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 stand-alone 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 (gly-oxal). '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

55   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.

60   (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

65   (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

70   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

75   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
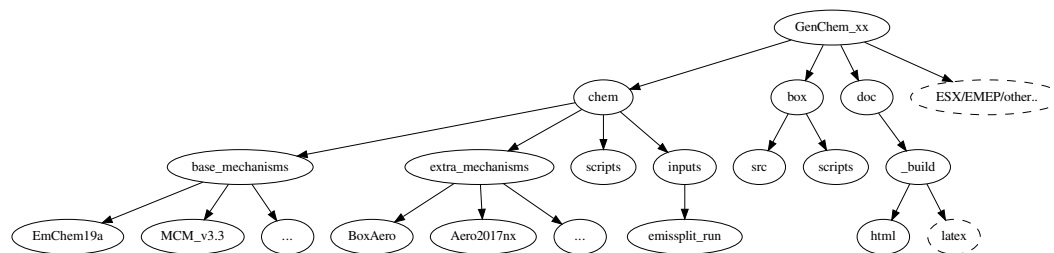
Figure 2. Directory structure of GenChem's chem and box directories. The dashed 'ESX/EMEP/other' directory indicates the possible placement of future EMEP, ESX or other model directories in this system.

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 emiss-plit_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 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
135   lines beginning:

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

with 'voc' emissions set on the next line as $15.4 \, \mathrm{kg \, m^{-2} \, day^{-1}}$. These emissions are converted by boxChem to instantaneous production rates in molecules $\mathrm{cm^{-3} \, s^{-1}}$, 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
140   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
145   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 $\mathrm{cm^{-3}}$, and for particulate matter $\mu\mathrm{g \, m^{-3}}$.

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

150   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*

155   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*

160   which results in ResConcs_boxEmChem19a_O3_ppb.txt
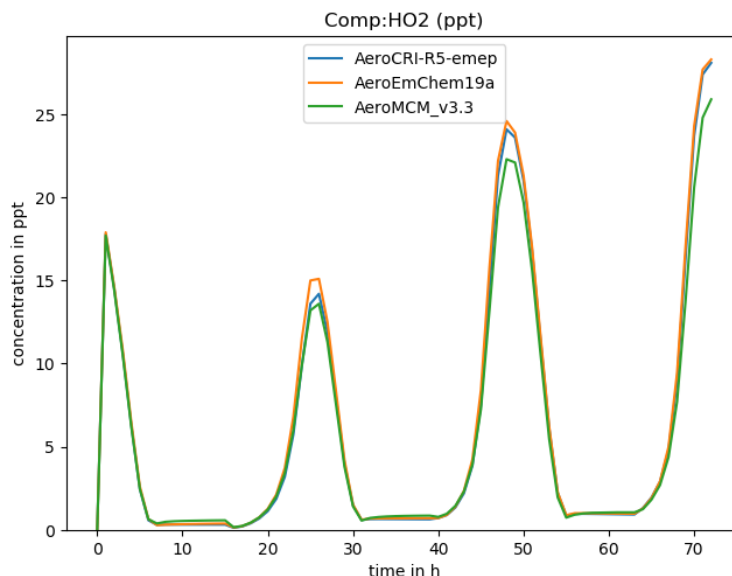
Figure 3. Example of comparison of three chemical schemes, produced for HO2 with the boxplots.py script

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-vbs 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 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

180 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

185 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

190 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

195 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

200 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.

205 – 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 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. CH4). 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. $\mu g(N)/m^3$) 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 caluclated 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 (ΔH_{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 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 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 semi-colon used to separate groups). For example, SOA species which use the VBS system require specification of their effective saturation concentrations at 298K (C^*, in $\mu g\,m^{-3}$) and the vaporization enthalpies (ΔH_{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 HO2 + 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 semi-colon 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 particlar reaction. In this way tracers are easily added. 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 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. 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 for emission input files, and also the file endings for the respective emissplit file, see Sect. 6.4. Other labels can easily be used

```
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*

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.).

385 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
390 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
395 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' depen-
400 dency 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
405 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

430   This file specifies basic information about the chemical compounds, in terms of number, indices and some chemical charac-
teristics. 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
435   '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.

440 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"
445 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 450 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 list of advected species, and the second entry is the

460 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
465 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:

470

```
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
475 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:

480   – 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.

485

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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