(1) SIM-BIM – Seasonal Isoprenoid synthase Model – Biochemical Isoprenoid biosynthesis Model

(2) EULS – Estonian University of Life Sciences, Estonia Steffen M. Noe <steffen.noe@emu.ee>

## (3) Available modes for the model runs: Research

(4) Components & processes: Atmosphere, Biosphere & Physical, Chemical, Biological.

## (5) Brief model description

The SIM-BIM model was developed since mid 1990ies and has been originally covered isoprene emission from leaves (Zimmer et al. 2000; Lehning et al. 2001). BIM implements the chloroplastic isoprene synthesis pathway by a coupled ordinary differential equation system and is linked to a seasonality module (SIM) that alters the activation state of the enzymatic reaction scheme mapped by BIM.

It was originally coupled to a photosynthesis model (Kirschbaum et al. 1997; Zimmer et al. 2003) that allowed using ambient temperature, photosynthetic active radiation (PAR) as driving parameters of isoprene emissions. Further enhancements covered the inclusion of monoterpene emissions (Grote et al. 2006). In the following years, the model was further developed independently by R. Grote (SIM-BIM2) and S. Noe (SIM-BIM). The latter model was further coupled to a simpler photosynthesis model (Noe and Giersch 2004) that allowed the explicit use of ambient carbon dioxide concentrations and the water vapor deficit (VPD) as additionally environmental driving factors.

The latest version of SIM-BIM was linked with the boundary layer transport model SOSA (Boy et al. 2011) in a comparison study (Smolander et al. 2014).

The challenge to run a model that employs first-order Michaelis-Menten enzyme kinetics lies in the multitude of enzyme kinetics parameters, which further need to be scaled to the gas exchanging surface area of trees and may vary for different species.

## References:

- Boy, M., A. Sogachev, J. Lauros, L. Zhou, A. Guenther, and S. Smolander. 2011. "SOSA a New Model to Simulate the Concentrations of Organic Vapours and Sulphuric Acid inside the ABL – Part 1: Model Description and Initial Evaluation." Atmospheric Chemistry and Physics 11 (1):43–51. https://doi.org/10.5194/acp-11-43-2011.
- Grote, R., S. Mayrhofer, R.J. Fischbach, R. Steinbrecher, M. Staudt, and J.-P. Schnitzler. 2006. "Process-Based Modelling of Isoprenoid Emissions from Evergreen Leaves of Quercus Ilex (L.)." Atmospheric Environment 40 (January). Pergamon:152–65. https://doi.org/10.1016/J.ATMOSENV.2005.10.071.
- Kirschbaum, M. U. F., M. Küppers, H. Schneider, C. Giersch, and S. Noe. 1997. "Modelling Photosynthesis in Fluctuating Light with Inclusion of Stomatal Conductance, Biochemical Activation and Pools of Key Photosynthetic Intermediates." Planta 31 (12):16–26. https://doi.org/10.1007/s004250050225.
- Lehning, A., W. Zimmer, I. Zimmer, and J.-P. Schnitzler. 2001. "Modeling of Annual Variations of Oak (Quercus Robur L.) Isoprene Synthase Activity to Predict Isoprene Emission Rates." Journal of Geophysical Research: Atmospheres 106 (D3):3157–66. https://doi.org/10.1029/2000JD900631.
- Noe, Steffen M., and Christoph Giersch. 2004. "A Simple Dynamic Model of Photosynthesis in Oak Leaves: Coupling Leaf Conductance and Photosynthetic Carbon Fixation by a Variable Intracellular CO2 Pool."

Functional Plant Biology 31 (12):1195–1204. https://doi.org/10.1071/FP03251.

- Smolander, S., Q. He, D. Mogensen, L. Zhou, J. Bäck, T. Ruuskanen, S. Noe, et al. 2014. "Comparing Three Vegetation Monoterpene Emission Models to Measured Gas Concentrations with a Model of Meteorology, Air Chemistry and Chemical Transport." Biogeosciences 11 (19). Copernicus GmbH:5425– 43. https://doi.org/10.5194/bg-11-5425-2014.
- Zimmer, W., N. Bruggemann, S. Emeis, C. Giersch, A. Lehning, R. Steinbrecher, and J-P. Schnitzler. 2000. "Process-Based Modelling of Isoprene Emission by Oak Leaves." Plant, Cell and Environment 23 (6). Blackwell Science Ltd:585–95. https://doi.org/10.1046/j.1365-3040.2000.00578.x.
- Zimmer, W., R. Steinbrecher, C. Körner, and J.-P. Schnitzler. 2003. "The Process-Based SIM–BIM Model: Towards More Realistic Prediction of Isoprene Emissions from Adult Quercus Petraea Forest Trees." Atmos Environment 37 (12). Pergamon:1665–71. https://doi.org/10.1016/S1352-2310(03)00013-X.