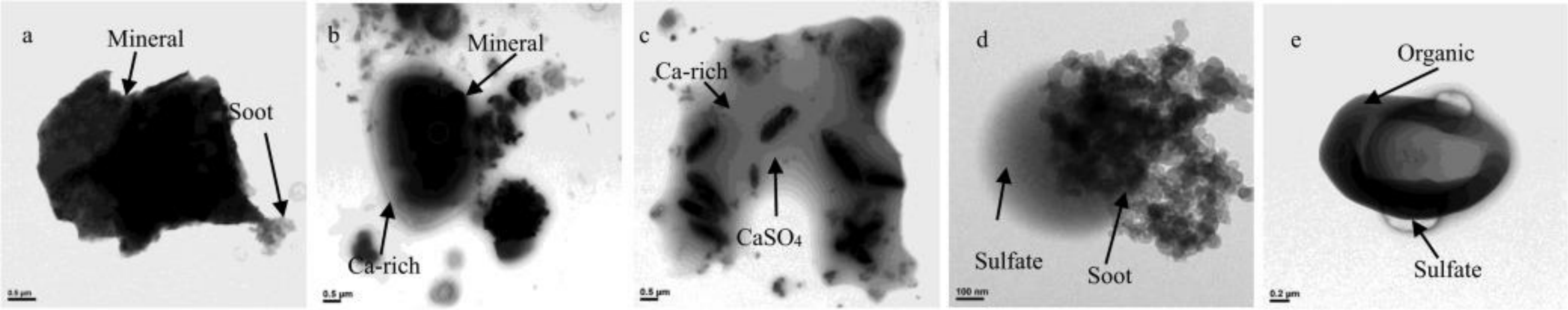
Representing the Optical Properties of Internally-Mixed Aerosols in Atmospheric models using Artificial Neural Networks

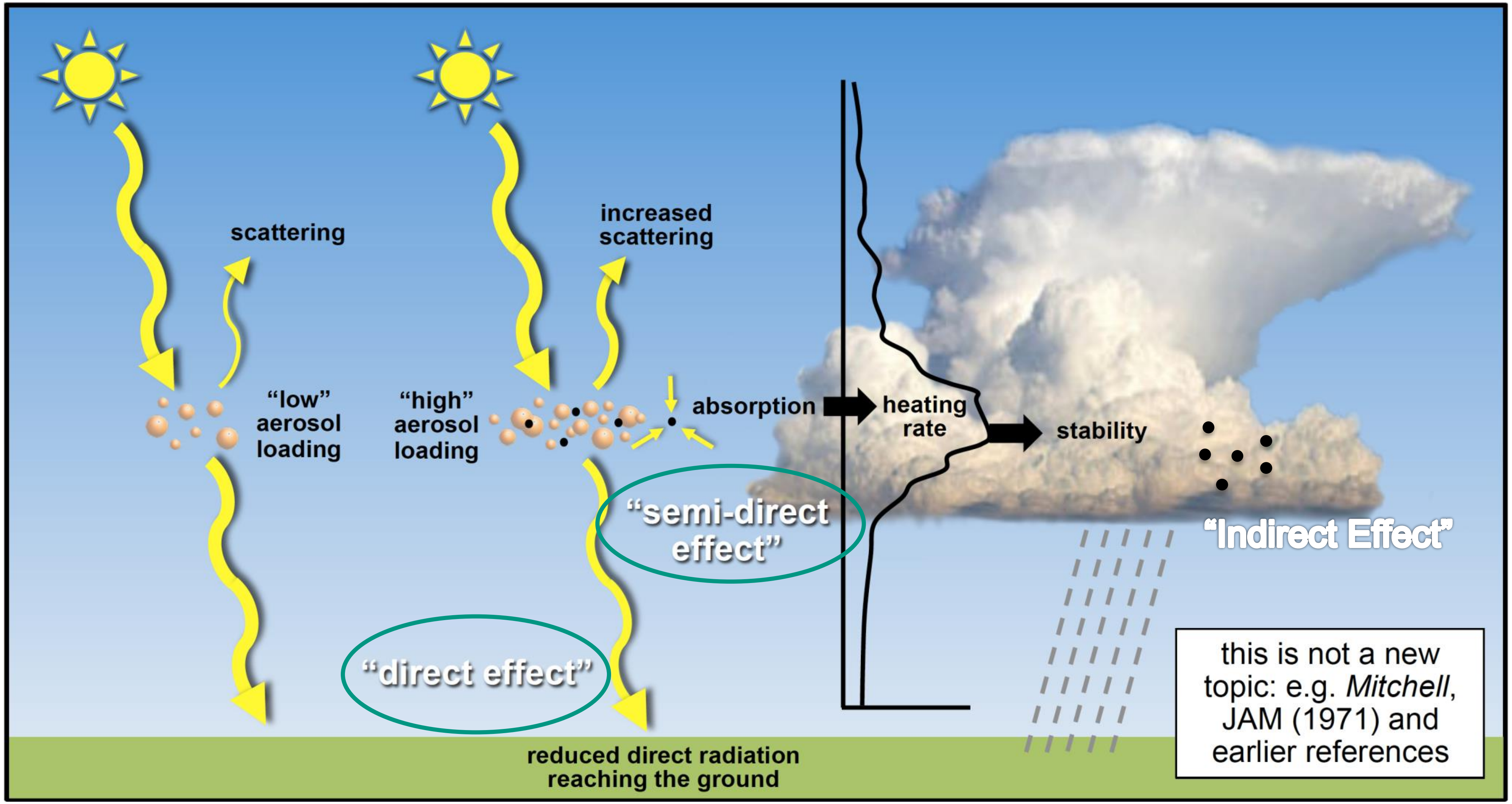
Ali Hoshyaripour[1*], Lukas Muser, Lisa Muth, Heike Vogel and Bernhard Vogel

[1]Institute of Meteorology and Climate Research, Karlsruhe Institute of Technology, Germany
*ali.hoshyaripour@kit.edu



Source: Fan et al 2016

Aerosol effects



this is not a new topic: e.g. *Mitchell*, JAM (1971) and earlier references

Source: Alma Hodzic, NCAR

Aerosol optical properties in models

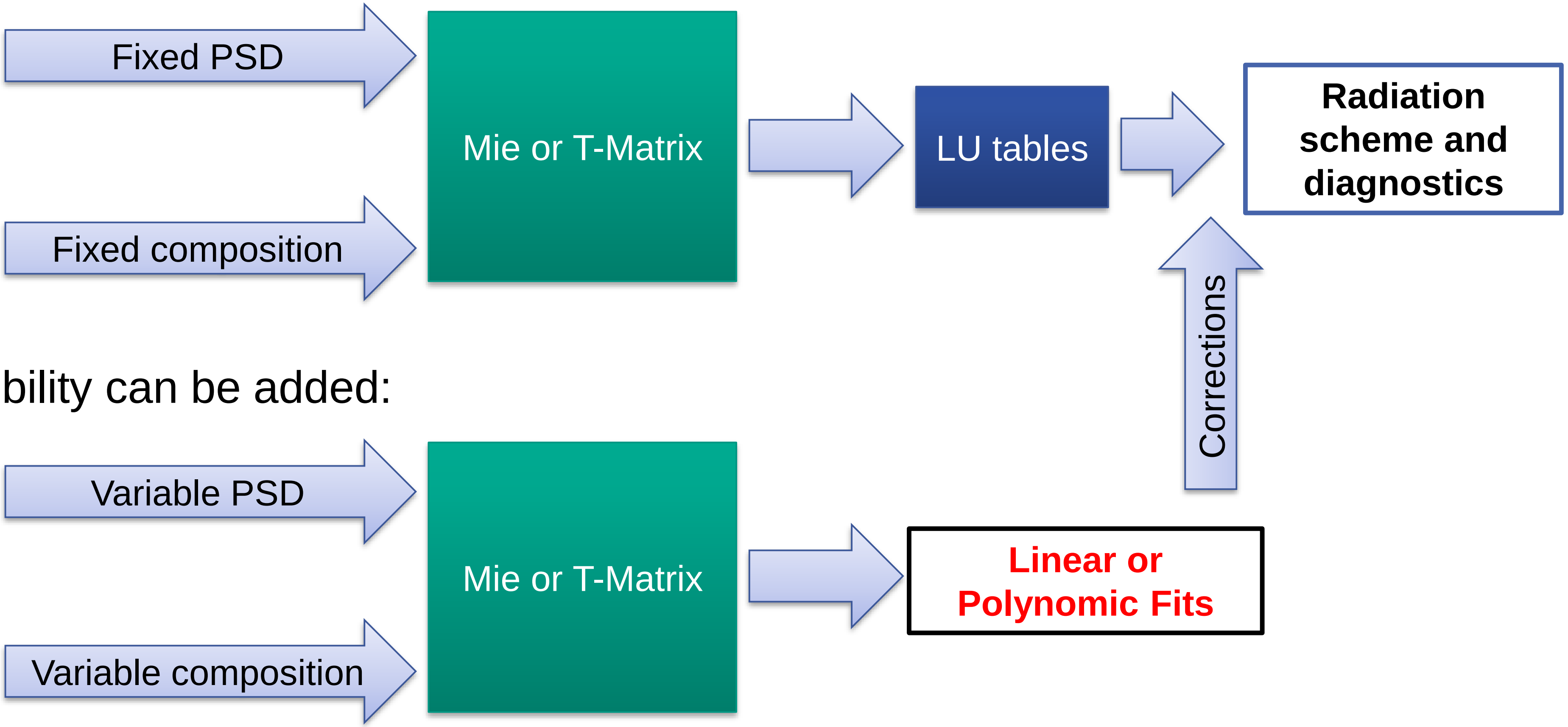
- **Extinction Coefficient (Q_{ext}):** fractional depletion of radiance per unit path length (m^{-1}) due to scattering and absorption by aerosols

- **Single Scattering Albedo (ω_o)**: ratio of scattering to extinction efficiency

- **Asymmetry Parameter (g):** Preferred scattering direction (forward or backward) for the light encountering the aerosol particles

The values of Q_{ext}, ω, and g depend on
Wavelength (λ),
Particle size distribution (PSD)
Mixing state (externally mixed, core-shell, well-mixed …)
Composition (refractive index)

Aerosol Optical Properties: Offline calculations



Fixed PSD

Fixed composition

Mie or T-Matrix

LU tables

Radiation scheme and diagnostics

Corrections

Some flexibility can be added:

Variable PSD

Variable composition

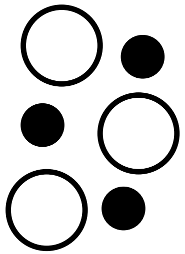
Mie or T-Matrix

Linear or Polynomic Fits

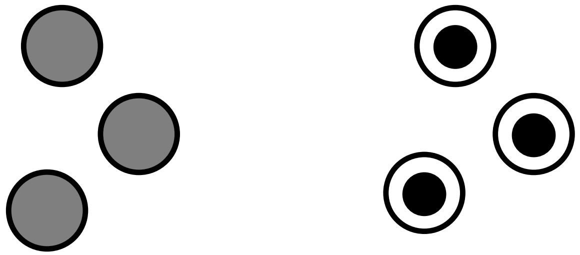
***n*-D look-up tables … revision is necessary by changing basic assumptions.**

Effect of Aerosol Dynamics (AeroDyn)

- So far: Externally mixed aerosols → fixed RI → lookup tables



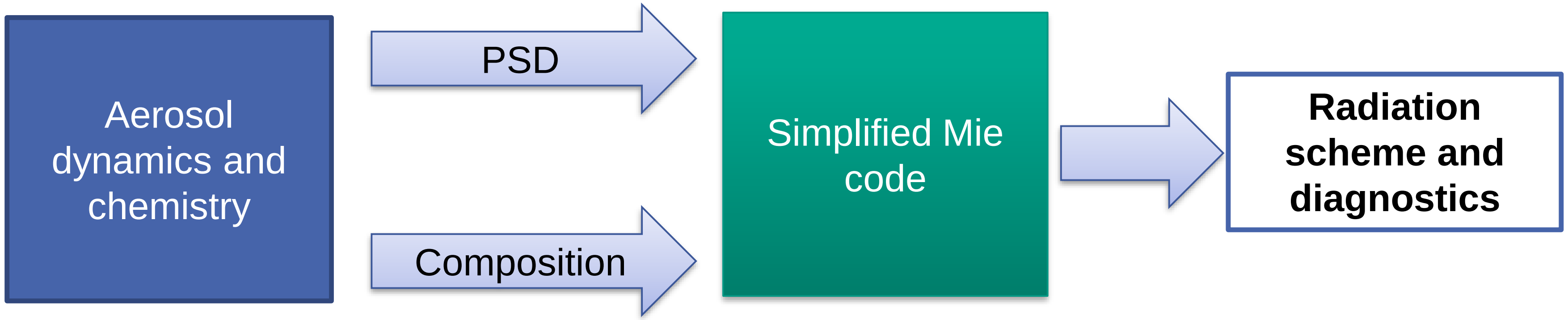
- **New:** Internally mixed aerosols → RI and D varies with composition → ??



Volume-average

Core-Shell

Aerosol Optical Properties: Online calculations


Aerosol dynamics and chemistry

PSD

Composition

Simplified Mie code

Radiation scheme and diagnostics

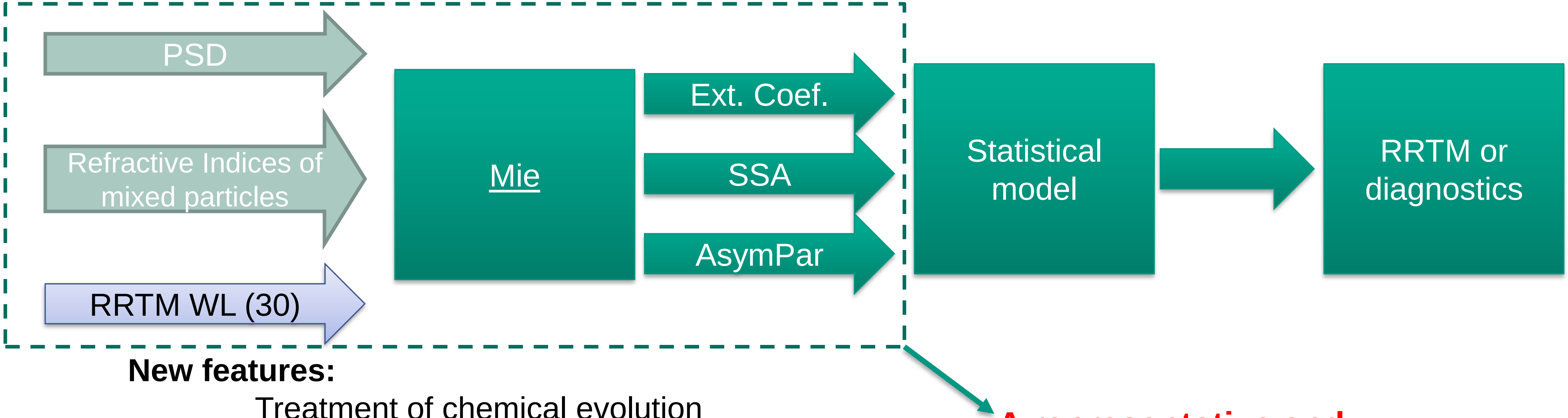
Mie codes can be computationally expensive, so an approximate version (*Ghan et al*. JGR, 2001) is also available.

Mie code is called infrequent for 3-5 WL only. For other WLs, inter- and extrapolation is necessary.

Computationally super expensive, with low precision for inter- and extrapolated WLs …

New concept

Karlsruhe Institute of Technology



New features:

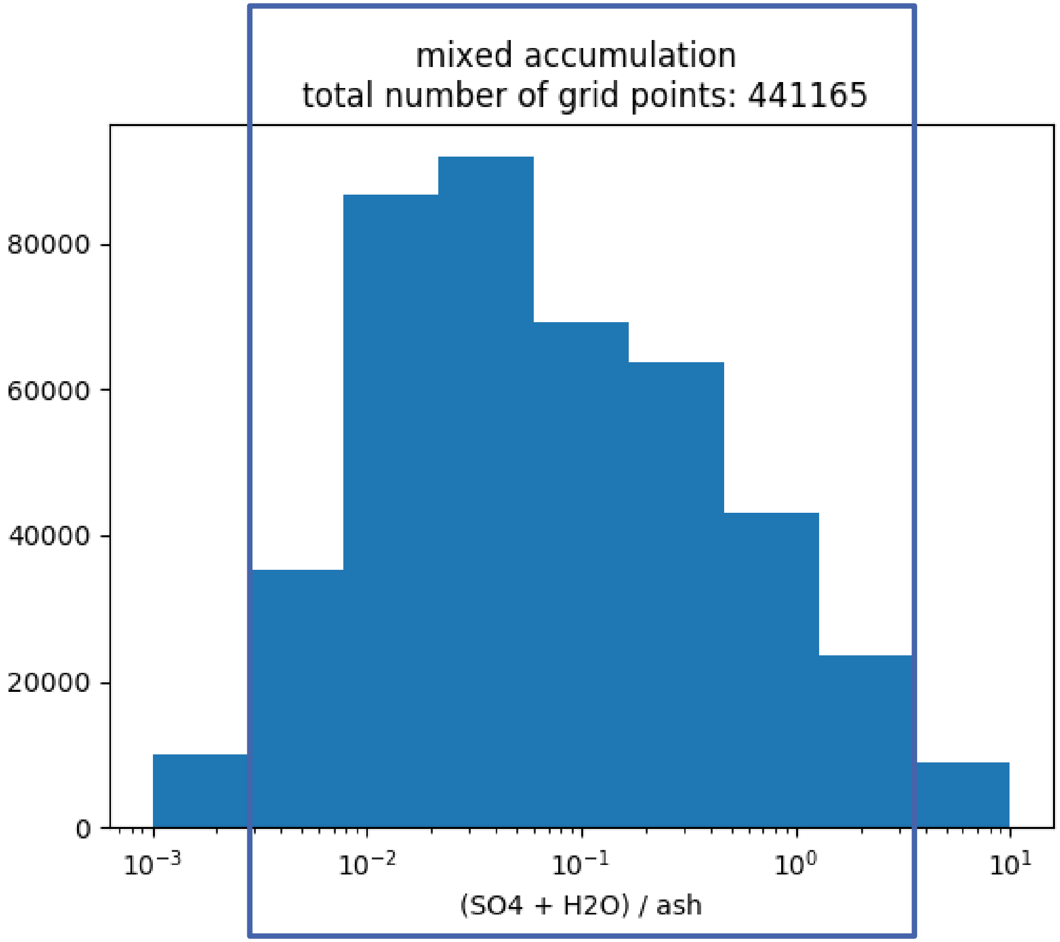
Treatment of chemical evolution
Treatment of PSD evolution
Treatment of core-shell state
One model/Fit for all

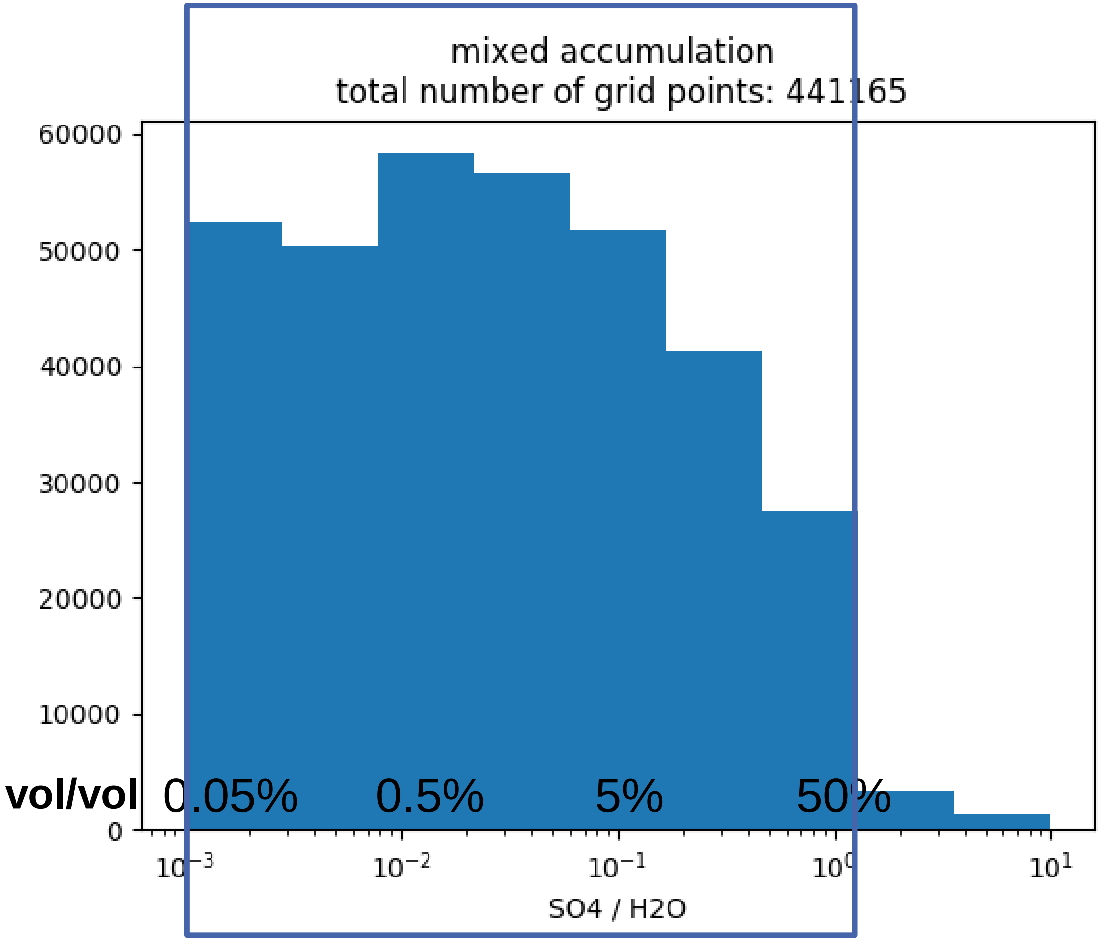
A representative and robust training dataset

Key challenge:

High degrees of freedom in all above parameters
Finding one global model/fit

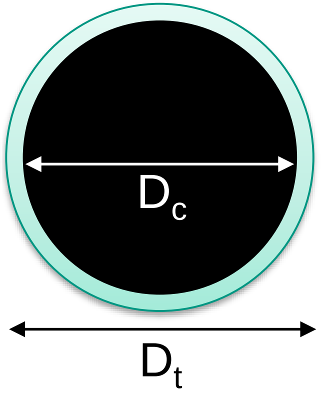
Constraining aerosol mixing state: volcanic aerosols

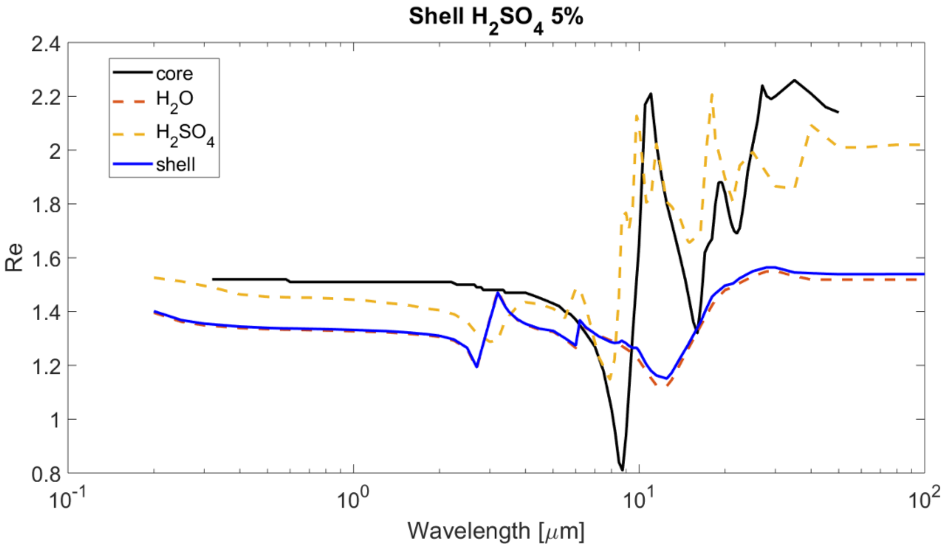


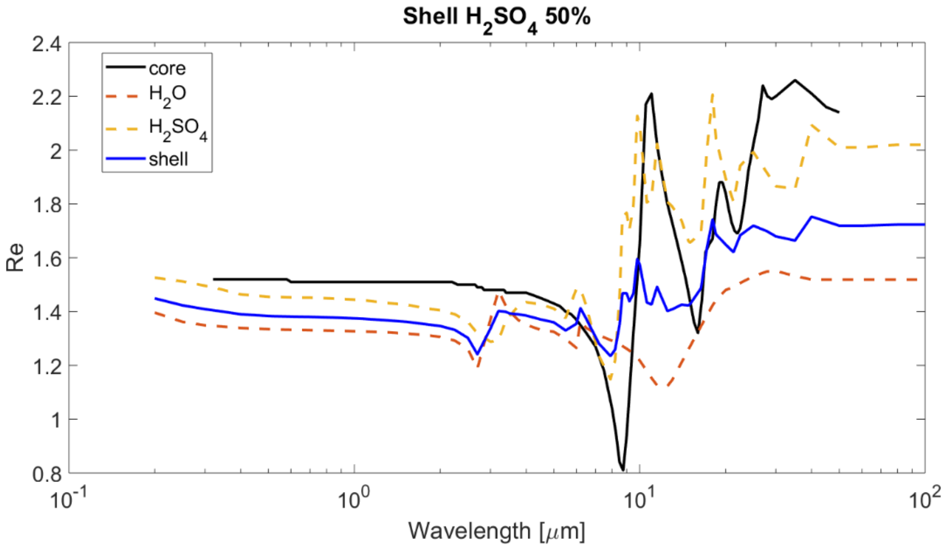


Input variables for Mie calculations

- **Variables**
  - X1 = D_c/D_t: 0.6 to 1 (Shell thickness 0-0.4*D_t)
  - X2 = D_t: 0.5*D to 1.5*D (Median diameter)
  - X3 = H2SO4/H2O: 1E-3 to 1 (Sulfate concentration)
  - X4 = λ: 0.2 to 100 µm (WL for RRTM)







Mie calculations

To calculate the extinction and scattering factors and the asymmetry parameter:

$$Q^{\text{ext}} = \frac{2}{x^2} \sum_{n=1}^{\infty} (2n+1)\, \text{Re}(a_n + b_n)$$

$$Q^{\text{sca}} = \frac{2}{x^2} \sum_{n=1}^{\infty} (|a_n|^2 + |b_n|^2)$$

$$g = \frac{4}{x^2 Q^{\text{sca}}} \sum_{n=1}^{\infty} (2n+1) \left[\frac{n(n+2)}{n+1} \text{Re}(a_n a_{n+1}^* + b_n b_{n+1}^*) + \frac{2n+1}{n(n+1)} \text{Re}(a_n b_n^*) \right]$$

$$x = \frac{2\,\pi\, r}{\lambda}$$

$$\begin{cases} a_n = \dfrac{\psi_n'(y)\, \psi_n(x) - m\, \psi_n(y)\, \psi_n'(x)}{\psi_n'(y)\, \xi_n(x) - m\, \psi_n(y)\, \xi_n'(x)} \\[2ex] b_n = \dfrac{m\, \psi_n'(y)\, \psi_n(x) - \psi_n(y)\, \psi_n'(x)}{m\, \psi_n'(y)\, \xi_n(x) - \psi_n(y)\, \xi_n'(x)} \end{cases}$$

The extinction, scattering and absorption factors based on complex refractive indices (m), y=mx; extension for core-shell

Once we have the Q^{ext}, the mass-extinction coefficient for every mode is:

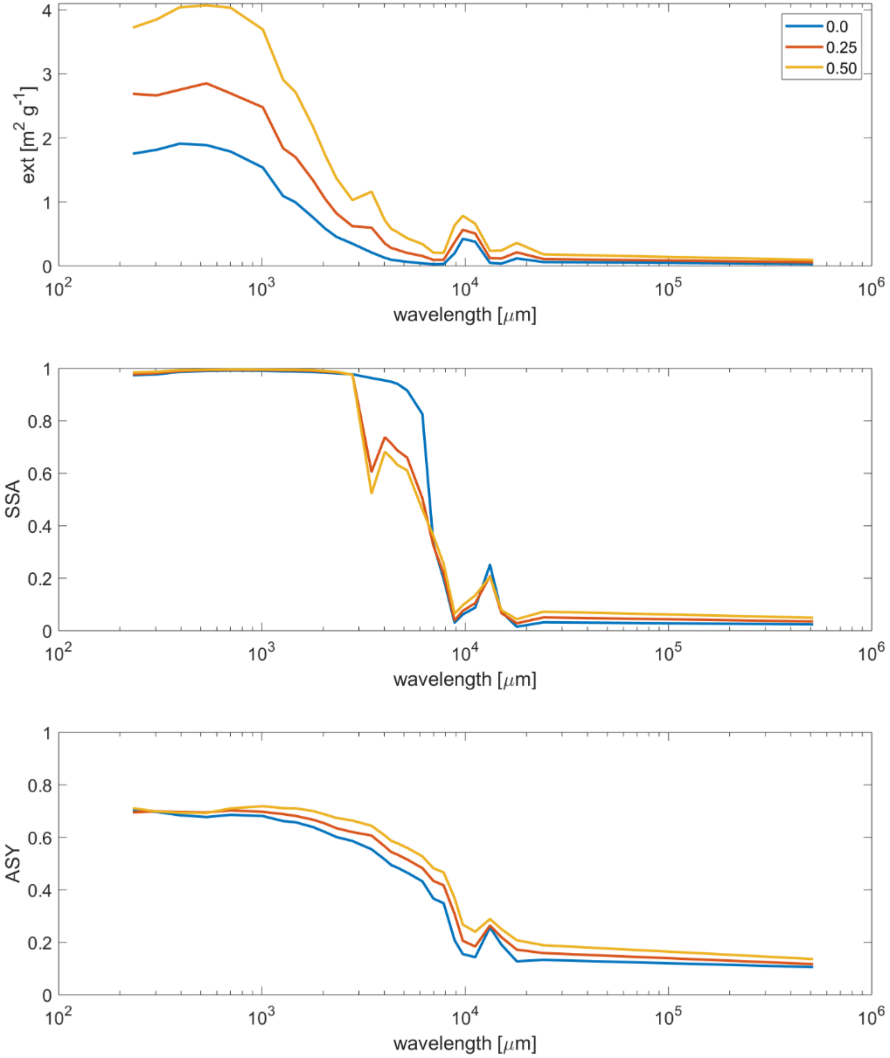
$$k_e(l, \lambda, B_\lambda) = \frac{\int_0^\infty \frac{\pi}{4} d_p^2 Q_e(d_p, \lambda, B_\lambda) \psi_{0,l}(d_p) \mathrm{d}d_p}{\int_0^\infty \psi_{3,l}(d_p) \mathrm{d}d_p}$$

Source: Boucher 2015; Petty 2006

Ash coated with 50% H_2SO_4-H_2O solution (D_s variable)

Increased coating to 0,5 of Dt leads to

- 2* extinction at SW
- Large effect on SSA and ASY at NIR

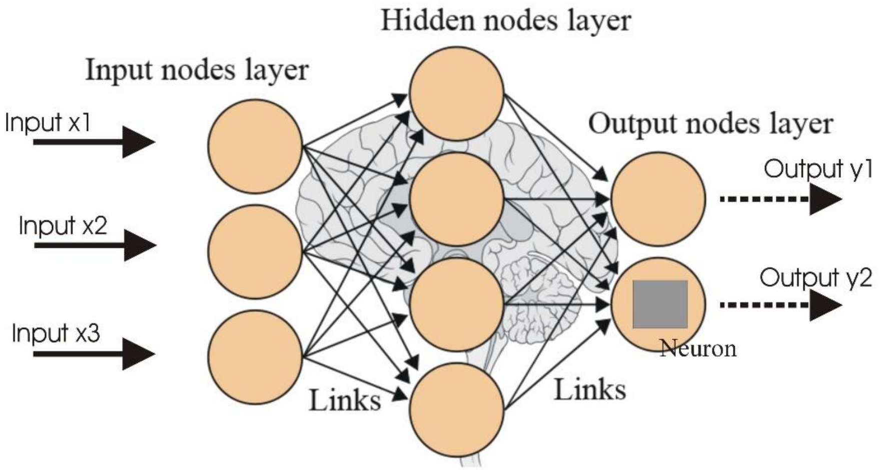


Statistical models

- From simple linear regression to complex artificial intelligence methods

- Chosen based on the system complexity (e.g. linear vs. nonlinear, static vs. dynamic), model performance and computational burden

- **Artificial Neural Network (ANN)**: “the most recommended AI technique” as it satisfactorily learns the associations, functional dependencies and patterns in nonlinear systems resulting in excellent prediction skill.

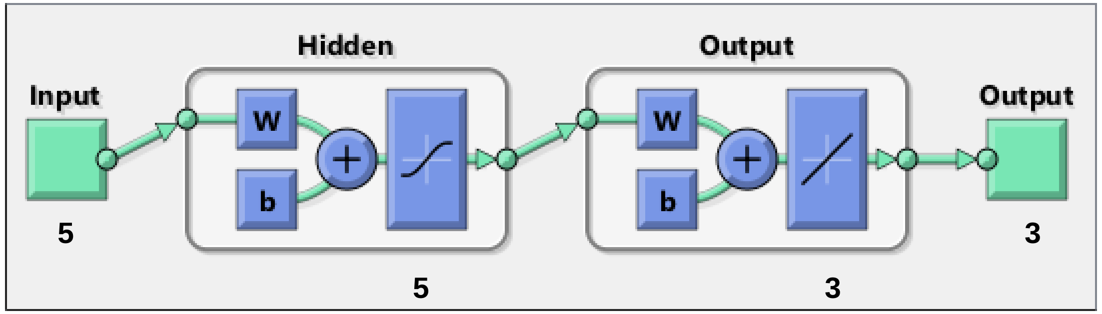


Source: https://www.analyticsvidhya.com

ANN development

- **Network architecture**
  - Two-layer feed-forward network with sigmoid hidden neurons and linear output neurons

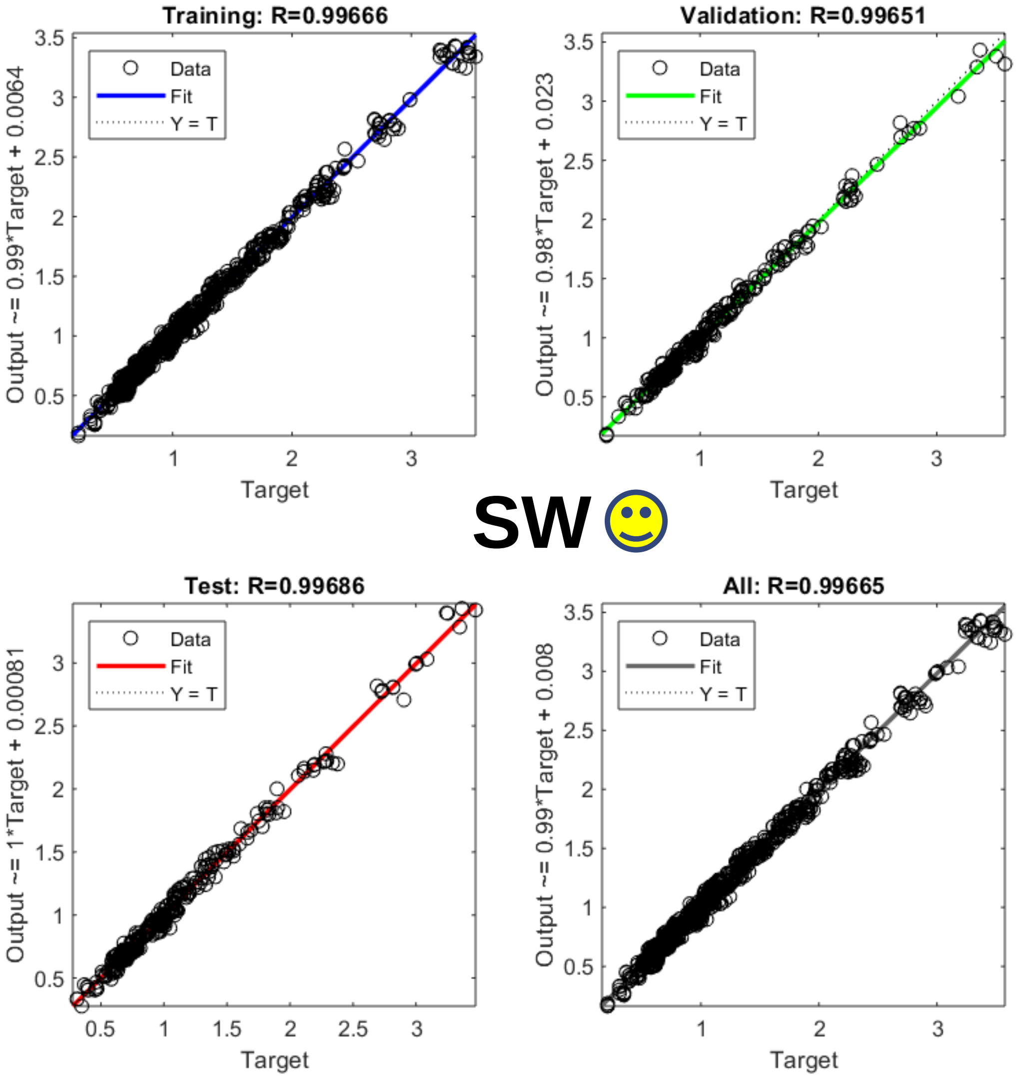
λ
D_c/D_t
D_t
n_s
k_s



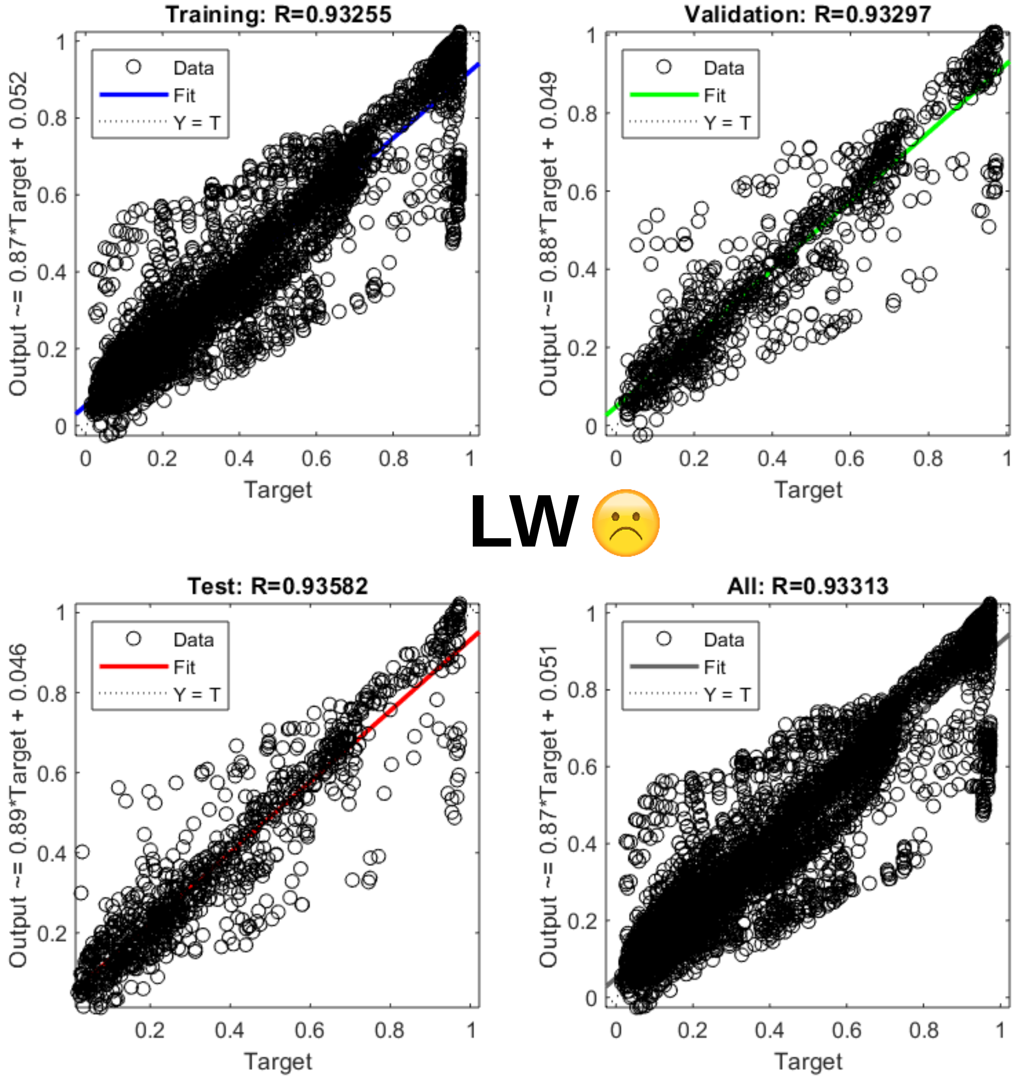
k_e
ω
g

- **Training algorithm:**
  - Data division: Random (70% for Training, 15% for validation, 15% for testing)
  - Training method: Levenberg-Marquardt
  - Performance: mean square error
  - Two networks are trained: one for SW and one for LW

Results of the training



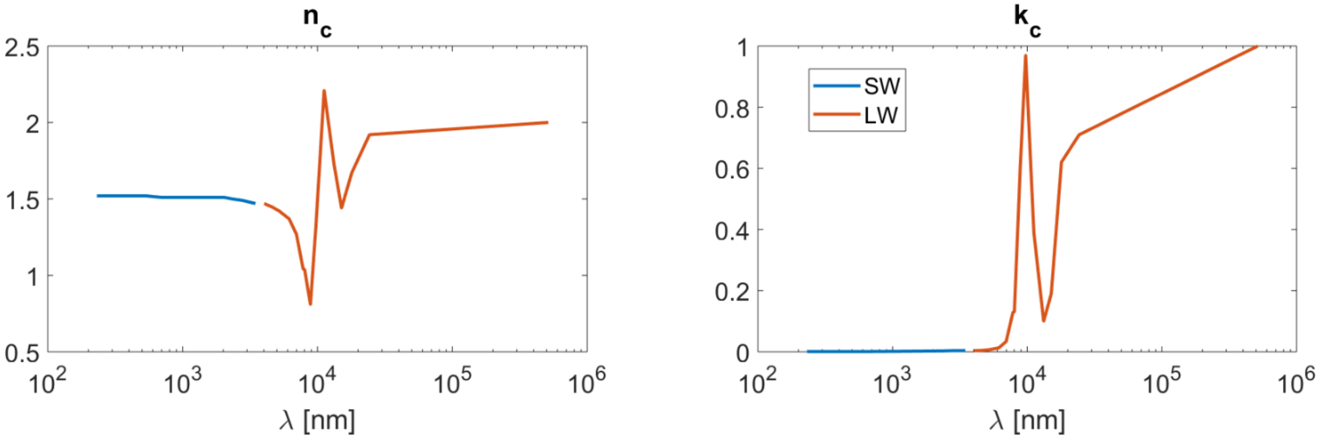
SW 🙂



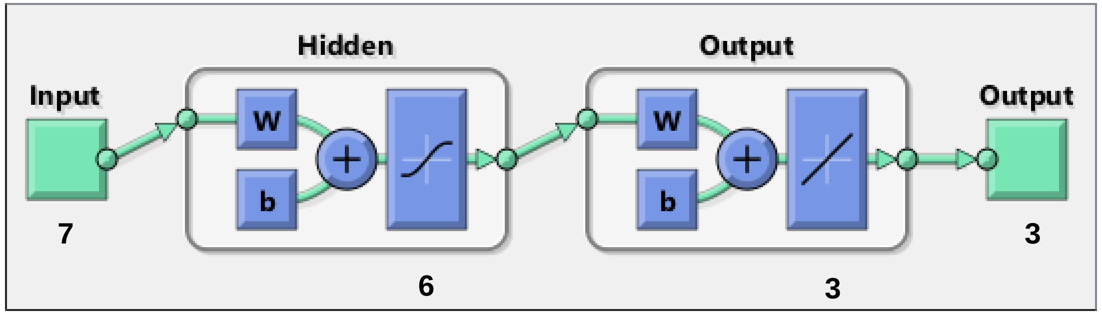
LW ☹

Why is the LW problematic?

- RI of the core (ash) are highly variable in LW → it should be added to the inputs

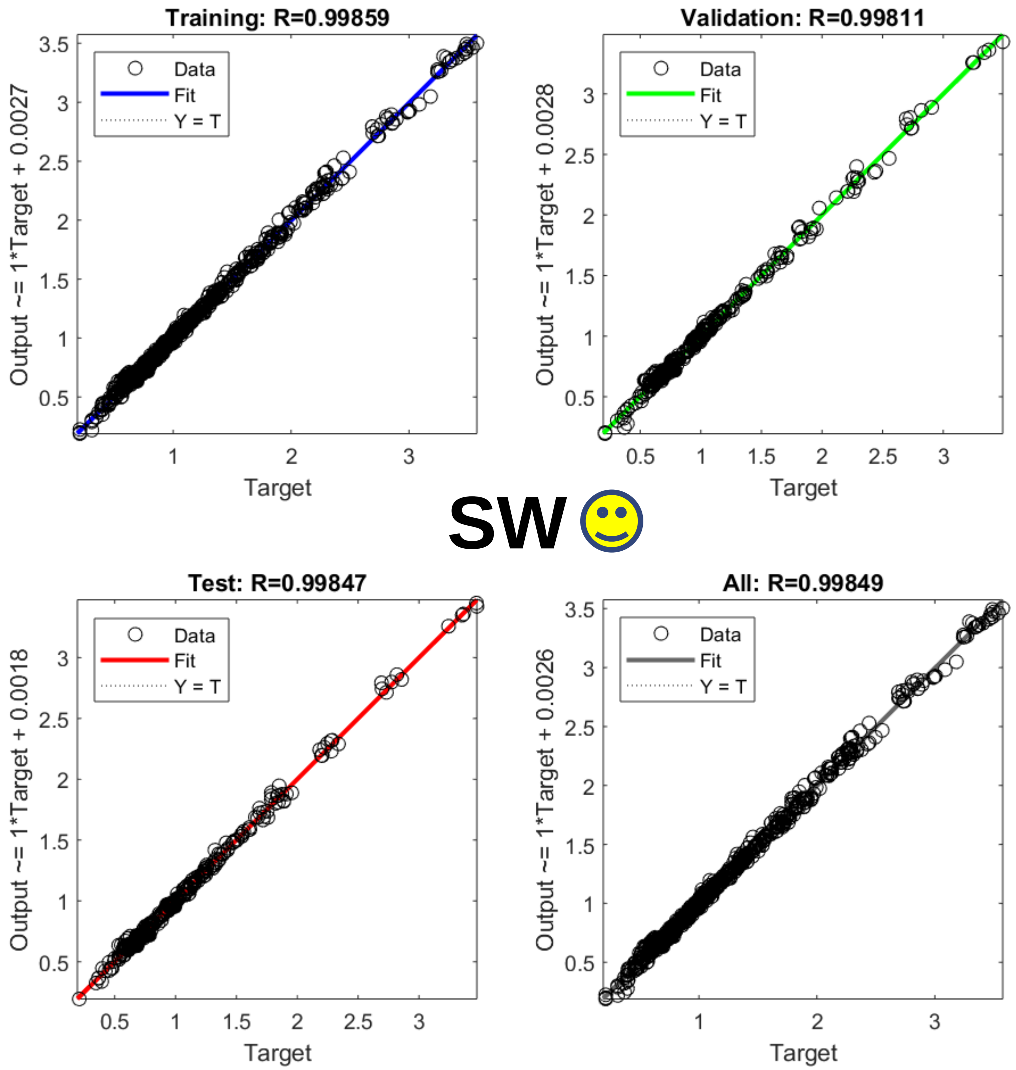


λ
D_c/D_t
D_t
n_s
k_s
n_c
k_c

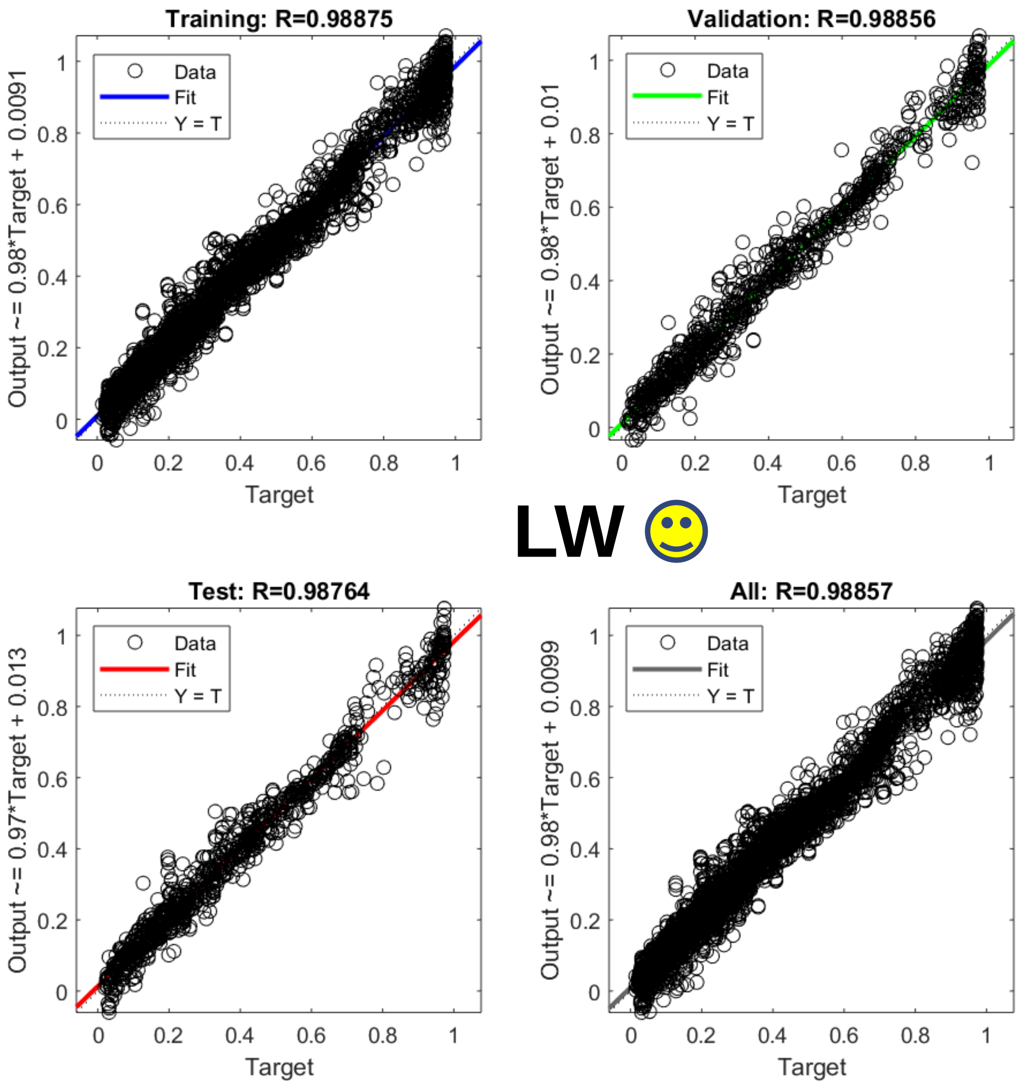


k_e
ω
g

Results of the NEW training

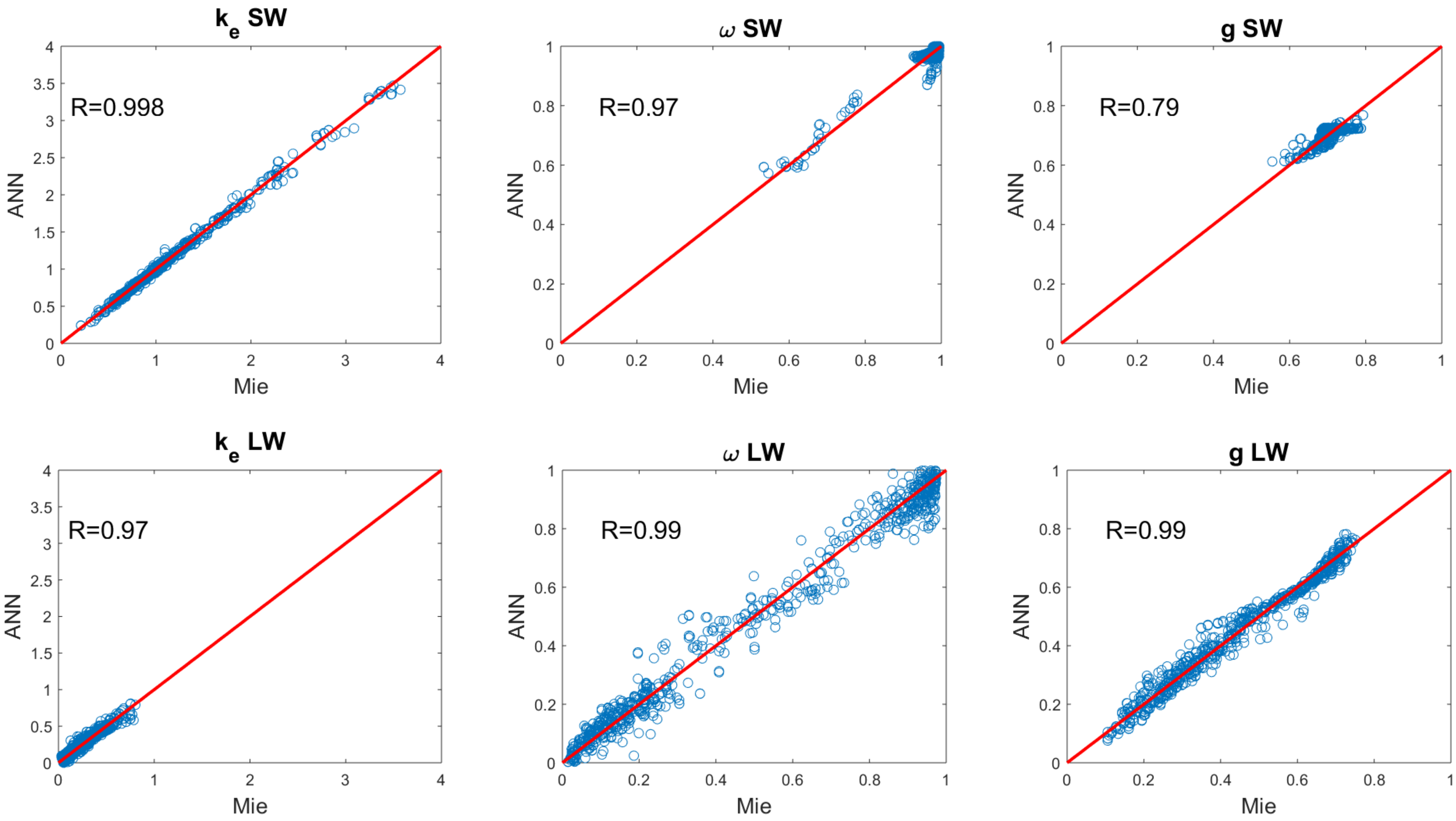


SW 🙂



LW 🙂

An independent test for individual parameters



Conclusions:

- ANN leads to R>0.95 for all parameters except *g* in SW with R~0.8
- Two ANNs for all optical parameters …
- Proof-of-concept for a flexible, generic and computationally affordable tool for online calculation of aerosol optical properties