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

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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

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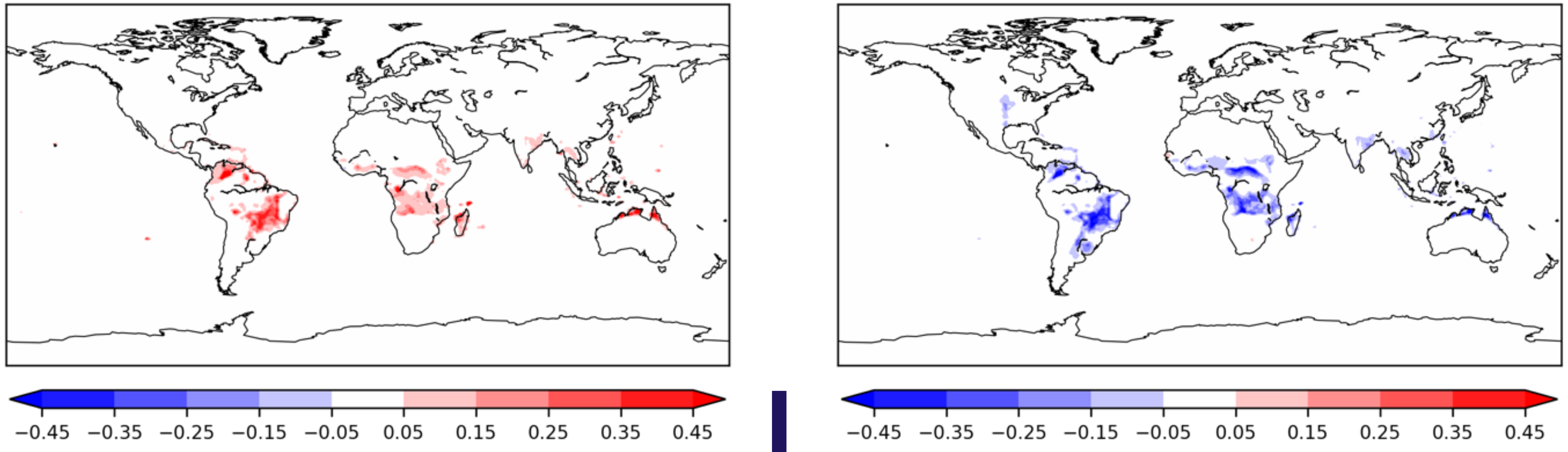
Convert MEGAN emission factors to work in iBVOC

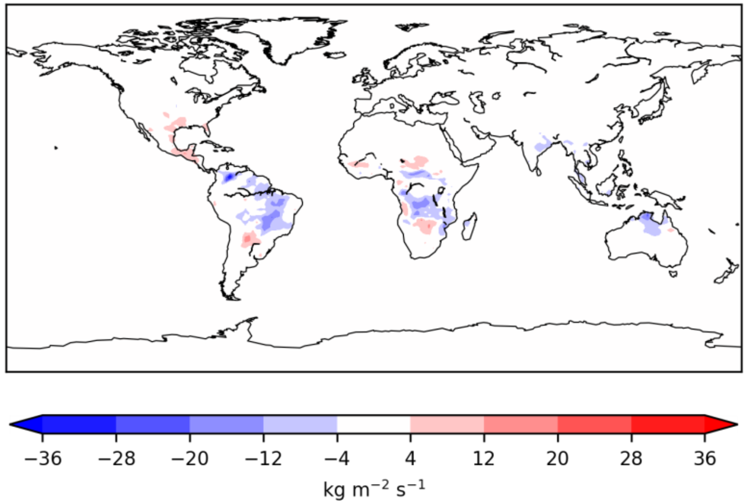
Reforestation Scenario

(a) Broadleaf Evergreen Tropical

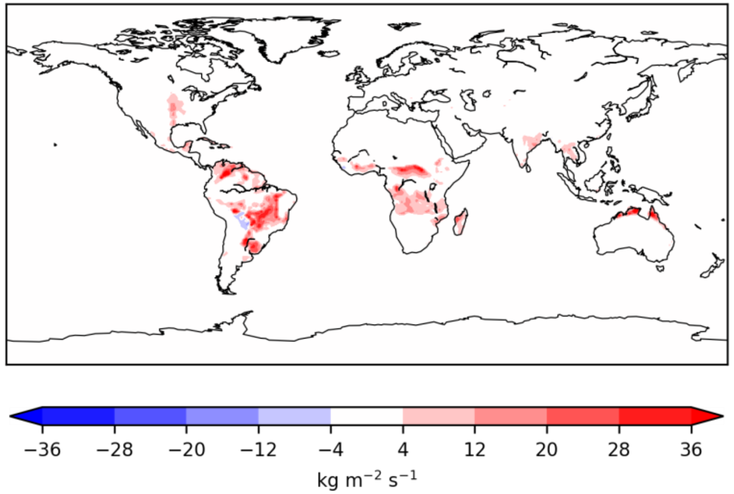
(b) C4 Grass



(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

$$\mathrm{Emiss_{PFT}} = \mathrm{EF_{PFT}} \times \mathrm{f_{CO_2}} \times \mathrm{f_{temp}} \times \mathrm{f_{photo}}$$

$\mu\mathrm{C}\ \mathrm{g_{dw}^{-1}}\ \mathrm{hr^{-1}}$

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

Current Implementation: 13-PFT setup

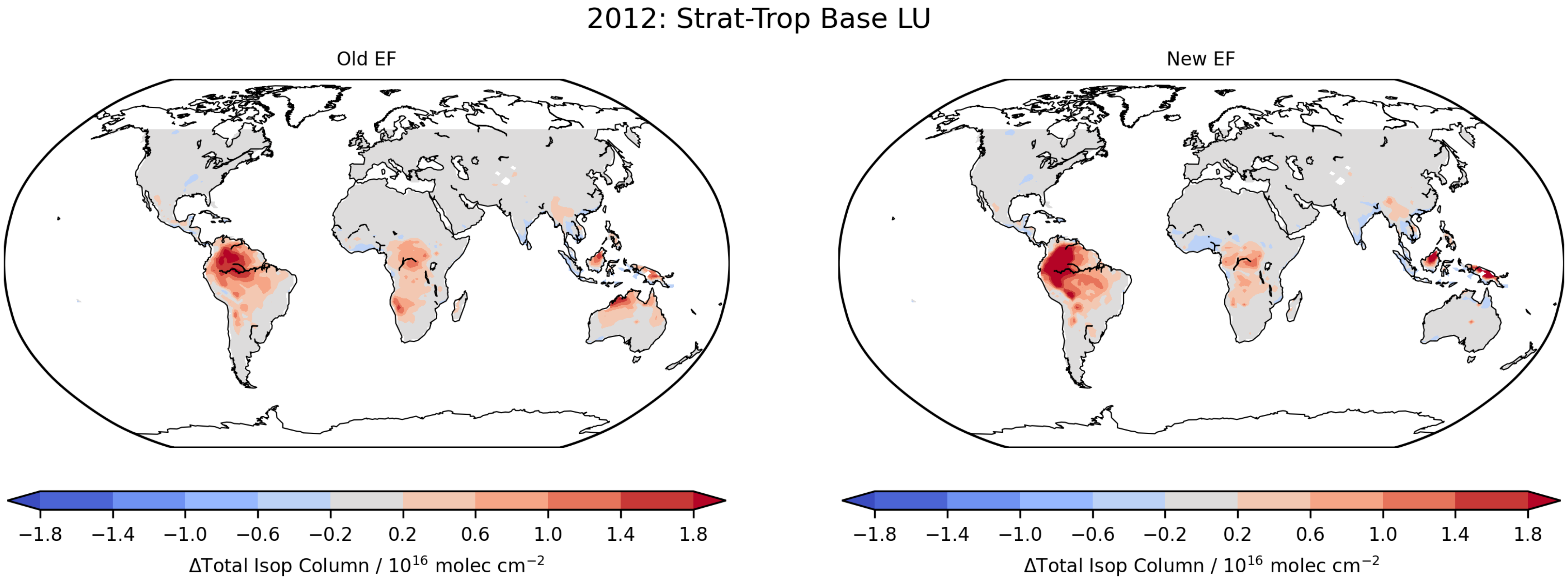
PFT	Abbreviation	iBVOC Std	ORCHIDEEv1 (Lathiere et al., 2006)
Broadleaf deciduous trees	Br-Dec	35	24/45/8[c]
Broadleaf evergreen tropical trees	Br-Ev-Trop	24	24
Broadleaf evergreen temperate trees	Br-Ev-Temp	16	16
Needleleaf deciduous trees	Ne-Dec	8	8
Needleleaf evergreen trees	Ne-Ev	8	8/8[d]
C3 grass	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)



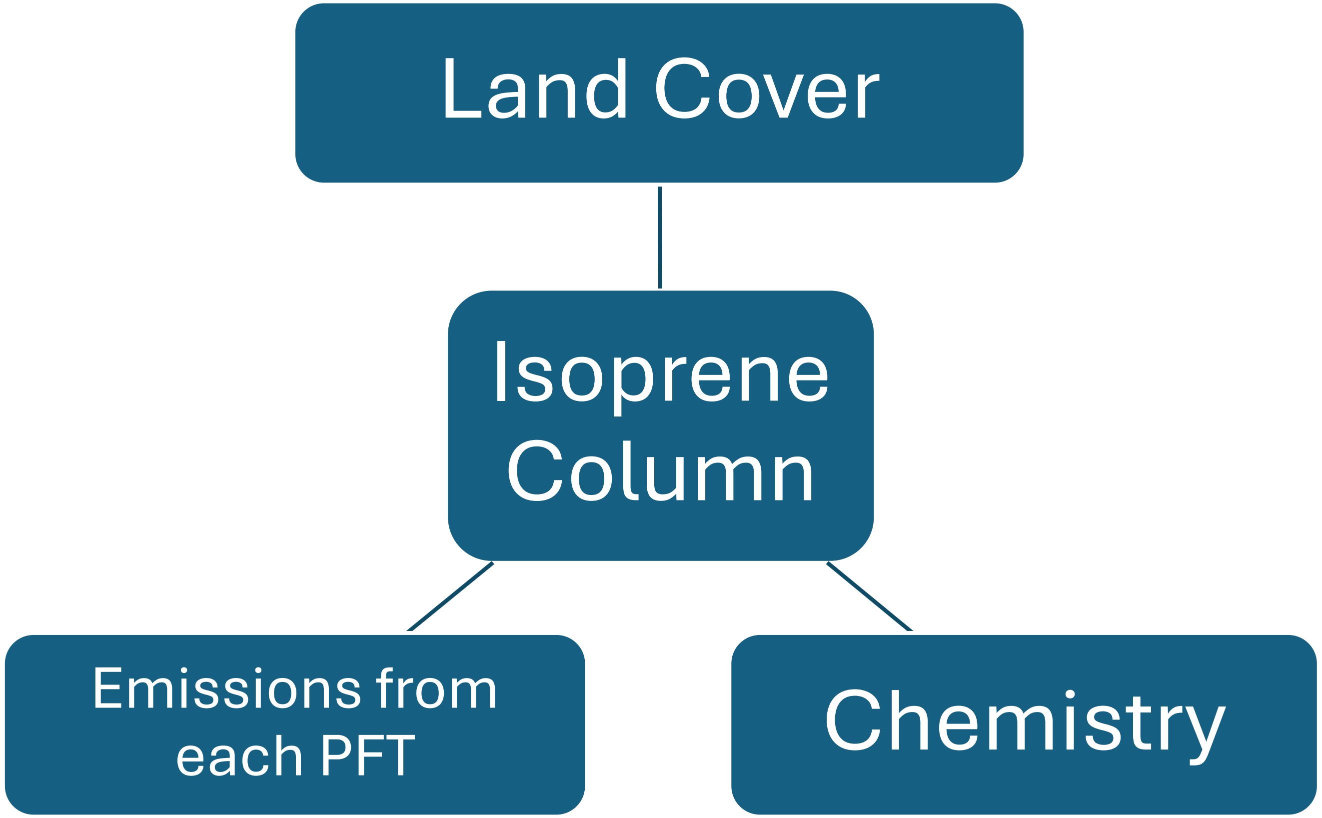
Article | Published: 09 September 2020

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?

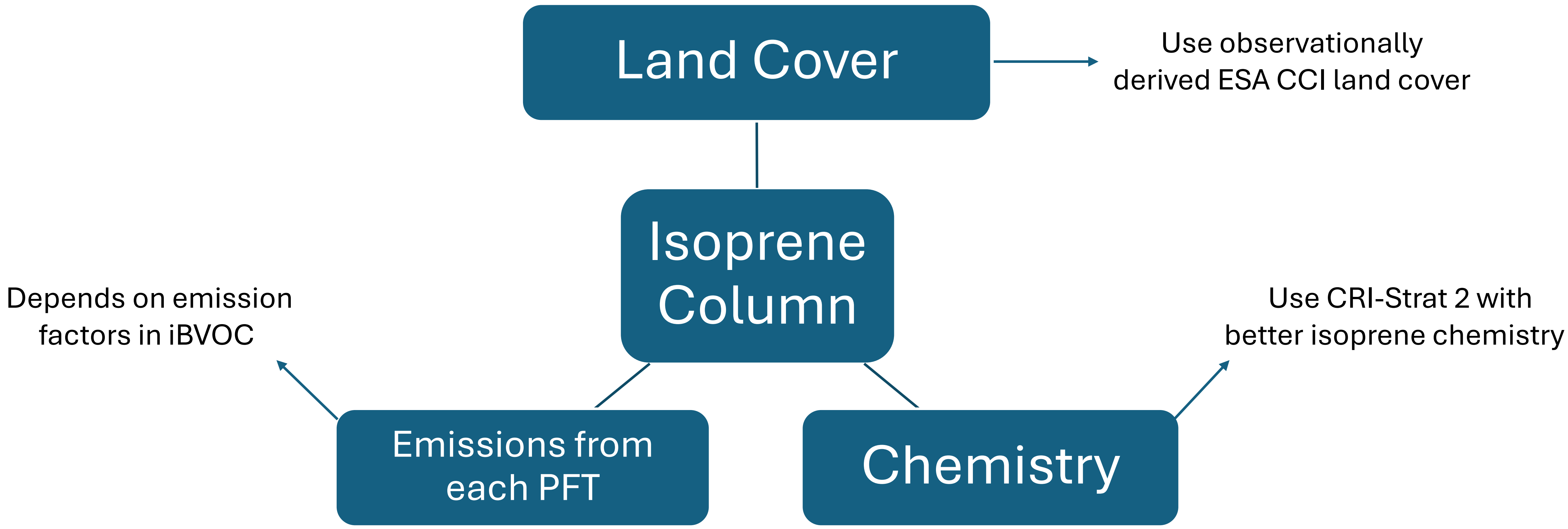


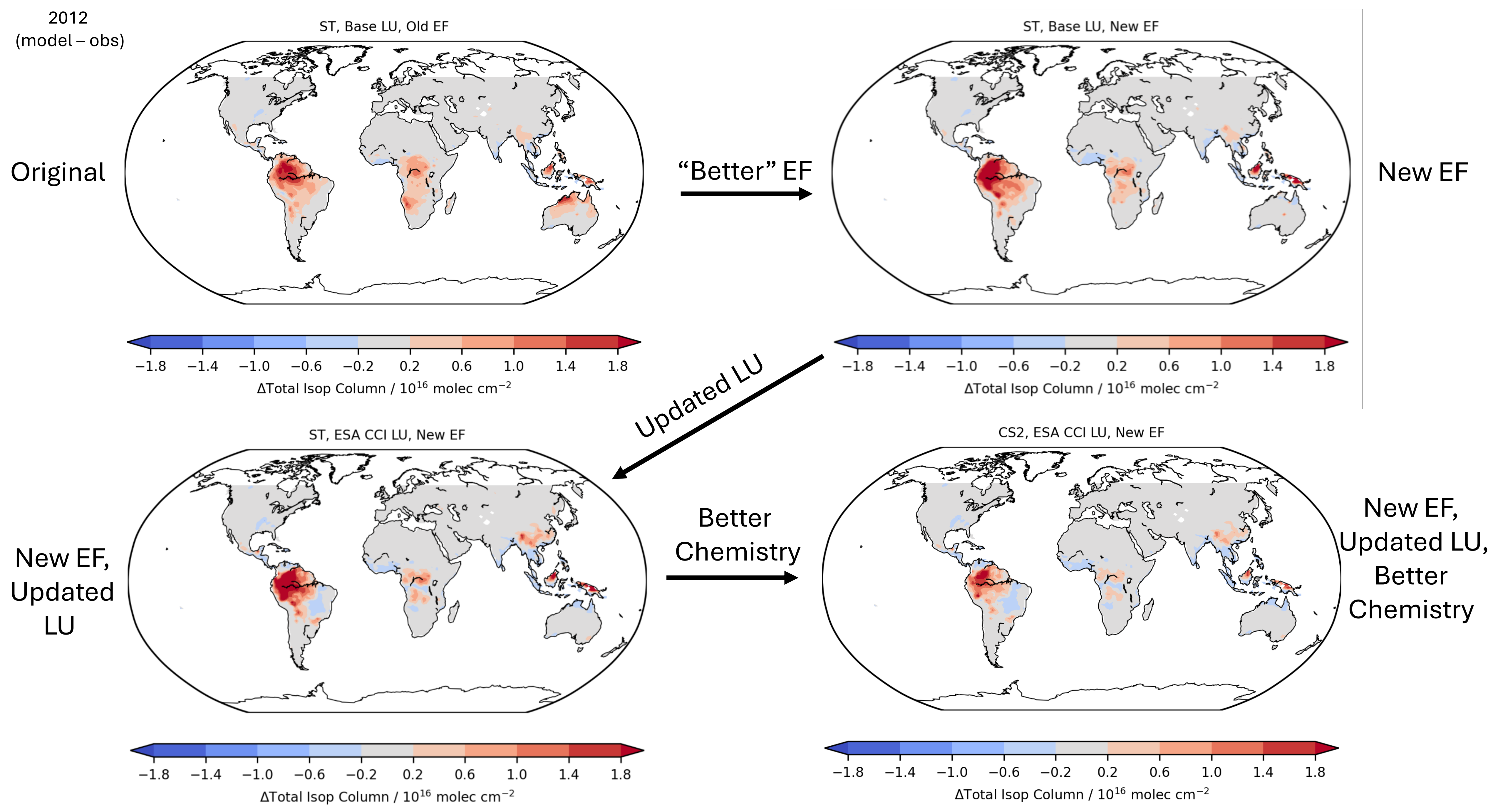
Emissions from each PFT

Chemistry

Land Cover

What is driving the bias?

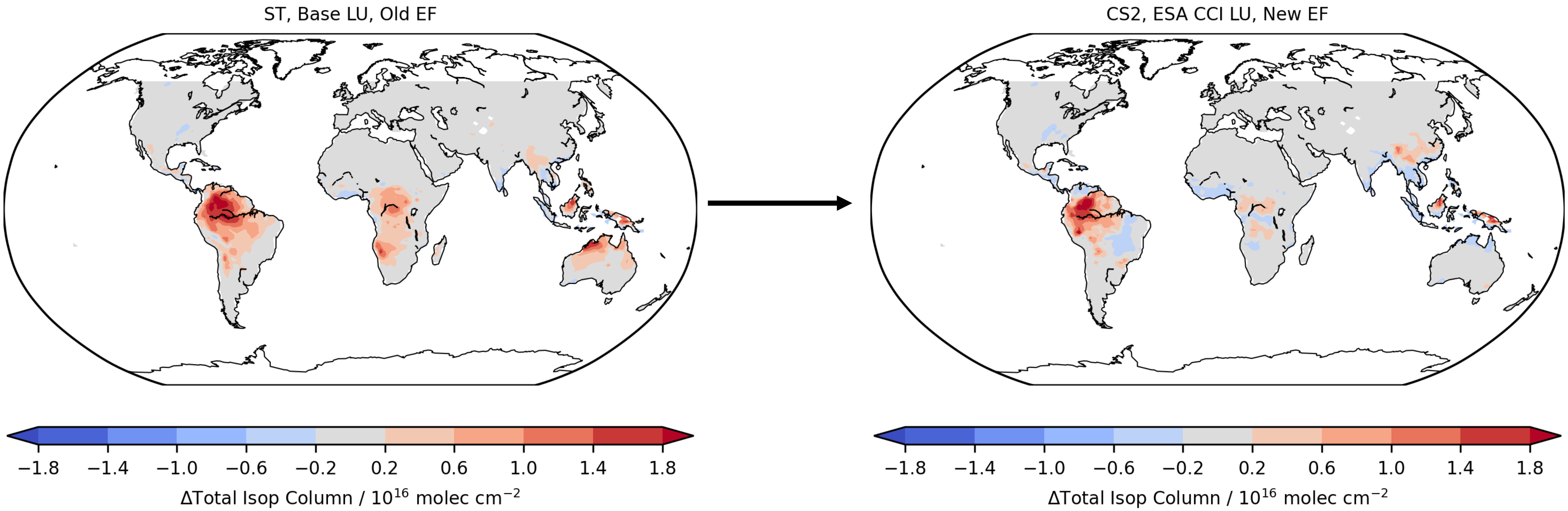


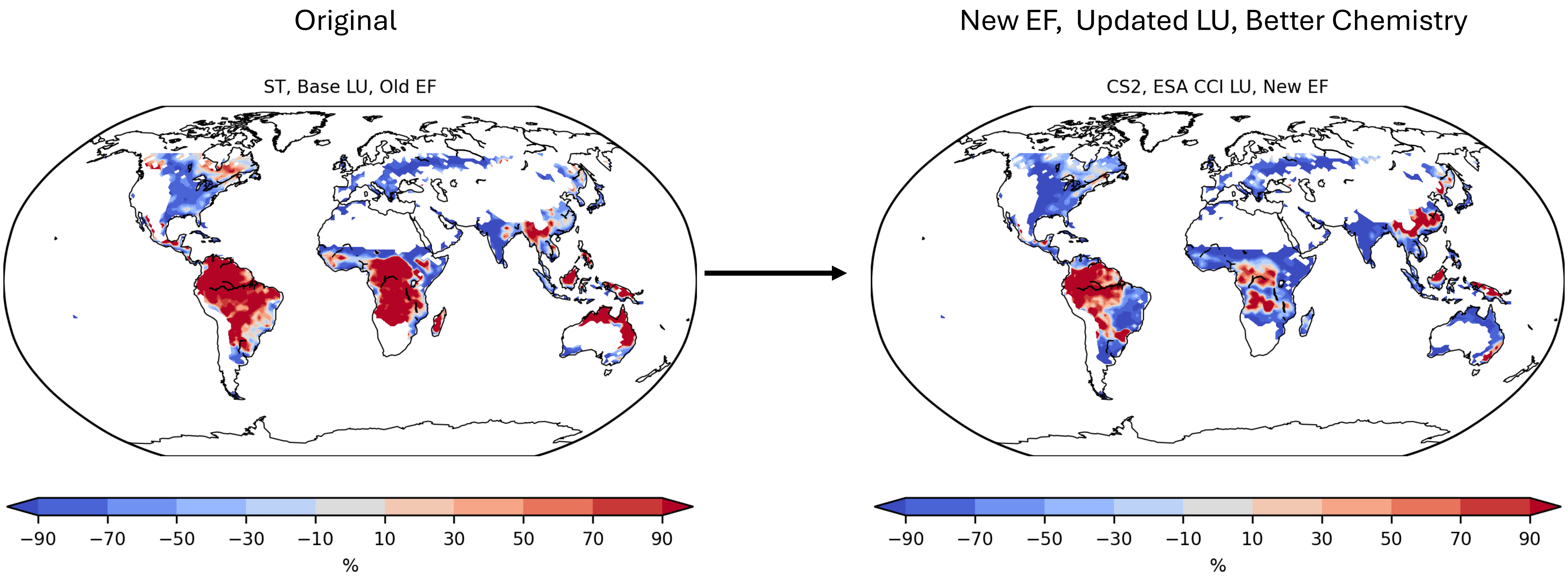


2012
(model – obs)
ST, Base LU, Old EF
Original
"Better" EF
ST, Base LU, New EF
New EF
ΔTotal Isop Column / 10^16 molec cm^−2
−1.8 −1.4 −1.0 −0.6 −0.2 0.2 0.6 1.0 1.4 1.8
Updated LU
ST, ESA CCI LU, New EF
New EF, Updated LU
Better Chemistry
CS2, ESA CCI LU, New EF
New EF, Updated LU, Better Chemistry

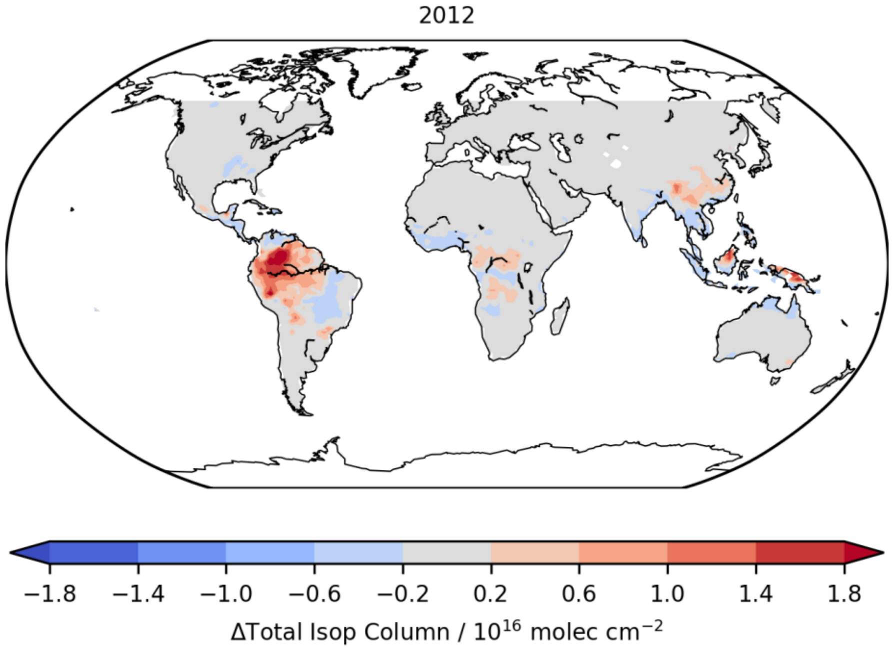
Original

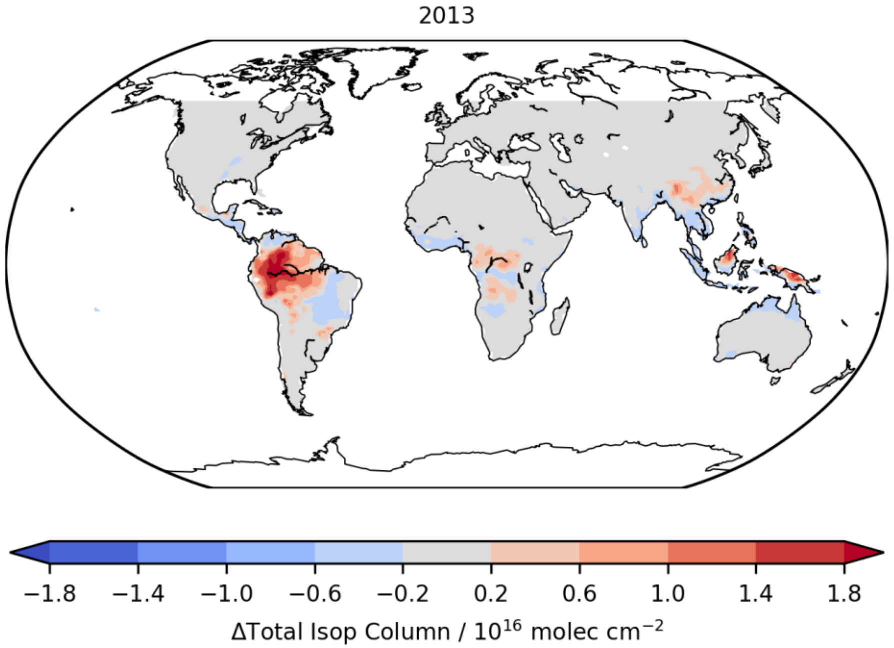
New EF, Updated LU, Better Chemistry

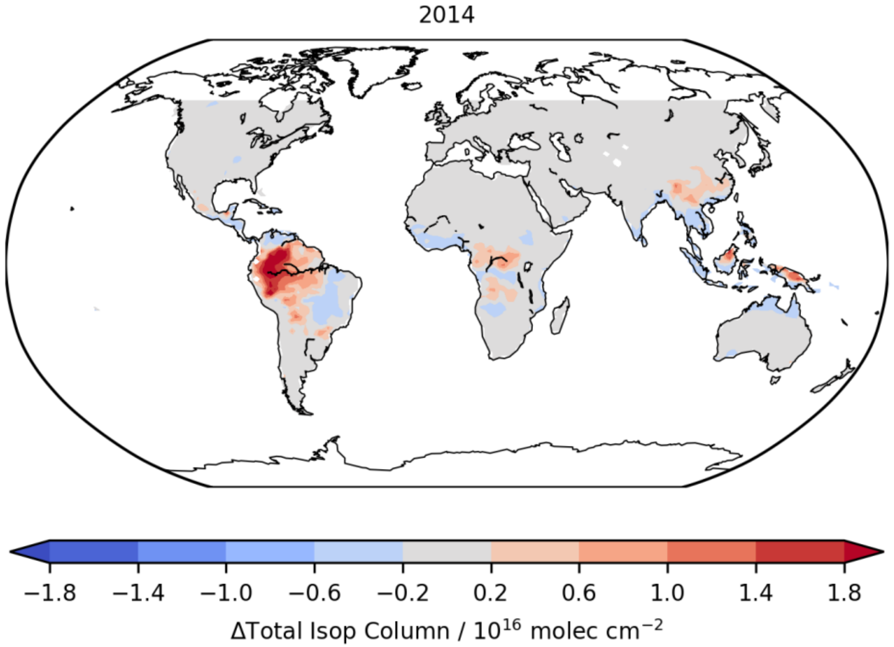



Original
New EF, Updated LU, Better Chemistry
ST, Base LU, Old EF
CS2, ESA CCI LU, New EF
−90 −70 −50 −30 −10 10 30 50 70 90
%
−90 −70 −50 −30 −10 10 30 50 70 90
%

New EF, Updated LU, Better Chemistry

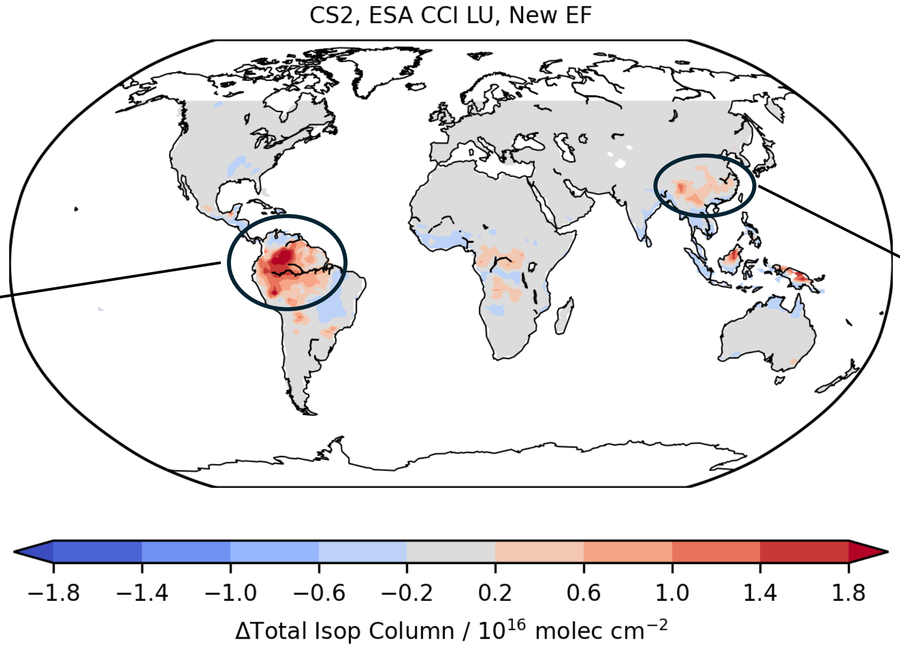






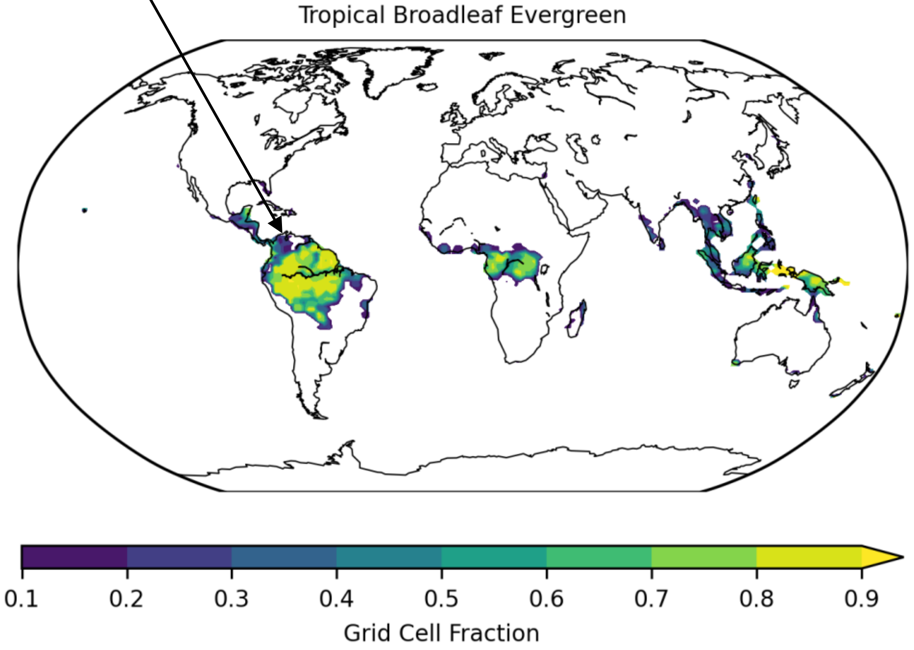
Still a lot of room for improvement!

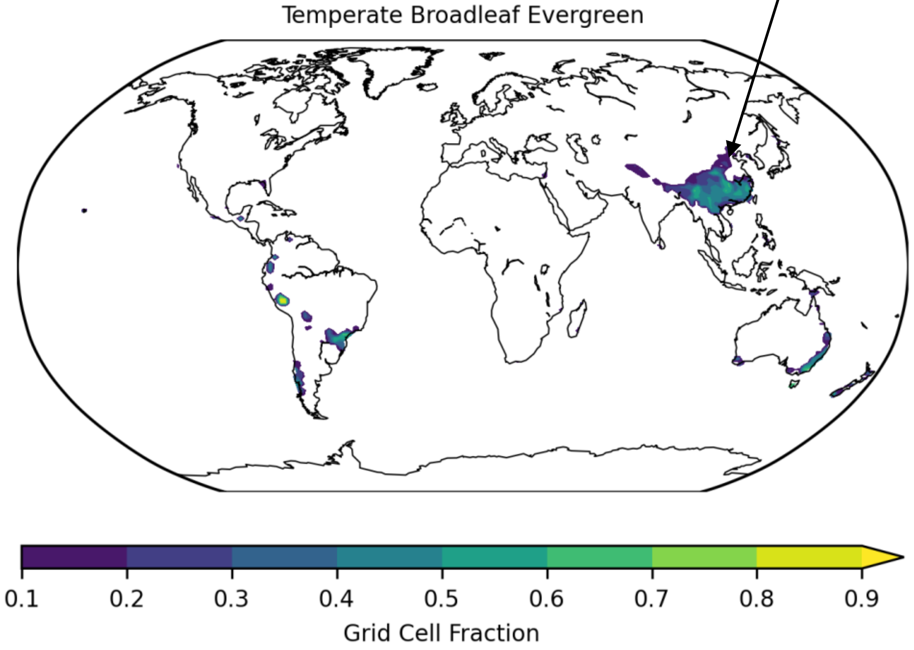
Brute Force / Educated Guess – adjust certain EF



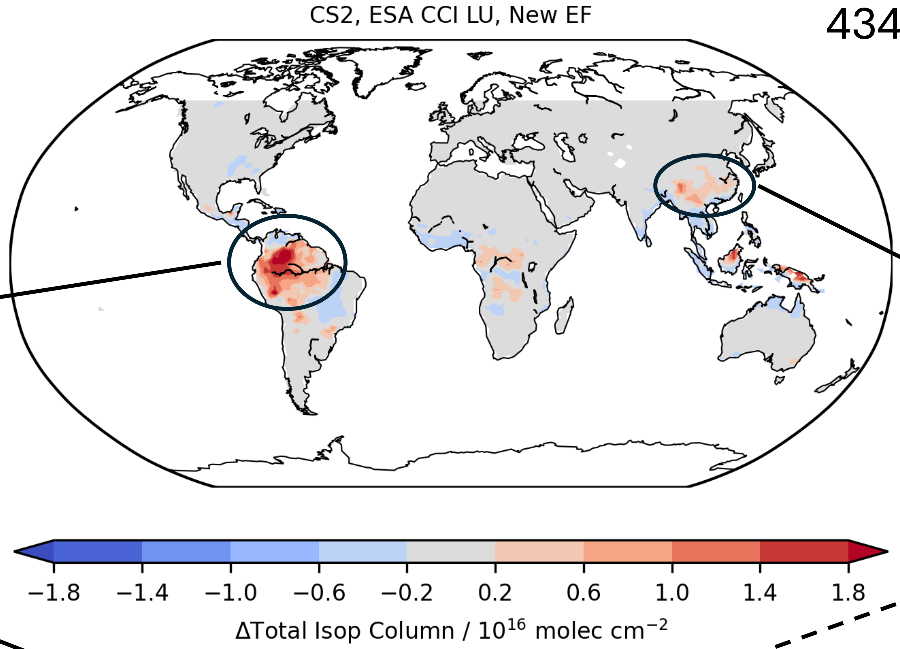
Focus on tropical evergreen broadleaf

Focus on temperate evergreen broadleaf





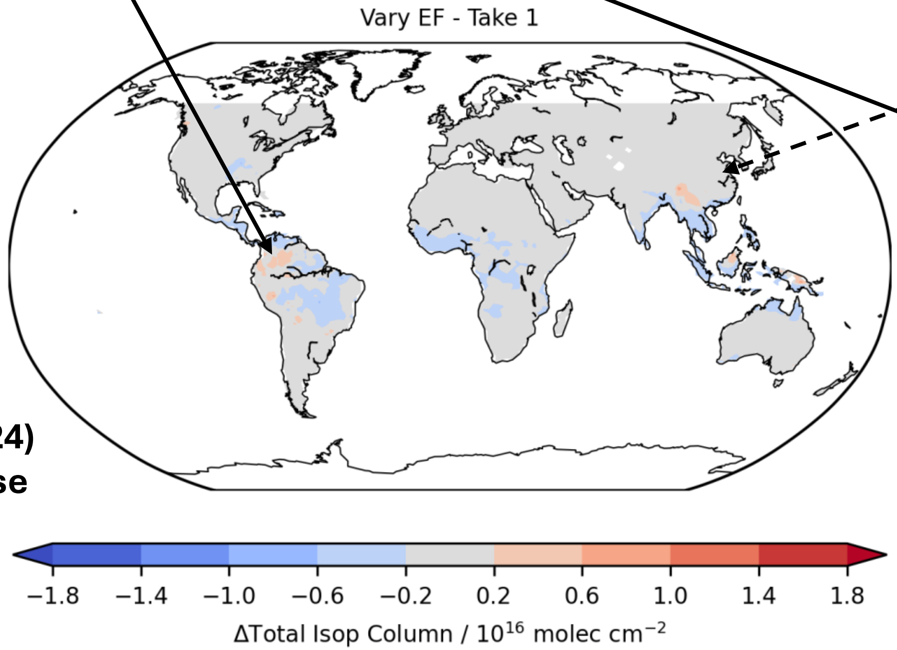
Brute Force / Educated Guess – adjust certain EF



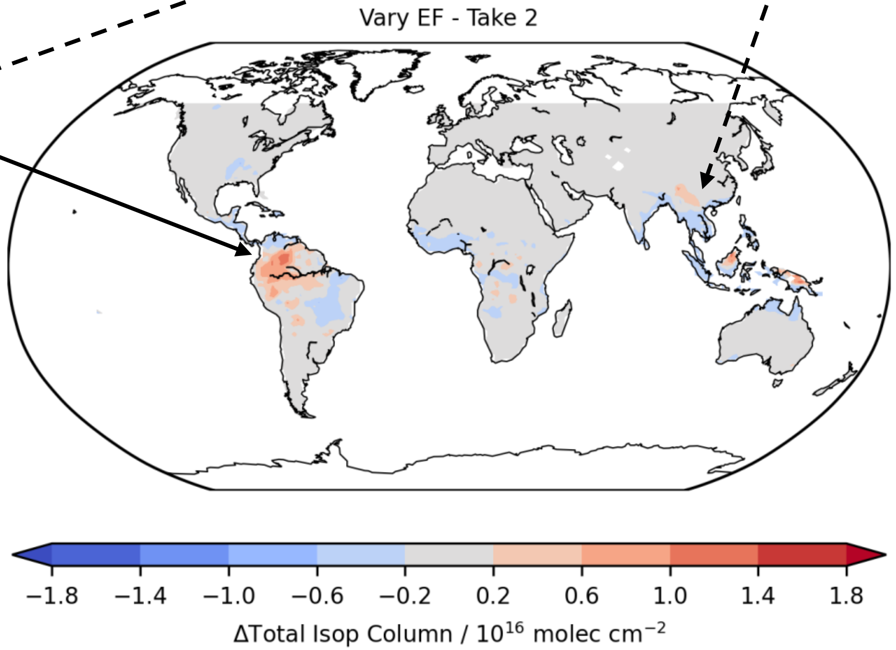
434 Tg yr^{-1}

Focus on tropical evergreen broadleaf

Focus on temperate evergreen broadleaf



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 CO_2 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.)

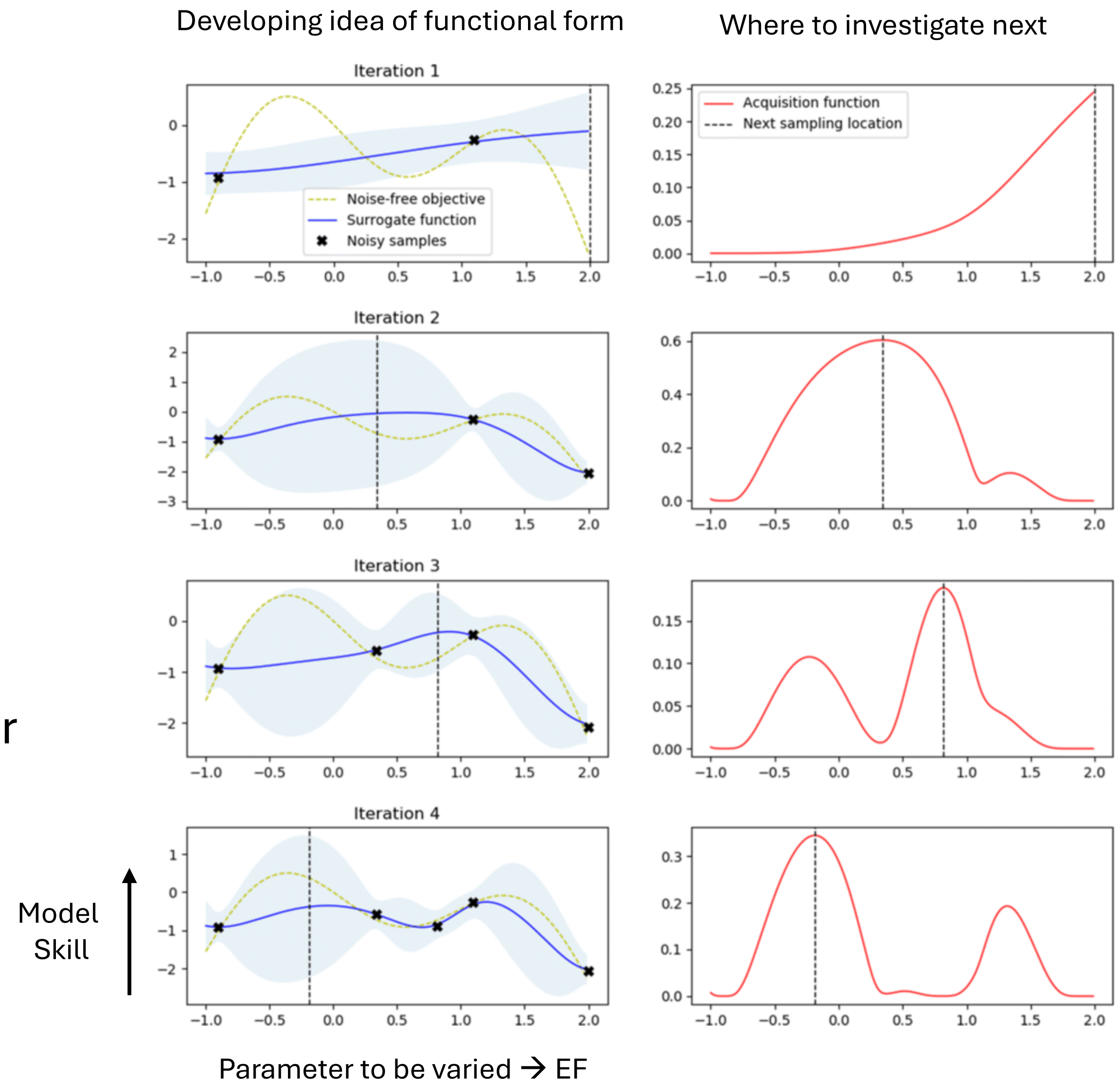
$$\mathrm{Column_i} = \underbrace{\sum_{\mathrm{PFT}} \alpha \mathrm{E_i}}_{\text{Emissions}} + \underbrace{\beta \mathrm{u_i} + \gamma \mathrm{v_i} + \delta \mathrm{w_i} + \cdots}_{\text{Meteorology}}$$

<u>If</u> the emulator can reproduce UKESM column values, changing PFT emission factors (→ emissions) could then be used to optimise model performance against observation → 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.



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!