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BOOK OF ABSTRACTS

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

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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). The $PM_{2.5}$ mass concentrations in collected samples have been determined following SRPS EN 12341:201 procedure, elemental concentrations were obtained by PIXE alanytical technique in the frame of the regional IAEA project, in the Institute of Nuclear Research, Hungarian Academy of Sciences, and soot concentrations were analyzed by smoke stain reflectometry in accordance with ISO 9835:1993 (E). The EPA PMF program ver 5.0, was used to solve the PMF model. Since the determination of an optimal PMF solution is a strongly heuristic procedure, there is a necessity of finding a more quantitative ways to reduce the arbitrariness of this technique. In order to reduce the range of possible solutions, we have analyzed how the values of model parameters changes as a function of the number of factors. PMF modeling was performed in a robust mode. For the purpose of finding the best fit solution wich minimize the object function Q, we varied the number of factors in the range from 4 to 8. Additionally, influence of rotations are also analyzed in iterative steps by varying FPEAK function in the range -1 to +1 with an increment of 0.5. Obtained results indicated significant role of Q/Q_{exp} ratio analysis for optimal solution choice. In optimization process, number of factors with Q/Q_{exp} ratio less than 1, were rejected as a possible solutions. 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.

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