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NEW INTEGRATED EMISSION PROCESSOR FOR AIR QUALITY MODELS

Nina Benešová[3], Ondřej Vlček[3], Michal Belda[2,4], Peter Huszár[2,4], Jaroslav Resler[1,2], Pavel Juruš[1,2], Pavel Krč[1,5], Kryštof Eben[1,5]

[1]Institute of Computer Science, Czech Academy of Sciences, Czech Republic
[2] Faculty of Transportation Sciences, Czech Technical University in Prague, Czech Republic
[3]Czech Hydrometeorological Institute, Czech Republic
[4]Faculty of Mathematics and Physics, Charles University, Czech Republic
[5] Czech Institute of Informatics, Robotics and Cybernetics, Czech Technical University in Prague, Czech Republic

Abstract: A structure of the emission processor being developed for the chemical transport model is described. Processor is based on free software (PostgreSQL, PostGIS, Python) and is not bound to any predefined fixed input file formats, where possible. It is planned that its source will be made available after the end of intensive model development phase.

Key words: *emission processor, air quality modelling, chemical transport models, air pollution.*

INTRODUCTION

Besides meteorology, emissions are another key input needed by air quality models. Level of detail on which emissions need to be prepared differs depending on the type of model. Generally chemical transport models (CTM) require the most elaborated inputs – annual emissions of main species need to be disaggregated in time and space and chemical speciation has to be applied. CTMs also usually work with huge amount and various types of sources (anthropogenic point, area, and line sources, biogenic sources, etc.). The only widely used open source emission preprocessor for CTMs is SMOKE (CMAS, 2017). Its main advantage is that it can be readily used with NWP model WRF (Skamarock et al., 2008) and chemical transport model CMAQ (Byun and Schere, 2006). Although SMOKE has been applied for Europe many times (e.g. Bieser et al., 2011; or Borge et al., 2008), its application with non-US data is quite complicated since it is designed for US-specific inputs. Therefore we decided to develop a new emission processor, which will be flexible and easily configurable for users using different NWP and CTM models. Its structure was presented at HARMO 17 conference (poster H17-130; Juruš et al., 2016). While the processor is still under intensive development, we would like to point out its main features (current or planned) and what are its main benefits compared to the SMOKE model.

STRUCTURE OF EMISSION PROCESSOR

Emission processor (EP) is based on free software (PostgreSQL, PostGIS, Python) and has a modular design which allows users to add their own modules. Structure of the EP can be divided into four main layers which corresponds to the three phases of emission processing: 1) inputs preprocessing and preparation, 2) scenario setup, 3) emission processor core, 4) outputs postprocessing. Figure 1 shows the schematic structure of the EP indicating the basic data flow and modules dependency of the processor.

Preprocessing and transformations of the input data

EP has to ingest heterogeneous primary information about the emissions. The role of this phase is to consolidate and unify the structure and format of emission inputs. Emission processor currently accepts two file formats the input data: GIS shapefiles and text files. In case of text files, the spatial information can be provided in a separate GIS shapefile (useful if multiple emission inventories have the same spatial

distribution) or can be read directly from the text file in case of point or regular grid sources based on its predefined parameters – in this way e.g. TNO MACC (Kuenen et al., 2014) emissions can be read from the ascii file standardly provided by TNO. Each input file or emission inventory is accompanied by the supplementary file, which holds information on the type of the input file, its geometry and coordinate system, type of emission sources (area/point/line), names of columns that contain necessary data (e.g. parameters of the point sources), and their units. Names of the source categories can be user-defined and are not bound to any fixed form.

Data are processed to unified format and stored in a PostGIS database. The same emission inventories can be used for different scenarios, therefore no further preprocessing is done at this stage.

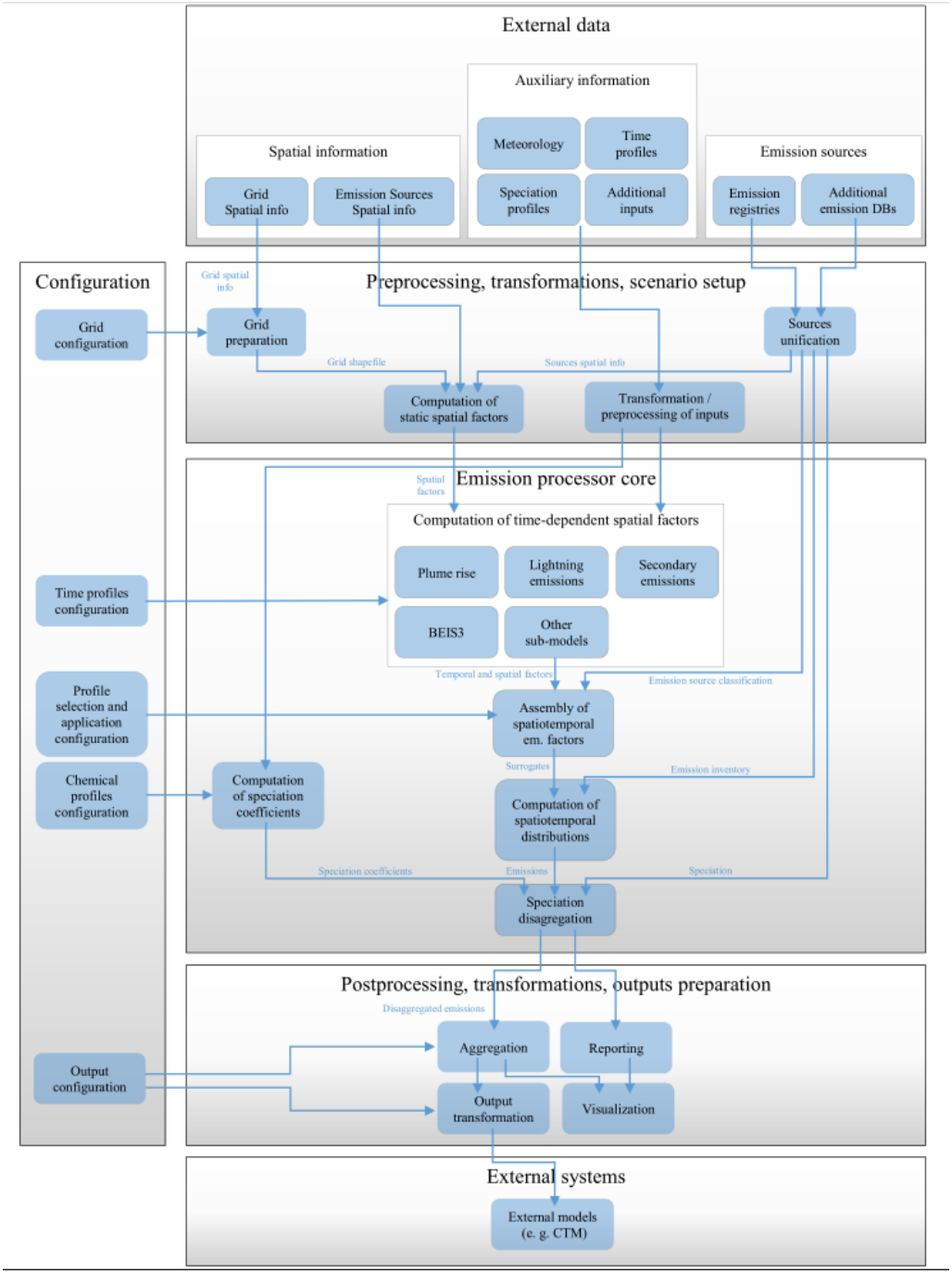

Figure 1 Structure of the new emission processor. The scheme shows basic layers of the processor, flow of the data and modules dependency (from Juruš et al., 2016).

Scenario setup

Based on the configuration setup, the desired scenario case is initialised. First the grid is created. Generally, this is not bound to a regular grid, EP can be used to generate emissions for any irregular polygons. Coordinate system parameters are also initialised. EP is not limited to any particular coordinate system and can process emissions in any known predefined or user-defined system.

One of the tasks solved by configuration is the setup of particular modules and adjustments to emission data based on simulation scenario. Configuration also decides which module implementation will be used in case of multiple implementations of particular submodule – e.g. different calculations of plume rise based on the availability of meteorological data and/or stack parameters.

Emission processor core

Emission processor core is a key part of the toolchain where the disaggregation of emission totals takes place. The central task is the processing of spatiotemporal factors for the disaggregation and consequent chemical speciation. The factors range from static profiles stored in database to less or more dynamic profiles which can be computed by complex models (e.g. for local heating or agriculture). Time variation of emissions based on continuous measurement is also possible to use. The emission processor should be also able to encapsulate external sub-models for the calculation of emission factors. The steps of emission processor core are:

- Spatial distribution – the factors describing the distribution of emissions into the user-defined grid or polygons are calculated;
- Computation of time dependent spatial factors – based on static time profiles, meteorology, mathematical models, GIS data etc.;
- Chemical speciation – the emission data are recalculated into modelled species or groups based on speciation coefficients;
- External submodules – currently biogenic emissions are calculated by the MEGAN model (Guenther et al., 2012).

Postprocessing, transformations, outputs preparation

The resulting raw data containing disaggregated emissions from emission processor core are aggregated according to the user requirements. The results are then transformed to desired data format which is used by external systems – e.g. by chemical transport models. Currently outputs for CAMx (ENVIRON, 2016) and CMAQ chemical transport models are the option. But users can define their output file formats. Various visualizations and reports are also the part of this phase.

CURRENT STATE AND OUTLOOK

At the moment the emission processor has been successfully used in combination with the CAMx model. It is planned to make the source code publically available after the end of intensive development. If you would like to be informed about the release of the source code, please send your request to Mr. Ondřej Vlček <vlcek@chmi.cz>.

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REFERENCES

Bieser, J., Aulinger, A., Matthias, V., Quante, M., and Builtjes, P., 2011: SMOKE for Europe – adaptation, modification and evaluation of a comprehensive emission model for Europe, *Geoscientific Model Development Discussions*, Volume **4**, 47-68, https://doi.org/10.5194/gmdd-3-949-2010

Borge, R., Lumbreras, J., and Rodríguez, E., 2008: Development of a high-resolution emission inventory for Spain using the SMOKE modelling system: A case study for the years 2000 and 2010, *Environmental Modelling & Software*, Volume **23**, Issue 8, 1026-1044, http://dx.doi.org/10.1016/j.envsoft.2007.11.002

Byun, D.W. and Schere, K.L., 2006: Review of the governing equations, computational algorithms, and other components of the Models-3 Community Multiscale Air Quality (CMAQ) modeling system. *Appl. Mech. Rev.*, Volume **59**, Issue 2, 51–77, http://dx.doi.org/10.1115/1.2128636

CMAS, 2017: Sparse Matrix Operator Kernel Emissions (SMOKE) Modeling System - official website of the model. WWW: https://www.cmascenter.org/smoke/

ENVIRON, 2017: CAMx – User's Guide to Comprehensive Air Quality Model with Extensions Version 6.40. WWW: http://www.camx.com

Guenther, A. B., Jiang, X., Heald, C. L., Sakulyanontvittaya, T., Duhl, T., Emmons, L. K., and Wang, X., 2012: The Model of Emissions of Gases and Aerosols from Nature version 2.1 (MEGAN2.1): an extended and updated framework for modeling biogenic emissions. *Geoscientific Model Development*, Volume **5**, 1471-1492, http://dx.doi.org/10.5194/gmd-5-1471-2012

Juruš, P., Karel, J., Jareš, R., Martinovský, J., Píša, V., Polák, R., Smolová, E., Pelikán, E., Brabec, M., Konár, O., Fuglík, V., Eben, K., Resler, J., Vlček, O., Machálek, P., Modlík, M., Hnilicová, H., Benešová, N., Srbová, D., Zapletal, M., Kadlubiec, R., Škarková, P., and Barnet, J., 2016: Emission Processor for Air Quality Models Utilizing Newly Availagle Data. In: László Bozó, Zita Ferenczi, and Márta T. Puskás eds. 17th International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes. Budapest: Hungarian Meteorological Service, 117–120. ISBN 978-963-9931-10-7.

Kuenen, J. J. P., Visschedijk, A. J. H., Jozwicka, M., and Denier van der Gon, H. A. C., 2014: TNO-MACC_II emission inventory; a multi-year (2003–2009) consistent high-resolution European emission inventory for air quality modelling. *Atmospheric Chemistry and Physics*, Volume **14**, 10963-10976, http://dx.doi.org/10.5194/acp-14-10963-2014

Skamarock, W. C., Klemp, J. B., Dudhia, J., Gill, D. O., Barker, D., Duda, M. G., yu Huang, X., Wang, W., and Powers, J. G., 2008: A Description of the Advanced Research WRF Version 3, NCAR Tech. Note NCAR/TN-475+STR, 113 pp., NCAR/UCAR, Boulder. WWW: http://www2.mmm.ucar.edu/wrf/users/docs/arw_v3.pdf