 2009–2018). In our implementation the MCM mechanism has over 5800 species and over 17000 reactions. See Jenkin et al. (2015), and references therein, for details about MCM, and Bergström et al. (2020a) for details about the revisions made for MCMv3.3Em. The MCM mechanism is too large for the EMEP CTM, but can be run with boxChem or ESX, and serves as an important reference mechanism.
  - CRIv2R5Em is an adaption of the 'Common Representative Intermediates' scheme, with a variant of the CRI v2.2 isoprene chemistry (Jenkin et al. 2008, 2019). In order to make the scheme manageable for 3D-modelling the full

CRI scheme is reduced by only including emissions from a limited set of different VOCs (the so called CRI_R5 reduction subset from Watson et al. 2008 is used in the EMEP adaption of CRI). Even with this reduction the CRI scheme is substantially larger than our EmChem schemes, but still well suited to 3-D modelling (see e.g. McFiggans et al., 2019 and Jenkin et al., 2019, for studies employing the CRI-R5 mechanism with the EMEP CTM). The EMEP version of CRI v2-R5 (CRIv2R5Em) is described in detail by Bergström et al. (2020a) and the revision of the isoprene chemistry by Jenkin et al. (2019).

- CB6r2Em — The ‘carbon-bond’ (CB) schemes have been developed over many years as an innovative solution for dealing with chemistry in 3-D CTMs (Gery et al., 1989; Yarwood et al., 2010a, b; Luecken et al., 2019). The CB6r2 chemical scheme has been implemented without any significant change in the GenChem, except that photolysis rates have been adjusted to use MCM (for boxChem usage) or EMEP CTM surrogates. Also, the biogenic VOCs of CB6r2, ISOP (isoprene) and TERP (representing all monoterpenes, MT), have been renamed to the C5H8 and APINENE (also a surrogate for all MT in this case), since this allows the same emission reaction equation to be used for all four mechanisms if desired.

- ***extra_mechanisms***

  In this directory we store sets of reactions and sometimes species that can be appended to the base mechanisms. Many of these are essential for 3-D chemical transport modelling, whilst others are used for box model simulations. With this release we provide mechanisms for sea-salt, dust, emissions from ships (EMEP uses a special ShipNOx species, see Simpson et al. 2015), and several organic aerosol and BVOC emission options. Comments on each scheme can be found in the appropriate README files. The organic aerosol schemes will be further discussed and compared in Bergström et al. (2020b).

  Tables S1–S2 in the Supplementary information provide brief explanations of the many currently implemented extra_mechanism packages, but we can give three important extra mechanisms as examples:

  - BoxAero

    Provides SO_2 gas phase chemistry and some reactions for very simple gas to aerosol conversion for SO_3, HNO_3 and N_2O_5. The reactions provide simplified chemical loss mechanisms for these species in the box model — they are calculated in a more complex way in the full EMEP CTM, which also includes NH_3 chemistry. This directory is intended only for boxChem usage, and is applied automatically when using the ***do.testChems*** script (see Sec.3).

  - PM_WoodFFuelInert

    PM emissions (fine and coarse) in the EMEP CTM are typically split into EC (elemental carbon), POM (primary particulate organic matter) and remaining PPM (remPPM) components. Different levels of detail are allowed, but this package enables the most common setup. POM and EC emissions are divided into those from biomass combustion (“wood-burning”) and fossil-fuel. POM are assumed inert, consistent with the ~~‘NPAS’~~ PM_VBS_-EmChem19 scheme discussed below. EC emissions are further divided into ‘new’ and ‘age’ components, to reflect the level of hydrophobicity (Tsyro et al., 2007; Genberg et al., 2013) In some inventories primary sulphate is also provided, represented here as pSO4 (if pSO4 is used, remPPM would then represent all PM components except EC, POM and pSO4).

- PM_VBS_EmChem19

  Provides additional organic aerosol reactions for EmChem19a. These reactions are currently (in version rv4.34) default in the EMEP CTM, and represent minor updates of the VBS schemes presented in Bergström et al. (2012, 2014); Simpson et al. (2012). The default scheme used in PM_VBS_EmChem19 uses the 'NPAS' version of the EMEP VBS mechanisms (with non-partitioning (i.e. inert) primary emissions and aging of SOA compounds) – see Simpson et al. (2012) (and its SI) for further details. Unlike the simple gas-phase compounds used elsewhere, SOA species are tracked as a true aerosol — with one compound representing the sum of gas and particle-phase compounds. These semi-volatile species and reaction formats are discussed more in Sect. 6.1.1 and Sect. 6.3.

Table 3 summarise the number of species and reactions involved in typical boxChem or EMEP CTM usage, and Tables 4–5 give examples of the combinations of base_ and extra_mechanisms packages. When a script such as ***do.testChems*** or ***emep_setup.py*** is run (Sects. 3,4), these scripts collect or concatenate inputs from the base directory together with those from the extra directories, to produce the input files (see Table 1) needed by GenChem. For example, running ***'emep_setup.py EmChem19a'*** would concatenate the file ***EmChem19a_Species.csv*** from the base directory with equivalent species files from ***PM_VBS_EmChem19***, ***BVOC_IsoMT1_emis***, etc (c.f. Table 5) to produce the input file ***GenIn_Species.txt*** needed by GenChem (Table 5).

It can be seen that the GenChem system allows a very flexible approach to explore different levels of chemical complexity, especially for EMEP CTM applications. Both base and extra mechanisms will be expanded in future GenChem versions, for example with further organic aerosol modules.

Table 3. Comparison of chemical mechanisms provided with GenChem 1.0, in either boxChem (mainly gas-phase) or EMEP CTM (with many particle and semivolatile compounds and tracers) configurations: number of species (N_s), number of rate-coefficients, (N_r, includes photolysis), number of photolysis reactions (N_j), number of anthropogenic emission terms (N_e), and computer execution time (T_e) for example run.

	boxChem$^{(a)}$					EMEP CTM$^{(b)}$				
	N_s	N_r	N_j	N_e	$T_e{}^{(c)}$	N_s	N_r	N_j	N_e	$T_e{}^{(d)}$
EmChem19a	80	171	34	21	3.56 s	127	198	34	48	7.3h
CB6r2Em	127	227	27	30	4.15 s	174	252	27	57	8.0h
CRIv2R5Em	225	575	111	35	26.7 s	272	602	111	62	10.2h
MCMv3.3Em$^{(e)}$	5842	17220	3120	141	4.72 h					–

Notes: (a) EmChem19a-box, CB6r2Em-box, CRIv2R5Em-box, cf. Table 4 (b) EmChem19a-vbs, CB6r2Em-vbs, CRIv2R5Em-vbs, cf. Table 5 (c) boxChem execution time is for default configuration, for a 24h run, on an x86 PC running Ubuntu-based linux, gfortran compiler. Times given are best of five simulations. (d) EMEP CTM execution time is for an annual global run with regular 0.5° lat/lon resolution grid, 20 model layers, and using 512 processors on a linux cluster, intel compiler. No time shown for MCM since this mechanism is too large for EMEP CTM runs. (e) Unlike the other provided schemes, MCMv3.3Em includes many halogen reactions. These are included for future developments. Further, MCM treats all individual reactions paths as separate reactions, whereas the other schemes frequently combine reactions into a single net reaction.

Table 4. Examples of Base and Extra mechanisms associated with boxChem configurations.

Label	base_mechanism	extra_mechanisms	Comment
EmChem19a-box	EmChem19a	BoxAero, BoxDep, BVOCemis	boxChem schemes all use same extras
CB6r2Em-box	CB6r2Em	as above	
CRIv2R5Em-box	CRIv2R5Em	as above	
MCMv3.3Em-box	MCMv3.3Em	as above	

Table 5. Examples of Base and Extra mechanisms associated with EMEP CTM configurations (via emep_setup.py).

Label	base_mechanism	extra_mechanisms	Comment
EmChem19a-vbs (or EmChem19a)$^{(a)}$	EmChem19a	PM_VBS_EmChem19$^{(b)}$, BVOC_IsoMT1_emis, +COMMON$^{(c)}$	Standard EMEP, VBS SOA for α-pinene surrogate
EmChem19p-vbs (or EmChem19p)$^{(a)}$	EmChem19a	As EmChem19a-vbs, + Pollen	Open-source EMEP has pollen
EmChem19a-vbs3	EmChem19a	As EmChem19a-vbs, + BVOC_ExtraMTs, PM_VBS_ExtraMTs, BVOC_IsoMT3_emis, +COMMON$^{(c)}$	with 3 mono-terpenes
CB6r2Em-vbs	CB6r2Em	PM_VBS_CB6r2Em, BVOC_IsoMT1_emis, +COMMON$^{(c)}$	CB6 gas-phase, VBS SOA for α-pinene surrogate
CB6r2Em-H	CB6r2Em	PM_Hodzic_CB6, BVOC_IsoMT1_emis, +COMMON$^{(c)}$	CB6 gas-phase, Hodzic-like SOA$^{(d)}$
CRIv2R5Em-vbs	CRIv2R5Em	PM_VBS_EmChem19, BVOC_IsoMT1_emis, +COMMON$^{(c)}$	CRI gas-phase, VBS SOA for α-pinene surrogate
CRIv2R5Em-M19	CRIv2R5Em	BVOC_XTERP_CRI, PM_Hodzic_Aromatics, PM_JPAC_MT3, BVOC_IsoMT3_emis, +COMMON$^{(c)}$	SOA as used in McFiggans et al. (2019)

Notes: $^{(a)}$ The simpler terms EmChem19a and EmChem19p are used in EMEP CTM rv4.35 (current at time of writing). $^{(b)}$ EMEP's default 'NPAS' scheme — see Sect. 5 and SI Table S2. $^{(c)}$ COMMON=Aqueous, Aero2017nx, ShipNOx, PM_FFireInert, SeaSalt, DustExtended, Ash, PM_WoodFFuelInert, BVOC_SQT_NV. See SI Table S1 for further explanation of these packages. $^{(d)}$ Loosely based upon Hodzic et al. (2016).

Table 6. Example content lines from ***GenIn_Species.csv*** input file.

Spec	Type	Formula	MW	DRY	WET	Groups	!Comments
OD	0	O	xx	xx	xx	xx	!
OH	0	OH	xx	xx	xx	xx	!
O3	1	O3	xx	O3	xx	OX	!
NO2	1	NO2	xx	NO2	xx	NOX;OX;OXN;daObs	!
HCHO	1	HCHO	xx	HCHO	HCHO	xx	!
CH3O2	1	CH3O2	xx	xx	xx	RO2	!
C2H5OOH	1	C2H5OOH	xx	ROOH	xx	xx	!
C5H8	1	C5H8	xx	xx	xx	BVOC	!
BVOCNO3	1	someNO3	199.99	xx	xx	nitrate;OXN	! demo species
C918NO3	1	C9H13NO5	215.2032	xx	xx	xx	!
RO2POOL	1	special	xx	xx	xx	xx	! Sum of RO2
BSOC_ng1e2	2	C	12	ALD	ROOH	CSTAR:0.1;DeltaH:30; OM25;PCM;BSOA	!
EC_f_wood_new	3	C	xx	PMf	ECfn	Extinc:ECn;EC_f;PMfine;...	!Primary wood burning $EC_{2.5}$

Note: commas and comment lines from file omitted for clarity.

6 Defining chemical mechanisms

Chemical mechanisms are defined in GenChem using three input files, which are themselves constructed from one or more files originating in the various sub-directories of the ***chem*** directory: ***GenIn_Species.csv***, ***GenIn_Shorthands.txt*** and ***GenIn_Reactions.txt***. In addition, a mechanism-specific emissplit file is needed in order to tell models how VOC emissions are to be split into individual compounds. These files are discussed below in Sect.6.1–6.4.

6.1 Chemical species and properties: *GenIn_Species.csv*

The ***GenIn_Species.csv*** file is typically created by either ***do.testChems*** or ***emep_setup.py***. As explained in Sect. 5 these scripts concatenate the Species.csv file from the 'base' mechanism with any 'Species' files found in the specified 'extra' mechanisms files. The resulting ***GenIn_Species.csv*** file is a spreadsheet-friendly comma-separated file where the characteristics of the chemical compounds are given. Table 6 gives some example entries, which we briefly discuss here. Referring to Table 6, the 'Spec' column is straightforward and gives the species name used in the model. The 'Type' is set to zero for short-lived (non-advected) species, 1 for simple advected species, 2 for semivolatile compounds (see Sect. 6.1.1), and 3 for compounds that react very slowly (e.g. CH_4). The chemical formula ('Formula') is mainly for information, though it can be used to estimate the molecular weight ('MW') if wanted, and can be used to keep track of e.g. the number of carbon atoms. The MW is also not essential for many compounds, but it is needed if compounds are emitted, or if outputs in mass-units (e.g. μg(N)/m^3) are wanted.

The ‘DRY’ and ‘WET’ deposition columns specify which compounds undergo such deposition, and which surrogate compounds are used, since the EMEP CTM calculates dry and wet deposition explicitly for only a limited number of compounds. For example, for dry deposition of O3 we simply use O3 since this is one of the explicitly calulated compounds, but for C2H5OOH we use the MEOOH surrogate. Note that for the semivolatile SOA species, the EMEP CTM will use this rate for the gas-phase fraction of the SOA; deposition of the particle phase is treated using the EMEP standard parameters for fine particles.

The ‘Groups’ column specifies which groups the species belongs to (e.g. OXN for oxidised nitrogen, RO2 for peroxy radicals) and allows surrogate species or factors to be assigned to these groups, e.g. Cstar:10.0;Extinc:0.4. It is important that these groups are separated by semi-colons, not commas. This rather powerful feature is discussed further in Sect. 6.1.2.

More detailed information on these entry types can be found in the readthedocs website (see Code Availabilty section at end).

6.1.1 Defining semivolatile species in ***GenIn_Species.csv***

As noted above, Type 2 in ***GenIn_Species.csv*** signifies semivolatile compounds, e.g. secondary organic aerosol (SOA) species. These are also subject to advection, but in addition they are semivolatile and exist in both gas and particulate phase. The EMEP CTM tracks such species by compound rather than phase, and calculates the partitioning between the phases dynamically, based upon the compound’s volatility (Bergström et al., 2012; Simpson et al., 2012). The approach used, the volatilty-basis-set (VBS) follows methods developed by Donahue et al. (2006), Robinson et al. (2007) and colleagues — see Bergström et al. (2012) and references therein for details. For GenChem purposes, species labelled with type 2 are accounted within the list of advected species, but the start and end of the semivolatile list is calculated by GenChem.py, to produce integer variables in the Fortran code which demarcate these semivolatile compounds, e.g. **FIRST_SEMIVOL=136** and **LAST_SEMIVOL=176**. (Note, GenChem will reorder different types of species to be consecutive, so despite the order of species in the ***GenIn_Species.csv*** file, all type-2 species will lie together in the index range **FIRST_SEMIVOL=136:LAST_SEMIVOL=176**.)

Type 2 (SOA) species require specification of their effective saturation concentrations (C^*) and the enthalpies of vaporization (Δ H_{vap}), following normal VBS principles. These specifications are made using the ‘Group’ methods described next.

6.1.2 Defining Groups in ***GenIn_Species.csv***

The ‘Groups’ mechanism plays an important role for feeding key information to the EMEP ~~/ESX~~ CTM or boxChem. Some groups are indeed essential — for example, in EmChem19a, CRIv2R5Em and MCMv3.3Em, the RO2_GROUP needs to be set correctly to get the correct concentrations of the special RO2POOL concentration, and the deposition of groups of compounds (e.g. oxidised nitrogen deposition) depends on those compounds being correctly identified by their groups. Groups have to be separated by a semicolon, and there are two types of group labels for a specific species:

(i) simple name, e.g. OXN — indicates here that this species ~~that belong to a group, in this case~~belongs to the group of oxidised nitrogen compounds. In the CTM code, the members of one group are easily accessible so they can be treated specially (see Sect. 7.3).

(ii) compound groups which specify numerical or character values to pass specific properties, e.g. the groups CSTAR:0.1 and DeltaH:30 for BSOC_ng100, or Extinc:ECn for EC_f_wood_new in Table 6.

If a species is both a member of a type (i) group and has a (wet or dry) deposition surrogate, additional WDEP or DDEP groups will be automatically generated, e.g. `DDEP_OXN_GROUP`.

The specification of numerical or character values (group type (ii)) is indicated with a colon notation (as opposed to the semicolon used to separate groups). For example, SOA species which use the VBS system require specification of their effective saturation concentrations at 298K (C*, in μg m^{-3}) and the vaporization enthalpies (Δ H$_{vap}$, in kJ mol^{-1}), or for aerosol optical absorption we need extinction coefficients. These specifications are simply set through the groupings Cstar, deltaH and Extinc, with e.g. Cstar:1.0e-2;deltaH:30.0 for SOA, and Extinc:SO4 for sulphate. Sect. 7.3 provides further explanation of such groups.

These groupings are not hard-coded in GenChem, and may or may not be used by any CTM, so this system provides an easily extensible mechanism for introducing new characteristics into modelling systems.

6.2 Defining Chemical reactions, A) *GenIn_Shorthands.txt*

Firstly, we can note that in the EMEP CTM and boxChem systems, some key variables have special names, and can be used in either the ***GenIn_Shorthands.txt*** or the ***GenIn_Reactions.txt*** files. The variables which are known to the EMEP CTM and GenChem codes are: **TEMP** (temperature), **TINV** (inverse temperature), **M**, **O2**, **N2** and **H2O** (concentrations of air, oxygen, nitrogen and water vapour).

Other short-hand notation is often used in ***GenIn_Reactions.txt*** (Sect. 6.3), and this has to be defined first in the ***GenIn_Shorthands.txt*** file. For example, we might use **KHO2RO2** as a generic rate coefficient for $\mathrm{HO2} + \mathrm{RO2}$ reactions. The shorthand **LogTdiv300** is also frequently used for the common expression log(TEMP/300). The ***GenIn_Shorthands.txt*** file is typically created by either ***do.testChems*** or ***emep_setup.py***, and these scripts concatenate the file generic_Shorthands.txt from the **chem** directory and the chemistry-specific files, e.g. **chem/base_mechanisms/EmChem19a_Shorthands.txt**, to produce the needed GenChem input file.

The name and the expression for a shorthand have to be separated by whitespace for GenChem to process it. Names of species can also be used in shorthands expressions. Figure 4 illustrates several examples, including how short-hands defined earlier can be re-used in the same system — as done for the MCM example in producing the KMT08 variable. The last example, for KMT3, also illustrates that the right-hand side can be a function, which of course needs to be compatible with the Fortran code of the calling code.

```
FH2O                 (1.0+1.4e-21*h2o*exp(2200*TINV))
*
K80                  3.2e-30*M*(TEMP/300)**(-4.5)
K8I                  3.0e-11
KR8                  K80/K8I
FC8                  0.41
NC8                  0.75-1.27*(LOG10(FC8))
F8                   10**(LOG10(FC8)/(1+(LOG10(KR8)/NC8)**2))
KMT08                (K80*K8I)*F8/(K80+K8I)
KMT3_OH_HNO3         KMT3(2.4e-14,460.,6.5e-34,1335.,2.7e-17,2199.)
```

Figure 4. Selected lines from the input file, ***GenIn_Shorthands.txt***

```
TROE_OH_NO              : OH + NO = HONO ; Ref1
1.44e-13+M*3.43e-33     : [OH]   + CO_FIRE   =    ;  tracer
2.2e-10                 : OD + <H2O> = 2. OH        ; A97,J
TROE_NO_OP              : OP + NO  + {M}   = NO2      ; A97,J
1.36e-11                : [OXYL] + [OH] = |YCOXY(0)|  ASOC_ug1  + ...
```

Figure 5. Selected lines from the input file, ***GenIn_Reactions.txt***

6.3 Defining Chemical reactions, B) *GenIn_Reactions.txt*

The ***GenIn_Reactions.txt*** file is typically created by either ***do.testChems*** or ***emep_setup.py***, which concatenate the appropriate ***Reactions.txt*** file from the wanted **chem/base_mechanisms** directory (e.g. **chem/base_mechanisms/EmChem19a_Reactions.txt**) and those from the wanted **chem/extra_mechanisms** directories. The ***GenIn_Reactions.txt*** file contains the chemical reactions, with format:

```
rate coefficient : reaction ; [optional comment]
```

and with the reaction consisting of reactants and products, along with their stoichiometric factors as appropriate. The semicolon marks the end of the reactions, and whitespace is needed between all terms, e.g. between a stoichiometric factor and a species. Some typical lines are given in Fig. 5. The first line here is trivial, in the sense that OH, NO, and HONO are all normal chemical species as defined in ***GenIn_Species.csv***, and GenChem will add production and loss terms appropriately for each, with a reaction rate given by the TROE_OH_NO shorthand.

GenChem is flexible as to whether products are written explicitly or with stoichiometric coefficients (i.e. 2 OH is the same as OH + OH). Non integer stoichiometric coefficients are allowed, since we often condense multiple branches of a reaction into one equation for CTM use.

6.3.1 The funny brackets [], <>, {} and ||: constant, fixed and helper species, and yield modifiers

Four types of brackets are used in ***GenChem_Reactions.txt*** files to modify the way compounds or yields are handled:

[*constant_species*]: The second reaction of Fig. 5 illustrates a nice feature of GenChem; concentrations of species such as OH which are key parts of the photochemical reaction mechanism can be treated as constants over a time-step in this particular reaction. In this way tracers are easily added. ~~here a tracer of biomass burning CO, which we can track in the EMEP CTM. This~~ In this example the CO_FIRE tracer is emitted along with the 'real' CO, but its existence is not allowed to affect the standard photochemistry. The [] around the OH signifies that this CO tracer has a chemical loss due to OH, but that we do not allow the model's OH to be degraded by this artificial species. The lack of products in this example also signifies that we do not track the products of this loss, just the CO_FIRE itself.

< *fixed_species* >: The third example from Fig. 5 illustrates the use of <> notation. In this case, the species within the angle-brackets is not one of the chemical compounds tracked or changed by the ~~CTM,~~chemical solver, but is rather a compound whose whose concentration is effectively constant during a simulation time step and set by the EMEP and/or boxChem codebased upon humidity and pressure from the meteorological model. (In the KPP system these species are defined as 'DEFFIX' compounds, Sandu and Sander 2006). The compounds used so far in this way are H2O, N2, O2 and M (air molecules). This last line could equivalently have been written:

Example 6.1. `2.2e-10*H2O : OD = 2. OH ;`

where the H2O concentration now applies as a simple part of the rate coefficient. (This is actually exactly the way GenChem handles this internally).

{ *helper_species* }: The fourth reaction in Fig. 5 shows another type of special notation. Species within curly brackets are not used in any way, but they can be added to the reactions as helpful comments illustrating reactants, whose concentrations are already included in the rate expression — in the example the TROE_NO_OP rate expression takes into account the pressure (i.e. [M]) dependence for this 3-body reaction.

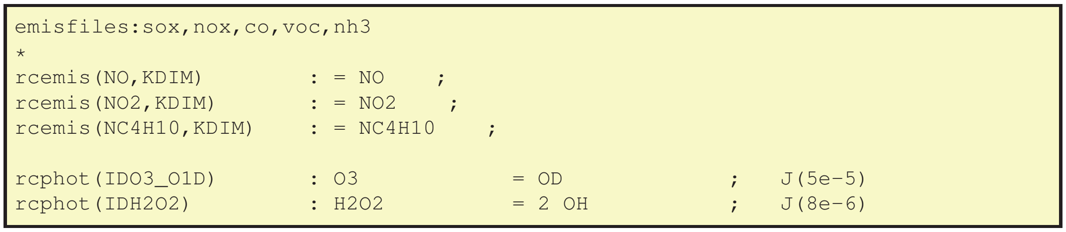
| *yield-modifier* |: The final reaction of Fig. 5 illustrates the use of || brackets. These are sometimes used in the reaction schemes for secondary organic aerosol, as seen here for the production of the semivolatile ASOC_ug1 species. The contents of || represent yield expressions which will be updated each time-step in the chemical solver. ~~boxChem or the EMEP CTM.~~ The output CM_Reactions2.inc file for this case includes the term:

Example 6.2. `P = YCOXY(0)* 1.36e-11 * xnew(OXYL) * xnew(OH)`

These variables (here YCOXY(0)) must be predefined in the appropriate Fortran system (boxChem or EMEP CTM) in order for box_setup.py or emep_setup.py to achieve successful compilation.

6.3.2 Adding emissions in *GenIn_Reactions.txt*

When using emissions in ***GenIn_Reactions.txt***, the labels used for associated emission files have to be defined in a special line, e.g. ***emisfiles:sox,nox,co,voc,nh3*** as in the first line of Fig. 6. These emission labels (e.g. nox) are those used in EMEP



```
emisfiles:sox,nox,co,voc,nh3
*
rcemis(NO,KDIM)         : = NO     ;
rcemis(NO2,KDIM)        : = NO2     ;
rcemis(NC4H10,KDIM)     : = NC4H10     ;

rcphot(IDO3_O1D)        : O3             = OD              ;    J(5e-5)
rcphot(IDH2O2)          : H2O2           = 2 OH            ;    J(8e-6)
```

Figure 6. Emissions and photolysis lines from the input file, ***GenIn_Reactions.txt***

for emission input files, and also the file endings for the respective emissplit file, see Sect. 6.4. Other labels can easily be used and defined, as long as the emissplit system exists to convert these groups into model species (e.g. nox into NO and NO2, or voc into C2H6, NC4H10, etc.).

The next three lines in Fig. 6 are examples for emission reactions: the reaction rate is denoted as **rcemis(SPECIES,KDIM)** and there is no reactant in the reaction. GenChem will replace KDIM with the vertical cordinate, assumed to be k, in the Fortran code, e.g. giving **rcemis(NO,k)**.

Biogenic VOC (BVOC) emissions are special, in that specific functions exist in the EMEP model for dealing with the light, temperature, and other dependencies of these (see e.g. Simpson et al., 2012). In the **extra_mechanisms** files used for the EMEP CTM setup, we use the 'rcbio' functions as shown in Fig. 7.

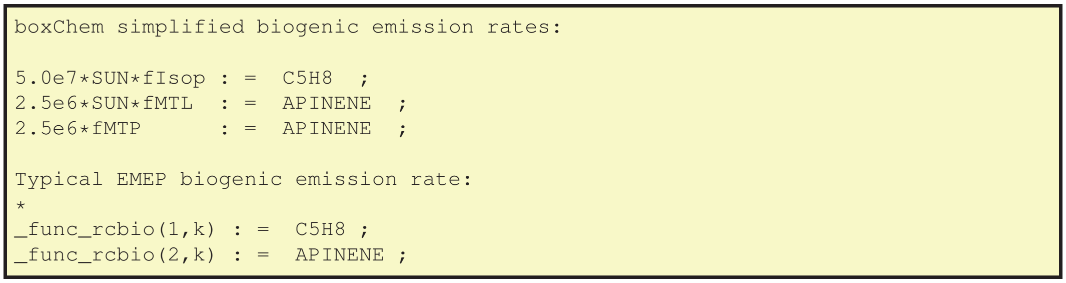
When using boxChem, a very simplified system is used for BVOC emissions, illustrated also in Fig. 7. The 'SUN' variable (borrowed from the KPP system) allows for simple variation of emissions with zenith angle (and gives zero emissions at night, when SUN=0, and maximal emissions at noon, when SUN=1). The numerical coefficients (5.0e7 or 2.5e6) correspond to typical emission rates (units are molecules cm^{3} s^{-1}, see the appropriate mechanism file for species), and the fIsop, fMTL and fMTP factors , which are set in config_box.nml, provide the possibility to scale these emissions. For example, light dependent emissions for MT can be reduced by 50% set using fMTL=0.5, and light-independent ('pool') emissions set to zero by setting fMTP=0.0.

6.3.3 Adding photolysis reactions in *GenIn_Reactions.txt*

The reaction rates of photolysis reactions are denoted as **rcphot(PHOT_ID)**. GenChem will automatically add the 'k' dependency on the vertical level to the photolysis rate (e.g. to give **rcphot(IDH2O2,k)**). The index variables (e.g. **IDO3_O1D**) refer to photolysis rates as defined in the EMEP/boxChem codes.

6.4 Emissions speciation: emissplit files

Emissions are often provided to models for groups of compounds, e.g. NOx for NO & NO$_2$, and NMVOC for non-methane volatile organic compounds. These emissions need to be assigned to individual chemical compounds, and converted from mass to number using the appropriate molecular weight.



```
boxChem simplified biogenic emission rates:

5.0e7*SUN*fIsop : =  C5H8  ;
2.5e6*SUN*fMTL  : =  APINENE  ;
2.5e6*fMTP      : =  APINENE  ;

Typical EMEP biogenic emission rate:
*
_func_rcbio(1,k) : =  C5H8 ;
_func_rcbio(2,k) : =  APINENE ;
```

Figure 7. Biogenic emissions lines from input files used in ***GenIn_Reactions.txt***, for either EMEP or boxChem setups

The default files for sox, nox, co and nh3 are identical across all provided schemes, and provided in the input/emissplit_defaults directory as files such as emissplit_defaults_nox.csv. For NMVOC and PM inventories specific files are needed for each chemical mechanism, and sometimes depending on available inventories.

Default NMVOC emission splits are provided in GenChem for 11 different source categories (covering traffic, agriculture, etc), according to the so called ‘SNAP’ classifications. The provided data are based upon average UK emission profiles from Passant (2002) and emissions from 2010, and have been adapted in this work for each base chemistry scheme.

For GenChem we provide such NMVOC files for all supported chemical mechanisms, in the appropriate directory. Thus, for EmChem19a the file for NMVOC emissions would be named EmChem19a_emissplit_defaults_voc.csv. For boxChem testing the do.GenChem or do.testChems scripts will move this file to inputs/emissplit_run and also copied to ZCMBOX_EmChem19a/emissplit_run and rename to simple emissplit_defaults_voc.csv. If emep_setup.py is used, the emissplit_run dircetory is copied to ZCM_EmChem19a/emissplit_run.

In the EMEP CTM it is common for these default values to be overridden by ‘emissplit_specials’ files which can assign country and sector-specific NOx, NMVOC and PM profiles. Such profiles need to be generated by the EMEP CTM user, however, and are not part of GenChem. An example of this system, and such emission splits, is given in the Supplementary Information, Table S5, of Simpson et al. (2012). Also in boxChem, users may of course modify any of these emissplit files - see Sect. S2.3 in Supplementary information.

7 GenChem outputs: Fortran modules and include files

The main purpose of the GenChem system is to convert chemical equations into Fortran code suitable for use in the boxChem and/or EMEP CTM systems. The output files, prefixed with CM_ to denote chemical mechanism, are summarised in Table 1, and discussed in the relevant section below.

7.1 CM_ChemDims_mod.f90 — the dimensions of the chemical system

The ***CM_ChemDims*** module provides basic information (Fig. 8) about the dimensioning of the chemical system, giving for example the total number of species (NSPEC_TOT), photolysis rates (NPHOTOLRATES) or emission files (NEMIS_File).

```
  ! NSPEC for TOT : All reacting species
  integer, public, parameter :: NSPEC_TOT=120
  integer, public, parameter :: NSPEC_ADV=117
  integer, public, parameter :: NSPEC_SHL=3
  integer, public, parameter :: NSPEC_SEMIVOL=23
  integer, public, parameter :: NDRYDEP_ADV = 55
  integer, parameter, public :: NPHOTOLRATES = 17
  integer, parameter, public :: NEMIS_File = 7
  integer, parameter, public :: NEMIS_Specs = 32
```

Figure 8. Selected lines from the output file CM_ChemDims_mod.f90 file. (The actual file has comments for each entry.)

```
  integer, public, parameter :: &
      OD           =   1  &
    , OP           =   2  &
    , OH           =   3  &
...
 !+ Defines indices and NSPEC for ADV : Advected species

  integer, public, parameter :: NSPEC_ADV=79
  integer, public, parameter :: FIRST_ADV=29, &
                                  LAST_ADV=79

  integer, public, parameter :: &
      IXSHL_OD           =    1   &
    , IXSHL_OP           =    2   &
...

  integer, public, parameter :: &
      IXADV_O3           =   29   &
    , IXADV_NO           =   30   &
...
SOMETHING ON  SEMIVOL
```

Figure 9. Selected lines from the GenChem-produced file, CM_ChemSpecs_mod.f90.

7.2 CM_ChemSpecs_mod.f90 — chemical compounds information

This file specifies basic information about the chemical compounds, in terms of number, indices and some chemical characteristics. Extracts of the file are shown in Fig. 9 and Fig. 10. As seen in Fig. 9, this module provides the simpe indices which represent the chemical compounds in the EMEP systems, e.g. OH = 3. Indices are additionally provided for the short-lived and advected species (IXSHL_ indices, and IXADV_ indices).

One subroutine, define_chemicals, is generated in this module, which sets the contents of a Fortran derived type array named 'species'. The 'species' derived type (c.f. Fig. 10) contains the following elements: name, molwt, nmhc, carbons, nitrogens, and sulphurs. This routine is called in the initialisation of the CTM, and thereafter this array provides useful information on each species, e.g. species(HNO3)%molwt is the molecular weight of HNO3 and species(C5H8)%carbons the number of carbon

```
   !+
   ! Assigns names, mol wts, carbon numbers, advec,  nmhc to user-defined Chemical
   !                                     MW  NM   C    N   S
    species(OD ) = Chemical("OD␣␣",  16.0000,  0,  0,   0,  0 )
...
    species(O3 ) = Chemical("O3␣␣",  48.0000,  0,  0,   0,  0 )
...
   SOME MORE COMPLEX; e.g. SOA

   THINK ABOUT Cstar here vs new GROUPs
```

Figure 10. Selected lines from the species array defined in the GenChem-produced file, CM_ChemSpecs_mod.f90

```
  integer, public, target, save, dimension (13) :: &
    RO2_GROUP = (/  &
      HO2, CH3O2, C2H5O2, SECC4H9O2, ISRO2, ETRO2, PRRO2, OXYO2,  &
      MEKO2, MALO2, MVKO2, MACRO2, MACO3  &
    /)
....
  integer, public, target, save, dimension (5) :: &
    WDEP_OXN_GROUP = (/ HNO3, HONO, NO3_f, NO3_c, XHNO3 /)

....
  integer, public, target, save, dimension (2) :: &
    BVOC_GROUP = (/ C5H8, APINENE /)
```

Figure 11. Selected lines from the GenChem-produced file, CM_ChemGroups.

atoms in C5H8. The nmhc element identifies if a species is a non-methane hydrocarbon (nmhc=1) or not (nmhc=0). This file also defines pointers to the advected, short-lived and semi-volatile species list, which are used in the EMEP CTM.

7.3 CM_ChemGroups_mod.f90 — Fortran arrays for the groups

As noted in Sect. 6.1.2, GenChem makes use of the information provided in the Groups column of GenIn_Species.txt to produce Fortran arrays, e.g. OXN_GROUP would include all oxidised nitrogen compounds specified with OXN in the Group column (See Fig. 11 for more examples). These groups are also accessible through a Fortran pointer system, e.g.

```
   chemgroups(1)%name="RO2"
   chemgroups(1)%ptr=>RO2_GROUP
...
   chemgroups(7)%name="DDEP_OXN"
   chemgroups(7)%ptr=>DDEP_OXN_GROUP
```

which allows the EMEP CTM to access and perform actions on these groups without having to 'know' the names of the species involved. For example, dry-deposition of all OXN species can be formulated in the model as a simple loop over all

```
...
real , public , target , save , dimension (23) :: &
   DELTAH_GROUP_FACTORS = (/   &
     30.0, 30.0, 30.0, 30.0, 30.0, 30.0, 30.0, 30.0, 30.0, 30.0,   &
     30.0, 30.0, 30.0, 30.0, 30.0, 30.0, 30.0, 30.0, 30.0, 30.0,   &
     112.0, 112.0, 112.0   &
   /)

...
real , public , target , save , dimension (23) :: &
 character(len=TXTLEN_SHORT), public , target , save , dimension (14) :: &
   EXTINC_GROUP_MAPBACK = [ character(len=TXTLEN_SHORT) :: &
   ”SO4”, ”NO3_f”, ”NO3_c”, ”NH4_f”, ”ECn”, ”ECa”, ”PMCO”,   &
     ”ECn”, ”ECa”, ”PMCO”, ”DDf”, ”DDc”, ”EC”, ”DDf”   &
   ]
```

Figure 12. Further lines from CM_ChemGroups_mod.f90, illustrating the numerical or string values associated with type (ii) compound groups, see Sect. 6.1.2.

```
integer, public, parameter :: NDRYDEP_ADV = 21
type(depmap), public, dimension(NDRYDEP_ADV), parameter :: DDepMap = (/ &
  depmap(IXADV_O3          , "O3␣␣␣␣␣␣␣␣", -1) &
 ...
, depmap(IXADV_HCHO        , "HCHO␣␣␣␣␣␣", -1) &
, depmap(IXADV_CH3CHO      , "ALD␣␣␣␣␣␣␣", -1) &
 ...
```

```
integer, public, parameter :: NWETDEP_ADV = 12
type(depmap), public, dimension(NWETDEP_ADV), parameter :: WDepMap = (/ &
  depmap(IXADV_HNO3        , "HNO3␣␣␣␣␣␣", -1) &
 ...
, depmap(IXADV_NH3         , "NH3␣␣␣␣␣␣␣", -1) &
 ...
```

Figure 13. Selected lines from the output file, CM_DryDep.inc, CM_WetDep.inc.

the compounds in either DDEP_OXN_GROUP_OXN or, equivalently, by finding the index of DDEP_OXN in chemgroups and following the Fortran pointer to the array of indices.

The more complex type (ii) compound groups discussed in Sect. 6.1.2, in which numbers or character strings are associated with a group, result in further arrays in CM_ChemGroup_mod.f90 which provide access to these data. Fig. 12 illustrates some examples of this.

7.4 CM_DryDep.inc, CM_WetDep.inc — mapping individual chemical species to dry and wet deposition surrogates

Species which have had dry or wet-deposition surrogates specified in the ’DRY’ or ’WET’ column of GenIn_Species.txt are listed as part of a Fortran derived type (depmap) in the output files CM_DryDep.inc and CM_WetDep.inc using code such as in Fig. 13, where the first entry is the index of the species in the ~~EMEP model’s~~ list of advected species, and the second entry is the surrogate species as discussed in Sect. 6.1. The last entry can be used to set fixed values of deposition velocity (although this is not typically done for the EMEP CTM). This listing is then used by the EMEP CTM as part of the standard deposition calculations.

7.5 CM_Reactions1(2).inc. CM_Reactions.log — the chemical reactions code

Sect. 1, Fig. 1, has already presented an example section from the file ***CM_Reactions1.inc***. This file generally comprises such production and loss terms (P, L) for all, or the majority, of the model's chemically reacting species. The terms xold and xnew in this example represent the original and updated concentrations arising from the TWOSTEP Gauss-Seidel calculations for the timestep dt2. For those slowly-reacting species such as CH4, a second file ***CM_Reactions2.inc*** is produced with the same type of equations, but which can lie outside of the iteration loop in the EMEP system, e.g. the EMEP CTM code can be summarised as:

```
do iter = 1, NITER
  include 'CM_Reactions1.inc'
end do
include 'CM_Reactions2.inc'
```

The file CM_Reactions.log is not needed by the EMEP CTM, but is output as a valuable help-file, containing a listing of all the chemical reactions, along with their index in the 'rct', 'rcphot' and 'rcemis' arrays as appropriate. Equations which were specified with simple constant values (e.g. 1.0e-5) are also reported here with the 'k' indicator and rate.

7.6 CM_ChemRates_mod.f90 — setting the reaction rates

CM_ChemRates_mod.f90 is the module where all chemical rate-coefficients and photolysis rates are calculated (this is done every advection step in the EMEP CTM for example). The module is entirely written by GenChem, and produces two subroutines:

- setChemRates
- setPhotolUsed

Typical lines of ***CM_ChemRates_mod.f90*** are shown in Fig. 14. This Figure also illustrates how the model makes use of the defined meteorology-associated arrays temp, tinv, rh and Log300divT (Sect. 6.2). The setPhotolUsed array routine is much simpler, in that it just lists the indices used, e.g.

Example 7.1. `photol_used = (/ IDO3_O3,IDO3_O1D, ... /)`

```
  subroutine setChemRates()

    rct(1,:) = ((5.681e-34*EXP(-2.6*(LOG(TEMP/300))))*O2)*M
    rct(2,:) = (1.8e-11*EXP(107.0*TINV))*N2
....
    rct(65,:) = KAERO(RH)
    rct(66,:) = (IUPAC_TROE(1.0e-31*EXP(1.6*LOG300DIVT),  &
              & 3.0e-11*EXP(-0.3*LOG300DIVT),  &
              & 0.85,  &
              & M,  &
              & 0.75-1.27*LOG10(0.85)))
....
```

Figure 14. Selected lines from the output file, CM_ChemRates_mod.f90.

```
integer, parameter, public :: NEMIS_File = 5
character(len=3), save, dimension(NEMIS_File), public :: EMIS_File = (/ &
  "sox" , "nox" , "co␣" , "voc" , "nh3"  /)
```

Figure 15. Selected lines from the output file, CM_EmisFile.inc.

7.7 CM_EmisFile.inc — listing emission files

The last file simply lists the names used for input emission files. By tradition the EMEP system has used lower case for these emission markers. The names used are triggered by the ’emisfiles:’ line of GenIn_Reactions.txt as discussed in Sect. 6.3. Other typical emissions that might be used, depending on the application and available inventories are pm25 (fine particulate matter), or ec, oc, or pom (elemental and organic carbon, or primary organic matter).

8 Conclusions

This paper outlines the structure and usage of the GenChem system, which includes a chemical pre-processor (GenChem.py) for converting chemical equations into differential form for use in atmospheric chemical transport models (CTMs). Although primarily intended for users of the EMEP CTM and related systems, GenChem also features a simple box-model testing system (boxChem), which can run as a stand-alone chemical solver, enabling for example easy testing of chemical mechanisms against each other. GenChem has been developed and tested in a Linux environment, but can be run in virtual environments on Windows or other architectures.

The mechanisms included now reflect those used or made available for the EMEP CTM, as well as the MCM scheme which works in the boxChem mode. The EmChem19a-vbs scheme is the default mechanism used in the EMEP CTM, but we include slightly adapted versions of CB6 which is used in the widely used CAMx model (http://www.camx.com) or CMAQ (Luecken et al., 2019), and CRIv2-R5 scheme which is used in STOCHEM (Archibald et al., 2010; Khan et al., 2015). It is hoped that some of the other widely-used mechanisms can be added in future, for example the MOZART scheme (Emmons et al., 2010;

Surendran et al., 2015), the RACM scheme (Stockwell et al., 1997; Goliff et al., 2013), or SAPRC-07 (Carter, 2010) which is also used in CMAQ (https://www.airqualitymodeling.org/index.php/CMAQv5.1_Mechanisms).

As provided here, GenChem is already a useful tool to explore different chemical mechanisms, both for gas-phase and simple (EMEP-compatible) aerosol phase systems. For example, Fig. 3 showed one comparison between the EMEP CTM's EmChem19a scheme and the far more advanced CRIv2R5Em and MCMv3.3Em schemes, and Bergström et al. (2020a) provide many more. Such comparisons will greatly aid the development of new EMEP mechanisms, or indeed for comparison of any mechanisms of interest to users.

In future new and/or updated chemical mechanisms will be added as well as utility scripts to simplify result analysis, and to convert between GenChem and other formats, such as those used in KPP (Damian et al., 2002), the MCM website, FACSIMILE (Curtiss and Sweetenham, 1987) or more recently PyBox (Topping et al., 2018).

Code availability. The code needed to run the GenChem system is released as open-source code under the GNU license, (https://github.com/metno/genchem), with the user-guide provided at https://genchem.readthedocs.io. The EMEP MSC-W CTM can be found at https://github.com/metno/emepctm

Author contributions. DS wrote the original perl version of the GenChem script, and has written much of the Fortran and python code of the more extensive GenChem/boxChem systems. AB wrote the first python version of GenChem.py. RB worked with the chemical mechanisms, HI, JJ worked with and improved many scripts from the GenChem system, including conversion of CRI and MCM codes to GenChem format. MP added the Docker functionality and helped test the code on Windows. AMV added the Pollen module, and also contributed to some code developments. All authors contributed to the paper.

Competing interests. The authors declare that they have no conflict of interest.

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Supplementary material:

GenChem v1.0 – a chemical pre-processing and testing system for atmospheric modelling

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S1. extra_mechanisms used in boxChem and EMEP

The ***extra_mechanisms*** system allows for a large number of extra chemical packages to be added to a given base mechanism, in a mix n' match system. Thus, one may include, exclude, or change various reaction and emissions schemes, for example related to SOA or PM. Tables S1–S2 give a brief summary of the main extra mechanisms available in the GenChem v1.0 release, as used in boxChem and EMEP CTM modelling. Extra information on each package can usually be found in the README.md files accompanying the Species and Reactions files of each mechanism.

S2. User-defined chemical schemes

Adding and modifying chemical mechanisms is rather easy in the GenChem system. We take the example of a gender-neutral user Jan, who wants to add a gas-phase chemistry ***JansChem*** ~~and a SOA mechanism~~ for EMEP usage. ~~JansSOA~~. The steps needed are as follows.

S2.1 Own chemical mechanisms

Jan is of course free to add new mechanisms to **base_mechanisms** and **extra_mechanisms**. Just follow the formatting guidelines and examples from the currently available mechanisms. Start testing from a temporary boxChem directory, following Sect. 3, which in our example means:

Example S1.1.

```
scripts/box_setup.py tmp_work
```

Then, from tmp_work:

Example S1.2.

```
./do.testChems JansChem
```

Once the code compiles and runs fine with do.testChems, the next step for those wanting to run the EMEP model is to modify emep_setup.py, as described below.

S2.2 Modification of emep_setup.py

Jan can then edit ***emep_setup.py*** (maybe renaming it as ***Jans_setup.py***, but we retain ***emep_setup.py*** below). If selecting from the provided base_mechanisms and extra_mechanisms you only need to extend the possible command lines as provided by the **cmdx** dictionary in that script.

The -b argument gives the base mechanism (only one allowed), and then the -e argument allows the addition of any number of compatible extra mechanisms. Any keys from ***cmdx*** can be used by ***emep_setup.py***, e.g. if our user Jan has their own gas-phase chemical scheme (***JansChem***) one could edit ***emep_setup.py*** a new option::

Example S2.3. ***`cmdx['JansChem'] ='-b JansChem -e common'`***

Jan could then do::

Example S2.4. ***`emep_setup.py JansChem`***

Example S2.4 creates the directory ZCM_JansChem with all the files needed for EMEP runs. These files can then be transferred directly to the EMEP system in the same way as is done for the pre-defined mechanisms (Sects. 3, 4). Note that ***emep_setup.py*** has a number of differently defined verions of ‘common’ with regard to extra mechanisms; the user should assess carefully which is needed.

S2.3 Modification of emissplit files

As noted in Sect. 6.4, the default emissplit files for sox, nox, co and nh3 are identical across all provided schemes, and provided in the input/emissplit_defaults directory as files such as emissplit_defaults_nox.csv. For NMVOC and PM inventories specific files are needed for each chemical mechanism, and sometimes depending on available inventories. In these emissplit files, splits are given for each of the 11 SNAP sectors, so that for example SNAP1 (power generation) has very different splits from SNAP7 (road traffic).

In the EMEP CTM these default speciations are usually replaced by country-specific values derived from more recent emission inventories, but for input to boxChem a much simpler procedure is used. For boxChem these SNAP splits are merged into one NMVOC speciation using the relative emissions for each SNAP given by average UK emission profiles from Passant (2002) and emissions from 2010. The procedure and SNAP fractions used can be found in the Fortran module ***EmisGet_mod.f90***. In principle the user could modify the numbers used in ***EmisGet_mod.f90***, but since boxChem users just need an overall NMVOC speciation the simplest approach is to give each SNAP sector the same NMVOC split. Then the weighted NMVOC split will also be given these values.

Thus, a user-configured emissplit file can be used, ideally stored with a different name and in a different directory to the boxChem defaults. The directory with these new emissplit files can be set in config_box.nml.

Table S1. extra_mechanism packages provided by GenChem 1.0 for boxChem

BoxAero	Simple reactions for SO2 oxidation and gas-aerosol uptake of N2O5 and HNO3.
BoxDep	Simple deposition reactions, for HNO3, SO2, O3, and NO2
BVOC_IsoMT1_emis	Emissions of isoprene and α-pinene†

Notes:

† This simple package is provided for both boxChem and EMEP since all base-mechanisms can handle isoprene and α-pinene chemistry, and often α-pinene is used as a surrogate for all monoterpenes. For use of more complex BVOC mixtures (e.g. with β-pinene, limonene, etc), the user may replace this package with a more complex emission package.

Table S2: extra_mechanism packages provided by GenChem 1.0 for EMEP CTM modelling

General extras	
Aero2017nx	Adds aerosol uptake[a] of N2O5, NO3, HNO3, HO2, H2O2 and CH3OOH
Ash	Volcanic ash tracers (fine and coarse)
Aqueous_EmChem16x	Gas and aqueous phase reactions converting SO2 to SO4
DustExtended	Emissions of Dust_f and Dust_c
PM_FFireInert	Emissions of inert species ffire_OM, ffire_BC and ffire_remPPM25
PM_WoodFFuelInert	Emissions of inert POM, EC and other components
Pollen	Emissions of pollen[b] from birch, olive, ragweed and grass
SeaSalt	Emissions of SeaSalt_f and SeaSalt_c
ShipNOx	Adds 'shipNOx' compound and its reactions for dealing with NOx plumes from shipping[c]
Biogenic VOC (BVOC) options	
BVOC_IsoMT1_emis	Emissions of C5H8 and α-pinene[d]
BVOC_IsoMT2_emis	Emis. C5H8, α-pinene, and β-pinene, can be used with CRIv2R5Em
BVOC_IsoMT3_emis	Emis. C5H8, α- and β-pinene, and other monoterpenes (XTERP), can be used with extended EmChem19 or CRIv2R5Em schemes
BVOC_XTERP_CRI	Reactions of "other monoterpenes" (XTERP) for use with CRIr2V5Em (optional)
BVOC_SQT_NV	Adds simple sesquiterpene emissions — treated as immediately transformed into non-volatile (particulate) secondary organic aerosol (SQT_SOA_NV)
BVOC_ExtraMTs	Reactions of β-pinene and XTERP for use with EmChem19a if BVOC_IsoMT3_emis is used
Secondary Organic Aerosol, SOA-associated extras	
PM_VBS_EmChem19	EMEP standard volatility basis set (VBS) SOA reactions for EmChem19-like chemistry[e] (can also be used with CRIv2R5Em); includes ASOA/BSOA from α-pinene surrogate
PM_VBS_ExtraMTs	VBS BSOA reactions for (extended) EmChem19 and CRIv2R5Em-like schemes, for β-pinene and XTERP; simple extension of [e] with additional monoterpenes

(continued on next page)

Table S2 cont.

PM_VBS_CB6r2Em	ASOA/BSOA reactions for CB6r2Em; adaption of PM_VBS_EmChem19 to CB6r2Em
PM_Hodzic_EmChem19	SOA formation reactions for EmChem19-like chemistry$^{(f)}$
PM_Hodzic_Aromatics	ASOA formation from aromatics, for CRIv2R5Em scheme$^{(f)}$
PM_Hodzic_BPINENE	BSOA formation from β-pinene, for extended EmChem19a (using BVOC_ExtraMTs) or CRI schemes$^{(f)}$
PM_Hodzic_XTERP	BSOA formation from XTERP monoterpene surrogate, for extended EmChem19a (using BVOC_ExtraMTs) or extended CRI schemes (using BVOC_XTERP_CRI)$^{(f)}$
PM_Hodzic_CB6	ASOA and BSOA formation reactions for CB6r2Em$^{(f)}$
PM_JPAC_MT3	Semi-empirical BSOA formation reaction for $\mathrm{C5H8}$, α- and β-pinene, and XTERP, as used in McFiggans et al. 2019 (combined with PM_Hodzic_Aromatics)

Notes: $^{(a)}$ c.f. Stadtler et al. (2018); Simpson et al. (2018); $^{(b)}$ c.f. Sofiev et al. 2017; $^{(c)}$ Simpson et al. (2015); $^{(d)}$ As in boxChem, Table S1. $^{(e)}$ Default is 'NPAS' VBS scheme used, see Sect. 5, Simpson et al. (2012); $^{(f)}$ Loosely based upon VBS system by Hodzic et al. (2016).

S3. Time-steps for boxChem simulations

The config_box.nml file allows for a user-defined 'external' time-step, dt, which is typically set at 30 seconds. This time-step governs the frequency at which emissions, photolysis, and rate-coefficients are updated. The chemical solver (ChemSolver) is called once per dt time-step, but then ChemSolver implements between 5–15 sub-timesteps. First, 5 very short time-steps (between 0.2 to 1 s, depending on dt) are used to bring the chemistry into rapid equilibrium, and then 5–10 longer timesteps are used for the remainder of dt.

Using calculations with dt=1 s as a reference (which gives an internal dif time-step dt_i of 0.2 s), we have calculated the relative root mean square error, $RRMS_k$, for several key species k for dt ranging from 3 s to 600 s. $RRMS_k$ is defined as:

$$RRMS_k = \sqrt{\frac{\sum_{n=1}^{N}(c_k^n(1) - c_k^n(dt))^2}{\sum_{n=1}^{N}(c_k^n(1))^2}}$$

where $c_k^n(dt)$ is the calculated concentration of species k at hour n with timestep dt (in seconds). In the examples presented here, we use a 24h (N=24) simulation, starting at noon.

Table S3. Calculated $RRMS_k$ values for a 24 hour simulation of EmChem19a, and external time-steps (dt) of between 1–600 s

		$RRMS_k$ (in %) values for dt=							
Species	$c(1)^{(a)}$ (ppb)	3	10	30	60	120	240	450	600
O3	3.473e+01	0.0021	0.0099	0.0326	0.0668	0.1362	0.2807	0.5570	0.7760
OH	2.077e-04	0.0043	0.0200	0.0600	0.1081	0.1793	0.2858	0.4957	0.6904
HO2	8.751e-03	0.0047	0.0235	0.0766	0.1504	0.2851	0.5360	0.9966	1.3778
NO	2.544e-01	0.0115	0.0556	0.1788	0.3463	0.6285	1.0537	1.7075	2.2788
NO2	1.911e+00	0.0027	0.0135	0.0452	0.0905	0.1758	0.3418	0.6613	0.9219
PAN	2.427e-01	0.0037	0.0175	0.0581	0.1194	0.2449	0.5112	1.0369	1.4660
NO3	5.235e-03	0.0041	0.0180	0.0571	0.1151	0.2298	0.4574	0.8673	1.1756
N2O5	1.046e-02	0.0028	0.0123	0.0396	0.0798	0.1572	0.2993	0.5334	0.7095
CPU$^{(b)}$:	10.17	3.38	2.02	1.00	0.52	0.25	0.13	0.07	0.05

Notes: (a) mean concentrations calculated for dt =1 s; (b) CPU time relative to dt =30 s run.

Tables S3–S4 illustrate the changes in $RRMS_k$ (in percent) with dt for some key species with EmChem19a and MCMv3.3Em systems. For our typical dt of 30 s, $RRMS_k$ are seen to be largest for NO and N2O5, but are $\leq$0.2% for those species in both schemes. Even with dt of 120 s $RRMS_k$ values don't exceed 1%. For dt=600 s the $RRMS_k$ are about 1–2% for EmChem19a, but much larger for the MCM scheme. Users may of course experiment with these choices, but the default dt=30 s seems adequate for normal boxChem usage.

Table S3 also illustrates the CPU required (relative to the dt=30 s case) for these runs (as calculated on a desktop PC, x86_64 linux processor, gfortran 5.4). The 30 s case is seen to require about 20 times more CPU than dt=600 s, but this corresponds to only 4 s real time. The dt=1 s case requires nearly 10 times more CPU than the 30 s, but for EmChem19a this is only 40 s real time. For MCMv3.3Em the CPU used is far greater, ca. 40 h for dt=1 s, ca. 4 h for dt=30 s, and ca. 1 hour for dt=120 s. (In future the MCM scheme might be made much more CPU efficient by omission of non-used VOC and halogen precursors.)

Table S4. Calculated $RRMS_k$ values for a 24 hour simulation with MCMv3.3Em, and external time-steps (dt) of between 1–600 s

	c(1)	$RRMS_k$ (in %) values for dt=							
Species	(ppb)	3	10	30	60	120	240	450	600
Species	1	3	10	30	60	120	240	450	600
O3	3.488e+01	0.0021	0.0097	0.0324	0.0675	0.1436	1.7375	0.5737	0.7631
OH	1.938e-04	0.0041	0.0191	0.0570	0.1026	0.1730	2.8830	3.2349	3.6909
HO2	7.948e-03	0.0051	0.0246	0.0802	0.1608	0.3289	7.4843	7.0996	8.2689
NO	2.546e-01	0.0115	0.0552	0.1774	0.3445	0.6351	4.5669	1.6685	3.3062
NO2	1.902e+00	0.0026	0.0133	0.0445	0.0900	0.1818	1.5367	0.5717	0.7002
PAN	2.337e-01	0.0039	0.0185	0.0624	0.1348	0.3027	8.8077	4.7753	4.4970
NO3	4.568e-03	0.0038	0.0171	0.0542	0.1113	0.2277	0.5133	0.6467	0.6832
N2O5	9.001e-03	0.0027	0.0119	0.0385	0.0780	0.1544	0.3114	0.4404	0.5226
CPU:	10.03	3.34	2.00	1.00	0.50	0.25	0.12	0.07	0.05

Notes: as Table S3