



## **Regional-scale simulation of transport and transformations of semi-volatile polycyclic aromatic hydrocarbons (PAHs) in East Asia: diurnal variations investigation**

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Semi-volatile PAHs are major pollutants of urban air, mostly regionally transported and reaching remote environments<sup>[1]</sup>. Some semi-volatile PAHs are carcinogenic. About 22% of global PAHs emissions are in China.

The transport and sinks (atmospheric reactions, deposition) of semi-volatile PAHs in East Asia are studied using a modified version of the Weather Research and Forecasting model coupled with chemistry (WRF/Chem<sup>[2]</sup>). For this purpose, PAHs' gas and particulate phase chemical reactions and dry and wet deposition processes are included. We use emissions of 2008<sup>[3]</sup> which include technical combustion processes (coal, oil, gas, waste and biomass) and open fires and apply diurnal time functions as those of black carbon.

The model was run for phenanthrene (3-ring PAH,  $p = 1.5 \times 10^{-2}$  Pa at 298 K) and benzo(a)pyrene (5-ring PAH,  $p = 7 \times 10^{-7}$  Pa) for July 2013 with hourly output and 27 km horizontal grid spacing. The comparison of model predicted phenanthrene concentrations with measurements at a rural site near Beijing (own data, unpublished) validates the model's ability to simulate diurnal variations of gaseous PAHs. The model's performance is better in simulating day time than night time gaseous PAHs. The concentrations of PAHs had experienced significant diurnal variations in rural and remote areas of China. Elevated concentration levels of 40-60 ng m<sup>-3</sup> for phenanthrene and 1-10 ng m<sup>-3</sup> for benzo(a)pyrene are predicted in Shanxi, Guizhou, the North China Plain, the Sichuan Basin and Chongqing metropolitan areas due to the high emission densities at those locations.

### References

- [1] Keyte, I.J., Harrison, R.M., and Lammel, G., 2013: Chemical reactivity and long-range transport potential of polycyclic aromatic hydrocarbons – a review, *Chem. Soc. Rev.*, 42, 9333-9391.
- [2] Grell, G.A., Peckham, S.E., Schmitz, R., McKeen, S.A., Frost, G., Skamarock, W.C., and Eder, B., 2005: Fully coupled online chemistry within the WRF model, *Atmos. Environ.*, 39, 6957-6975.
- [3] Shen, H. Z., Huang, Y., Wang, R., Zhu, D., Li, W., Shen, G. F., Wang, B., Zhang, Y. Y., Chen, Y. C., Lu, Y., Chen, H., Li, T. C., Sun, K., Li, B. G., Liu, W. X., Liu, J. F., and Tao, S., 2013: Global atmospheric emissions of polycyclic aromatic hydrocarbons from 1960 to 2008 and future predictions, *Environ. Sci. Technol.*, 47, 6415-6424.