How to model the evolution of the polluted PBL?

Exploring a new approach

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The presentation plan

1. Introduction
2. What is the Eddy Diffusivity/Mass Flux scheme?
3. What is the LaFuLiou Radiation transfer model?
4. How were these two models joined together?
5. A quick look at the results + Bonus (?)
6. Summary and references

1. Introduction

Motivation

- Cities of Poland often experience a carbon-based pollution, concentrated mainly in the PBL
- The PBL diurnal cycles and its evolution affects the aerosol spatial distribution and therefore influences the radiation transfer
- Our group collected a lot of data concerning the radiation fluxes and aerosol concentration in the PBL

Idea: Let's try to join a model describing the PBL evolution and the radiative transfer model

fig. 1 - The panorama of Krakow, Poland on 29th Nov 2019. Taken from the deck of an observation balloon located near the Wawel Castle

Scientific motivation

- There exists the feedback loop between the height of the planetary boundary layer (PBL) and the concentration of absorbing aerosols
- When a decreasing aerosol structure is present, the heating effect strengthens vertical convection
- When an inverse aerosol structure is present, the heating effect facilitate the formation of temperature inversion

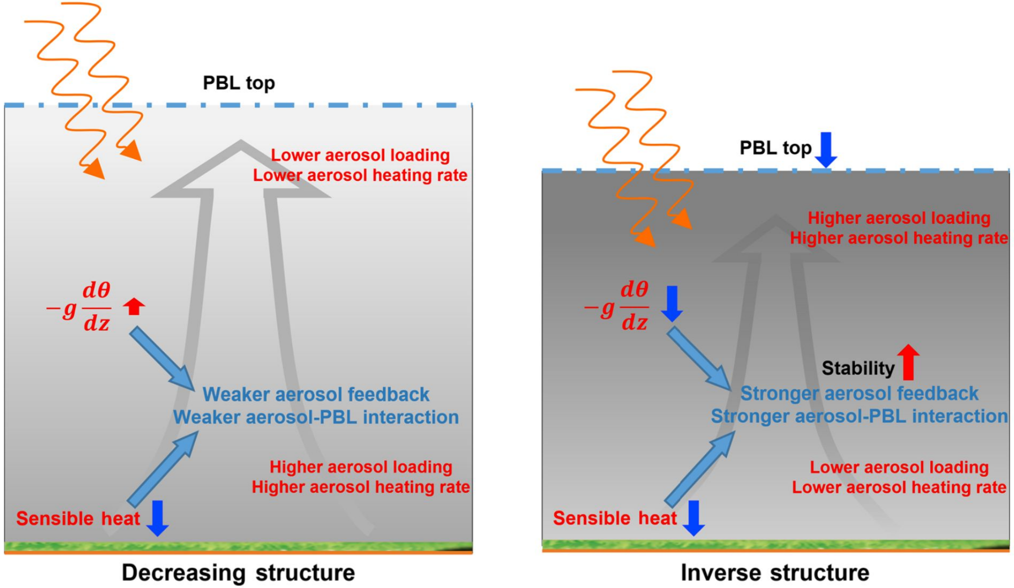

fig. 2 - Schematic diagrams describing aerosol–PBL interactions when decreasing and inverse aerosol structures are present[1].

What is Polluted PBL?

Planetary Boundary Layer, in which there is a non-zero concentration of absorbing aerosol.

Other descriptions found in literature:

- All-sky conditions
- Aerosol-filled PBL
- PBL with aerosols
- Avoiding directly referring to it and insead using ‘Aerosol-PBL interactions’ (API).
- PBL

2. Eddy Diffusivity/Mass Flux scheme

What is the EDMF model?

- Eddy Diffusivity: addressing downward fluxes

- Mass Flux: addressing the limitations of the ED. Introducing a strong thermal updraft motion

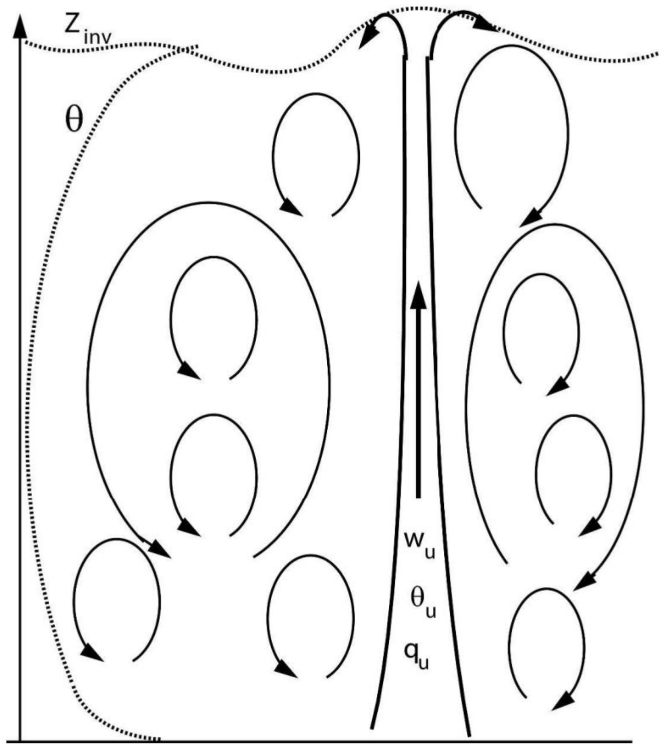

fig. 3 - The simplistic drawing depicting the EDMF framework[1]

The core idea behind EDMF

In the Eddy diffusivity scheme, normally we would have:

$$\overline{w'\theta'} = -K\frac{\partial\bar{\theta}}{\partial z} \quad (1)$$

Where K is eddy diffusivity coefficient. Unfortunately, this approach gives wrong predictions on the top of the PBL. In order to solve this, the EDMF scheme proposes a following decomposition:

$$\overline{w'\theta'} = a_u\overline{w'\theta'}^u + (1-a_u)\overline{w'\theta'}^e + a_u(w_u - \bar{w})(\theta_u - \theta_e) \quad (2)$$

where a_u is a small surface area, much smaller than the model domain. This surface is occupied by a strong thermal updrafts penetrating the top of the PBL.

The core idea behind EDMF

$$\overline{w'\theta'} = a_u \overline{w'\theta'}^u + (1 - a_u)\overline{w'\theta'}^e + a_u(w_u - \bar{w})(\theta_u - \theta_e) \quad (2)$$

We can further simplify by:

- taking into account that $a_u << 1$
- approximating θ_e by its mean value
- defining mass flux $M = a_u(w_u - \underline{w})$

$$\overline{w'\theta'} \approx \overline{w'\theta'}^e + M(\theta_u - \bar{\theta}) \quad (3)$$

The core idea behind EDMF

$$\overline{w'\theta'} \approx \overline{w'\theta'}^e + M(\theta_u - \bar{\theta}) \tag{3}$$

Finally, we plug back the original eddy diffusivity scheme and get:

$$\overline{w'\theta'} \approx -K\frac{\partial\bar{\theta}}{\partial z} + M(\theta_u - \bar{\theta}) \tag{4}$$

We can now plug it in into the time evolution of the scalar field ϕ[2] and get the final prognostic equation in the EDMF framework.

Equations in the EDMF with TKE closure (EDMF-TKE)

The prognostic equation for a scalar field ϕ[2]:

$$\frac{\partial \bar{\phi}}{\partial t} = \frac{\partial}{\partial z}\left[-K_{\phi}\frac{\partial \bar{\phi}}{\partial z} + M(\phi_u - \bar{\phi})\right] + F \tag{5}$$

The additional prognostic equation for TKE closure[2]:

$$\frac{\partial e}{\partial t} = -\frac{\partial}{\partial z}\left(-K_e\frac{\partial e}{\partial z}\right) + \frac{g}{\bar{\theta}_v}\overline{w'\theta'_v} - D \tag{6}$$

+ additional equations for K, M, D, F, ϕ_u etc.

Short description of the implementation

- Written fully in MATLAB
- The model operates in one dimension
- The spatial range: [0; 4] km, the spatial resolution: 20m
- The temporal resolution: 1 min
- Modelling the dry conditions
- The **clear-sky** case (with the aerosol present)

and other, less relevant settings...

3. LaFuLiou radiation transfer model

LaFuLiou (Ed4-LaRC-FuLiou) radiation transfer model

- developed in NASA Langley Research Center
- Uses the δ-four-stream approach which is a **natural extension** of the popular two-stream radiative transfer model commonly used in atmospheric sciences
- Uses the parameterization proposed by Fu, Liou and Ackermann[4] which proves to be **relatively accurate and not much more complex**
- The legacy code in fortran works **relatively fast**
- The fortran solver was embedded in the MATLAB shell to make it more **user friendly**
- Is **available** for everyone on github*

*given that you have tools and are able to compile multi-file fortran code

What parameters were used?

- Spectral resolution: 6 short wave and 12 long wave bands
- Spatial resolution: 78 levels from 0 to 100 km above the ground
- Near the ground (>600 hPa) the grid is denser. In the range [0; 4] km the spatial resolution is 80m
- The **clear-sky** case (with the aerosol present)
- The sun position was calculated for a user defined DOY and location

and other, less relevant settings…

4. EMDF-TKE/LaFuLiou Coupling

How were these two models combined?

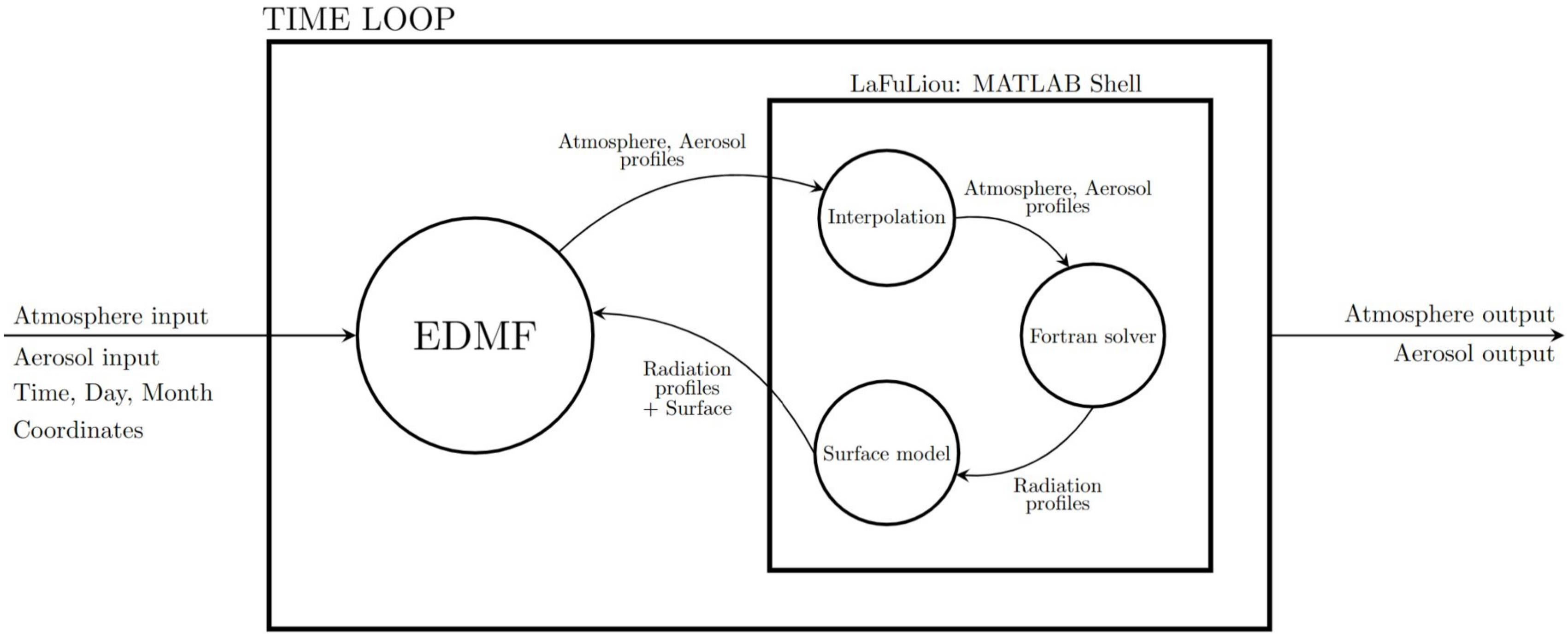

fig. 4 - The block diagram showing how two models were joined together in one time loop and how they exchange data

Initial profiles: Potential temperature and Heating rate

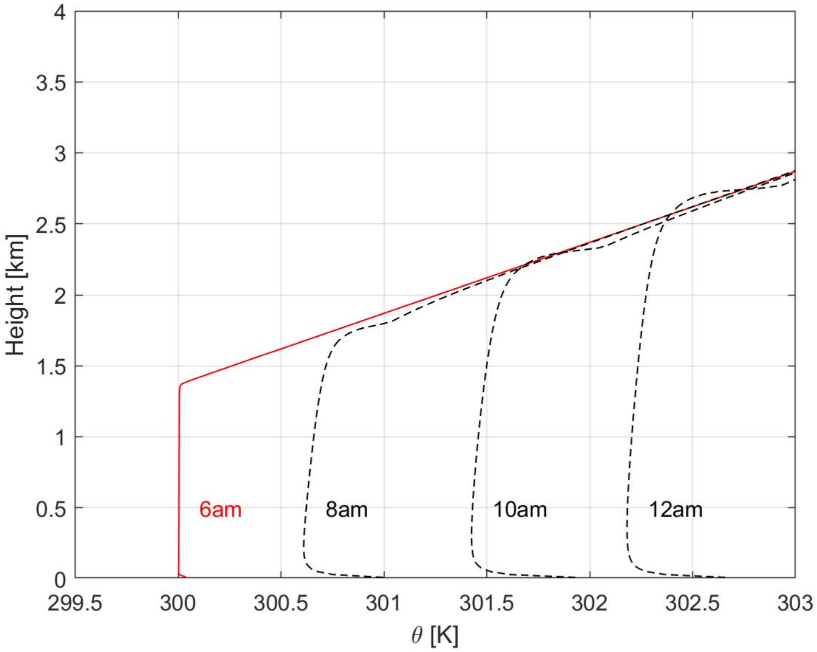

fig. 5a - An example of the model output: evolution of the potential temperature with time

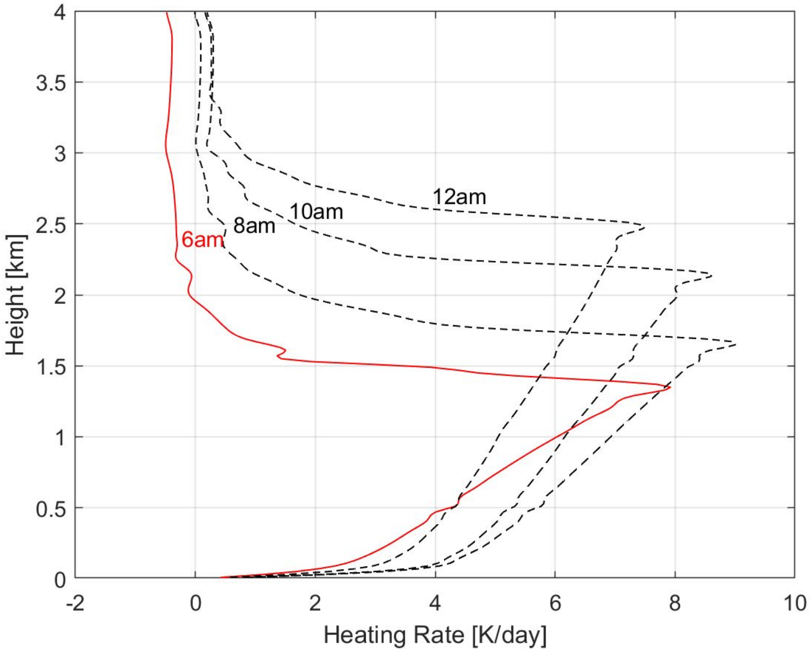

fig. 5b - An example of the model output: The evolution of the heating rate with time

Additional remark no. 1: The extinction suppression

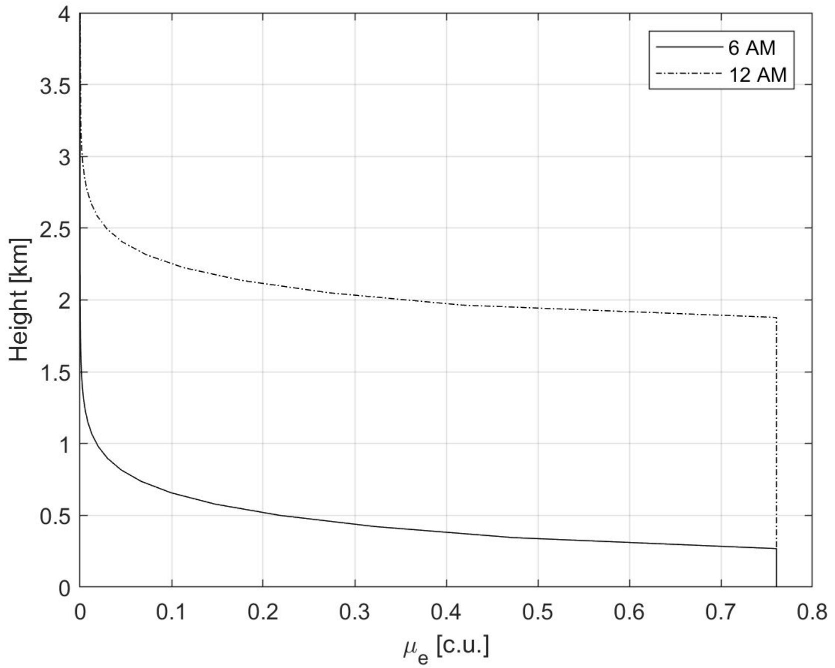

fig. 6 - An example of extinction profile. Dashed line denote profile at the end of the simulation.

The extinction profile was calculated as follows:

$$\mu_e(z) = \begin{cases} \mu_{e,0} & , \text{if } z \leq z^* \\ \mu_{e,0} \int_{z*}^{\infty} e^{-\frac{z-z^*}{H}} & , \text{if } z > z^*. \end{cases} \quad (7)$$

with the normalisation condition:

$$\tau_a = \int_0^{\infty} \mu_e(z) dz \quad (8)$$

or after the integration:

$$\tau_a = \mu_{e,0}(z^* + H) \quad (9)$$

Additional remark no. 2: The scattering enhancement factor

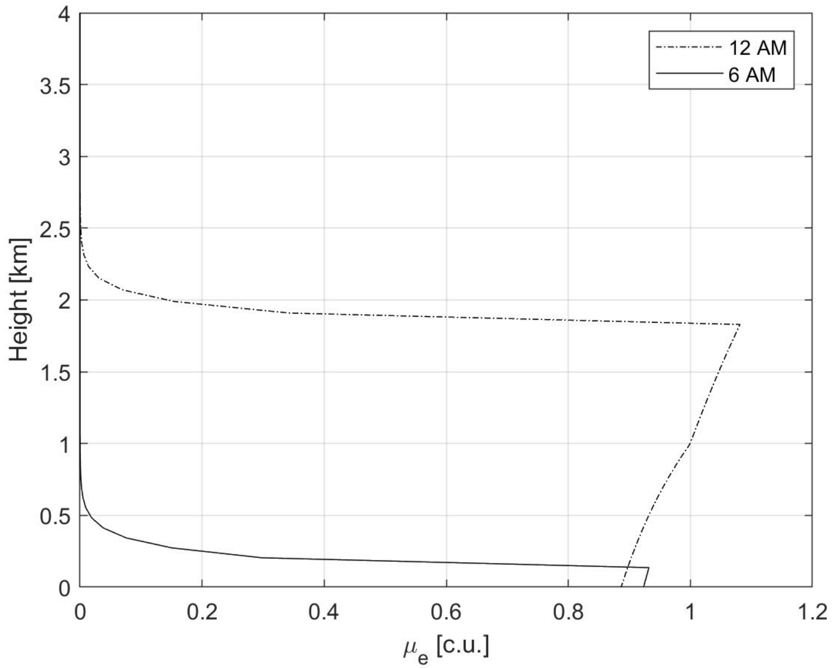

fig. 7 - An example of extinction profile after the scattering enhancement correction.

The extinction profile was additionally multiplied by:

$$f(RH) = \left(\frac{1 - RH}{1 - RH_{REF}} \right)^{\gamma} \quad (10)$$

Where ɣ is the scattering enhancement coefficient and RH_{REF} is the reference relative humidity for which the ɣ was derived experimentally.

In our simulations:

- $RH_{REF} = 0$
- ɣ = 0.5

5. Results

Polluted PBL evolution under different pollution levels.

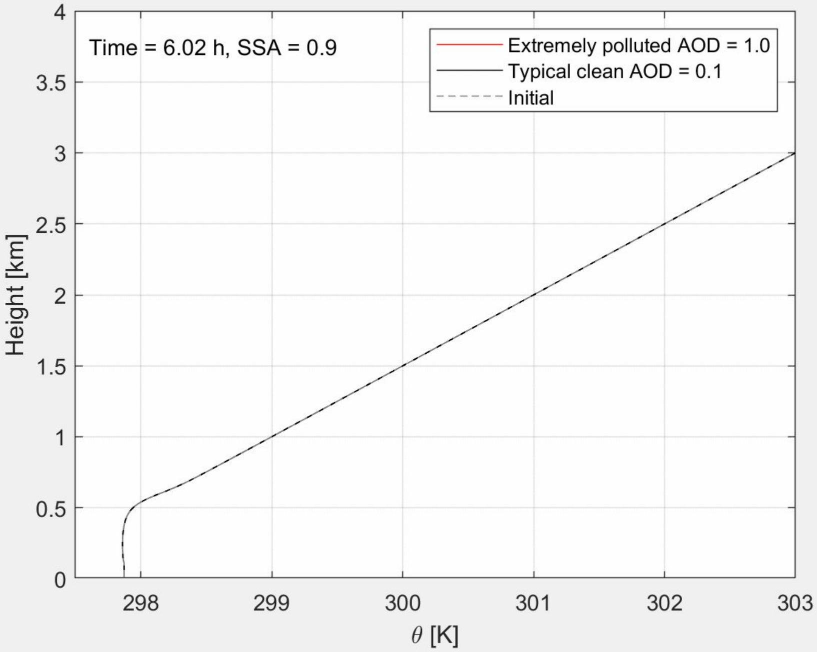

fig. 8a - The evolution of the PBL temperature with time

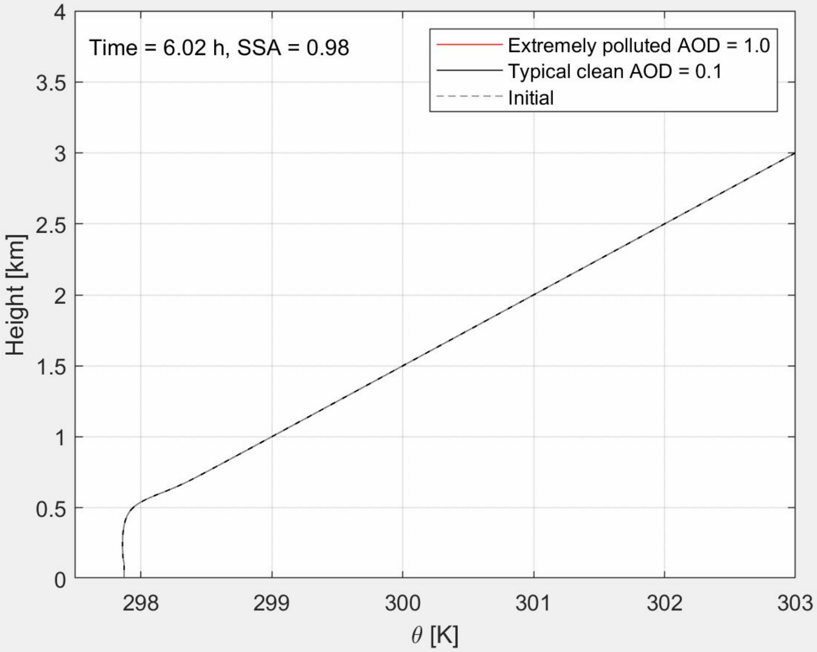

fig. 8b - The evolution of the PBL temperature with time

Polluted PBL evolution under different pollution levels.

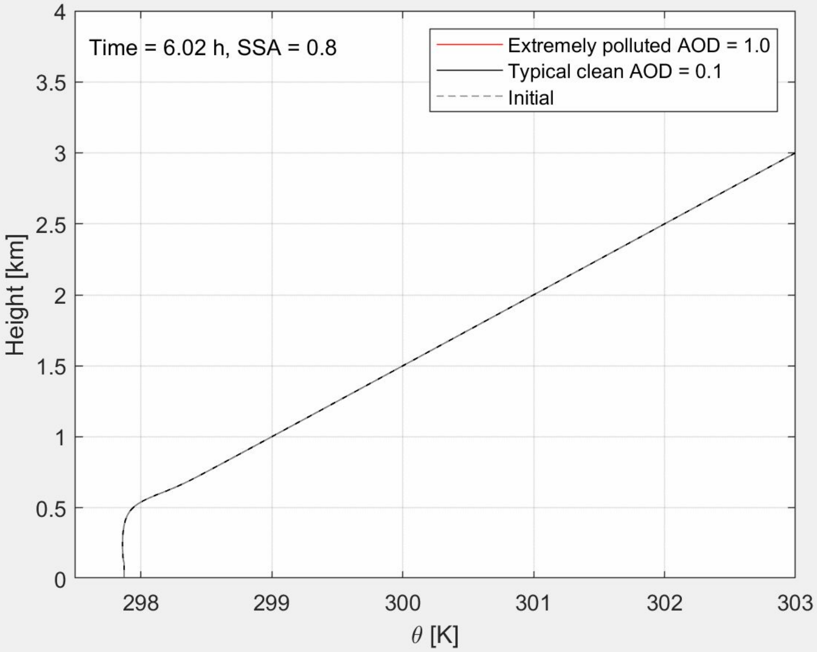

fig. 9a - The evolution of the PBL temperature with time

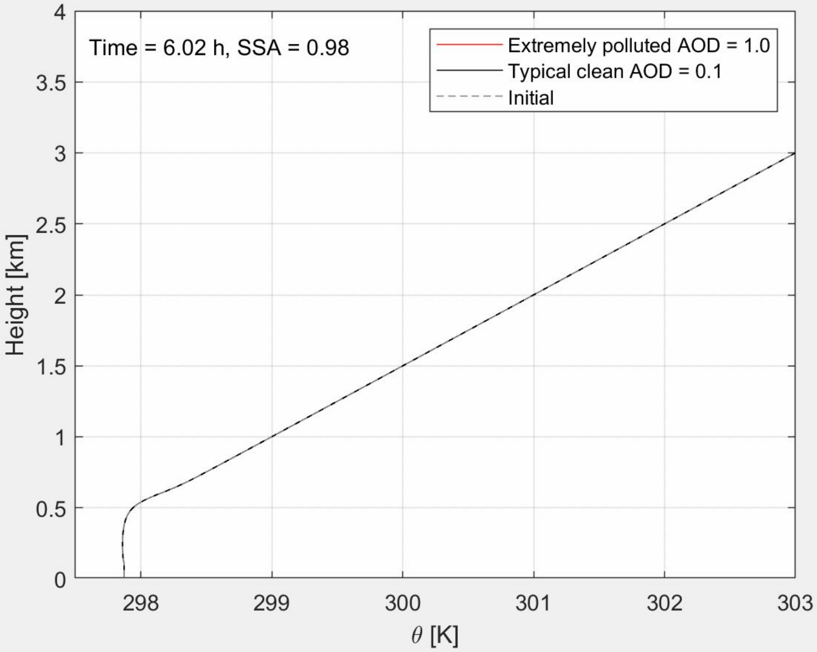

fig. 9b - The evolution of the PBL temperature with time

Polluted PBL evolution under different aerosol compositions

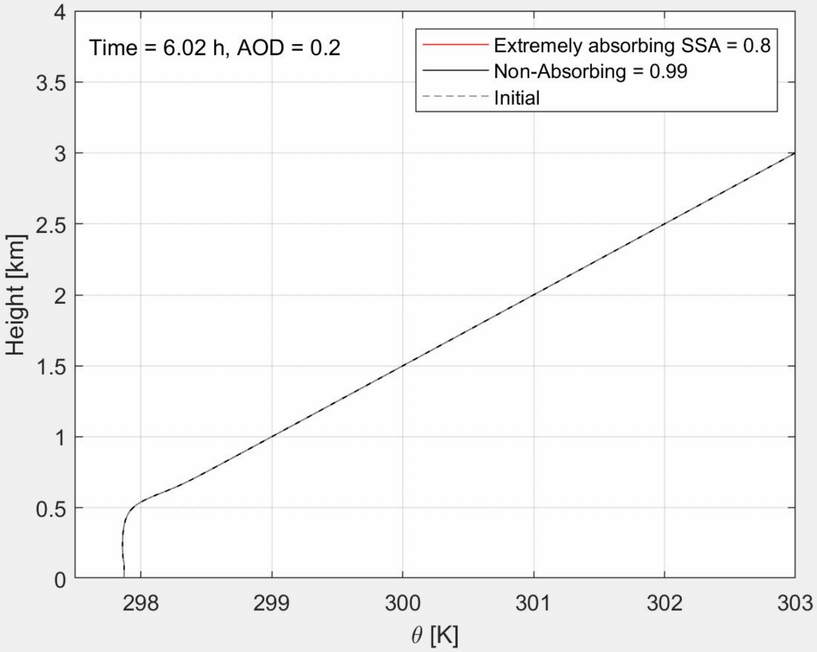

fig. 10a - The evolution of the PBL temperature with time

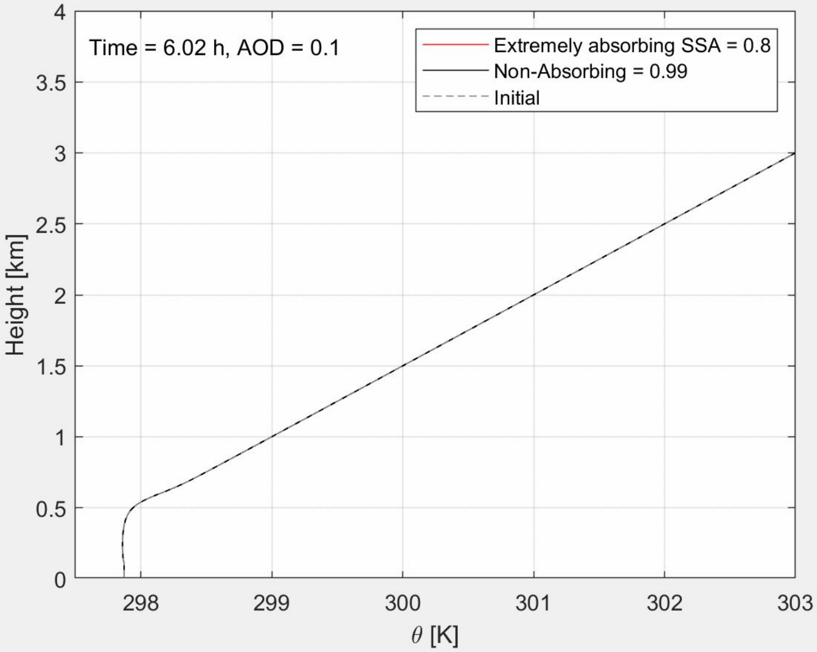

fig. 10b - The evolution of the PBL temperature with time

Polluted PBL evolution under different aerosol compositions

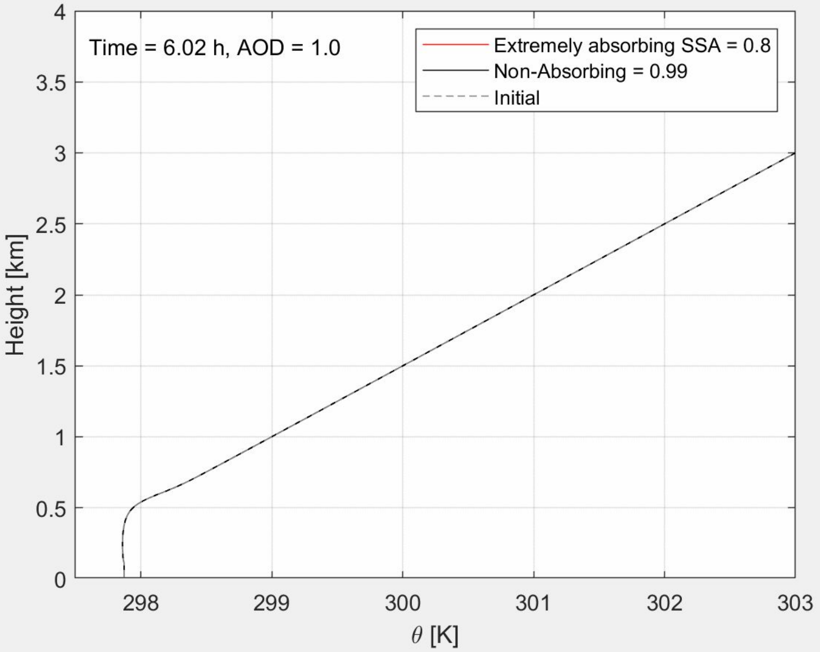

fig. 11a - The evolution of the PBL temperature with time

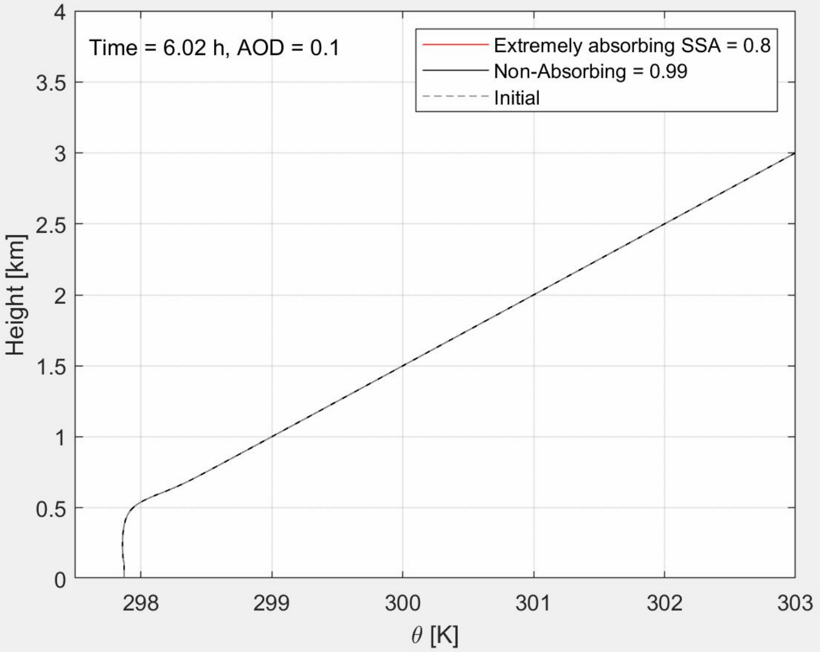

fig.11b - The evolution of the PBL temperature with time

Additional remark no. 3: Explaining additional parameters

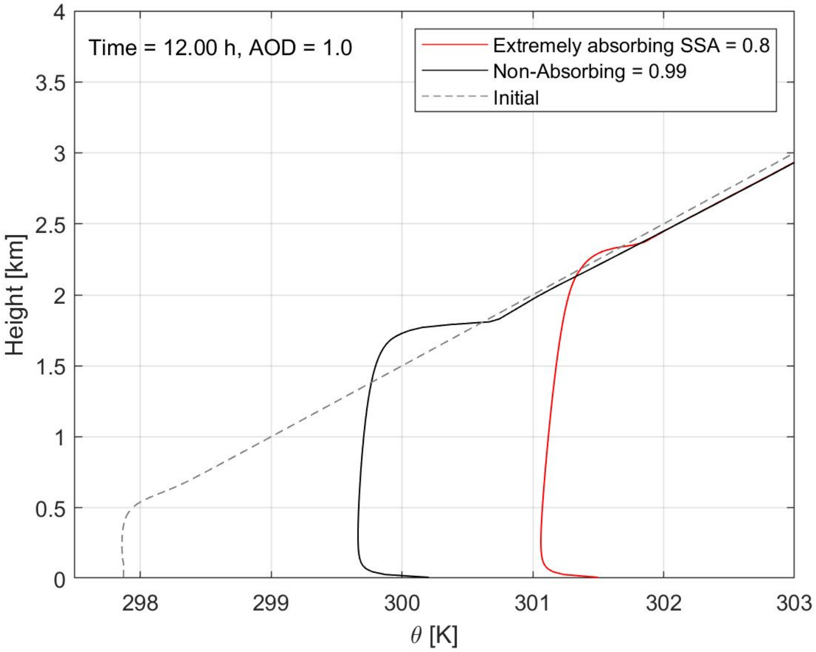

fig. 12 - Snapshot from the end of one of the previous animations.

Additional remark no. 3: Explaining additional parameters

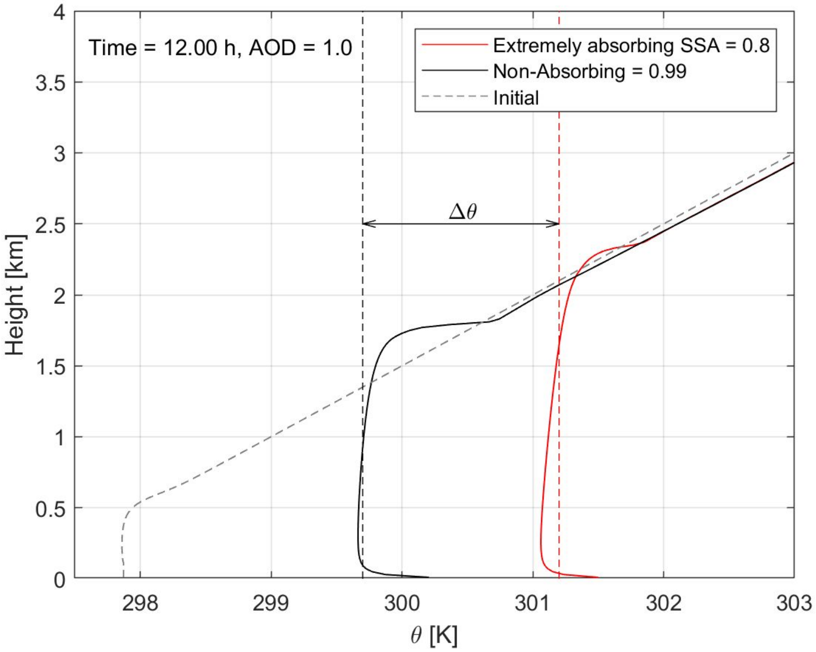

fig. 12 - Snapshot from the end of one of the previous animations.

Additional remark no. 3: Explaining additional parameters

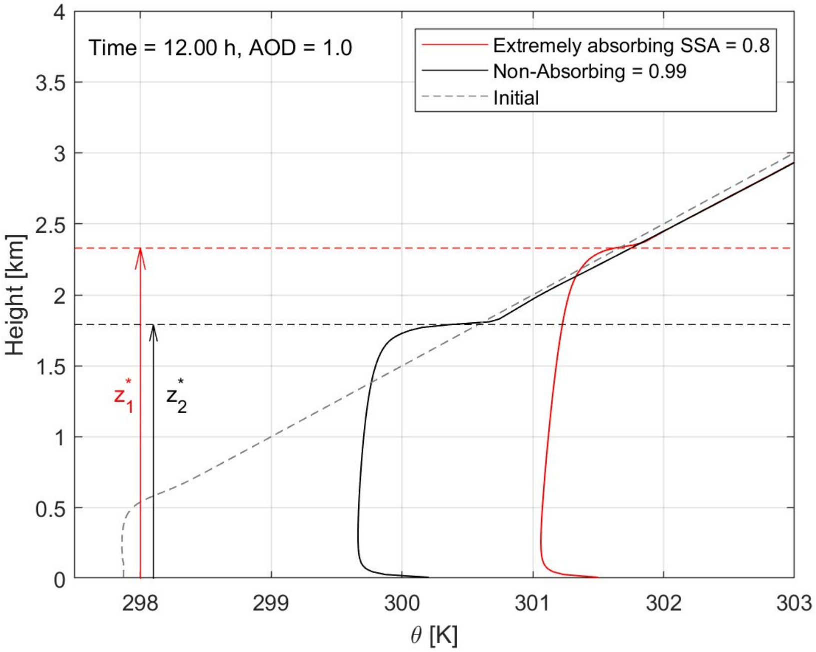

fig. 12 - Snapshot from the end of one of the previous animations.

The PBL Height vs Aerosol optical depth

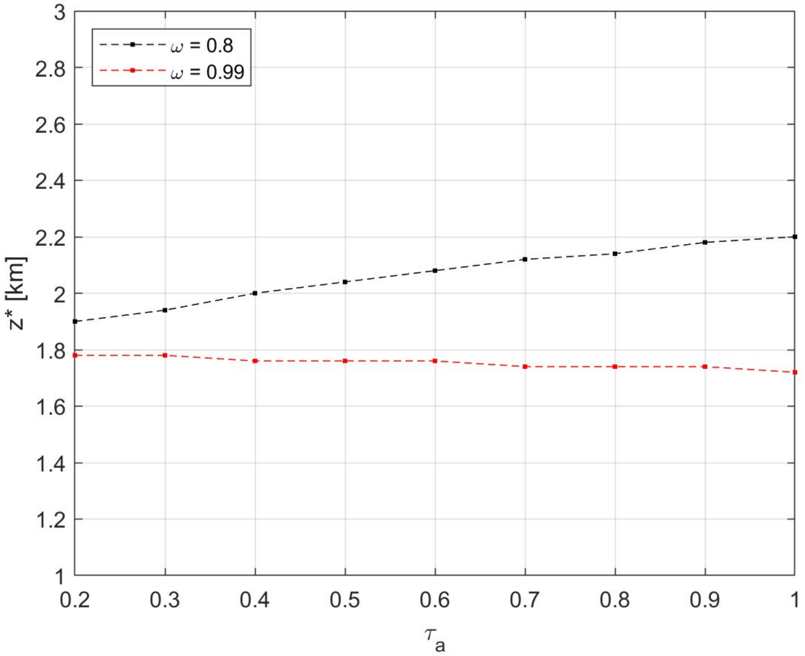

fig. 13a - The PBLH vs AOD.
The extinction suppression: 0.1 km

The PBL mean temperature difference vs Aerosol optical depth

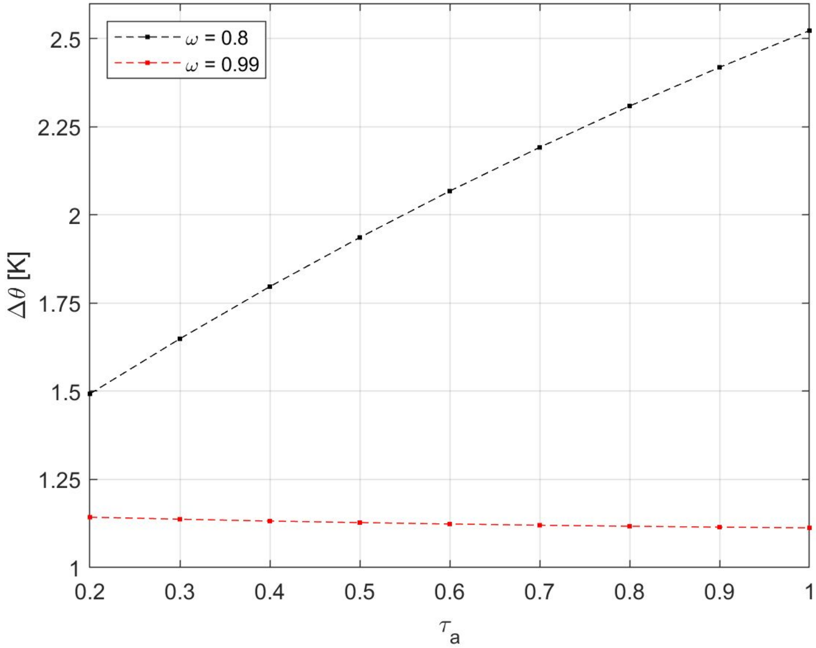

fig. 14a - The PBL mean temp. difference vs AOD.
The extinction suppression: 0.1 km

The PBL Height vs Aerosol single scattering albedo

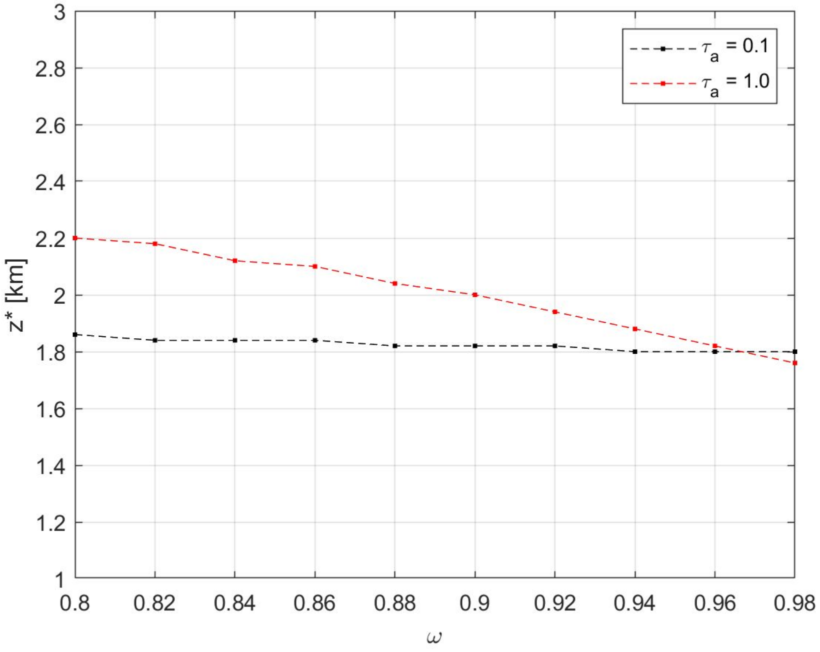

fig. 15a - The PBLH vs SSA.
The extinction suppression: 0.1 km

The PBL mean temperature difference vs Aerosol single scattering albedo

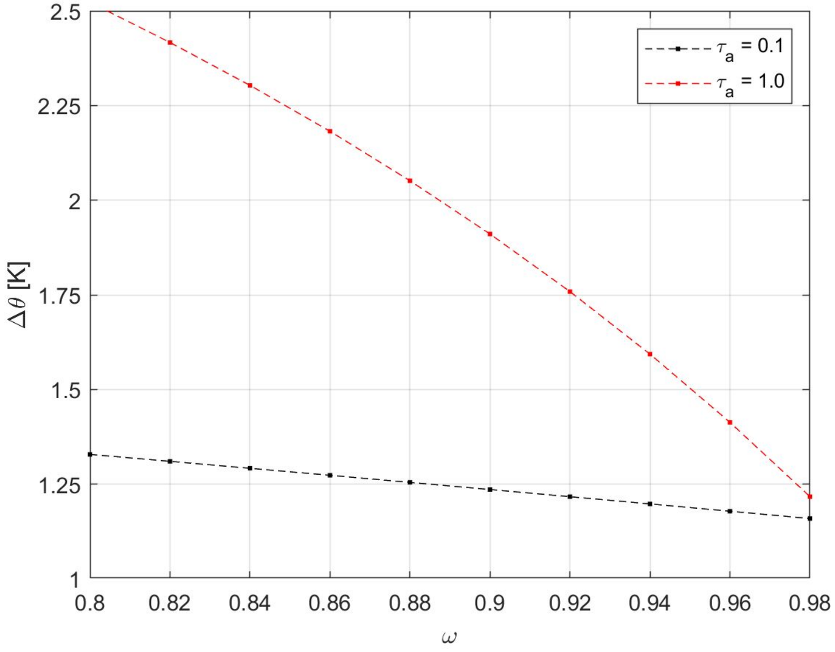

fig. 16a - The PBL mean temp. difference vs SSA.
The extinction suppression: 0.1 km

5+. Bonus - The extinction suppression

Additional remark no. 4: The extinction suppression H

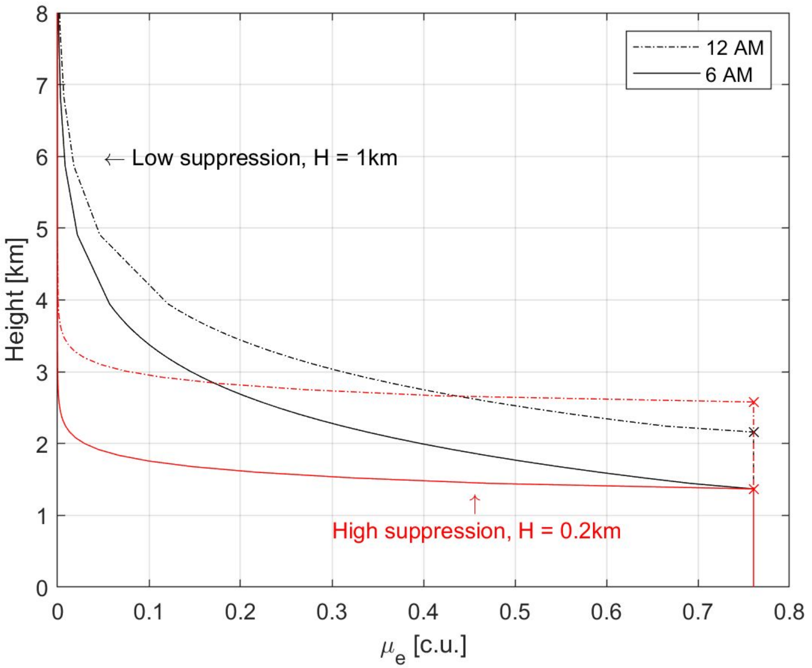

fig. 17 - Examples of extinction profiles. Dashed lines denote profiles at the end of the simulation. 'x' denotes the PBL top

The extinction profile was calculated as follows:

$$\mu_e(z) = \begin{cases} \mu_{e,0} & \text{, if } z \leq z^* \\ \mu_{e,0} \int_{z*}^{\infty} e^{-\frac{z-z^*}{H}} & \text{, if } z > z^*. \end{cases} \quad (7)$$

with the normalisation condition:

$$\tau_a = \int_0^{\infty} \mu_e(z) dz \quad (8)$$

or after the integration:

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PBL Evolution under different pollution levels

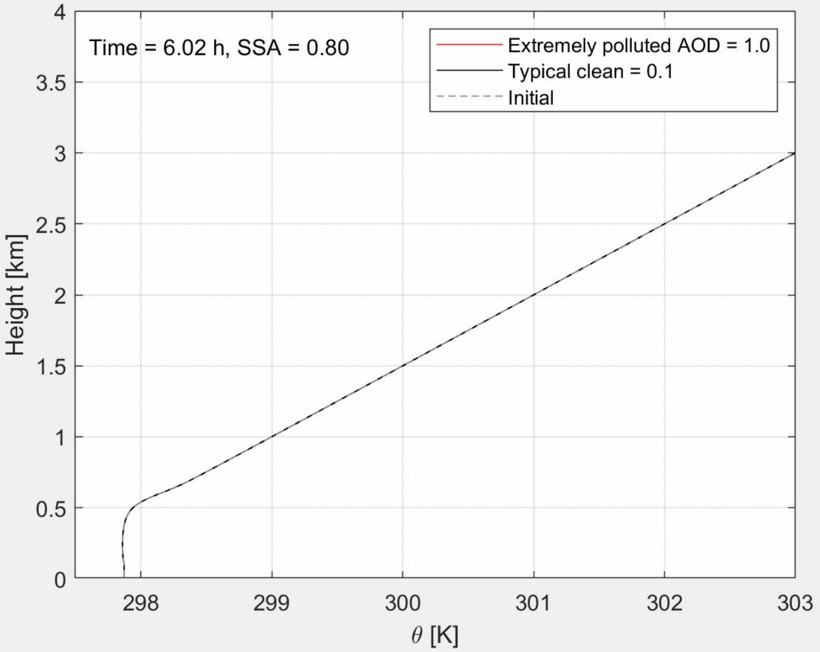

fig. 18a - The evolution of the PBL temperature with time.
SSA = 0.8, H = 1 km

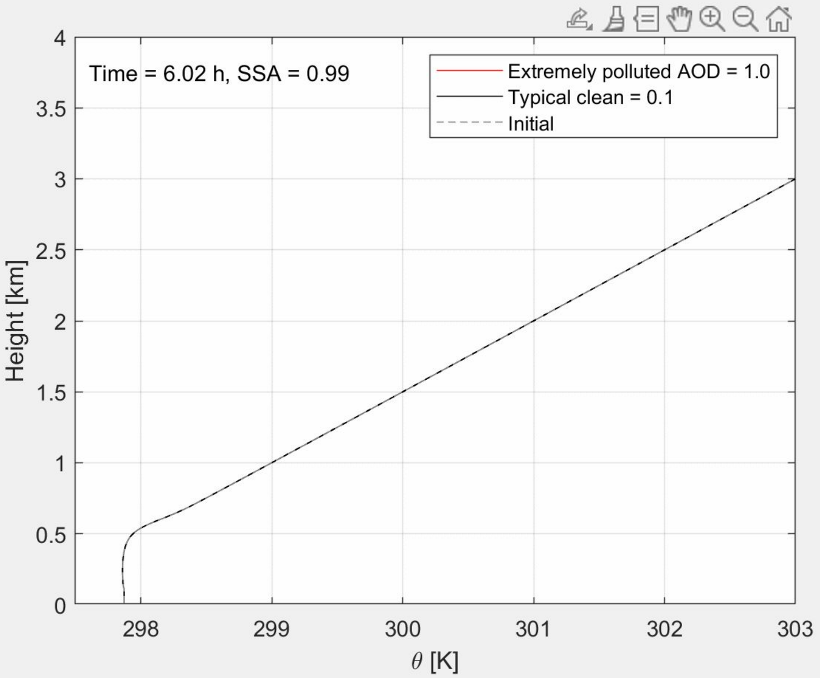

fig. 18b - The evolution of the PBL temperature with time.
SSA = 0.99, H = 1 km

PBL Evolution under different aerosol compositions

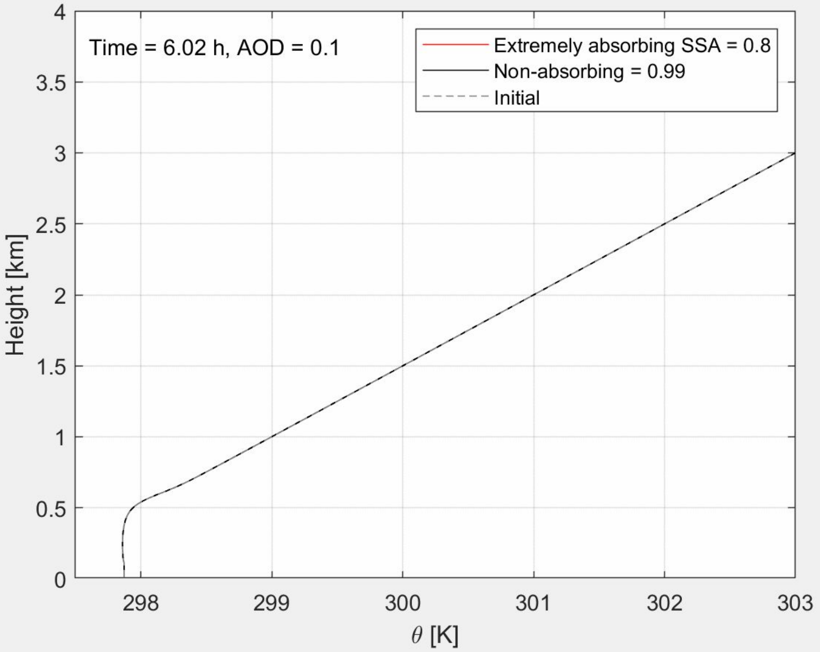

fig. 19a - The evolution of the PBL temperature with time.
AOD = 0.1, H = 1 km

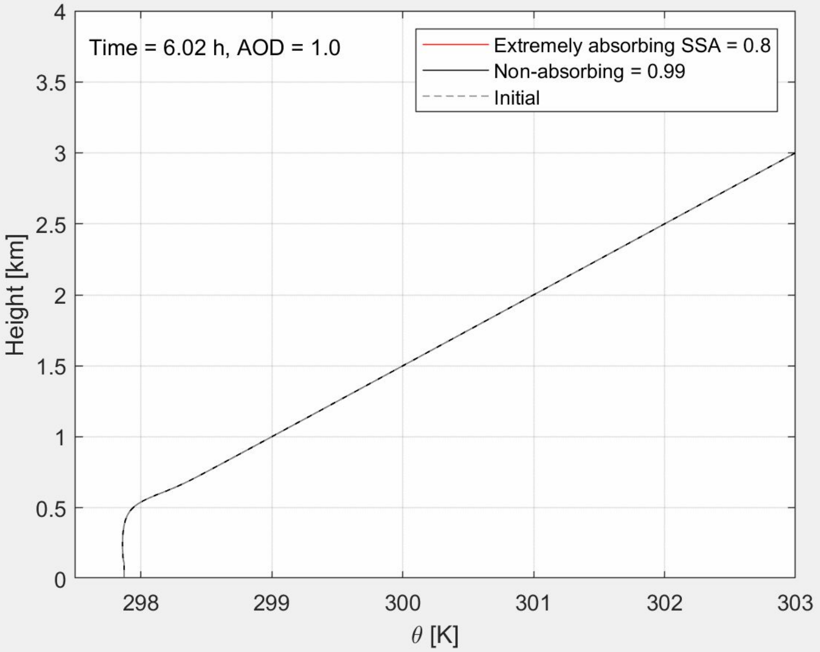

fig. 19b - The evolution of the PBL temperature with time.
AOD = 1.0, H = 1 km

The PBL Height vs Aerosol optical depth

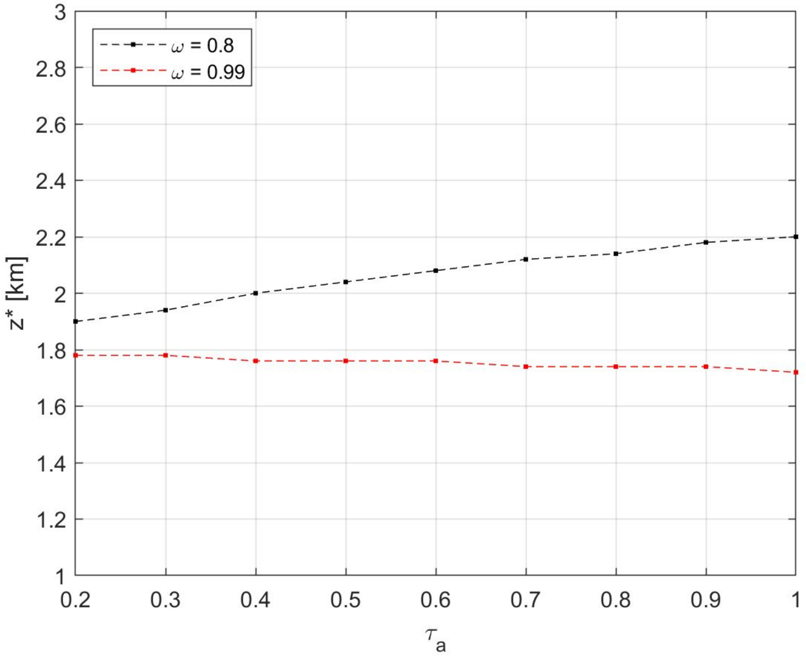

fig. 13a - The PBLH vs AOD.
The extinction suppression: 0.1 km

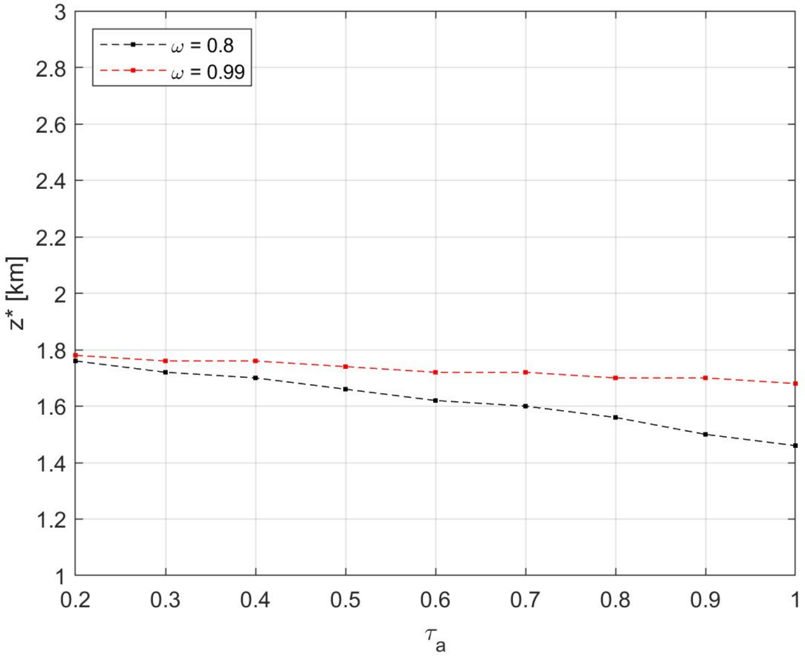

fig. 13b - The PBLH vs AOD.
The extinction suppression: 1 km

The PBL mean temperature difference vs Aerosol optical depth

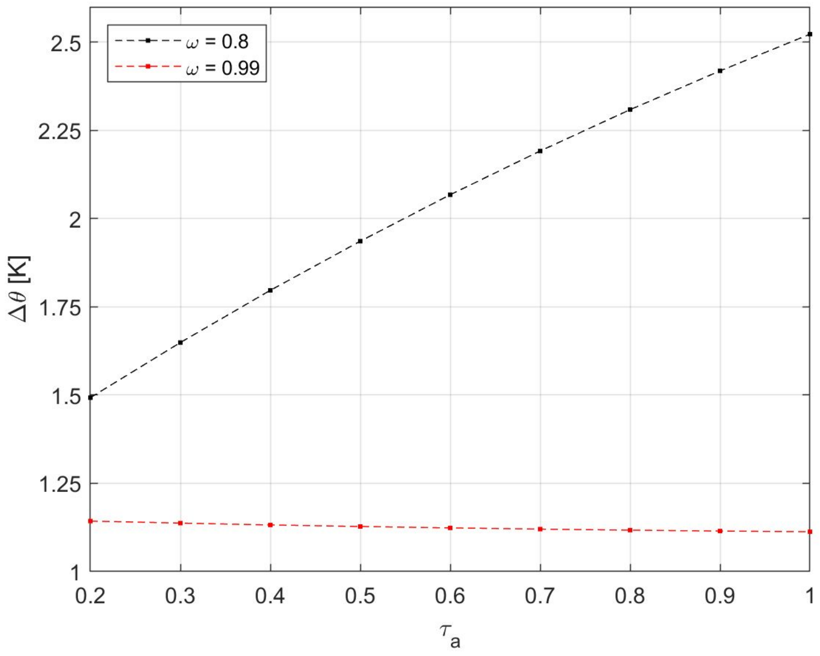

fig. 14a - The PBL mean temp. difference vs AOD.
The extinction suppression: 0.1 km

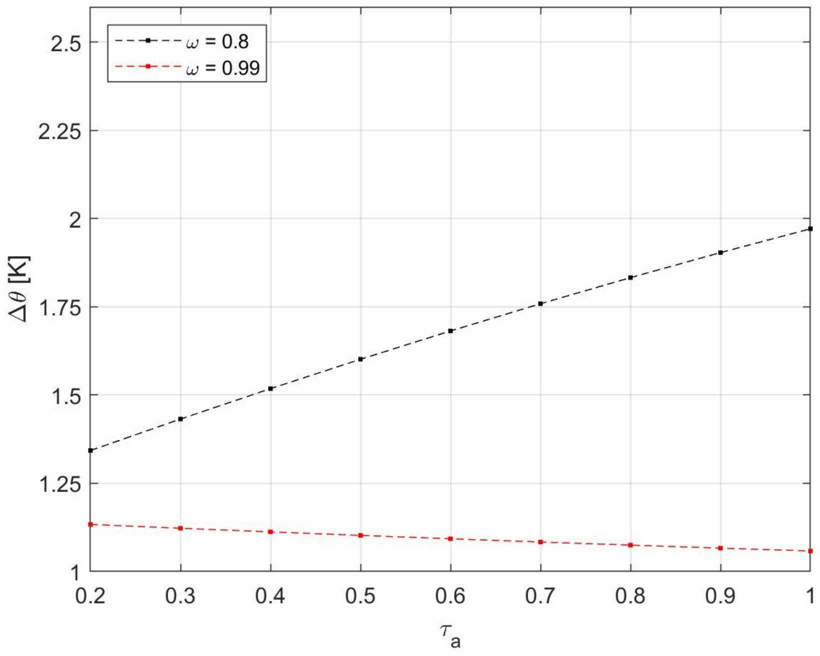

fig. 14b - The PBL mean temp. difference vs AOD.
Case for the extinction suppression: 1 km

The PBL Height vs Aerosol single scattering albedo

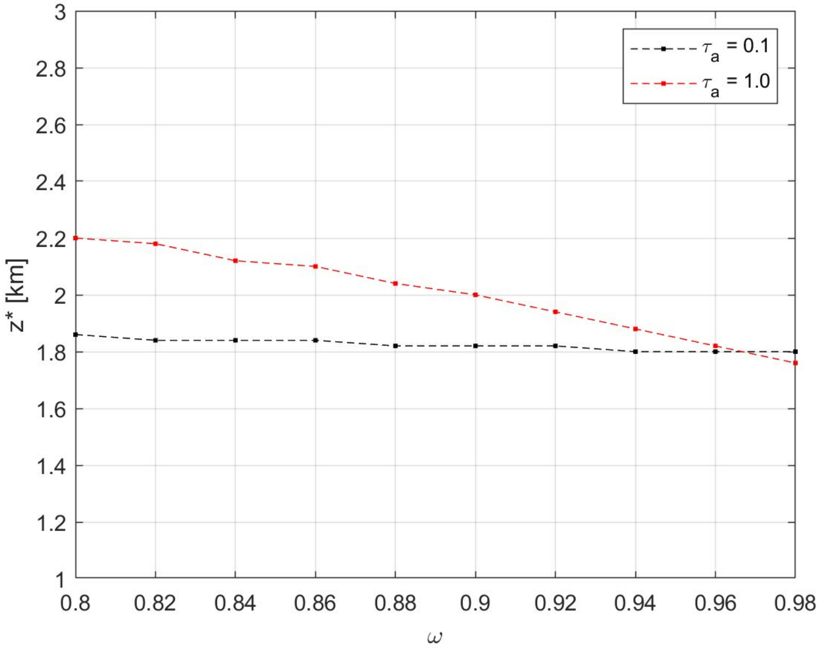

fig. 15a - The PBLH vs SSA.
The extinction suppression: 0.1 km

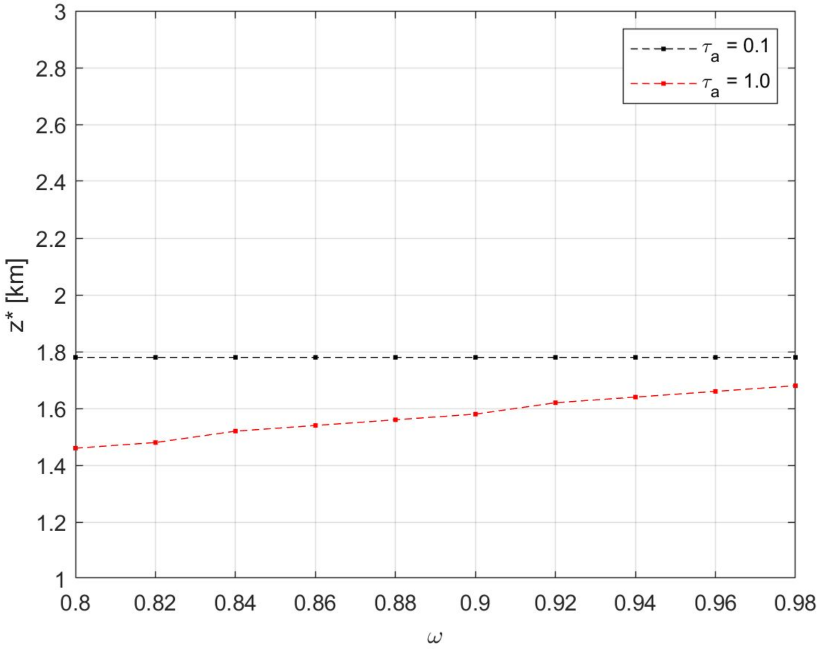

fig. 15b - The PBLH vs SSA.
The extinction suppression: 1 km

The PBL mean temperature difference vs Aerosol single scattering albedo

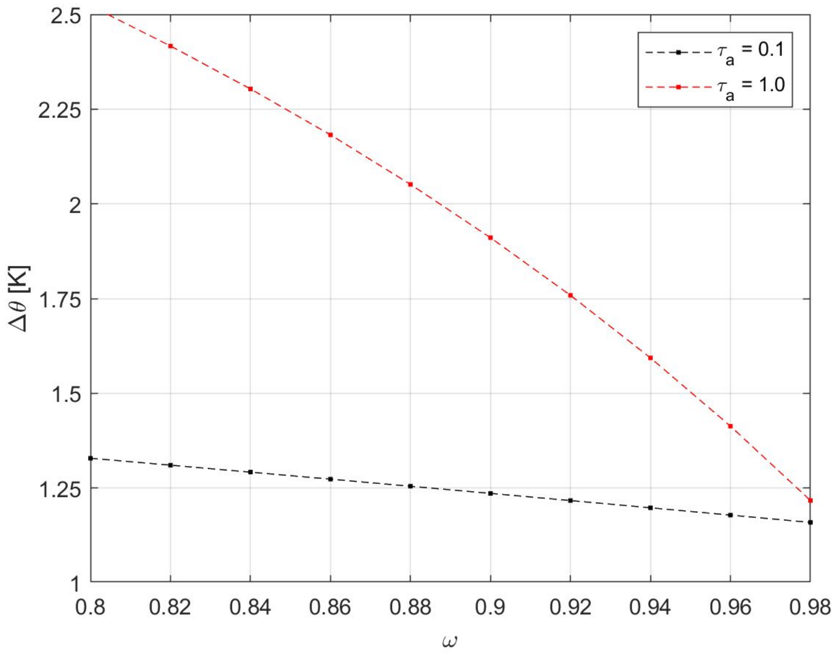

fig. 16a - The PBL mean temp. difference vs SSA.
The extinction suppression: 0.1 km

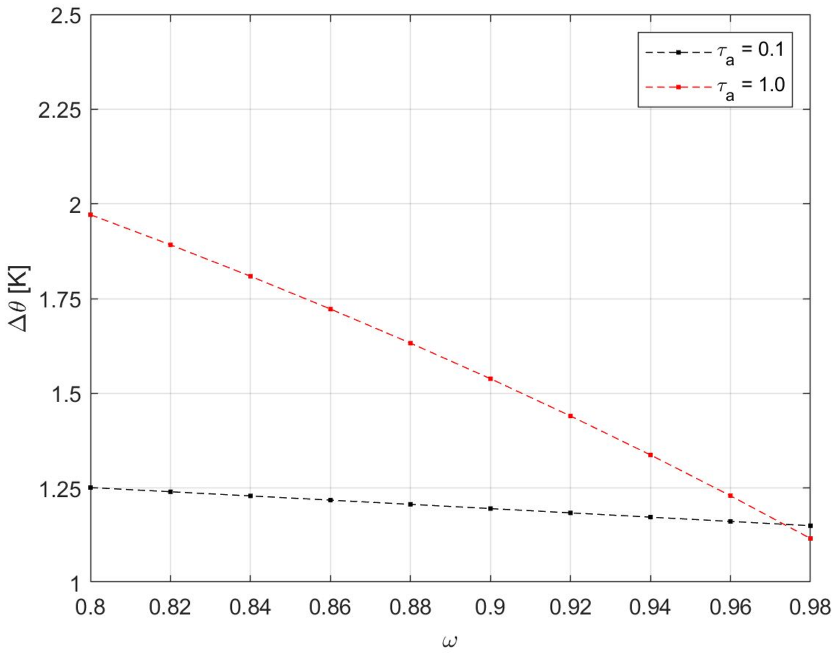

fig. 16b - The PBL mean temp. difference vs SSA.
The extinction suppression: 1 km

6. Summary

Summary

- The coupled model is relatively fast: 6 h of simulation with 1 min time step took about 1 min to run on a standard personal PC
- Output suggests:
  - Non-absorbing aerosol and low amounts of aerosol have a small impact on the PBLH and the temperature difference
  - The more absorbing the aerosol, the higher the temperature of the PBL
  - The more polluted the PBL the higher its temperature
- The extinction profile suppression effect:
  - Low suppression → Aerosol above the PBL → Smaller PBLH, Lower Temperature
  - High suppression → Aerosol only in PBL → Higher PBLH, Higher Temperature

Further possible improvements

- Implementation of a better surface model
- Improvements of the PBLH calculation
- Adding a faster way of data exchange between the MATLAB Shell and Fortran solver
- Verifying the model with experimental data
- Maybe (?) refactoring the Fortran solver. Update from Fortran 77 and Fortran 90 to Fortran 2018
- Providing more user friendly interface

References

[1] Su, T., Li, Z., Li, C., Li, J., Han, W., Shen, C., Tan, W., Wei, J., & Guo, J. (2020). The significant impact of aerosol vertical structure on lower atmosphere stability and its critical role in aerosol-planetary boundary layer (PBL) interactions. Atmospheric Chemistry and Physics, 20(6), 3713–3724. https://doi.org/10.5194/acp-20-3713-2020

[2] Siebesma, A. P., Soares, P. M. M., Teixeira, João (2007) A Combined Eddy-Diffusivity Mass-Flux Approach for the Convective Boundary Layer. *Journal of The Atmospheric Sciences*, 64, 1230–1248, doi: 10.1175/JAS3888.1

[3] Witek, M., L., J. Teixeira, G. Matheou (2010), An Integrated TKE-Based Eddy Diffusivity/Mass Flux Boundary Layer Closure for the Dry Convective Boundary Layer, *Journal of the Atmospheric Sciences*, 68, 1526, doi: 10.1175/2011JAS3548.1

[4] Liou, K. & Fu, Q. & Ackerman, T. (1988). A Simple Formulation of the Delta-Four-Stream Approximation for Radiative Transfer Parameterizations. Journal of the Atmospheric Sciences. 45. doi: 10.1175/1520-0469(1988)045<1940:ASFOTD>2.0.CO;2.

[5] GitHub - fredgrose/Ed4_LaRC_FuLiou: Edition 4 version of LaRC FuuLiou Broadband Correlated K Sw & Lw Radiative Transfer code

Thank you for your attention!

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Acknowledgements:

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fig. 1 - The panorama of Krakow, Poland on 29th Nov 2019. Taken from the deck of an observation balloon located near the Wawel Castle