“Applying PMF receptor model for PM$_{2.5}$ source appointment”

AND

“Processing MODIS AOD products for assessing biomass burning-related air pollution”
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INTRODUCTION

These training workshops were parts of the activities under the research project “Integrated Approach of In-situ Measurement, Modelling Techniques, and Advanced Satellite Remote Sensing for Mapping and Quantifying Contribution of Local and Regional Biomass Burning Sources to Air Pollution in Southeast Asian Countries” (Project Reference Number: CRRP2019-11MY-Nguyen) which supported by the Asia Pacific Network for Global Change Research (APN). The training workshops were successfully organized with the mixed online and offline mode by the Institute of Environmental Science and Engineering (IESE), Vietnam in September and October, 2021.

The trainings aimed to provide the young and early-career scientists from the local agencies, academic and research institutions, professional associations, and private sector with the opportunities to develop their knowledge and skills with respect to applying the PMF receptor model for PM$_{2.5}$ source appointment and using MODIS AOD products for assessing biomass burning-related air pollution. The trainings not only enhanced the technical capacity and capability of the young and early-career scientists to apply the advanced technical tools in studying biomass burning and air pollution issues, but also provided the good opportunities for establishing the collaborative network among the participants for future researches, thus directly contributed to the APN Capacity Development Agenda.
BACKGROUND & RATIONALE

Southeast Asia (SEA) has been reported as one of the largest biomass burning source regions in the world. The regional haze known as “Asian Brown Cloud” resulting from biomass burning sources occurs almost every year in SEA, which has strong impacts on human health, environment, and global climate variations. In addition to biomass burning, the increased air pollution in the SEA countries has been also significantly influenced by a number of local emission sources such as transport, industry, construction, and long-range transported air pollutants from regional sources.

In order to provide strong evidences on the impacts of diverse sources (including biomass burning) to the local air quality for supporting policy- and decision-making activities in the SEA countries, there is a critical need to employ different technical tools for exploring and assessing the contribution of emission sources to the measured air quality. Among the useful tools commonly applied in air quality studies, the Positive Matrix Factorization (PMF) is a multivariate factor analysis technique used successfully among others at the US Environmental Protection Agency (US EPA) for the chemometric evaluation and modelling of air quality datasets. Meanwhile, the Moderate Resolution Imaging Spectroradiometers (MODIS) aboard U.S. National Aeronautics and Space Administration (NASA)’s Terra and Aqua satellites has been widely used as a cost-effective method to monitor the highly variable air pollution at both local and regional scales, which could complement the spatially limited coverage of traditional ground-based air quality monitoring stations and/or in-situ measurements. Despite of this, the application of these useful tools for air quality studies in the SEA countries has been limited due to the lack of technical capacity and capability. Therefore, it is necessary to develop and enhance the technical capacity and capability of scientists in the SEA countries, especially the young and early-career ones, for using those tools in air quality studies, towards providing the improved scientific evidences which needed for local and regional policy- and decision-making communities in developing effective policies and strategies for reducing air pollution in the region.
SUMMARY OF TRAINING WORKSHOPS

Training Workshop 1: “Applying PMF receptor model for PM$_{2.5}$ source appointment”.

During the two-day training workshop (23-24 September 2021), the participants (mainly the young and early-career scientists from the local agencies, academic and research institutions, professional associations, and private sector) were provided with the knowledge and skills for applying PMF receptor model for PM$_{2.5}$ source appointment, including: preparing the input files required by PMF model and analysing the input data (PM$_{2.5}$ chemical data and uncertainty, plots); processing the model output files; handling the configuration file; initiating a base model run and analysing the base model results (residual analysis, observed/predicted scatter plot, observed/predicted time series, profiles/contributions, factor fingerprints, G-Space plot, factor contributions, base model displacement error, BS error, and BS-DISP error estimation, interpreting error estimate results); applying the rotational tools for advanced model run (Fpeak model run specification, constrained model operation); and model troubleshooting. The participants were trained on the job with “hands-on experience” using a real PM$_{2.5}$ datasets for the case of Hanoi City.

Training Workshop 2: “Processing MODIS AOD products for assessing biomass burning-related air pollution”.

During the one-day training workshop (15 October 2021), the participants (mainly the young and early-career scientists from the local agencies, academic and research institutions, professional associations, and private sector) were provided with the basic knowledge and skills for processing MODIS AOD products for assessing biomass burning-related air pollution, including: how MODIS AOD (aerosol optical depth) products can be used for studying biomass burning-related air pollution; how to create a new user account, download, and process MODIS AOD products obtained from NASA website, and the software needed for processing the data; handling and processing the multi MODIS aerosol products with different resolutions using several algorithms (Dark Target, Deep Blue, and Dark Target Deep Blue Combined); using visualization tools (software and programming languages) to temporally and spatially interpret the MODIS AOD datasets. The participants were trained on the job with “hands-on experience” using a real MODIS AOD datasets for the case of Vietnam.

Key feedbacks from the participants through the two training workshops

- **Training Workshop 1**: the training materials were prepared with the understandable and detail information level for the trainee; the contents were well organised and focused on basic knowledge and practical skills for PMF base model run which appropriate to the capacity of the participants; the participants would need more real practices in order to master the rotational tools for advanced model run after the training.

- **Training Workshop 2**: the training materials were well prepared with the practical information which appropriate to the trainee for the step by step exercises in accessing, downloading, processing, and interpreting MODIS AOD datasets; there should be more similar trainings in the future on the topics of processing and using other parameters from MODIS satellite as well as datasets provided by the other satellites, that can be used in air quality studies.
ANNEXES

Annex 1: Workshop agenda
Annex 2: List of participants
Annex 3: Presentation of Training Workshop 1
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ANNEX 1: WORKSHOP AGENDA

Training Workshop 1: “Applying PMF receptor model for PM$_{2.5}$ source appointment” (23-24 September 2021)

<table>
<thead>
<tr>
<th>Time</th>
<th>Contents</th>
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<tbody>
<tr>
<td><strong>23 September 2021</strong></td>
<td></td>
</tr>
<tr>
<td>8h30 – 8h40</td>
<td>Opening &amp; Welcome</td>
</tr>
<tr>
<td>8h40 – 9h00</td>
<td>Introduction of PMF model</td>
</tr>
<tr>
<td>9h00 – 10h15</td>
<td>Preparation of model input files and analysis of model input data</td>
</tr>
<tr>
<td>10h15 – 10h30</td>
<td>Break time</td>
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<tr>
<td>10h30 – 12h30</td>
<td>PMF base model run</td>
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<tr>
<td>12h30 – 13h30</td>
<td>Lunch break</td>
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<tr>
<td>13h30 – 14h30</td>
<td>Error estimation for PMF base model run</td>
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<tr>
<td>14h30 – 14h45</td>
<td>Break time</td>
</tr>
<tr>
<td>14h45 – 16h30</td>
<td>Exercises for PMF base model run</td>
</tr>
<tr>
<td>16h30 – 17h00</td>
<td>Q&amp;A</td>
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<tr>
<td><strong>24 September 2021</strong></td>
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<tr>
<td>8h30 – 10h15</td>
<td>Use of rotational tools for advanced model run</td>
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<tr>
<td>10h15 – 10h30</td>
<td>Break time</td>
</tr>
<tr>
<td>10h30 – 12h30</td>
<td>Troubleshooting; Q&amp;A</td>
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<tr>
<td>12h30 – 13h30</td>
<td>Lunch break</td>
</tr>
<tr>
<td>13h30 – 15h30</td>
<td>Case study &amp; Exercises for PMF model run</td>
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<tr>
<td>15h30 – 15h45</td>
<td>Break time</td>
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<tr>
<td>15h45 – 16h30</td>
<td>Discussions; feedbacks of the participants</td>
</tr>
<tr>
<td>16h30</td>
<td>Closing of the workshop</td>
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Training Workshop 2: “Processing MODIS AOD products for assessing biomass burning-related air pollution” (15 October 2021)

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<td>8h30 – 8h40</td>
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<td>8h40 – 9h00</td>
<td>Introduction of MODIS AOD products used for air pollution studies</td>
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<tr>
<td>9h00 – 10h00</td>
<td>Creating user account &amp; downloading MODIS AOD datasets</td>
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<td>10h00 – 10h15</td>
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<tr>
<td>10h15 – 10h45</td>
<td>Resolution of MODIS AOD data &amp; algorithms</td>
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<tr>
<td>10h45 – 12h30</td>
<td>MODIS AOD data processing</td>
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<td>12h30 – 13h30</td>
<td>Lunch break</td>
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<tr>
<td>13h30 – 14h30</td>
<td>Data visualization tools</td>
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<td>14h30 – 14h45</td>
<td>Break time</td>
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<tr>
<td>14h45 – 16h30</td>
<td>Assignment &amp; exercises with a real MODIS AOD datasets</td>
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<tr>
<td>16h30 – 17h00</td>
<td>Discussions; feedbacks of the participants</td>
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<tr>
<td>17h00</td>
<td>Closing of the workshop</td>
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<thead>
<tr>
<th>No</th>
<th>Name of participant</th>
<th>Institution/Organization</th>
<th>Email</th>
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ANNEX 3: PRESENTATION OF TRAINING WORKSHOP 1

Contents
- Introduction on PMF
- Getting Started
- Rotational Tools
- Troubleshooting
- Training Exercises

1. GETTING STARTED

Positive Matrix Factorization (PMF)
- Multivariate (statistical) model
- Does not require comprehensive advance information
- Incorporate time variation
- Non-negativity constraints (only non-negative factors)
- Rotation can be controlled by user
- Explicit least-squares approach to solving the factor analysis problem
- Individual data point weights
- Imposition of natural and other constraints, and
- Flexibility to build more complicated models
- On line information

1. Input Files

Two input files are required by PMF:
1. Sample species concentration values
2. Sample species uncertainty values or parameters for calculating uncertainty

Example of formatting of the input concentration file.
Input Files (cont.)

Two input files are required by PNP:
1. sample species concentration values
2. sample species uncertainty values or parameters for calculating uncertainty

Example of an equation-based uncertainty file:

\[ \text{Unc} = \frac{3 \times \text{MDL}}{\text{concentration}} \]

\[ \text{Unc} = \sqrt{\text{Error Fraction} \times \text{concentration}} = (0.5 \times \text{MDL})^2 \]

2. Output Files

The user can specify the output directory ("Output Folder"), choose the EFA, PNP output file types ("Output File Type" radio buttons) and define prefixes for output files ("Output File Prefix").

- _base.xlsx - Profiles, Contributions, Residual, Run Comparison
- _regression.xlsx - Summary, Input, Base Runs

3. Configuration Files

Q The user must provide a name for a configuration file on the Input File Screen to create a configuration file.

Q To choose a configuration file, the user can click on "Browse" to browse to the correct path or type in a path and name. The user can also press the "Load" button or simply press "Enter" on the keyboard to load the most recently used configuration file.

Q The "Save" and "Save As" buttons can be used to save the current settings to an existing or new configuration file.

4. Suggested Order of Operations

Flow chart of operations within EPA PNP - [Image]

5. Analyze Input Data: Concentration/Uncertainty

Flow chart of operations within EPA PNP - [Image]

Example of the Concentration/Uncertainty screen.
5. Analyze Input Data: Concentration Scatter Plots

Example of a concentration scatter plot.

5. Analyze Input Data: Concentration Time Series

Example of the Concentration Time Series screen with excluded and selected samples.

6. Base Model Runs: Initiating a Base Run

Example of the Base Model Runs screen showing Random Start (1) and Fixed Start (2).

6. Base Model Runs: Base Model Run Summary

Example of the Base Model Runs screen after base runs have been completed.

6. Base Model Runs: Base Model Results

Example of the Residual Analysis screen.

Base Model Runs: Base Model Results

Example of the Observed/Predicted Scatter Plot screen.
Base Model Runs: Base Model Results

Observed/Predicted Time Series

Example of the Observed Time Series screen.

Base Model Runs: Base Model Results

Profile/Contributions

Example of the Profile/Contributions screen.

Base Model Runs: Base Model Results

Profile/Contributions

Example of the Profile/Contributions screen with "Concentration Limits" selected.

Base Model Runs: Base Model Results

Profile/Contributions

Example of the Profile/Contributions screen with "P/E" selected.

Base Model Runs: Base Model Results

Factor Fingerprints

Example of the Factor Fingerprints screen.

Base Model Runs: Base Model Results

O-Space Plot

Example of the O-Space Plot screen with a red line indicating an edge.
6. Base Model Runs: Factor Names on Base Model Runs Screen

Example of the Base Model Runs screen with default base model run factor names.

7. Base Model Displacement Error Estimation

Example of the Base Model Displacement Summary screen.

8. Base Model BS Error Estimation

Example of the Base Model Runs screen highlighting the Base Model Bootstrap Method box.
1. Fpeak Model Run Specification

Example of the Fpeak Model Run Summary in the Fpeak Model Run screen

II. ROTATIONAL TOOLS

1. Fpeak Model Run Specification: Fpeak Results

Example of the Fpeak Profiles/Contributions screen
III. TROUBLESHOOTING
IV. TRAINING EXERCISES

References
- USEPA, 2014. EPA Positive Matrix Factorization (PMF) 5.0 Fundamentals and User Guide

Q & A Assignment & Practices
ANNEX 4: PRESENTATION OF TRAINING WORKSHOP 2

--- List of Content ---
1. Overview
2. Account registration
3. Data description
4. Data collection
5. Data processing
6. Data visualization

--- Overviews ---
- The tutorial presents a tour how to download and process MODIS AOD product with Dark Target Deep Blue Combine algorithm at 10km resolution (MOD04_L2).
- With the other products, please refers website: https://modis.gsfc.nasa.gov/data/dataprod/.
- Users should take a fundamental for GIS processing.
- Required software: ArcGIS or QGIS.

--- Account registration ---
1. Create a new account: https://urs.earthdata.nasa.gov/users/new

--- Account registration (cont.) ---
1. User login: https://urs.earthdata.nasa.gov/home
Account registration (cont.)

1. Check and modify the personal profile (optional)

--- Data description ---

MODIS Aerosol product is provided with three types of resolution including:
(1) Coarse-resolution : 10km (MOD04_L2 and MYD04_L2)
(2) Medium resolution : 3km (MOD04_3K and MYD04_3K)
(3) Fine resolution : 1km (MCD19A2)

--- Data description (cont.) ---

Several algorithms used to estimate the Aerosol Optical Depth (AODs) including:
(1) Dark Target
(2) Deep Blue
(3) Dark Target and Deep Blue Combined

--- Data description (cont.) ---

In addition, MODIS AOD products provides other parameters depending on each product. For instance:
- MOD04_L2 and MYD04_L2 provide the AODs loading with three algorithm
- MOD04_3K and MYD04_3K provide the AODs loading with only Dark Target algorithm
- MCD19A2 provide AODs loading with two band (470nm and 550nm)

--- Data collection ---

1. Access a link: https://ladsweb.modaps.eosdis.nasa.gov/search/
2. Select the product collections with multi versions (v5, v6, v6.1)
3. Select the type of sensor (MOD/Terra or MYD/Aqua)
4. Select the MODIS AOD product
5. Select the time period
6. Select the area
7. Download the MODIS AOD product

--- Data collection (cont.) ---

Web application to download MODIS database under NASA service
Data collection (cont.)
Select the newest collection: v6.1 (MODIS Collection 6.1)

Data collection (cont.)
Select the Terra sensor (MODIS: Terra)

Data collection (cont.)
Select MODIS AOD product: MOD04_L2 with resolution at 10km

Data collection (cont.)
Select time period by yourself (ex., 01/11 - 02/11, 2021)

Data collection (cont.)
Select research area using drawing tool.

Data collection (cont.)
Download the MODIS AOD Terra product at 10km
### Data collection (cont.)

MODIS AOD product (MOD04 L2) is stored under HDF format files.

### Data processing (cont.)

1. Extract the Aerosol Optical Depth (AODs) value
2. Extract the Quality Flag for each pixel
3. Store the database under CSV format and RASTER format
4. Calculate the AODs value at a specific location (e.g., Hanoi)

### Data processing (cont.)

Import the HDF file into ArcGIS software with any version (9.x or 10.x)

### Data processing (cont.)

Select the type of dataset: AOD 550nm Dark Target Dark Blue
Combine (subdataset 135)

### Data processing (cont.)

If software shows a warning message, ignore it.

### Data processing (cont.)

Change color bar to good display dataset
Data processing (cont.)

High and low AODs loading are blue and brown color, respectively

Data processing (cont.)

Extract the database under RASTER format

Data processing (cont.)

Add the setting to export the RASTER image

Data processing (cont.)

Extract the database under SHAPEFILE format

--- Data visualization ---

Several software and programming language can present the MODIS AODs product:

1. Software: Techplot, Paraview, HDFview
2. Programming language:
   - Python using package seaborn, geopandas
   - R using package ggplot2,
   - MATLAB, Javascript, Julia

Data visualization (cont.)
Data visualization (cont.)

Q & A
Assignment & Practices
ANNEX 5:
TRAINING WORKSHOP PHOTOS

Training Workshop 1: Applying PMF receptor model for PM$_{2.5}$ source appointment

Training Workshop 2: Processing MODIS AOD products for assessing biomass burning-related air pollution