

Supplement of Atmos. Meas. Tech., 13, 4885–4898, 2020  
<https://doi.org/10.5194/amt-13-4885-2020-supplement>  
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*Supplement of*

## **Assessment of particle size magnifier inversion methods to obtain the particle size distribution from atmospheric measurements**

**Tommy Chan et al.**

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## 1. Derivation of the step-wise method

The derivation of the step-wise method is as follows:

$$\begin{aligned}
 \frac{dR}{ds}(s_i) &= \int_0^{+\infty} K(s_i, d_p) \times \frac{dN}{dd_p} dd_p \\
 s_i \Leftrightarrow d_i : \int_0^{+\infty} K(s_i, d_p) \times dd_p &= \int_{d_i-\delta}^{d_i+\delta} K(s_i, d_p) \times dd_p, \delta \rightarrow 0 \\
 \therefore \frac{dR}{dd_p}(d_i) &= \frac{dR}{ds}(s_i) \times \frac{ds}{dd_p} = \frac{ds}{dd_p} \int_0^{+\infty} K(s_i, d_p) \times \frac{dN}{dd_p} dd_p \\
 &= \int_{d_i-\delta}^{d_i+\delta} K(s_i, d_p) \times \frac{dN}{dd_p} \times \frac{ds}{dd_p} \times dd_p \\
 &= \frac{dN}{dd_p}(d_i) \int_{s_i-\varepsilon}^{s_i+\varepsilon} K(s_i, d_i) \times ds \\
 &= \frac{dN}{dd_p}(d_i) \int_0^{+\infty} K(s_i, d_i) \times ds \\
 &= \frac{dN}{dd_p}(d_i) \times \eta(d_i, s_{\max}),
 \end{aligned}$$

where  $d$  is the derivate symbol;  $R$  is the raw concentration;  $s$  is the saturator flow rate;  $K$  is the kernel;  $dp$  is the particle diameter;  $s_i$  and  $d_i$  are the saturator flow rate and diameter at the  $i$ th point, respectively;  $\delta$  is Cauchy's definition of the limit;  $\varepsilon$  is the error;  $s_{\max}$  is the maximum saturator flow rate;  $\eta$  is the overall detection efficiency; and  $\int$  is the integral symbol. In the stepwise method, the resolution of the kernel is assumed to be positive infinity and hence, there is a one-to-one relationship between each saturator flow rate and the retrieved particle diameter.

## 2. Supplementary Figures

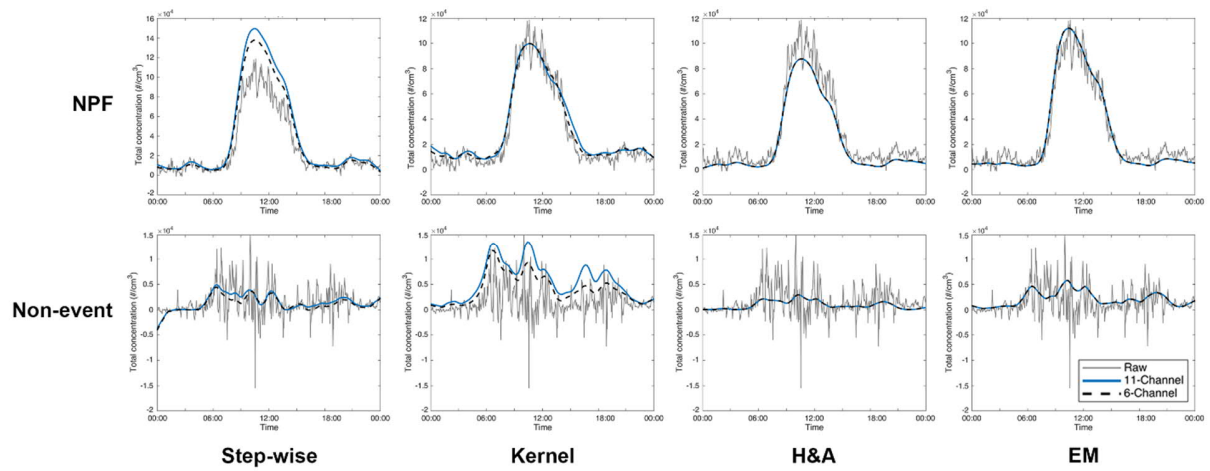


Fig. S1. Comparison of the 6- (dotted) and 11-channel (solid) size bins. The grey line indicates the raw estimation,  $R_{1.2-2.8}$  (calculated as difference between saturator flow rate at 1.3 lpm and 0.1 lpm). Top figures are during an NPF event (30 Jan.) and bottom figures are from a non-event day (6 Mar.).

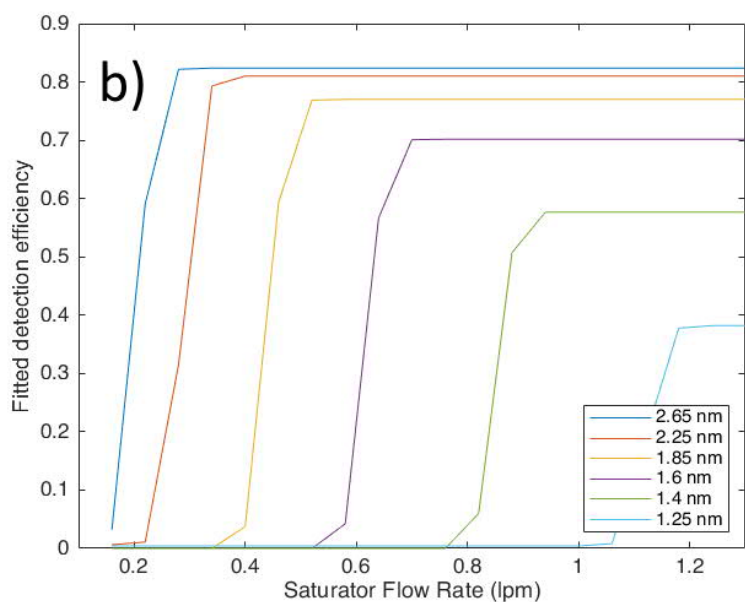
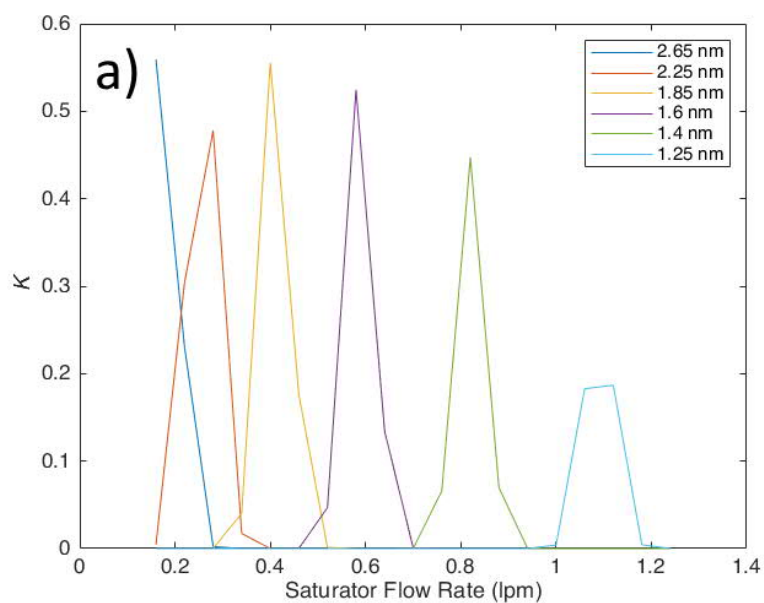


Fig. S2. The 6-channel a) kernel function curve ( $K$ ) and b) fitted detection efficiency curves for this study.

### 3. PSM inversion code usage (MATLAB)

This section is a step-by-step instruction on how to use the MATLAB code to invert PSM data.

Notes:

- Link: <https://github.com/tommychan-dev/PSM-Inversion>
- Script written using MATLAB 2018a and later
- Sample PSM data files (and PSM calibration file) included

- 1) Extract files your desired folder location and ensure the folder is added to the MATLAB search path (Home → Set Path → Add with subfolders)
- 2) Run the code with: Inversion\_Comp\_Run.m
- 3) All user parameters are from L9–60, as seen below:

```
%% User inputs

% Enter data directory *place all raw PSM dat to be analyzed
DatFolder = 'C:\DataFolderLocation\';

% Enter saving directory
paths.save='C:\DataFolderLocation\';

% Enter calibration file
path_calib = 'DataFileLocation.txt';

% Enter inversion method
% (1: Step-wise, 2: Kernel, 3: Hagen and Alofs, 4: Expectation-maximization algorithm)
method = 1;

% Enter PSM instrument
% (1: Normal, 2: Correction)
psm = 1; % Correction for A20s with older firmware

% Enter PSM data recording mode
% (1: stepping, 2: scanning)
mode = 2; % Only scanning mode at the moment!!

% Saving (1/0; on/off)
wanttosave = 1;

% Smoothen raw data (1/0; on/off)
pre_filtering = 1; % filter before inversion
pre_method = 'lowess'; % 'lowess' | 'moving' - loess or moving average
window_pre = 6; % span of the filtering (in seconds)
post_filtering = 1; % filter after inversion

% Data quality pre-treatment (1/0; on/off)
qualitycheck = 1;

% Fitting model profile for calibration file
% (1: exponential (2nd deg), 2: power, 3: polynomial (5 deg), 4:
% exponential (1st deg), 4: polynomial (3 deg)
fitting = 2;

% Enter diameter size bins (largest to smallest)
% Note errors may arise during inversion process: adjust max and min bins
dia = [3.1 2.8 2.5 2.0 1.7 1.5 1.35 1.25];

% Line losses correction (0:1:2 - None:Xue Mo:Lehtipalo)
% Xue Mo = with core sampler
% Lehtipalo = Gormley-Kennedy
core_sampling = 0;

% Diluter installation (1/0; on/off)
diluter = 0;
dilution = 10; % Dilution factor
```

- 4) Enter folder location of PSM data files (all files in the folder will be inverted)
- 5) Enter the saving and calibration file folder location
- 6) Choose the inversion method desired
- 7) Enter the PSM instrument. Generally, this is “1”, but if your A20 CPC is running an older firmware version, the select “2”. This has to do with the coincidence correction calculation
- 8) The PSM recording mode should be set to scanning mode. The current version (v1.0) can only invert PSM data running in scanning mode
- 9) If you wish to save the figures and inverted files, select “1”
- 10) L36-39 adjusts the smoothing/noise reduction of the data file, before and after data processing. The smoothing type and span can be adjusted
- 11) Data quality pre-treatment setting and fitting profile of the calibration can be adjusted
- 12) Enter the desired number of cut-off points by adjusting the diameter sizes (nm). This must be done from the largest to smallest, and separated by a space and enclosed in square brackets. Errors may arise and so adjust the largest and smallest cut-off sizes
- 13) Finally, if you have a core sampler (see Fu et al. 2019) and/or diluter installed on your PSM, these options can be selected. If using any line loss correction, change the parameters in the Loss\_Correction.m file (found in the Toolbox folder); e.g. length of tubes and flows