Optimization of the PMF source apportionment solution based on the rotational tools in US EPA PMF 5.0 software

Dušan B. Topalović1, Mirjana B. Radenković1, Viša Tasić2 and Predrag Božović1

1 Vinča Institute of Nuclear Sciences, National Institute of the Republic of Serbia, University of Belgrade, Serbia; 2 Mining and Metallurgy Institute, Bor, Serbia

Introduction
Positive matrix factorization (PMF) is a dimension reduction method used to model the covariance structures of observable variables in order to impel a smaller number of latent non-negative factors. It resolves receptor modeling problem, which is based on the chemical mass balance equation (CMB) and may discover hidden patterns in the environmental data, where each extracted factor is accompanied by an actual source of emission. In this paper, PMF source apportionment analyses of fine aerosol fraction (PM$_{2.5}$ mode) at Belgrade suburban background site, in 2016/17 year, have been performed by processing a data set of 130 PM$_{2.5}$ mass concentrations and twenty-one elemental concentrations and soot concentrations in each PM$_{2.5}$ sample (mode).

Theoretical model
The PMF model may be described in the following way:

$$x_{n,m} = \sum_{k=1}^{K} g_{n,k} f_{k,m} + e_{n,m},$$

where: $K$ is the number of major source groups, $f_{k,m}$ is a relative concentration of chemical species $m$ in the chemical profile of source group $k$, $g_{n,k}$ is a contribution of source $k$ to the sample $n$, and $e_{n,m}$ is the residual of species $m$ for sample $n$. The PMF algorithm calculates a weighted least squares fit through minimizing $Q$:

$$Q = \sum_{n=1}^{N} \sum_{m=1}^{M} x_{n,m} - \sum_{k=1}^{K} g_{n,k} f_{k,m},$$

where $u_{n,m}$ is uncertainty. BS and DISP method-capture the uncertainty due to both random errors and rotational ambiguity.

Conclusion
Obtained results indicated significant role of $Q/Q_{exp}$ ratio analysis for optimal solution choice. This paper shows that optimization procedure should include examination of rotational matrix in which the rotational degree of freedom of solution is considered. Solutions with a steep change in their rotational degree of freedom were rejected. Finally, the additional improvement can be done by optimizing the parameters representing the scaled mean value (IM) and the scaled standard deviation (IS) of the each individual column in scaled residual matrix.

References
[1] Paatero P and Tapper U 1994 Environmetrics 5 111

Acknowledgements
This research was funded by the Ministry of Education, Science and Technological Development of the Republic of Serbia.