

# ICLASS, a variational Inverse modelling framework for the Chemistry Land-surface Atmosphere Soil Slab model

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## Background

Surface heating under sunny daytime conditions usually leads to the growth of a relatively well-mixed layer close to the land surface, the **convective boundary layer** (CBL). Modelling the composition and thermodynamic state of the CBL in its interaction with the land surface is the target of the Chemistry Land-surface Atmosphere Soil Slab model (CLASS; Vilà-Guerau De Arellano et al., 2015; see next section). However, an important difficulty in the application of a model like CLASS concerns **parameter tuning** to obtain a good fit to observations. We present here a description of ICLASS, an **inverse modelling framework** built around the CLASS model. This framework serves as a tool to study the **atmospheric boundary layer** and/or **land-atmosphere exchange**.

## Model

-CLASS model (Vilà-Guerau De Arellano et al., 2015), slightly adapted  
-Several parts: mixed layer, surface layer and the land surface, including soil  
-CBL-model physics relatively **simple**, only includes the **essential boundary layer processes**.

## Inverse modelling framework

-Variational, iteratively minimising cost function  
-Non-linear model -> adjoint used  
-Monte-Carlo mode for uncertainties

### Key strengths

-**Allows to incorporate several streams of observations**  
-**Error statistics that are estimated provide information about the constraints the measurements place on the model parameters.**  
-**Bias correction for specific bias patterns, e.g. energy balance closure problem**  
-**surface layer profiles can be taken into account**  
-**Observation system simulation experiments using ICLASS can help in the planning of observational campaigns**  
-**allows to integrate knowledge from ecosystem-level studies (fluxes) and global studies (mixing ratios).**  
-**a tool that maximises the use of available observational data at CBL/ecosystem level**

## Application example: ICLASS applied to grassland in the Netherlands (Cabauw).

-'Golden' day  
-Optimised run much better fit than prior run  
-Substantial energy balance closure gap  
-Correcting biases critical in inverse modelling



Figure 5: KNMI measurement tower at Cabauw (source: KNMI website, Raymond Sluiter)

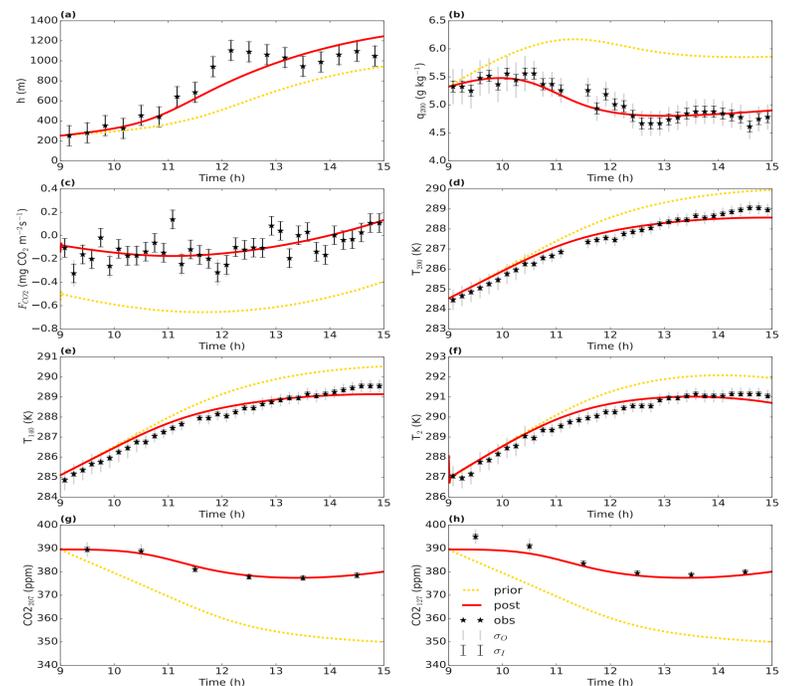


Figure 6: Optimisation for the Cabauw data. The full red line shows the optimised model ("post" meaning posterior), the dotted yellow line is the prior model. The observations are shown by a black star, the error bars show the measurement error standard deviation  $\sigma_o$ , and total error standard deviation  $\sigma_o$  on the observations.

- To conclude, we show examples of posterior pdfs that can be created using the Monte-Carlo way of running ICLASS, and a posterior correlation matrix for the state variables.

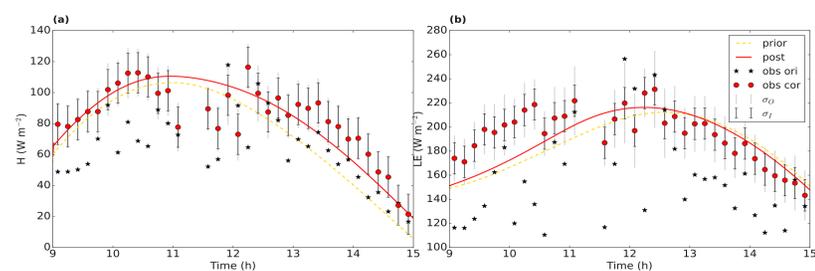


Figure 7: Energy balance data (left: sensible heat flux, right: latent heat flux) for the Cabauw case. The black stars are the original observations, the red dots the observations after forced closure of the energy balance. The error bars indicate the measurement error standard deviation  $\sigma_o$ , and the total observational error standard deviation  $\sigma_o$ . The full red line shows the optimised model ("post" meaning posterior), the dashed yellow line is the prior model.

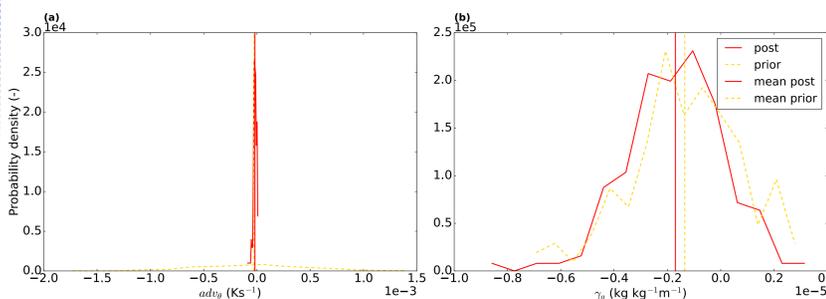


Figure 8: Probability density functions for the  $adv_0$  (left) and  $\gamma_0$  (right) parameters, the red full line is for the posterior and the yellow dashed line for the prior distribution. The vertical lines represent the mean of the distributions. 15 bins were used. Note that the prior distribution is determined from the sample of priors, which has a component of randomness.

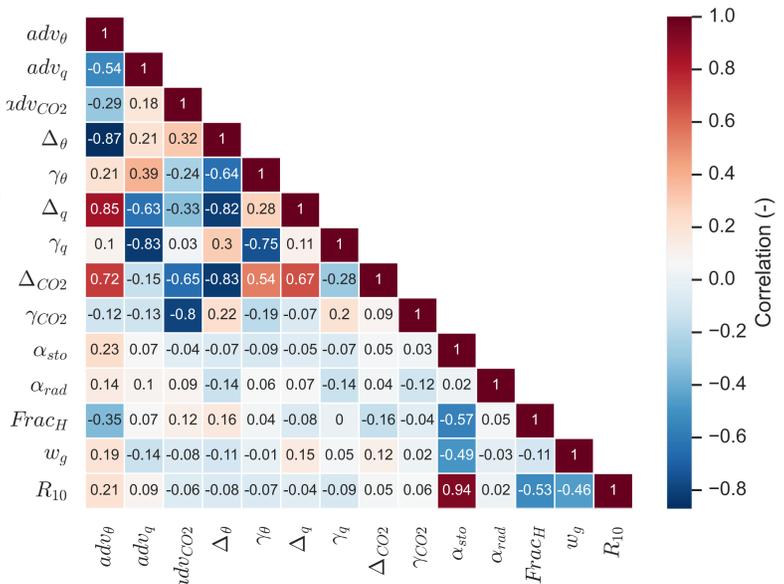


Figure 9: Correlation matrix for the optimised state parameters for the Cabauw case.

## References

Vilà-Guerau De Arellano, J., Van Heerwaarden, C. C., Van Stratum, B. J., and Van Den Dries, K.: Atmospheric boundary layer: Integrating air chemistry and land interactions, Cambridge University Press, <https://doi.org/10.1017/CBO9781316117422>, 2015.

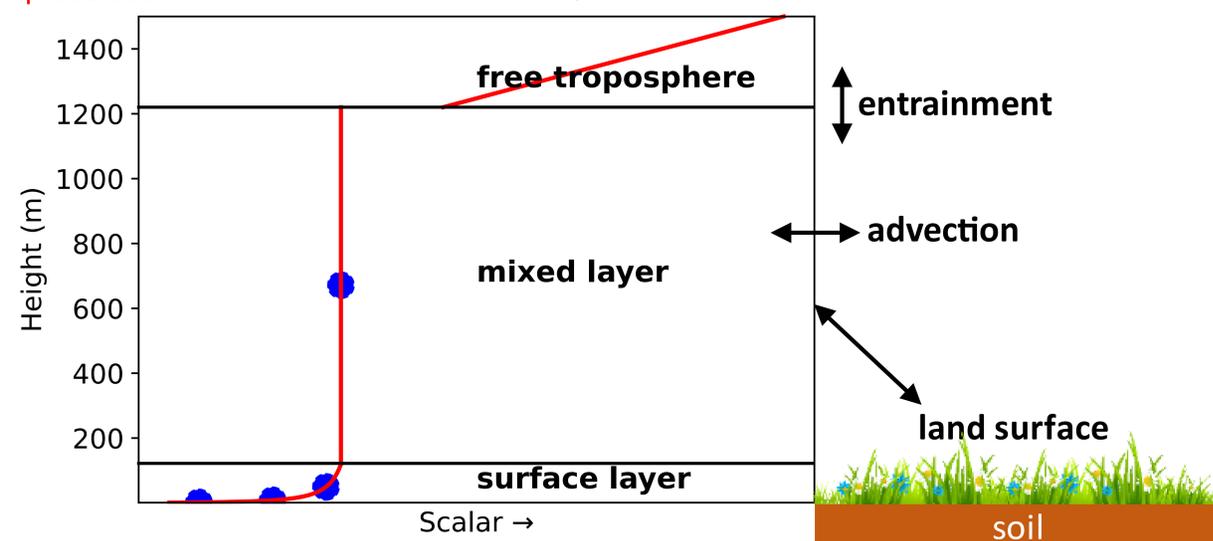


Figure 1: Sketch of the employed forward model: the (slightly adapted) CLASS model. The blue dots in the surface layer represent user-specified heights where the model calculates scalars, e.g. the  $CO_2$  mixing ratio. The mixed layer is represented by a single bulk value in the model (blue dot in mixed layer). At the top of the mixed layer, a discontinuity (jump) occurs in the profiles. The free troposphere is not explicitly modelled, but is taken into account for the exchange with the mixed layer (entrainment). The slope of the free troposphere line is the free tropospheric lapse rate. A constant advection can be taken into account as a source/sink.

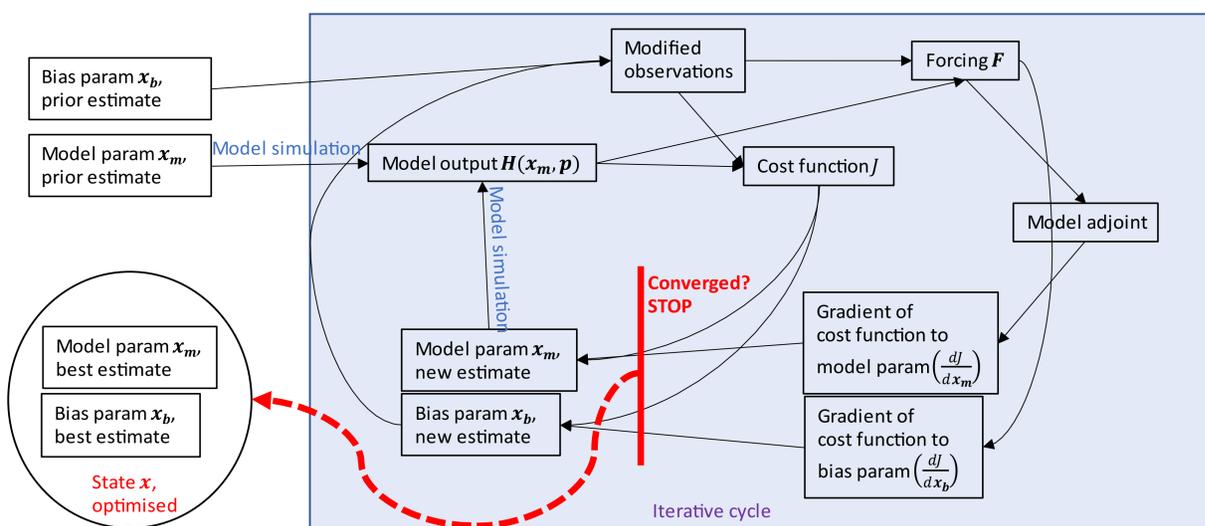


Figure 2: Slightly simplified sketch of the workflow of the inverse modelling framework, when using the adjoint model for the derivatives with respect to model parameters. Note that, for clarity of the figure, direct arrows between the parameters and the cost function and its gradients are not drawn. These arrows arise via the background part of the cost function (see equations in text). Everything within the shaded rectangle is part of the iterative cycle of optimisation. Model parameters that are not optimised are in vector  $p$ , this vector is used together with  $x_m$  in every model simulation. In case ICLASS is run in Monte-Carlo mode, this figure applies to the individual ensemble members.

### Ensemble of (variational) optimisations: (Co)variances and correlations derived from posterior ensemble

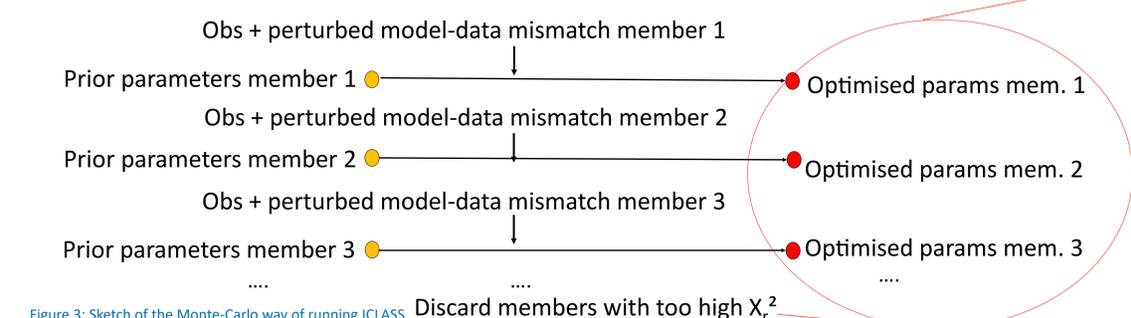


Figure 3: Sketch of the Monte-Carlo way of running ICLASS