

Evaluating isoprene columns in UKESM and exploring the use of ML to improve emission factors

James Weber, Seb Hickman, Simon Driscoll

Updated Isoprene and Terpene Emission Factors for the Interactive BVOC Emission Scheme (iBVOC) in the Joint UK Land Environment Simulator (JULES)

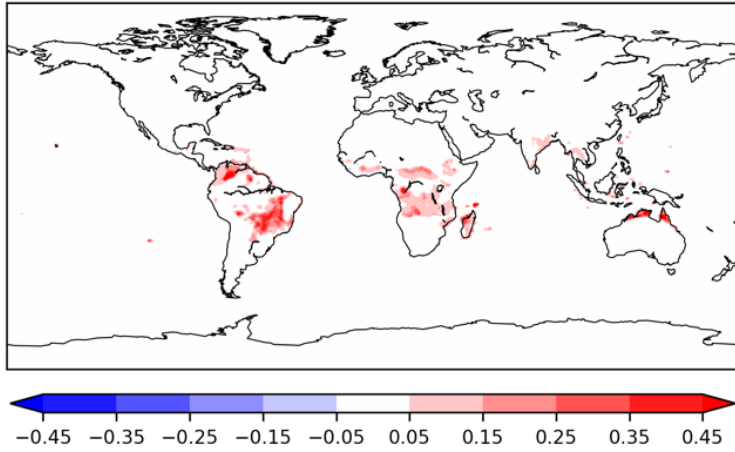
JULES Science Meeting Oxford 2022

Dr James Weber
University of Sheffield

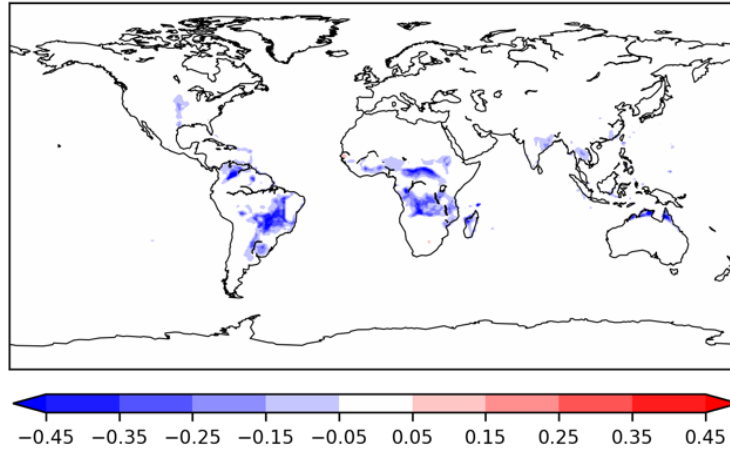
Dr James A. King, Dr Katerina Sindelarova, Dr Maria Val Martin

Convert MEGAN emission factors to work in iBVOC

(a) Broadleaf Evergreen Tropical

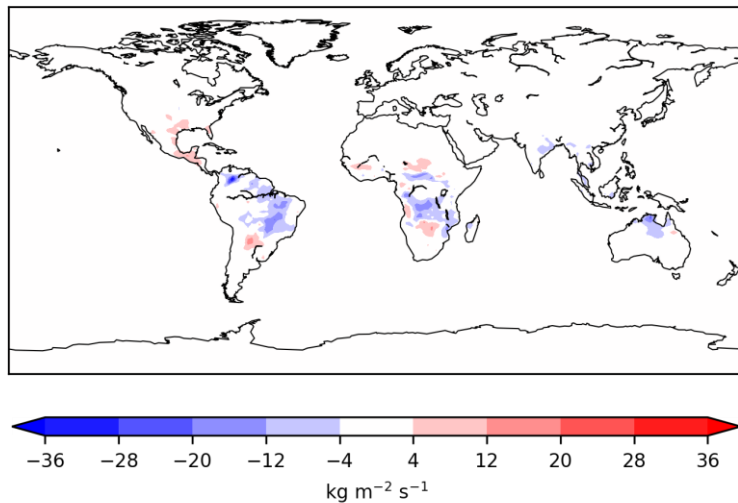


(b) C4 Grass

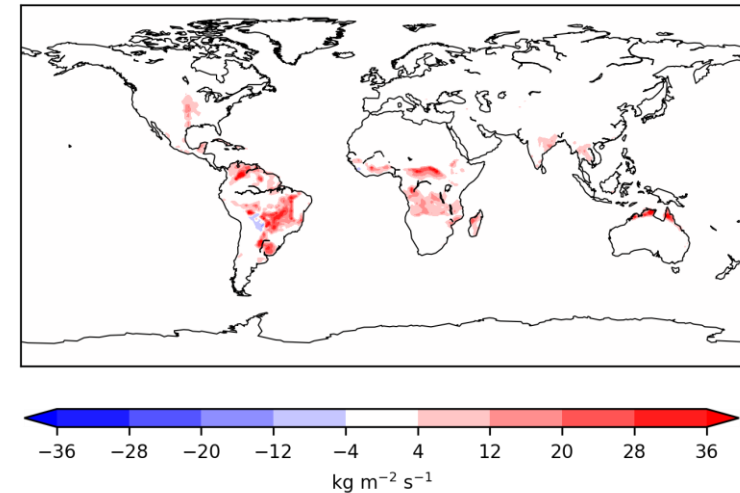


Reforestation Scenario

(a) UKESM_default_2050 - UKESM_default_2010 (-25 Tg yr⁻¹)



(c) CESM_2050 - CESM_2010 (+65 Tg yr⁻¹)



Increase in tree cover → decrease in isoprene emissions?! → update emissions factors

Weber et al (2023)

iBVOC Emission Model

$$\text{Emiss}_{\text{PFT}} = \text{EF}_{\text{PFT}} \times f_{\text{CO}_2} \times f_{\text{temp}} \times f_{\text{photo}}$$



$\mu\text{C g}_{\text{dw}}^{-1} \text{hr}^{-1}$

PFT-specific emission factor, EF_{PFT} , derived from emission measurements from surrogate species → “bottom up”

Current Implementation: 13-PFT setup

PFT	Abbreviation	iBVOC Std	ORCHIDEEv1 (Lathiere et al., 2006)
Broadleaf deciduous trees	Br-Dec	35	24/45/8 ^c
Broadleaf evergreen tropical trees	Br-Ev-Trop	24	24
Broadleaf evergreen temperate trees	Br-Ev-Temp	16	16
Needleleaf deciduous trees	Ne-Dec	8	8
Needleleaf evergreen trees	Ne-Ev	8	8/8 ^d
C3 grass	C3 grass	16	16
C3 crop	C3 crop	5	5
C3 pasture	C3 pasture	5	5
C4 grass	C4 grass	24	24
C4 crop	C4 crop	5	5
C4 pasture	C4 pasture	5	5
Shrub deciduous	Shrub-Dec	10	Not in scheme
Shrub evergreen	Shrub-Ev	20	Not in scheme

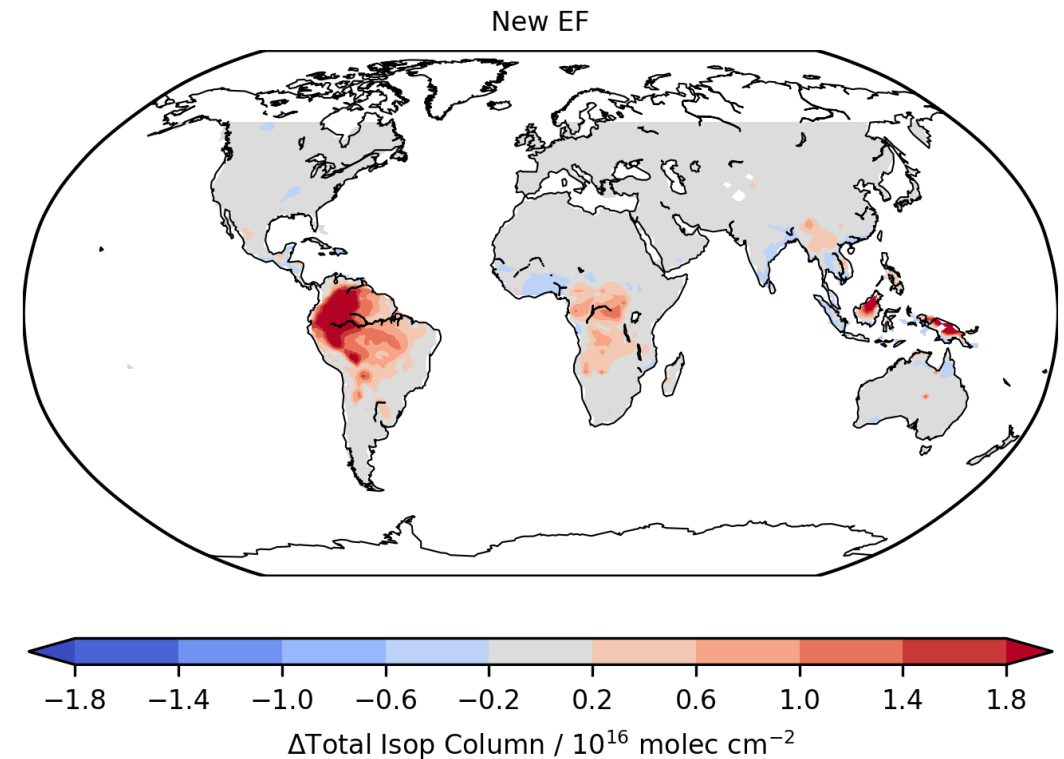
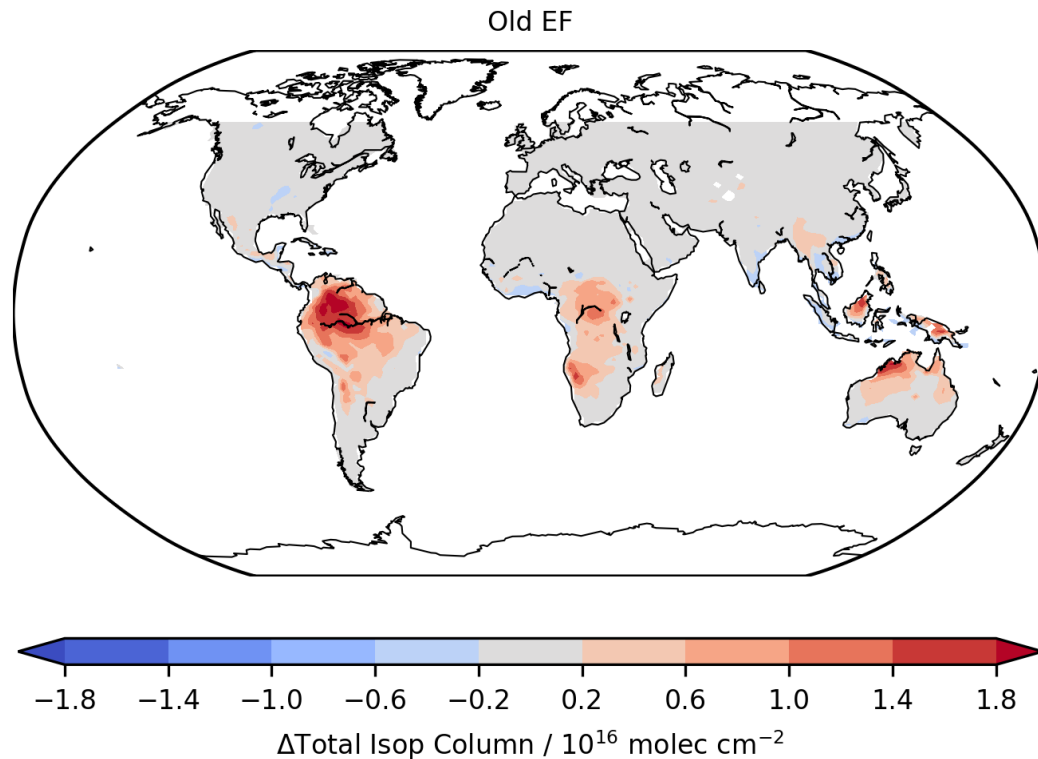
40% of isoprene from C4 grass in UKESM vs. 1% in MEGAN

Messina et al (2016) – ORCHIDEE v2

In ORCHIDEE, shrubs are not represented by one particular PFT but are included partly in the PFTs 10 and 11 related to grasses (C3Gr and C4Gr). In order to determine the EF for grass, we collect the data available for shrub plant species.

UKESM performance against observations (model – obs)

2012: Strat-Trop Base LU



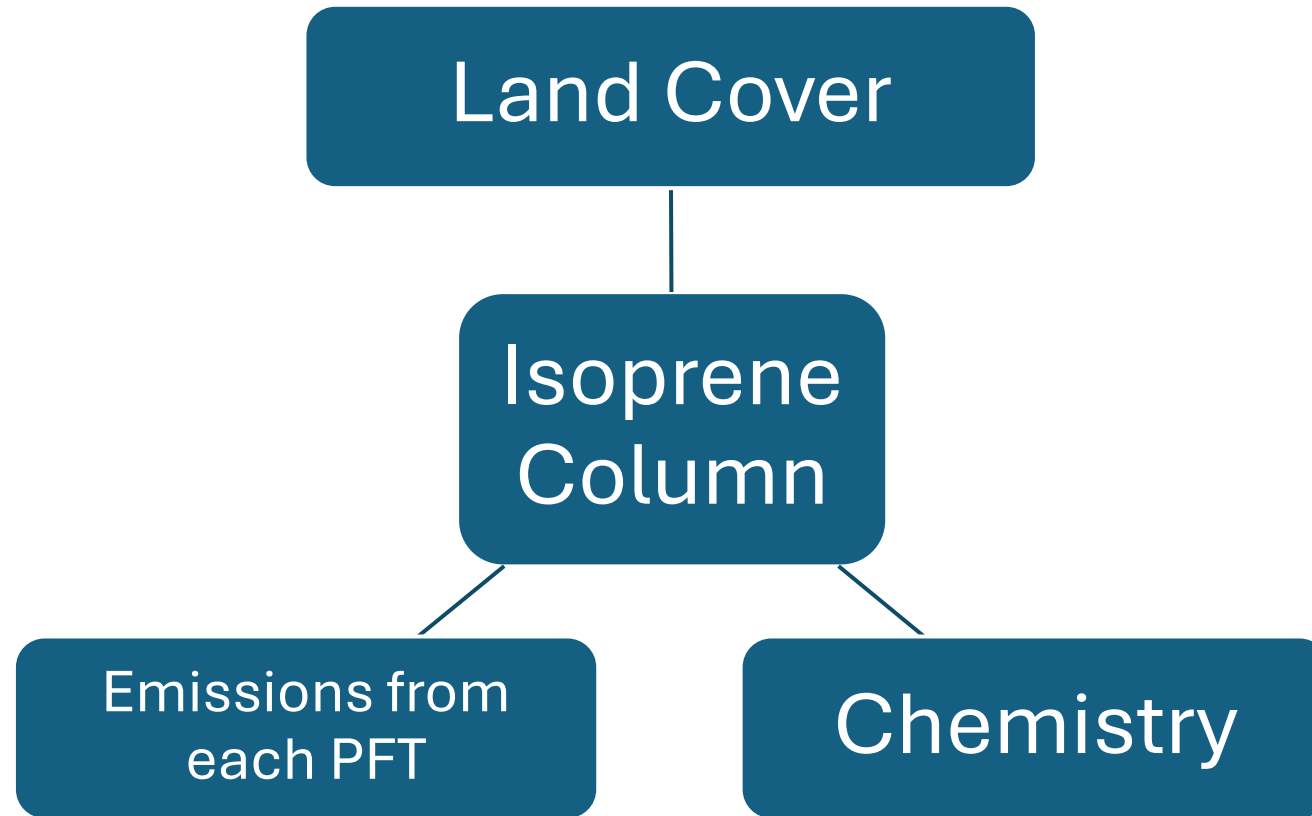
Article | Published: 09 September 2020

Satellite isoprene retrievals constrain emissions and atmospheric oxidation

[Kelley C. Wells](#), [Dylan B. Millet](#) , [Vivienne H. Payne](#), [M. Julian Deventer](#), [Kelvin H. Bates](#), [Joost A. de Gouw](#), [Martin Graus](#), [Carsten Warneke](#), [Armin Wisthaler](#) & [Jose D. Fuentes](#)

Maybe a bit worse?!

What is driving the bias?



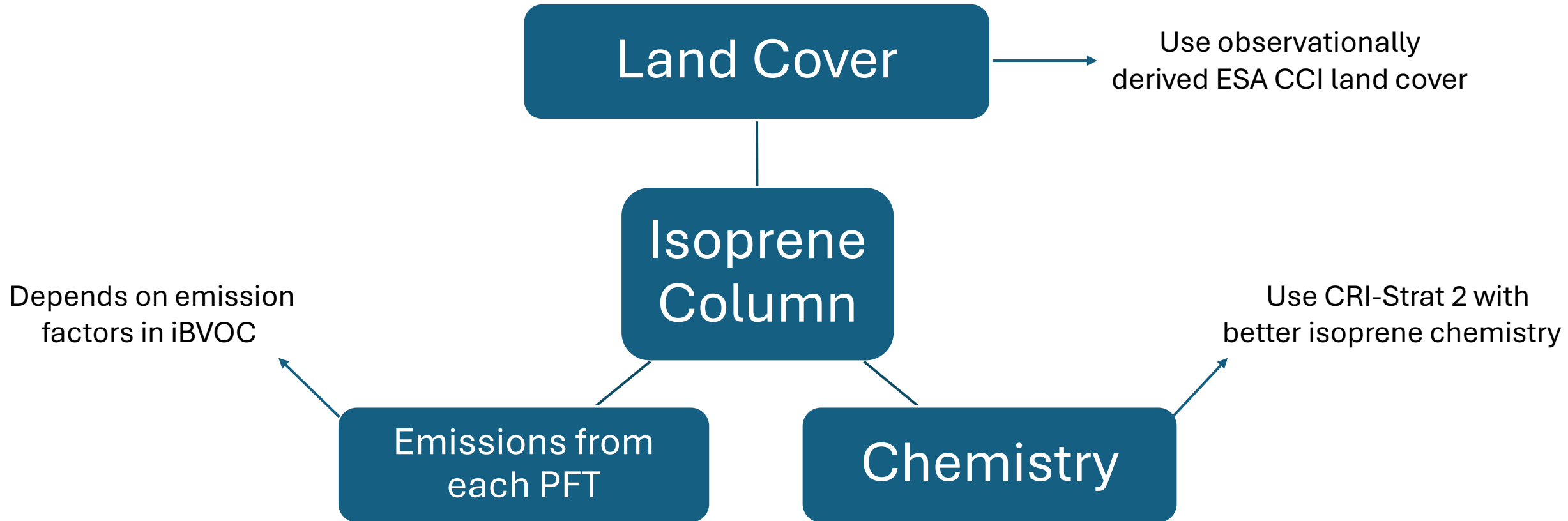


Emissions from
each PFT

Chemistry

Land Cover

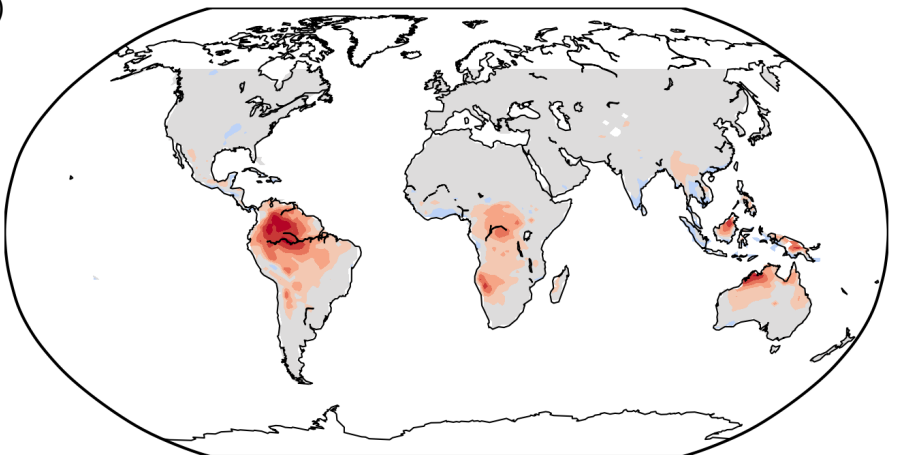
What is driving the bias?



2012
(model – obs)

Original

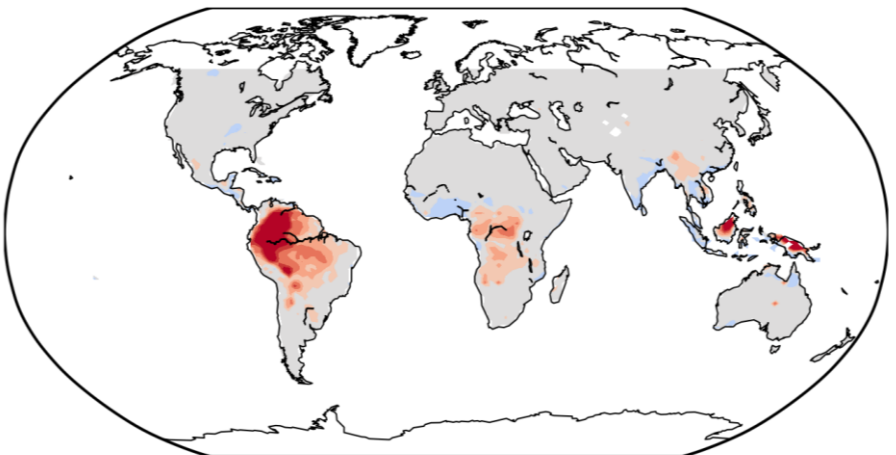
ST, Base LU, Old EF



“Better” EF

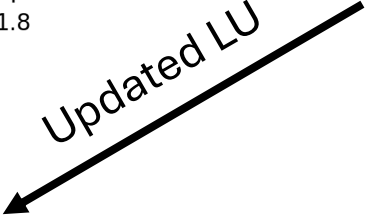


ST, Base LU, New EF



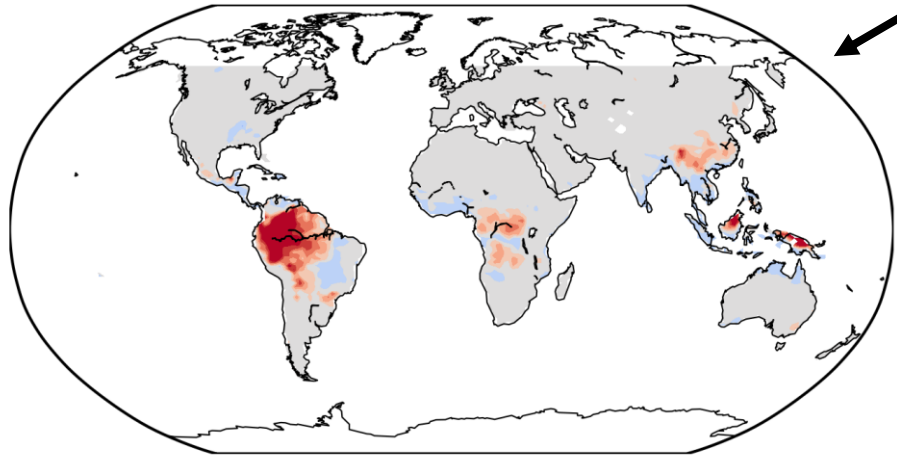
New EF

Updated LU



New EF,
Updated
LU

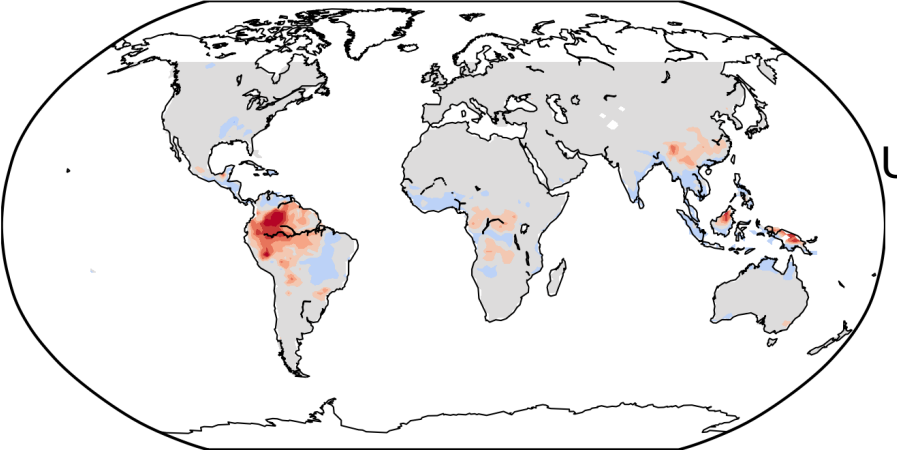
ST, ESA CCI LU, New EF



Better
Chemistry



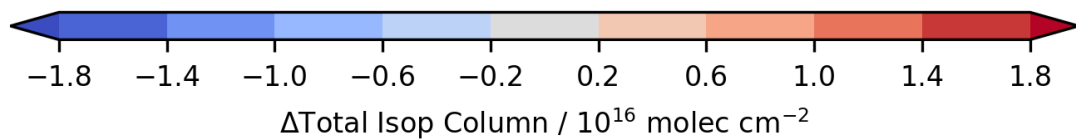
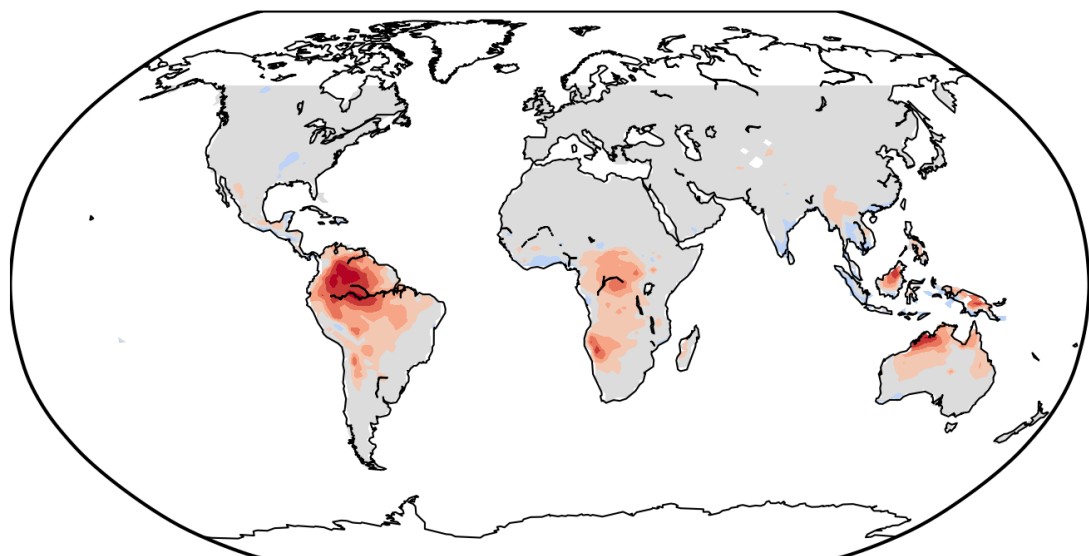
CS2, ESA CCI LU, New EF



New EF,
Updated LU,
Better
Chemistry

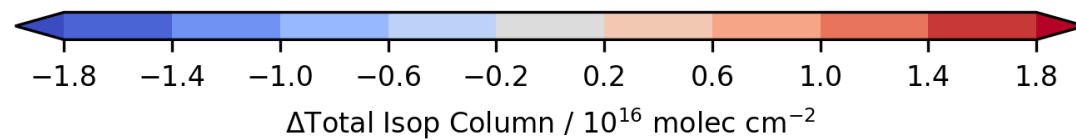
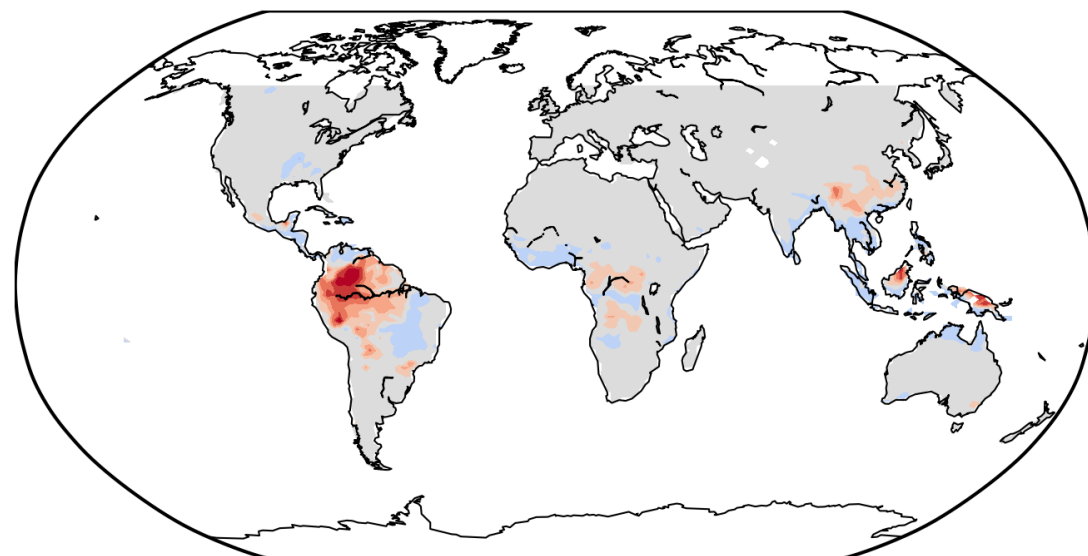
Original

ST, Base LU, Old EF



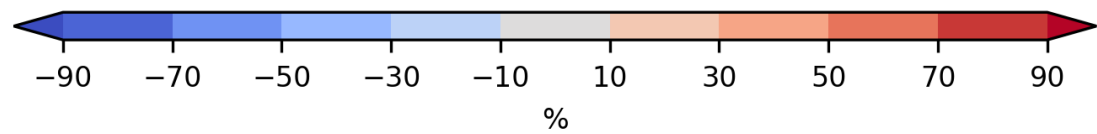
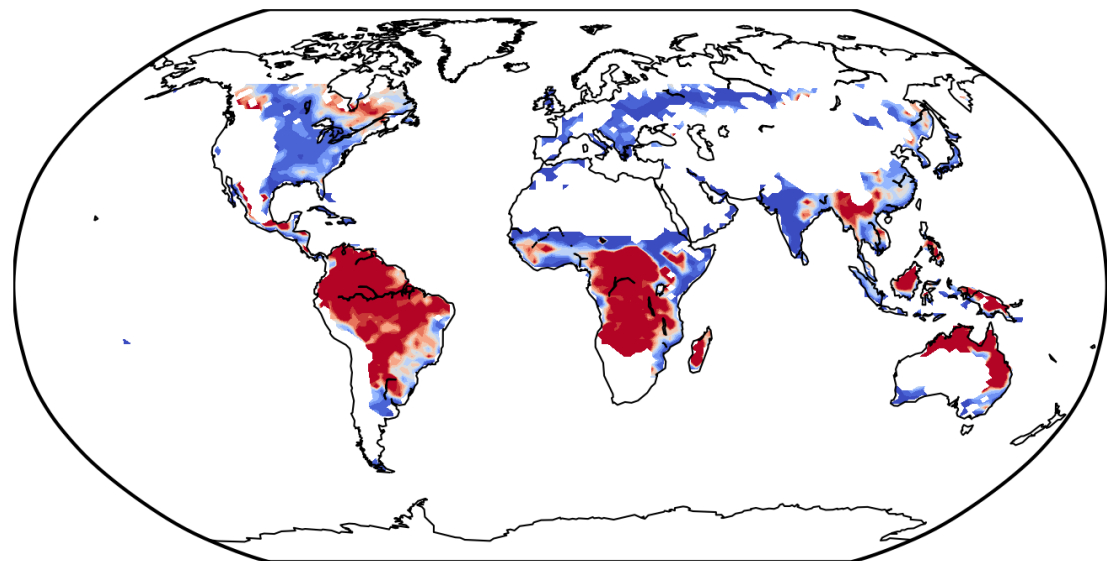
New EF, Updated LU, Better Chemistry

CS2, ESA CCI LU, New EF



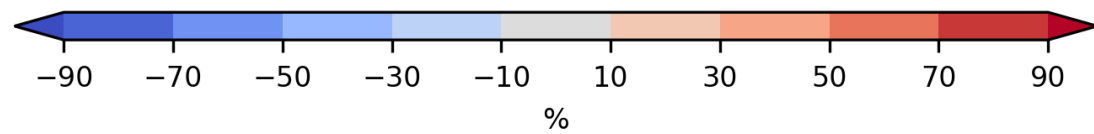
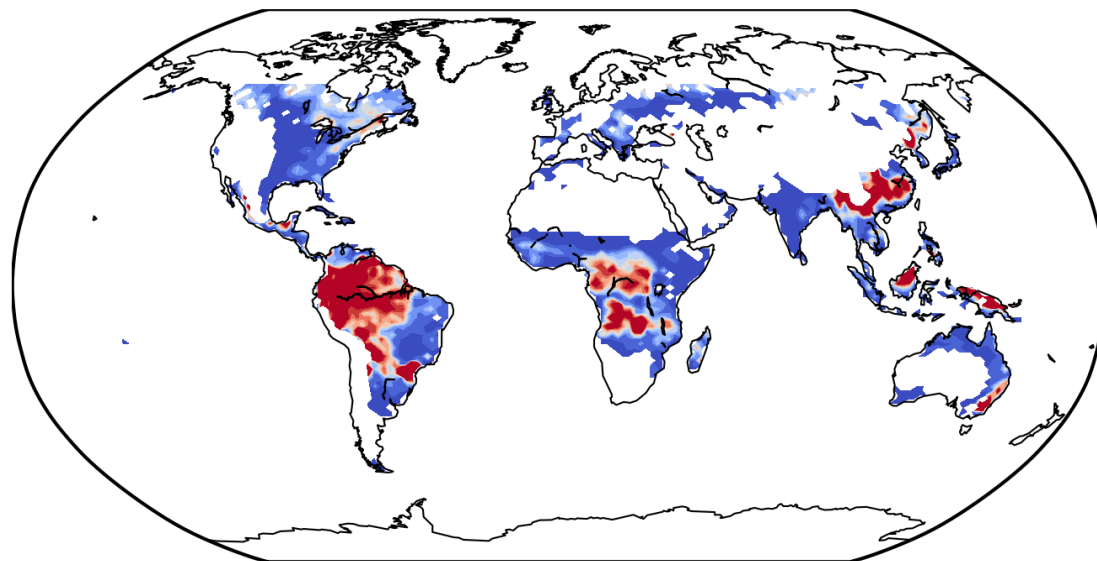
Original

ST, Base LU, Old EF

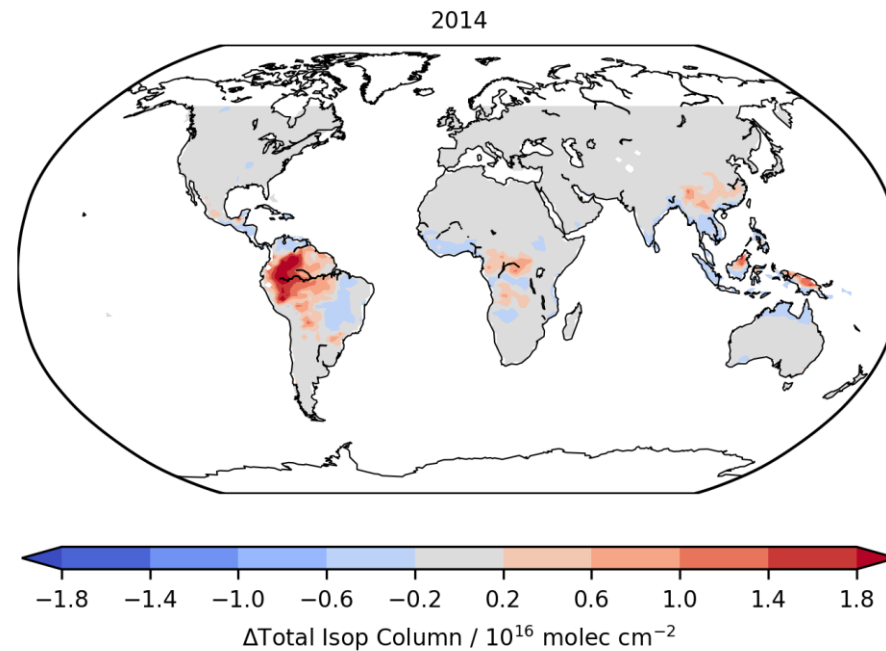
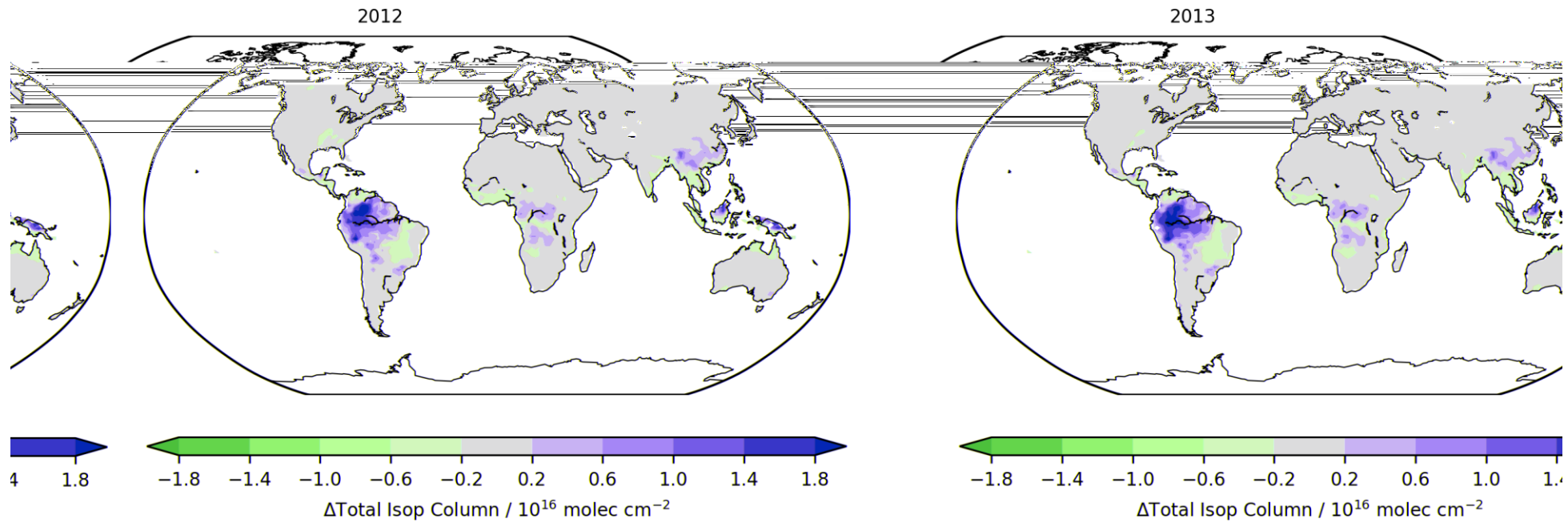


New EF, Updated LU, Better Chemistry

CS2, ESA CCI LU, New EF



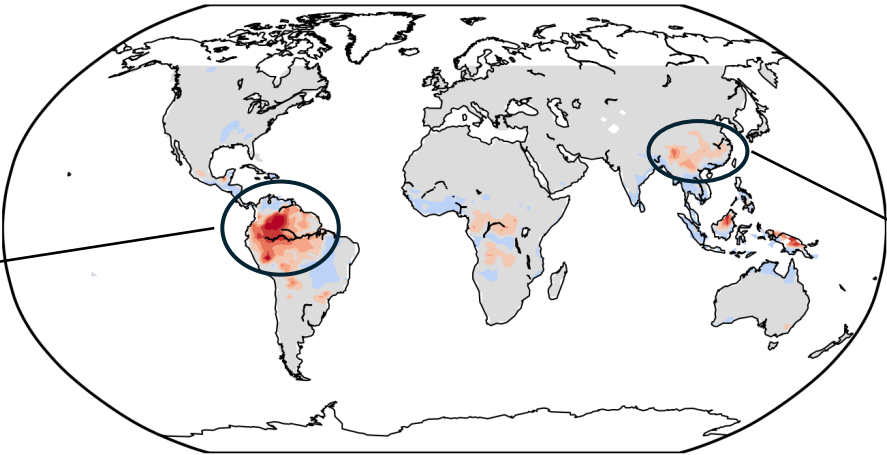
New EF, Updated LU, Better Chemistry



Still a lot of room for improvement!

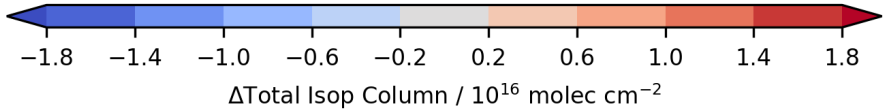
Brute Force / Educated Guess – adjust certain EF

CS2, ESA CCI LU, New EF

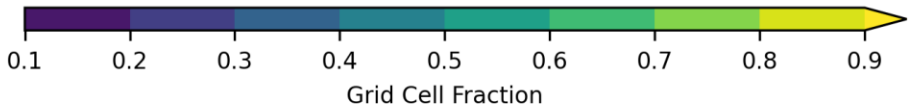
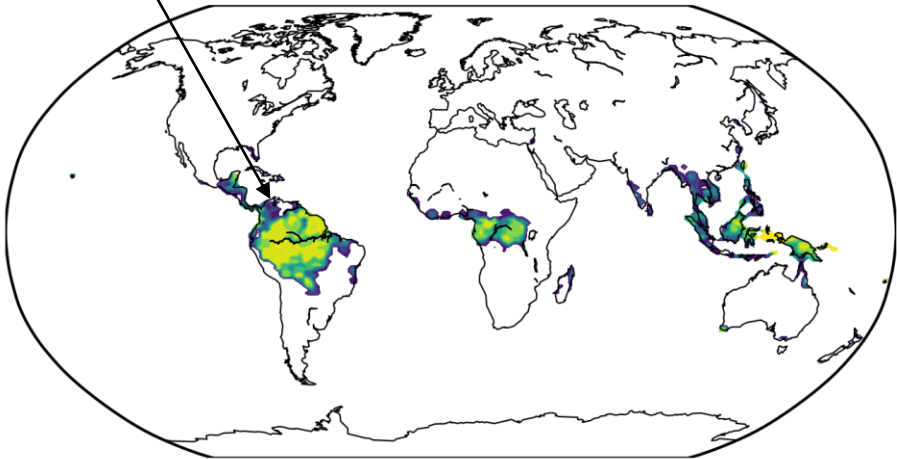


Focus on tropical
evergreen broadleaf

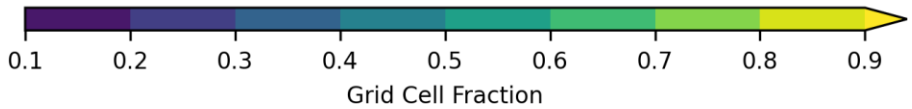
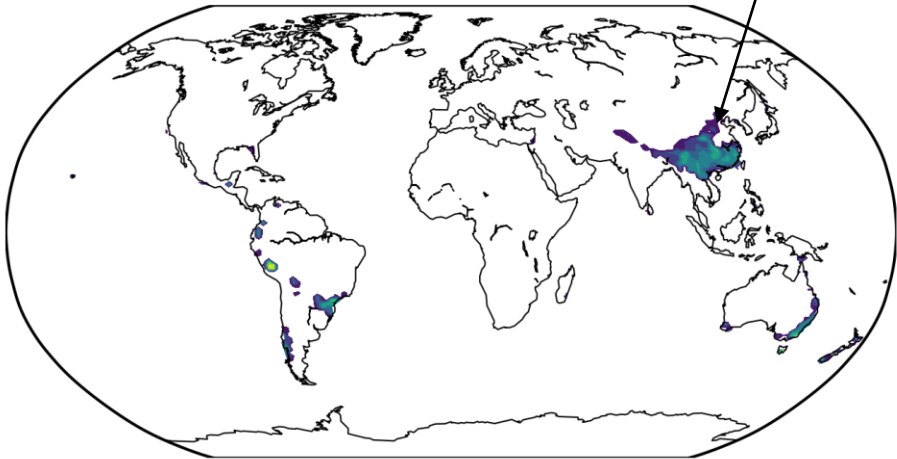
Focus on temperate
evergreen broadleaf



Tropical Broadleaf Evergreen



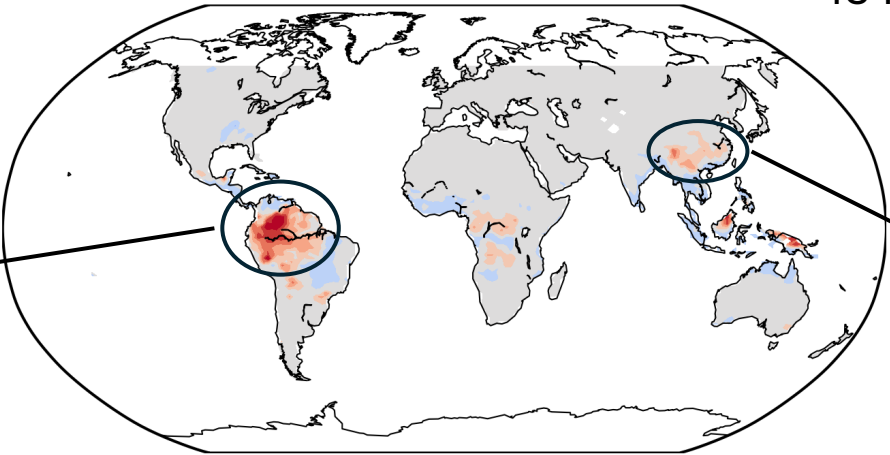
Temperate Broadleaf Evergreen



Brute Force / Educated Guess – adjust certain EF

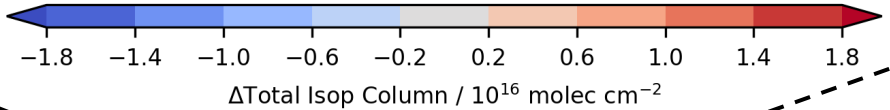
CS2, ESA CCI LU, New EF

434 Tg yr⁻¹



Focus on tropical
evergreen broadleaf

Focus on temperate
evergreen broadleaf

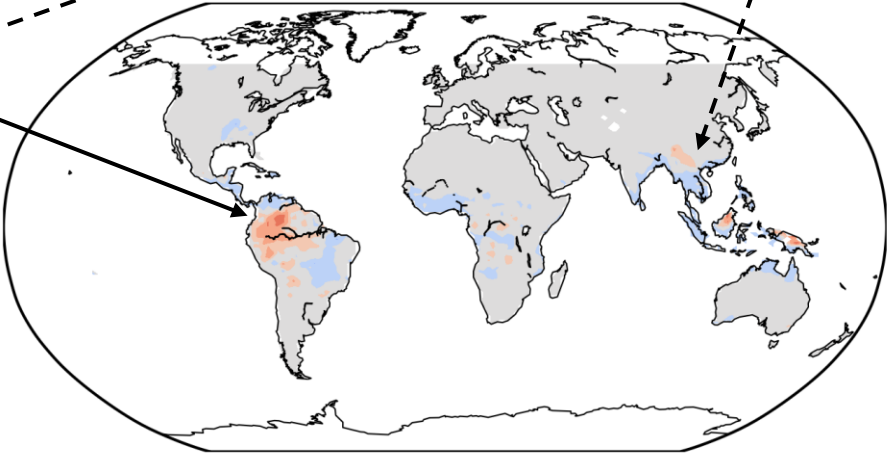
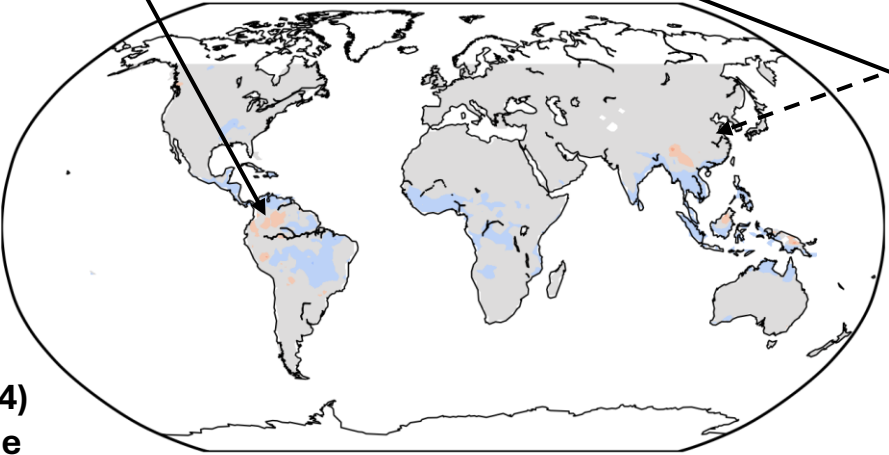


Vary EF - Take 1

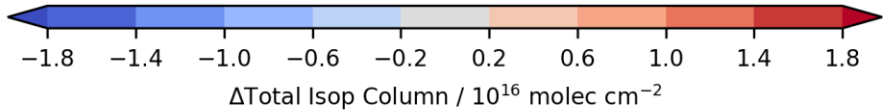
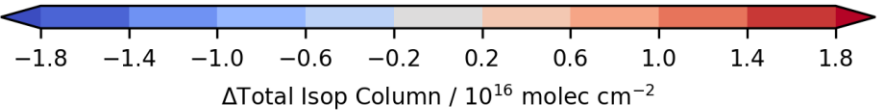
Vary EF - Take 2

310 Tg yr⁻¹

363 Tg yr⁻¹



Sindelarova (2024)
ESA CCI land use
→ 299 Tg yr⁻¹



How could ML help?

- Use observationally-derived land use (ESA CCI) and “best available” BVOC chemistry (CS2) → assume only bias in isoprene column is due to emissions.
 - Assume temperature, photosynthesis and CO₂ dependencies in iBVOC are suitable.
- Could use “brute force” method with lots of combinations of EF but time consuming and expensive
- (At least) 2 ML options

ML Option 1: Build “emulator”

Predict UKESM's isoprene column on a grid-by-grid basis firstly as a function of each grid cell's emissions and local meteorology.
(extensions to include neighbouring grid cells etc.)

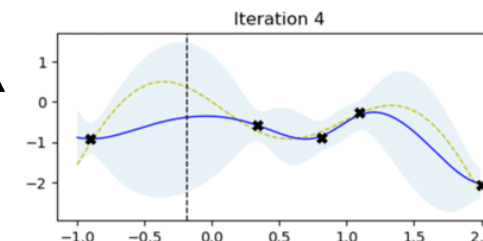
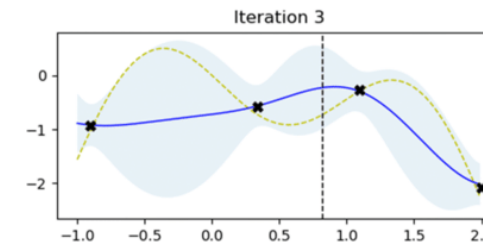
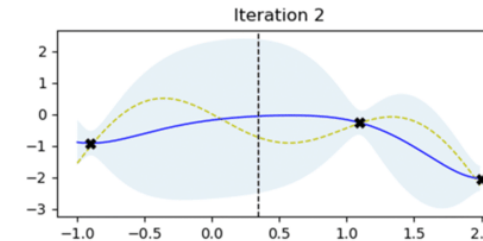
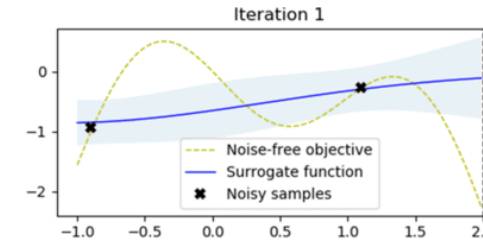
$$\text{Column}_i = \underbrace{\sum_{\text{PFT}} \alpha E_i}_{\text{Emissions}} + \underbrace{\beta u_i + \gamma v_i + \delta w_i + \dots}_{\text{Meteorology}}$$

If the emulator can reproduce UKESM column values, changing PFT emission factors ($\rightarrow$ emissions) could then be used to optimise model performance against observation $\rightarrow$ optimal EF combination.

ML Option 2: Bayesian Optimisation

- Learn a machine learning model that predicts accuracy (e.g. RMSE between UKESM isoprene column and observed isoprene column) based on some changeable parameters (e.g. PFT1 emission scaling factor)
- The model must also quantify uncertainty in its prediction
- We then use the ML model to predict **both**:
 - The best value of the parameter based on what we currently know
 - And the most useful next value of the parameter to try to see if it improves the model
- Choice of metric to be optimised needs careful consideration.

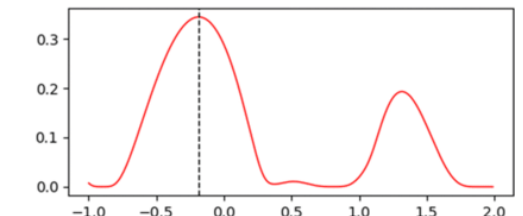
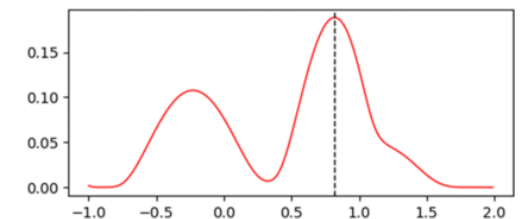
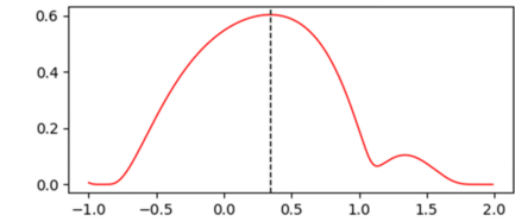
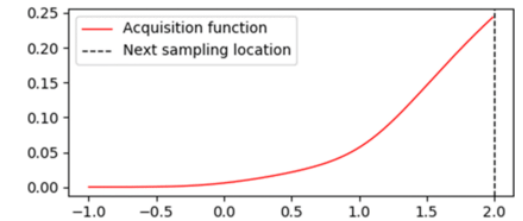
Developing idea of functional form



Model
Skill
↑

Parameter to be varied → EF

Where to investigate next



Summary

- Updates to EF derived from MEGAN resolves land use issue but still leaves bias vs. obs – could be problem for UKESM2
- Land use (PFT distribution), EF and simulated chemistry all influential in bias – when LU and chemistry are “optimised” bias is reduced but still present
- Try to derive “top down” estimate of EF for PFTs – has typically been done using “bottom up” approaches in the past.
- Brute force / educated guess approach (change certain EF) can reduce bias further
- Exploring 2 ML options to optimise EFs still further – other ML approach suggestions and/or observations very welcome!