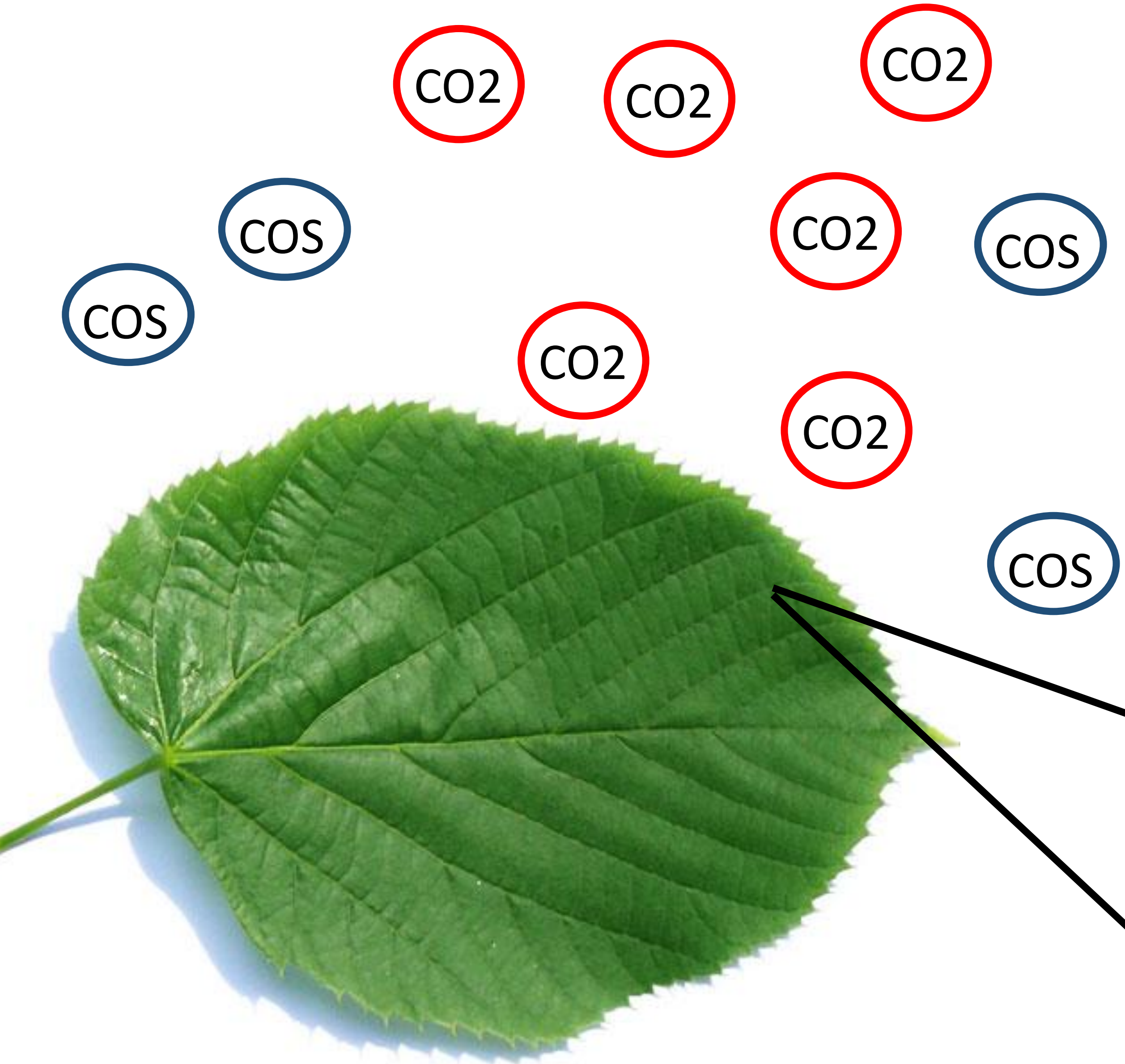
Inverse modelling with a coupled COS-CO_2 mixed-layer model

Peter Bosman, Maarten Krol

Overview of internship + current work in progress

Jan 27, 2020

Vegetation uptake



Largest COS sink

Uptake by diffusion

COS within leaves destroyed by enzymes

Leaf stomata

COS uptake and photosynthesis coupled to stomatal conductance -> crucial link between COS and photosynthesis

A-gs approach:

Low for COS

$$Flux = conductance * (concentration\ in\ air - internal\ concentration)$$

Stomatal + internal

COS

CO2

Canopy scale: integration over leaf area index

CO_2 and COS often coupled via ratio of deposition velocities, in this study coupled via conductance

Inverse modelling vegetation fluxes with a coupled COS-CO_2 mixed-layer model

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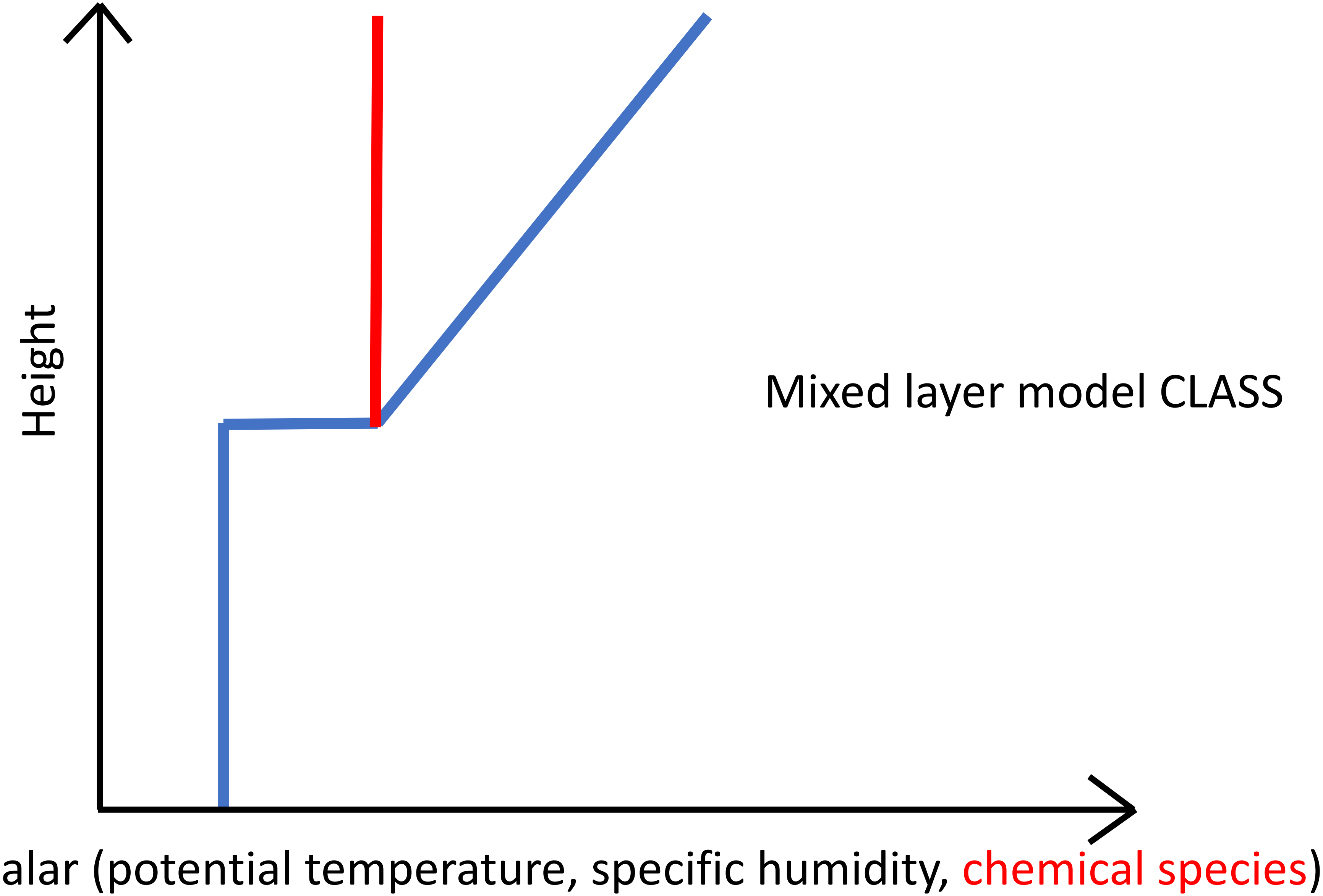
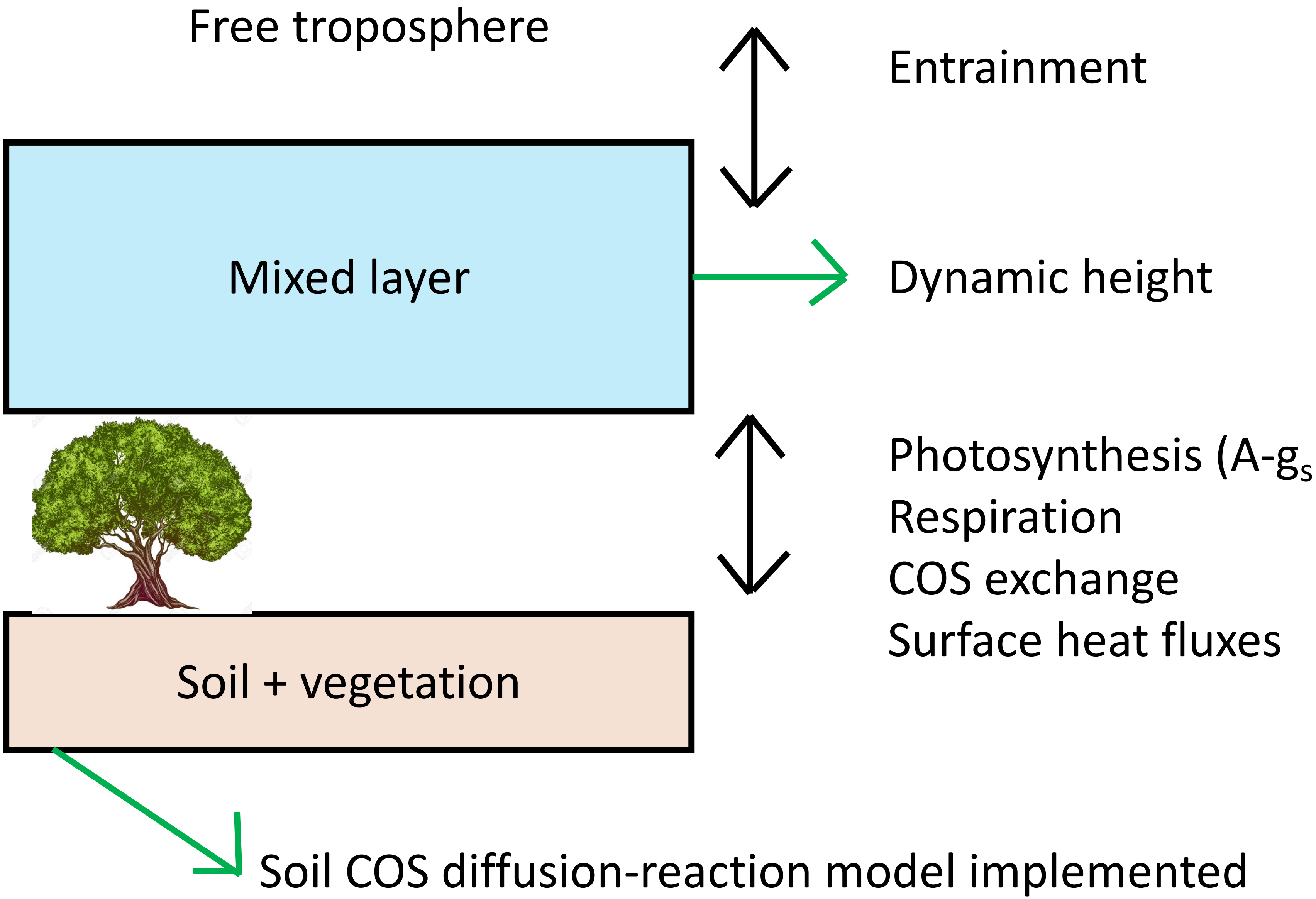
The model


Height
Mixed layer model CLASS
Scalar (potential temperature, specific humidity, chemical species)

The model



Free troposphere
Entrainment
Mixed layer
Dynamic height
Photosynthesis (A-g_s)
Respiration
COS exchange
Surface heat fluxes
Soil + vegetation
Soil COS diffusion-reaction model implemented

This research

Specific aim: Build an inverse modelling framework with a flexible cost function that allows for optimising different types of variables, including variables relating to the boundary layer dynamics

simple approach!

The optimisation

(max) 4 parameters optimised in this study:

- alfa_plant → scaling conductance
  influences COS and CO_2 uptake
  Main link with boundary layer dynamics removed

- alfa_soil → scaling soil COS uptake/emission
  influences COS uptake only

- FTC_COS → free tropospheric concentration of COS

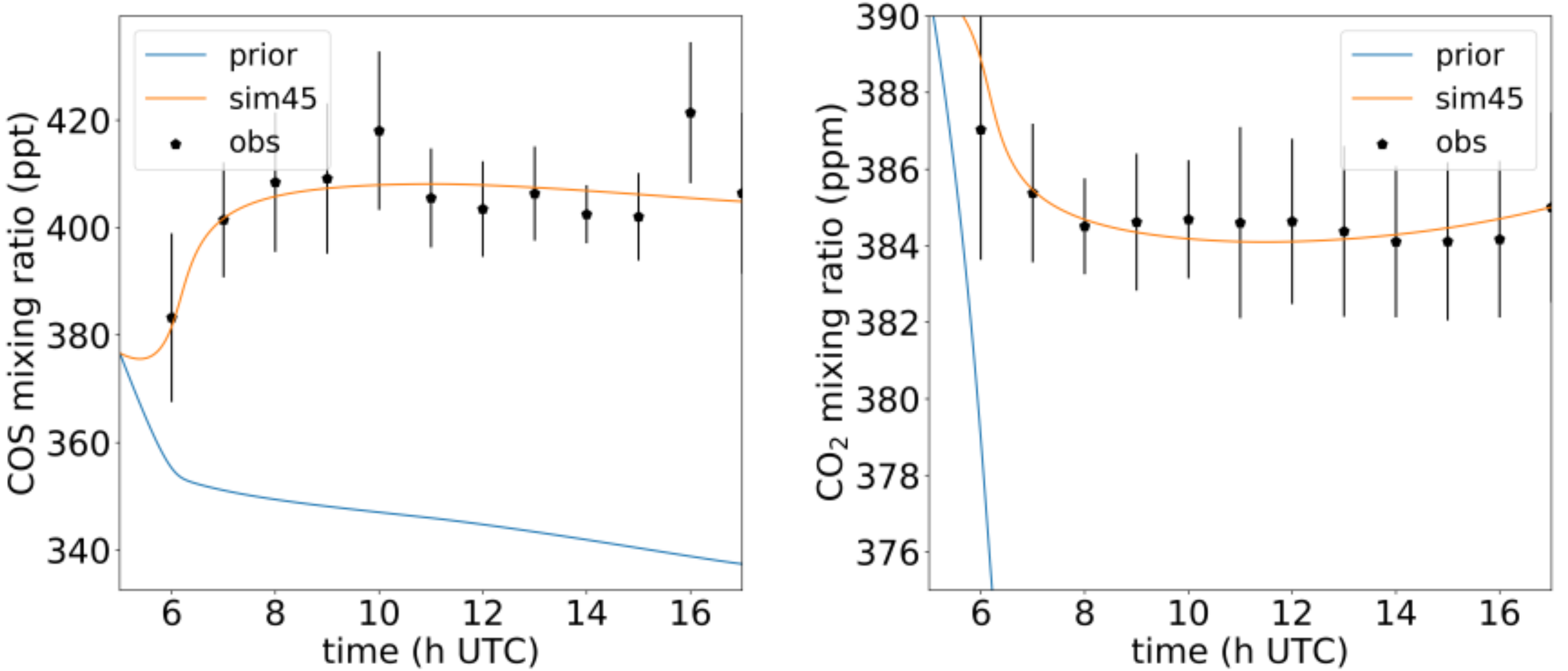
- FTC_CO2_scale → scale for free tropospheric concentration of CO_2

Observations - Hyytiälä

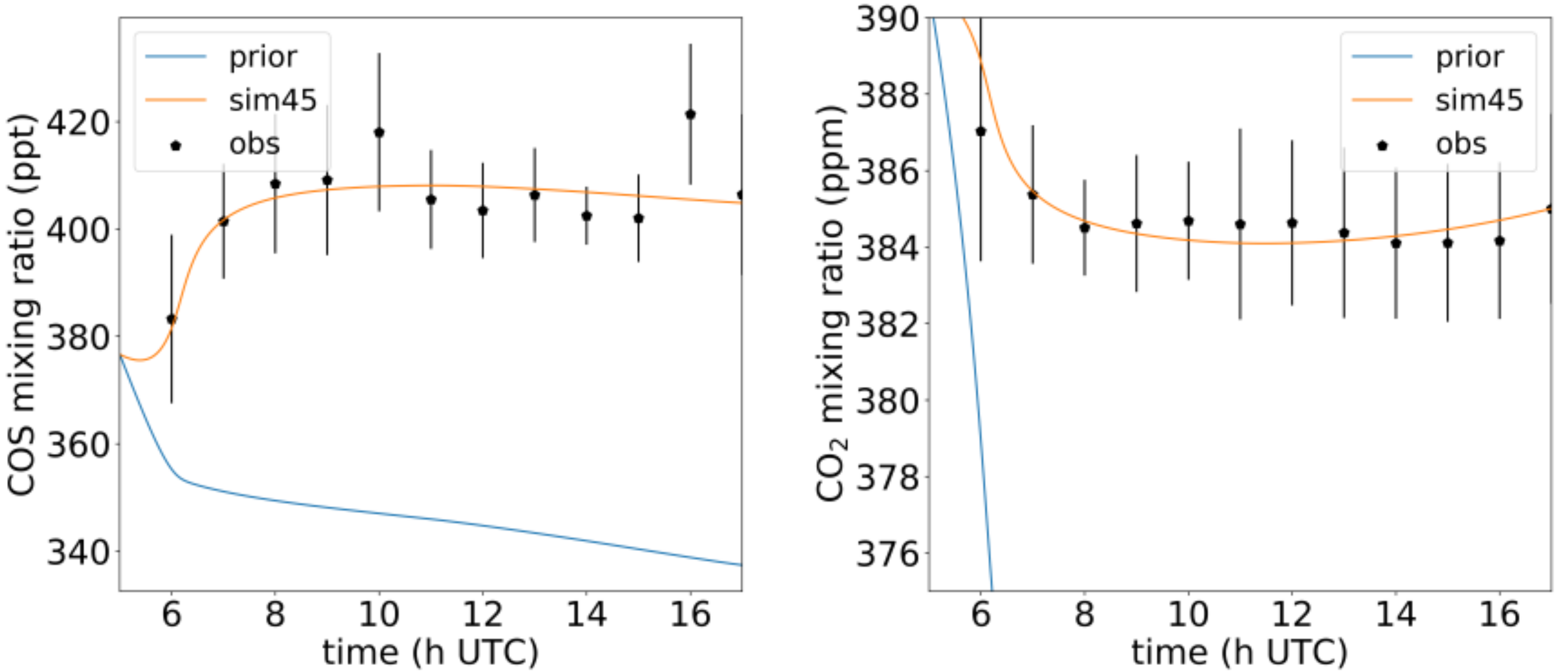
Dataset from boreal forest in Finland – Linda Kooijmans

COS and CO_2 mixing ratios at 125 m
eddy-covariance fluxes at 23 m
+…
Averaged over 7 sunny August days

Observations - Hyytiälä



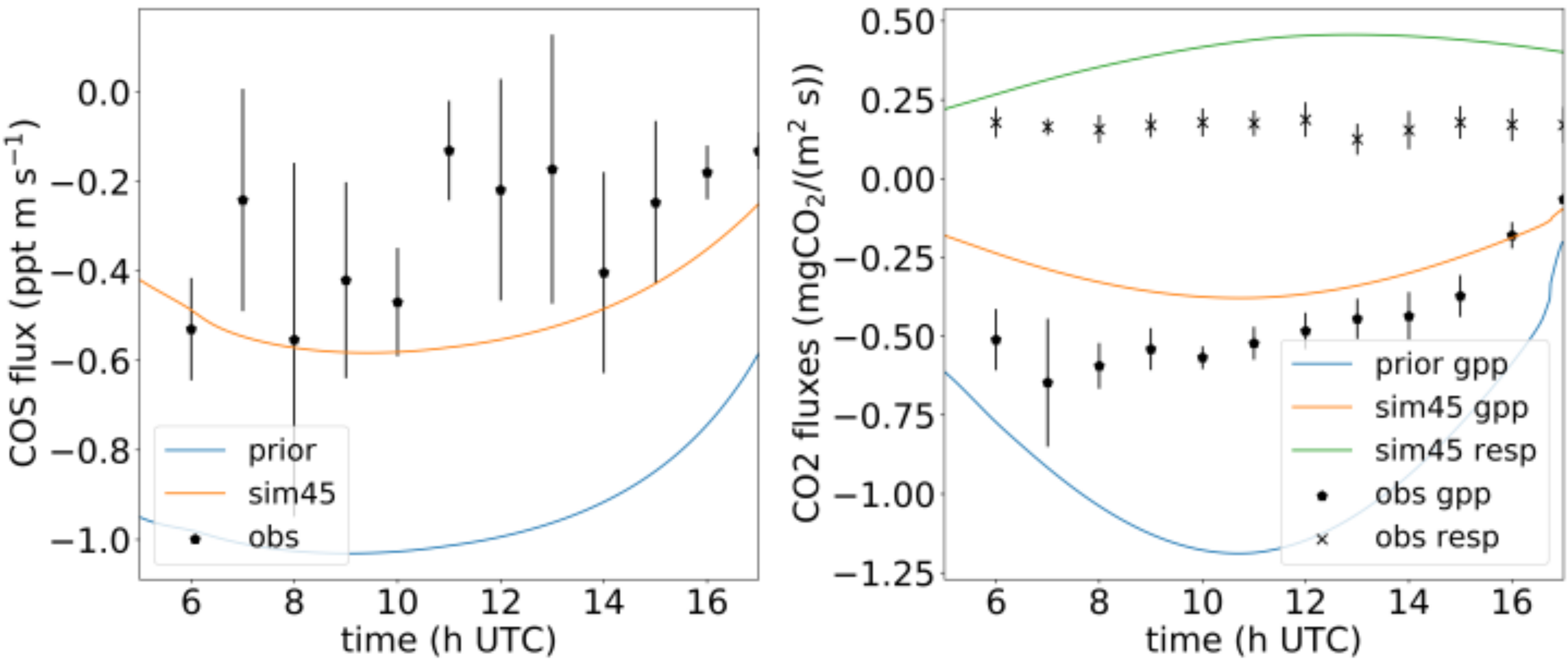
Observations - Hyytiälä



Cost function prior: 2067.45

Cost function optimised: 3.95

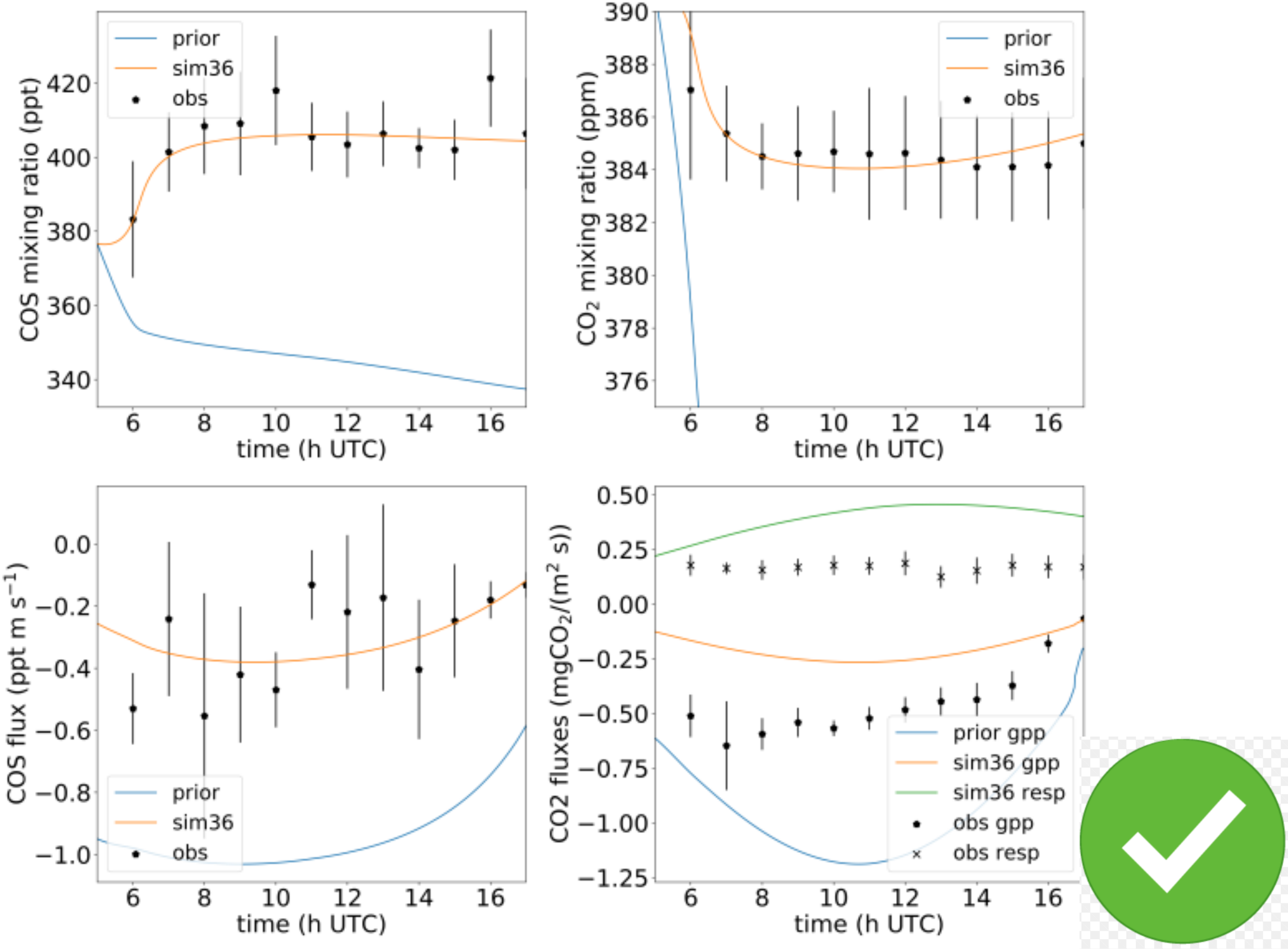
Observations - Hyytiälä



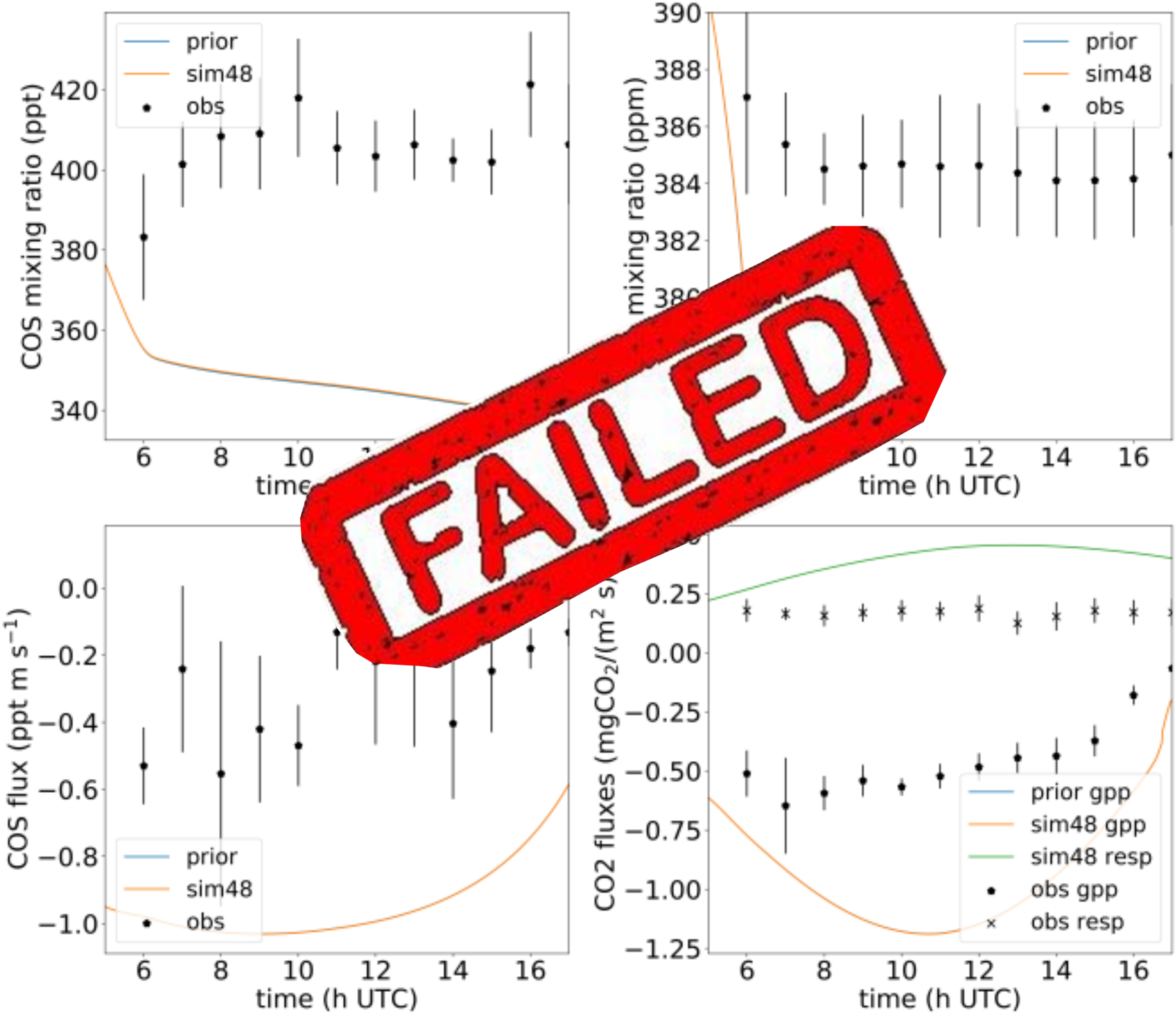
Fluxes can be improved

--> Add to cost function!

With net COS flux in cost function:



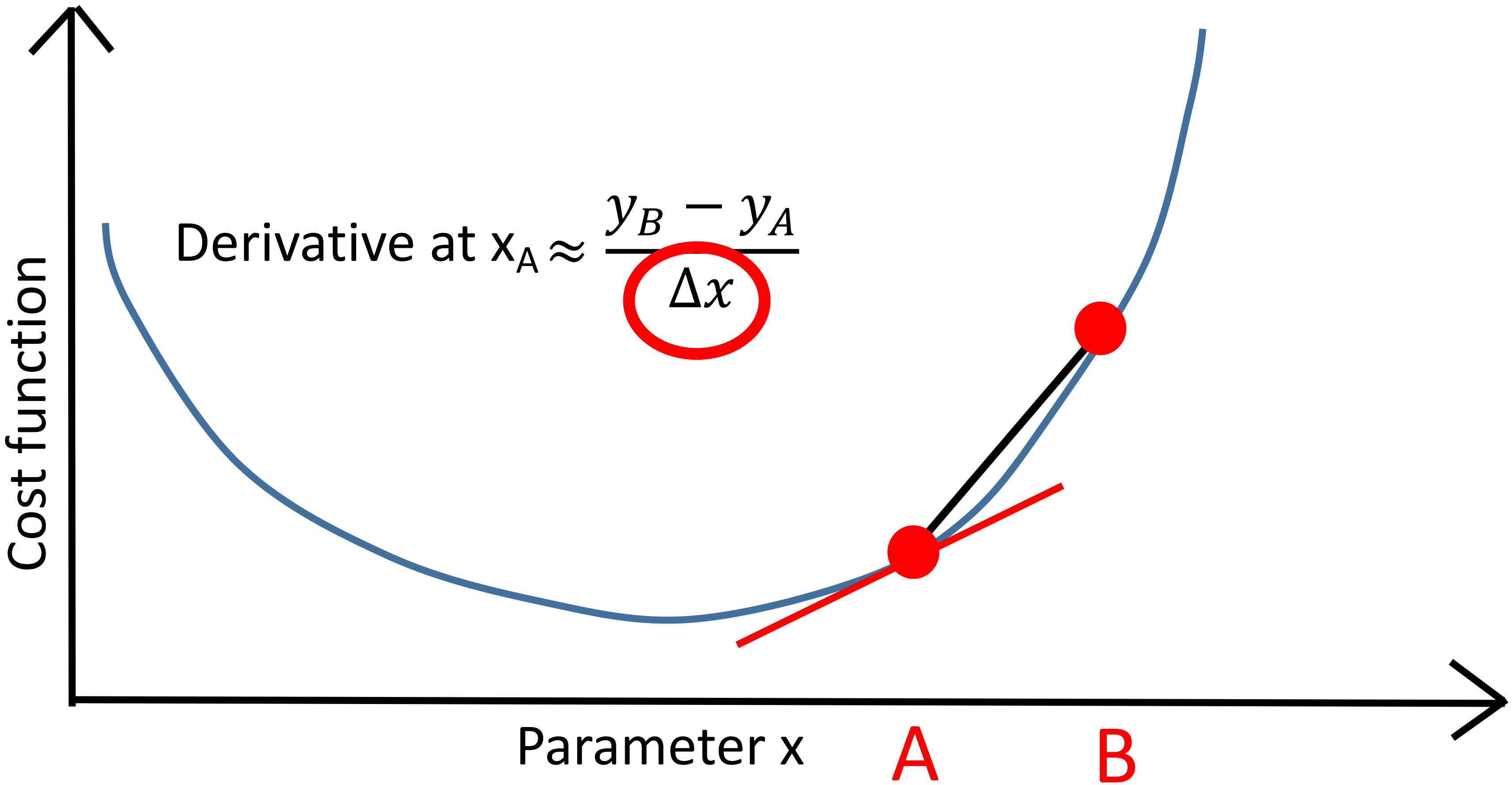
With net COS flux and gpp in cost function:



Challenges

Derivative is approximated numerically (forward perturbation only)

Analytical derivative requires construction of the *adjoint model*

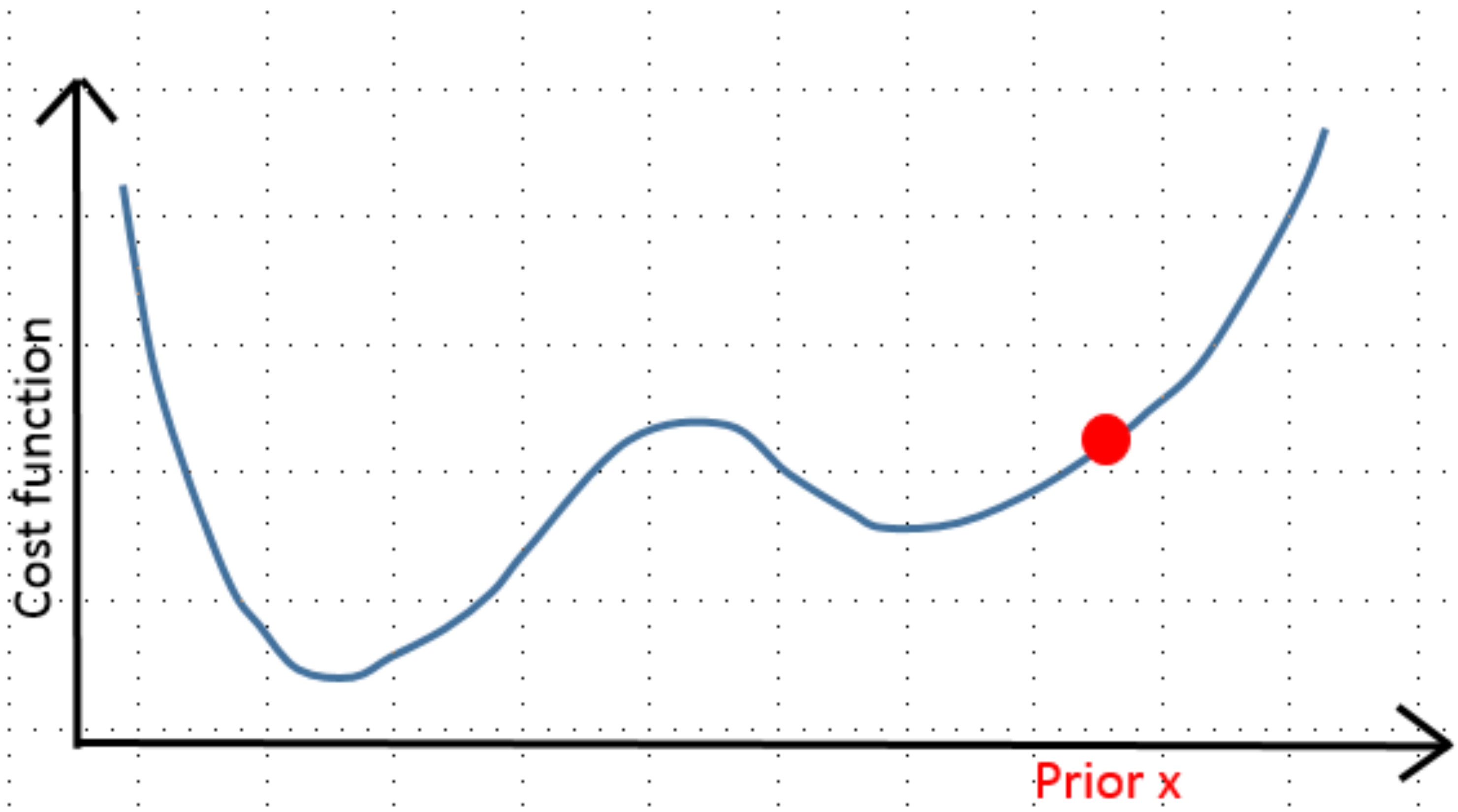


Challenges

Derivative is approximated numerically (forward perturbation only)

Analytical derivative requires construction of the *adjoint model*

Model is non-linear



Benefits of the framework

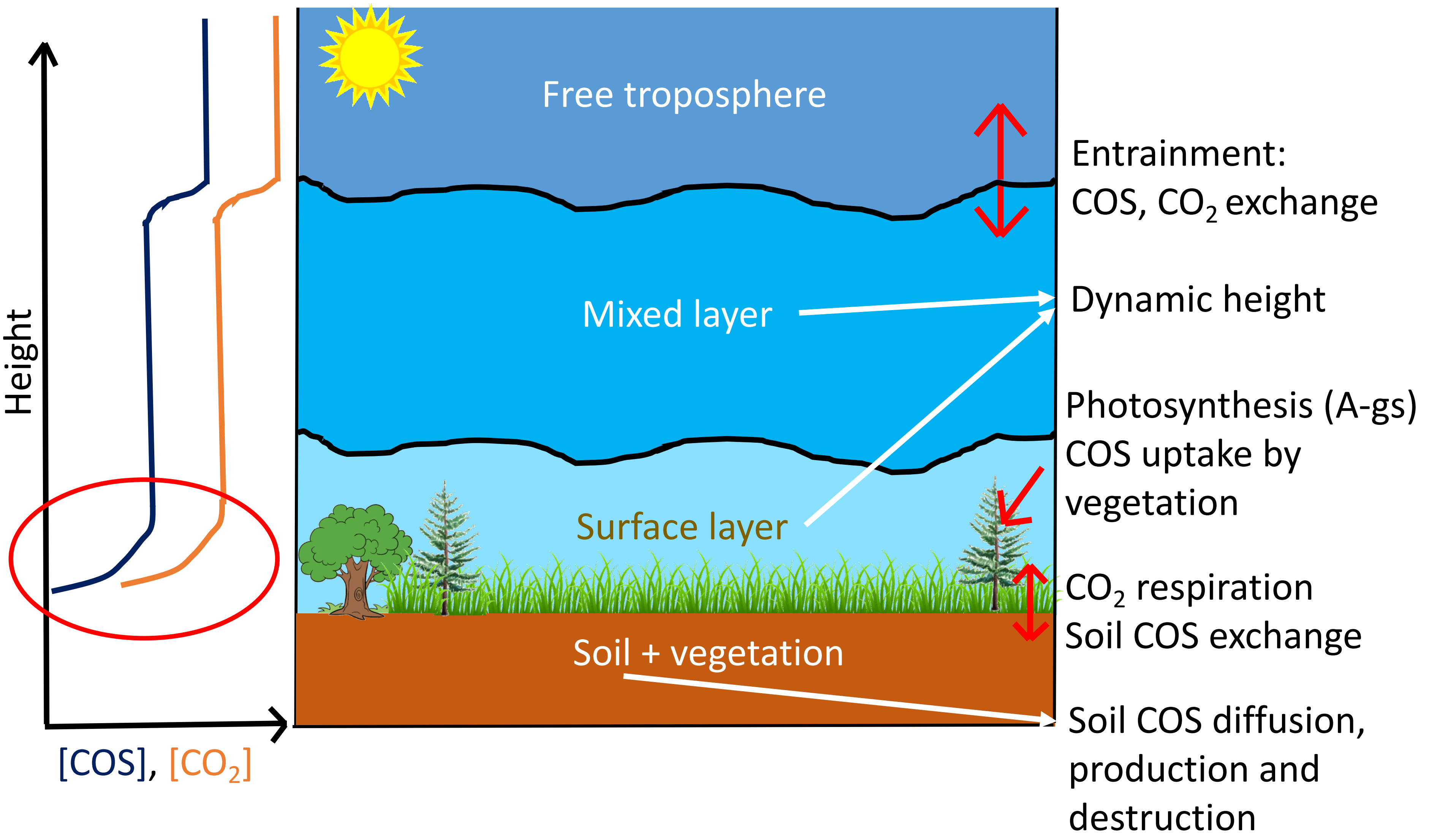
Cost function can contain any variable with observations

Any parameter can be optimised

Future goal:
No more messing with manual parameter fitting!!

Challenges remain
→ Switch to analytical derivative?

Current work



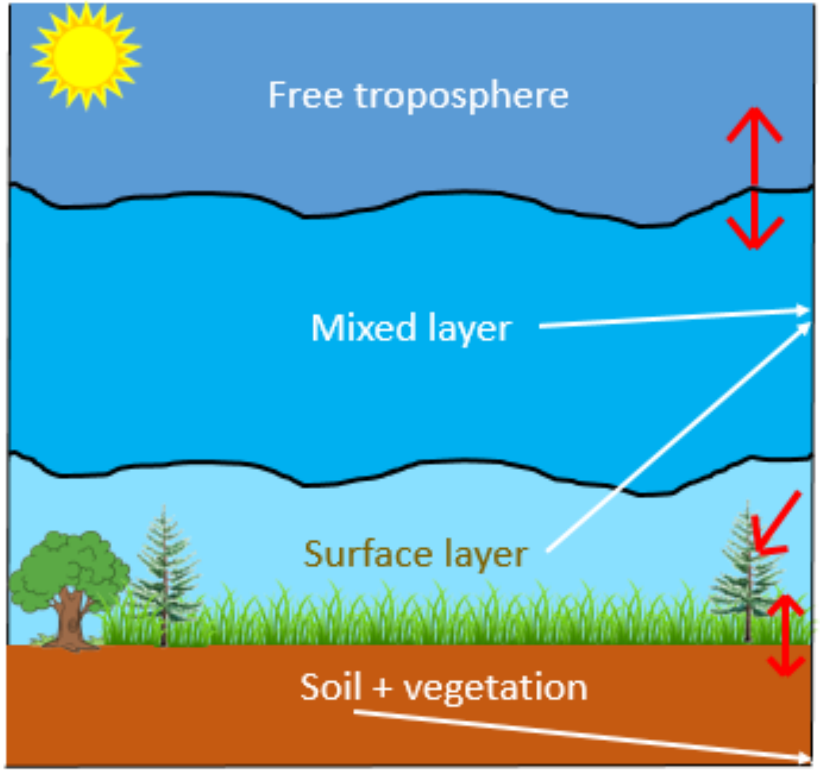
Novelties and challenges

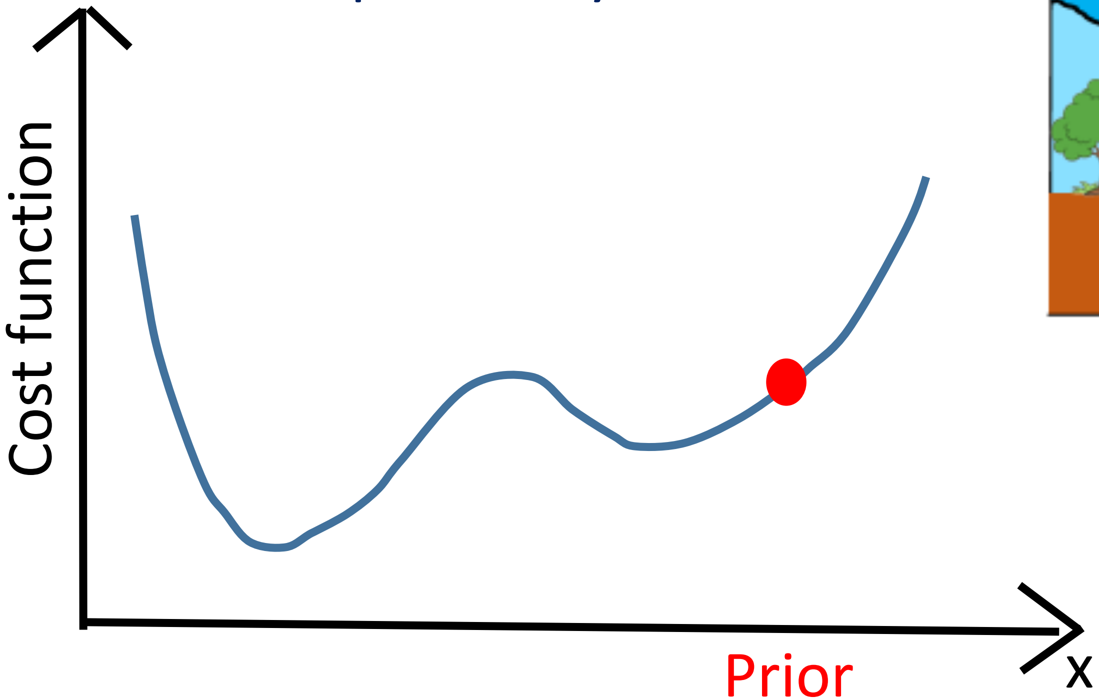
In between ecosystem and global study

Incorporate several type of obs

Strongly nonlinear model

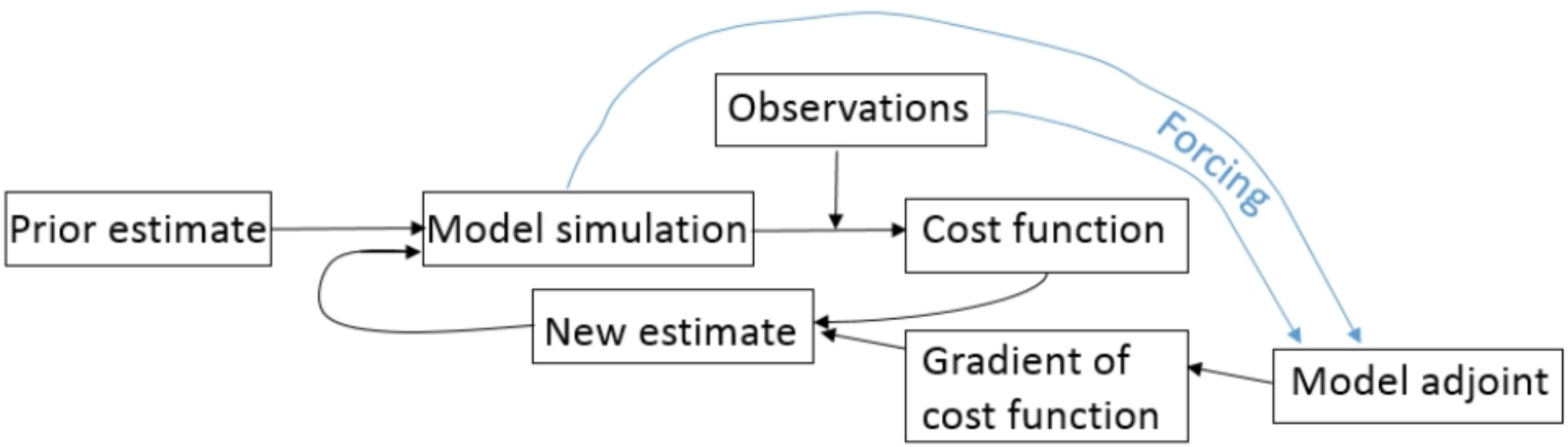
Parameter dependency





Current work

Analytical derivative : construction of the mixed-layer adjoint



Adjoint modelling

Model code:

$$C = 3 * A + 5 * B$$

Tangent linear model code:

$$dC = 3 * dA + 5 * dB$$

$$\begin{bmatrix} dC \\ dB \\ dA \end{bmatrix} = \begin{bmatrix} 0 & 5 & 3 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} dC \\ dB \\ dA \end{bmatrix}$$

Transpose matrix:

$$\begin{bmatrix} adC \\ adB \\ adA \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 \\ 5 & 1 & 0 \\ 3 & 0 & 1 \end{bmatrix} \begin{bmatrix} adC \\ adB \\ adA \end{bmatrix}$$

Adjoint model code:

$$adA = 3 * adC + adA$$

$$adB = 5 * adC + adB$$

$$adC = 0$$

Adjoint model code example

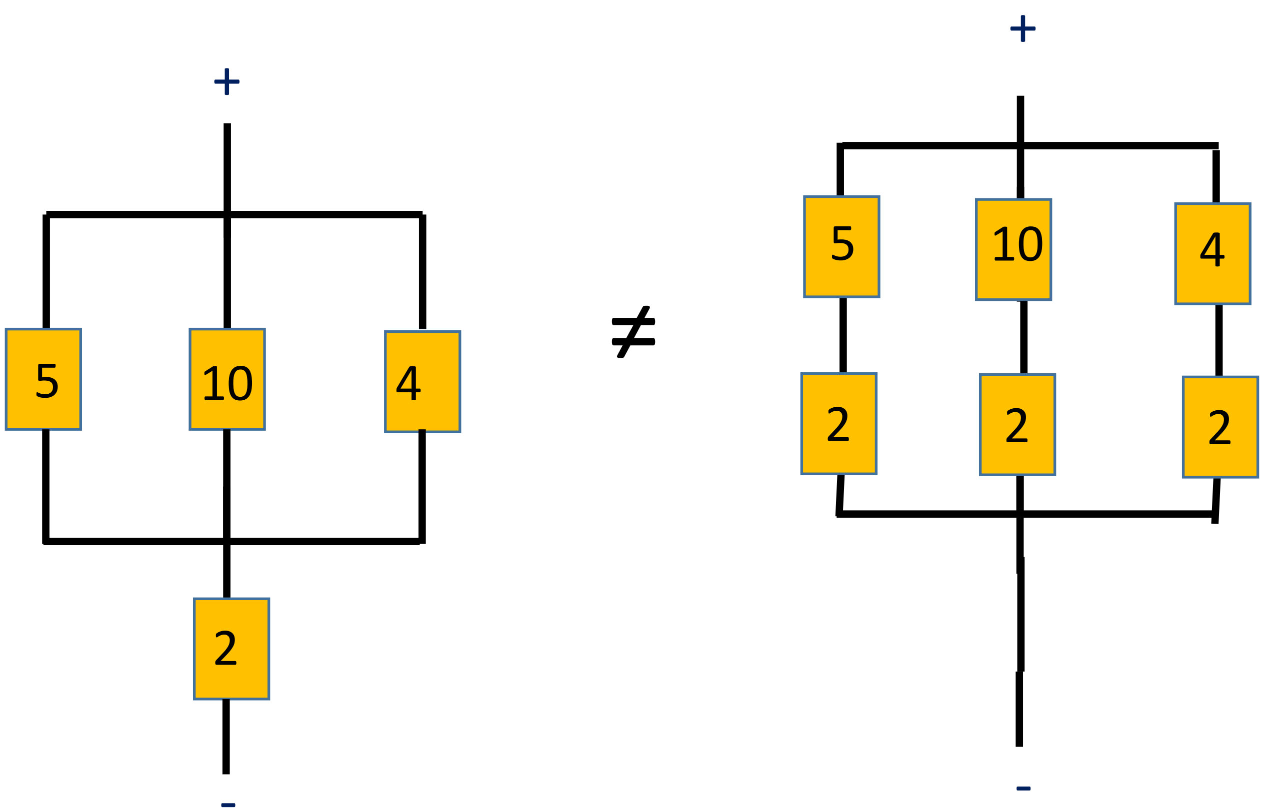
```
#statement ddeltaqtend = model.gammaq * (dwe + dwf_ddeltatheta - self.dM)
# - dqtend + dw_q_ft_dh
self.adwe += model.gammaq * self.addeltaqtend
self.adwf_ddeltatheta += model.gammaq * self.addeltaqtend
self.adM += -model.gammaq * self.addeltaqtend
self.adqtend += - self.addeltaqtend
self.adw_q_ft_dh += self.addeltaqtend
self.addeltaqtend = 0
#statement ddeltathetatend = model.gammatheta * (dwe + dwf_ddeltatheta - self.dM)
#- dthetatend + dw_th_ft_dh
self.adwe += model.gammatheta * self.addeltathetatend
self.adwf_ddeltatheta += model.gammatheta * self.addeltathetatend
self.adM += -model.gammatheta * self.addeltathetatend
self.adthetatend += - self.addeltathetatend
self.adw_theta_ft_dh += self.addeltathetatend
self.addeltathetatend = 0
#statement dCOStend = (self.dwCOS - dwCOSe - self.dwCOSM) / h + (wCOS - wCOSe - wCOSM)
#* (-1) * h**(-2) * self.dh + self.dadvCOS
self.adwCOS += 1 / h * self.adCOStend
self.adwCOSe += - 1 / h * self.adCOStend
self.adwCOSM += - 1 / h * self.adCOStend
self.adh += (wCOS - wCOSe - wCOSM) * (-1) * h**(-2) * self.adCOStend
self.adadvCOS += self.adCOStend
self.adCOStend = 0
```

Adjoint modelling

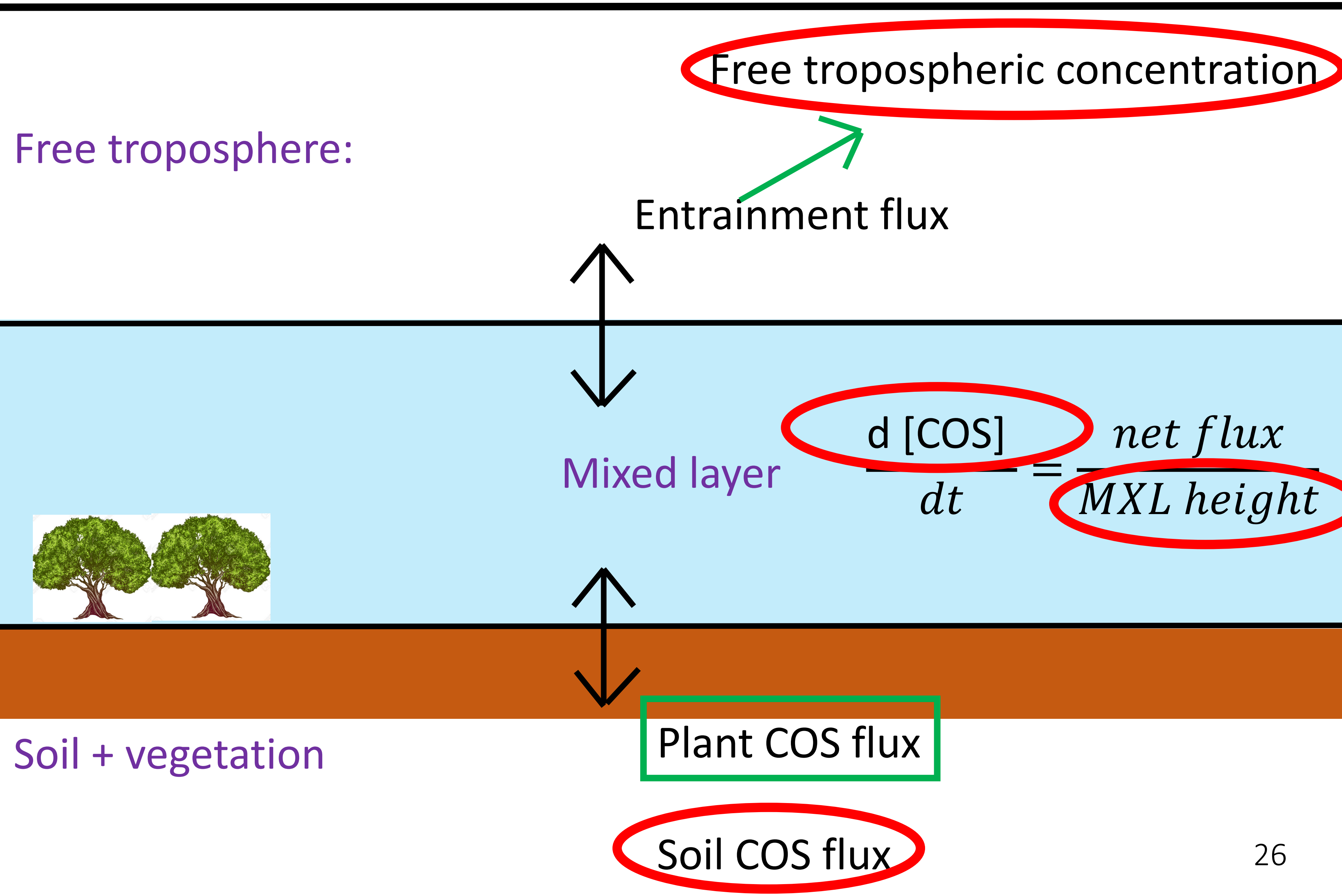
Extra slides

COS conductance issues

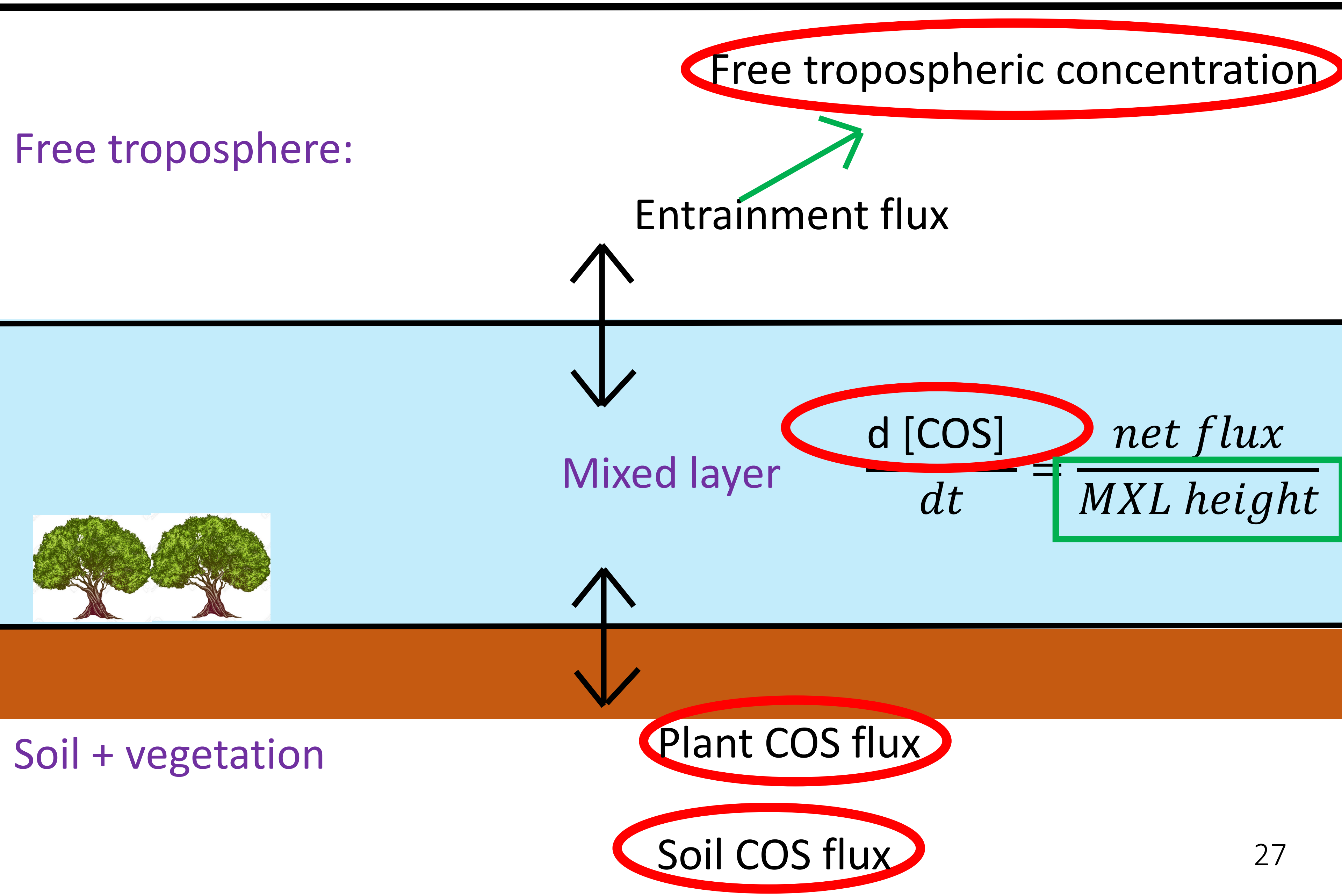
Assume canopy consists of three leaves of same size, different stom resistance
And C_air = 10



Potential of the framework



Potential of the framework



COS conductance issues

Assume canopy consists of three leaves of same size, different stom resistance
And C_air = 10

ri:	2	2	2
rs:	3	8	2
rtot	5	10	4
Flux(= C_air/rtot)	2	1	2.5
Flux_avg		1.8333	
Tot flux		3* 1.8333	
rs_avg		4.3333	
rtot_avg		6.3333	
flux_avg		1.578947	
Tot flux		3*1.578947	

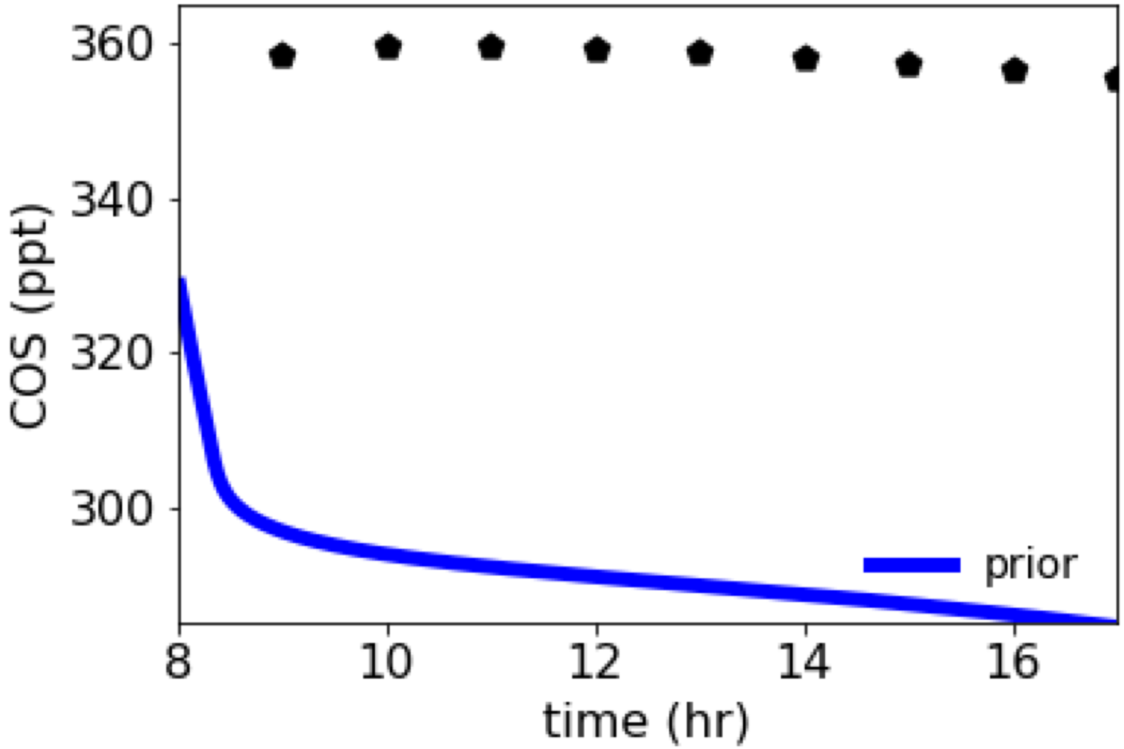
Parameters Harvard

Harvard four parameters optimised, two fluxes in cost function

	alfa_plant	alfa_soil	FTC_COS (ppb)	FTC_CO2_scale
Prior	0.8	0.5	0.380	1 (364 ppm)
Optimised	0.822	-4.674	0.361	1.063 (387 ppm)

Optimiser performance test

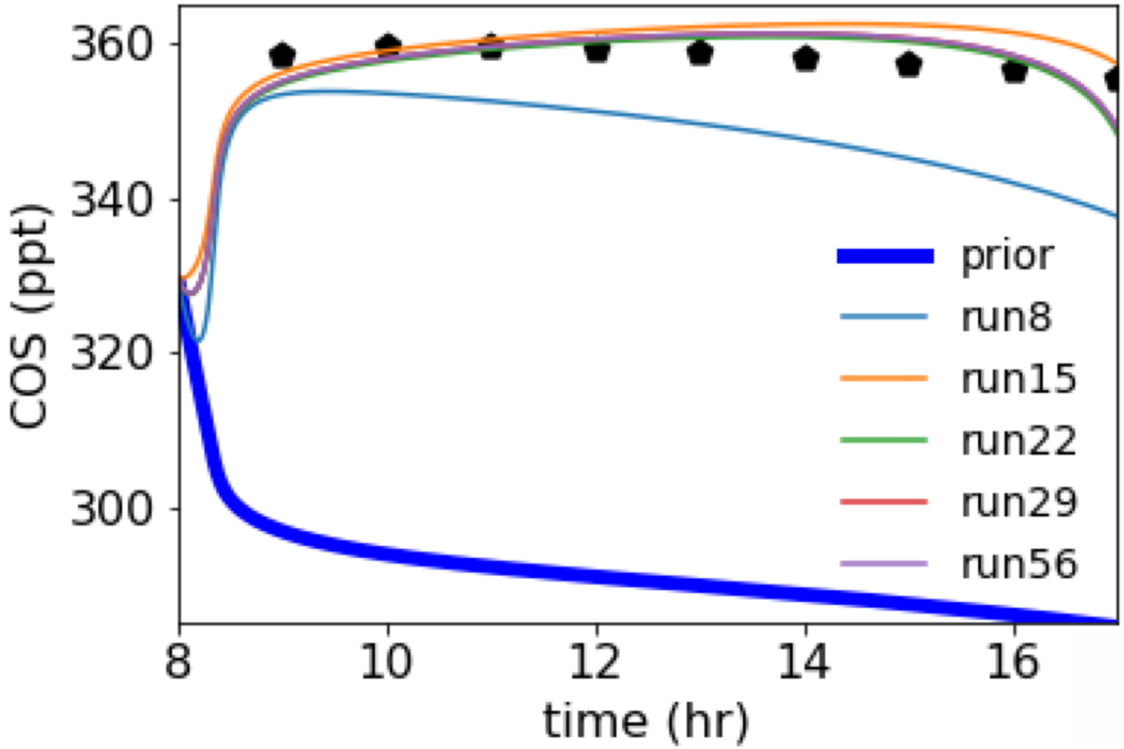
Now three parameters



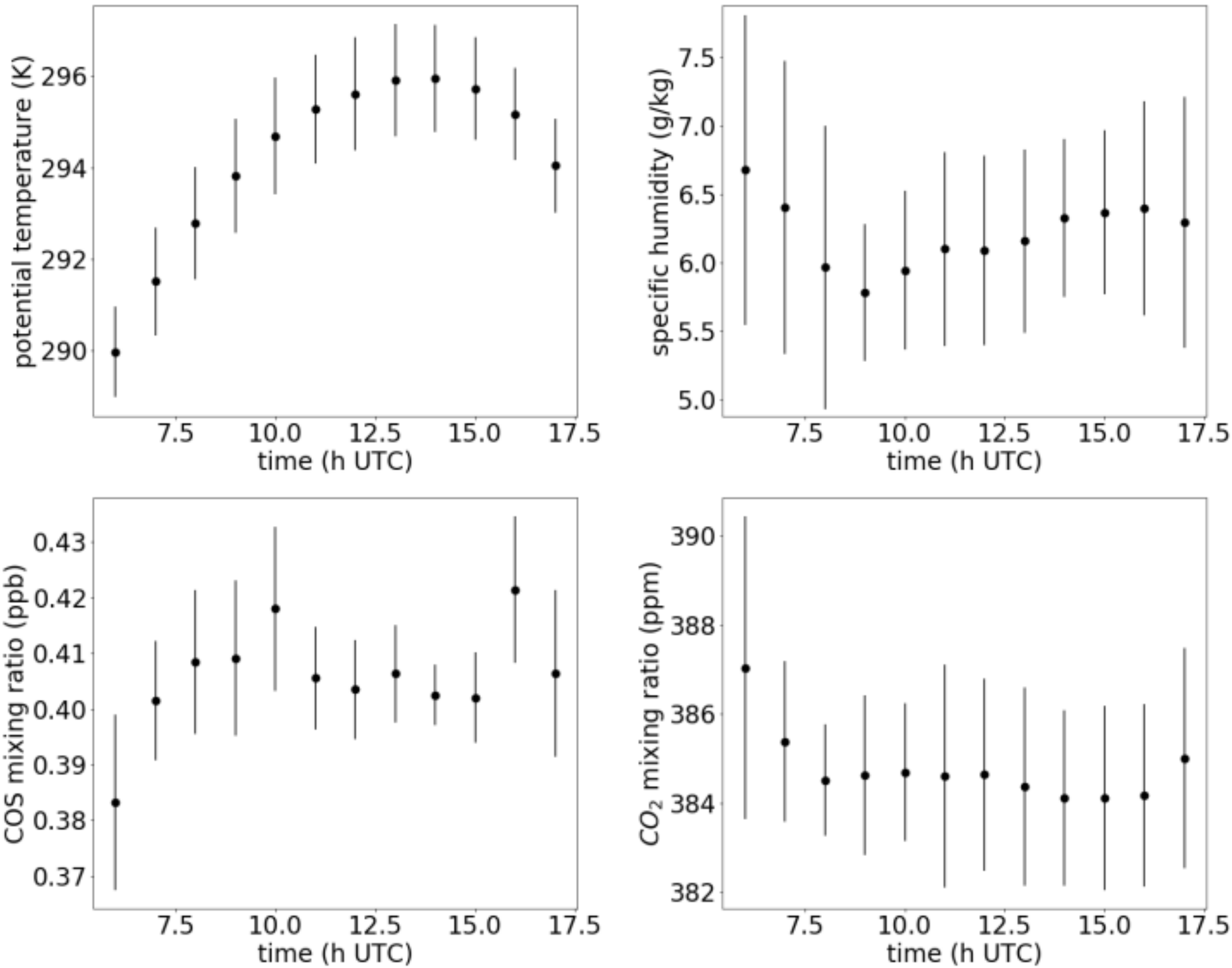
	alfa_plant	alfa_soil	FTC_COS
Truth	1	1	0.37 ppb
Prior	23	-1	0.3 ppb
Optimised			

Optimiser performance test

Now three parameters



	alfa_plant	alfa_soil	FTC_COS
Truth	1	1	0.37 ppb
Prior	23	-1	0.3 ppb
Optimised	-1.10	-94.62	0.364 ppb



potential temperature (K)
290
292
294
296
time (h UTC)
7.5
10.0
12.5
15.0
17.5
specific humidity (g/kg)
5.0
5.5
6.0
6.5
7.0
7.5
time (h UTC)
COS mixing ratio (ppb)
0.37
0.38
0.39
0.40
0.41
0.42
0.43
time (h UTC)
CO_2 mixing ratio (ppm)
382
384
386
388
390
time (h UTC)

Current coupling COS-CO_2

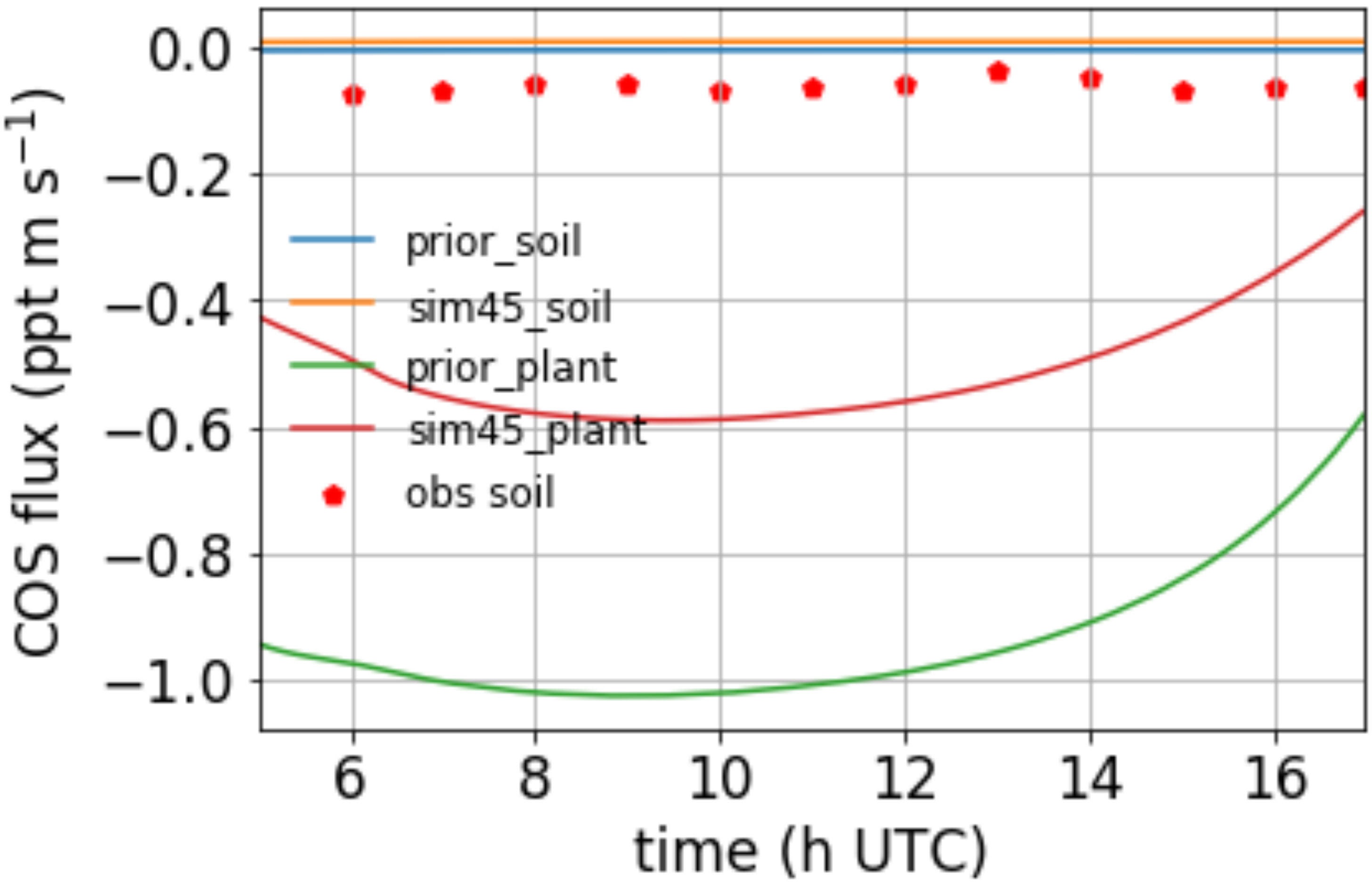
$$gCO_2\_can = gmin * LAI + \frac{f_{str} * a_1 \int_0^{LAI} A_g dL}{(C_{ext} - C_{comp})\left(1 + \frac{D_s}{D_*}\right)}$$

$$gsCO_2\_can = gCO_2\_can$$

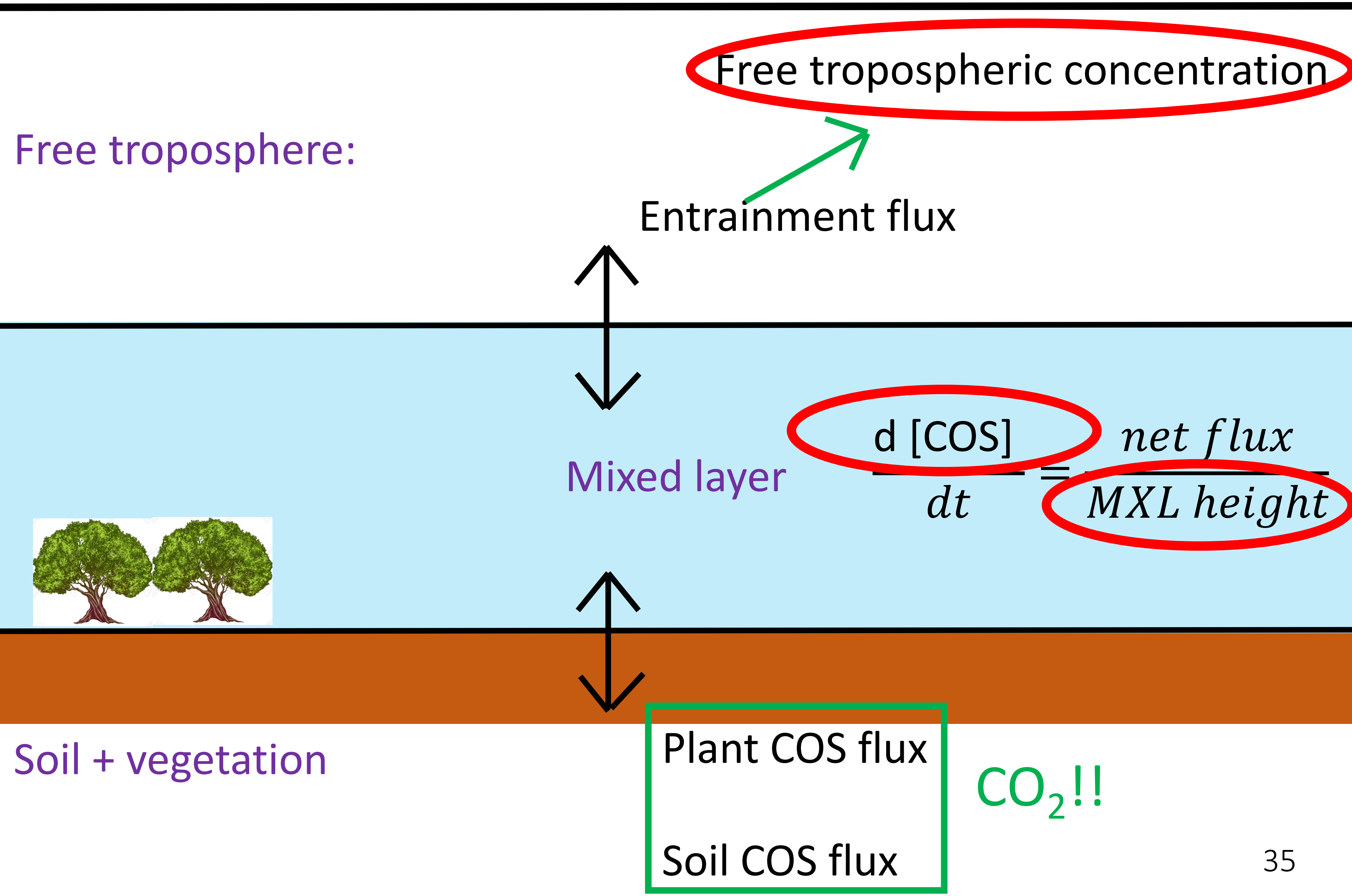
$$gsCOS\_can = \frac{gsCO_2\_can}{1.21}$$

$$gCOS\_can = \frac{1}{\left(\frac{1}{gsCOS\_can} + \frac{1}{giCOS}\right)}$$

Soil flux Hyytiala



Potential of the framework



Vegetation uptake

COS uptake and photosynthesis coupled to stomatal conductance -> crucial link between COS and photosynthesis

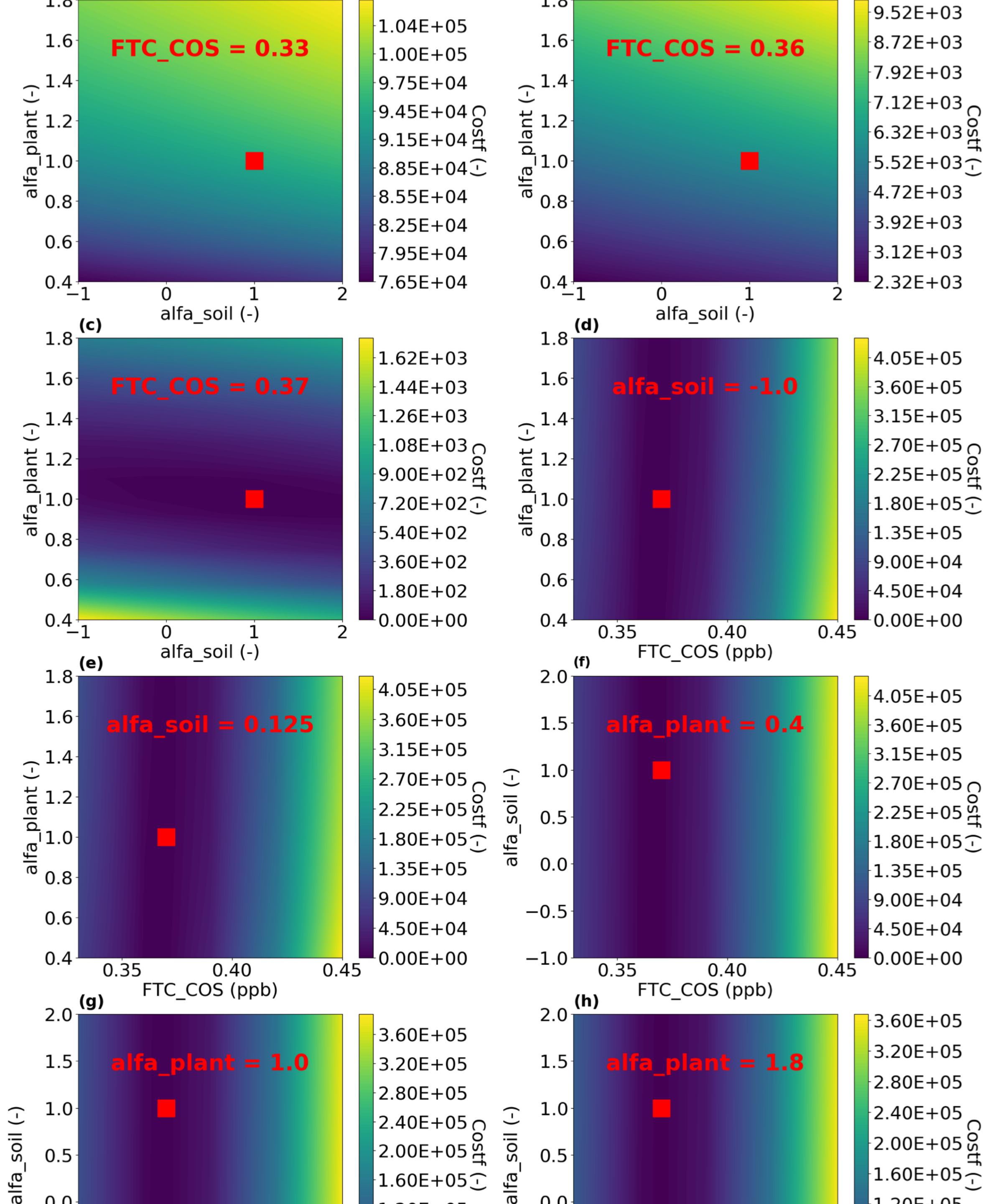
Often a simple relation assumed:

$$photosynthesis = \frac{COS\ uptake}{LRU}\frac{[CO_2]}{[COS]}$$

LRU = Leaf Relative Uptake

COS in leaves destroyed by enzymes, with limited backward diffusion

CO_2 in leaves often assimilated, but backward diffusion can be significant



FTC_COS = 0.33
alfa_plant (-)
alfa_soil (-)
Costf (-)
1.04E+05
1.00E+05
9.75E+04
9.45E+04
9.15E+04
8.85E+04
8.55E+04
8.25E+04
7.95E+04
7.65E+04
FTC_COS = 0.36
9.52E+03
8.72E+03
7.92E+03
7.12E+03
6.32E+03
5.52E+03
4.72E+03
3.92E+03
3.12E+03
2.32E+03
(c)
FTC_COS = 0.37
1.62E+03
1.44E+03
1.26E+03
1.08E+03
9.00E+02
7.20E+02
5.40E+02
3.60E+02
1.80E+02
0.00E+00
(d)
alfa_soil = -1.0
FTC_COS (ppb)
4.05E+05
3.60E+05
3.15E+05
2.70E+05
2.25E+05
1.80E+05
1.35E+05
9.00E+04
4.50E+04
0.00E+00
(e)
alfa_soil = 0.125
(f)
alfa_plant = 0.4
(g)
alfa_plant = 1.0
3.60E+05
3.20E+05
2.80E+05
2.40E+05
2.00E+05
1.60E+05
(h)
alfa_plant = 1.8