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Evaluation of BVOC Emission parametrization against local flux observations.

Jhilik Majumdar and Vincent Huijnen

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Introduction

- Biogenic Volatile Organic Compounds (BVOCs) are non-methane hydrocarbons emitted by vegetation and soils, constituting roughly 90 % of the total atmospheric VOC budget. They are highly reactive, influencing tropospheric photochemistry, ozone formation, and secondary organic aerosol production.
- Emission rates are driven by environmental factors—primarily temperature, solar radiation, vegetation type, seasonal cycles, leaf age, and ambient CO_2 levels—that modulate enzymatic activity in plants.
- Recent advances now allow dynamic, daily-updated simulations of biogenic sources (e.g., CAMS global analyses) to be coupled with chemistry models, improving air-quality forecasting.
- The MEGAN-style online BVOC model integrates vegetation characteristics (Leaf Area Index, plant functional types) with activity factors (temperature response, light scaling, LAI, leaf age, CO_2 inhibition) to compute net isoprene emissions under variable meteorology.
- By combining a predetermined base emission factor with these multiplicative modifiers, the model yields a total emission estimate that reflects both canopy environment and seasonal dynamics.

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Isoperene Daily emission : model vs data.

- b20d: Uses standard surface fluxes for each land use category, serving as a baseline for comparison.

  b2ow: Incorporates offline emission potential fields (EPF) specifically for isoprene emissions, refining biogenic VOC estimates..

- Observed isoperene emissions from the data show a significantly higher peak emission rate compared to the modeled values, particularly during midday (around 12:00–15:00 UTC).
- The model underestimates the emission intensity during peak daylight hours.
- Modelled emissions closely follow the expected diurnal pattern, with near-zero values during nighttime and a clear peak during midday due to higher sunlight and temperature activity.
- The observed data suggests a higher emission peak that the model does not capture. This discrepancy might be due to underestimations in the input activity factors like leaf age, LAI, or light activity factors.

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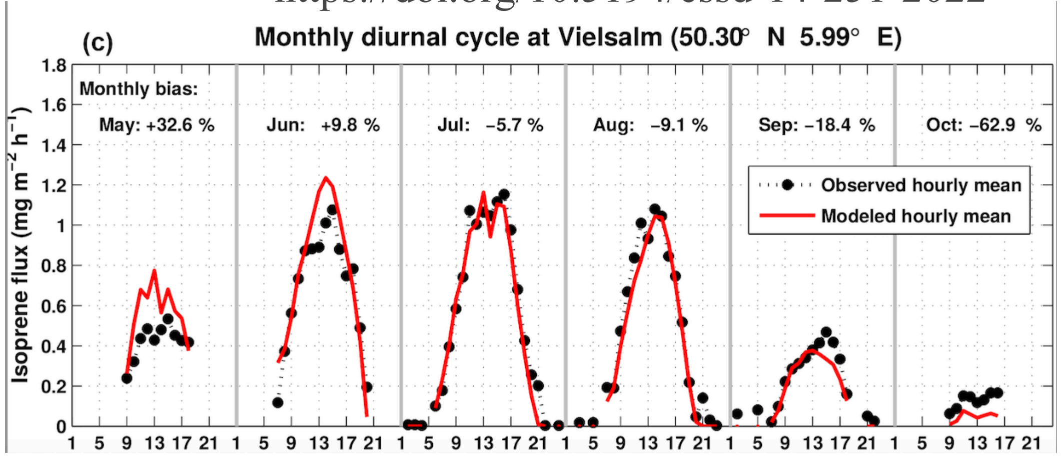
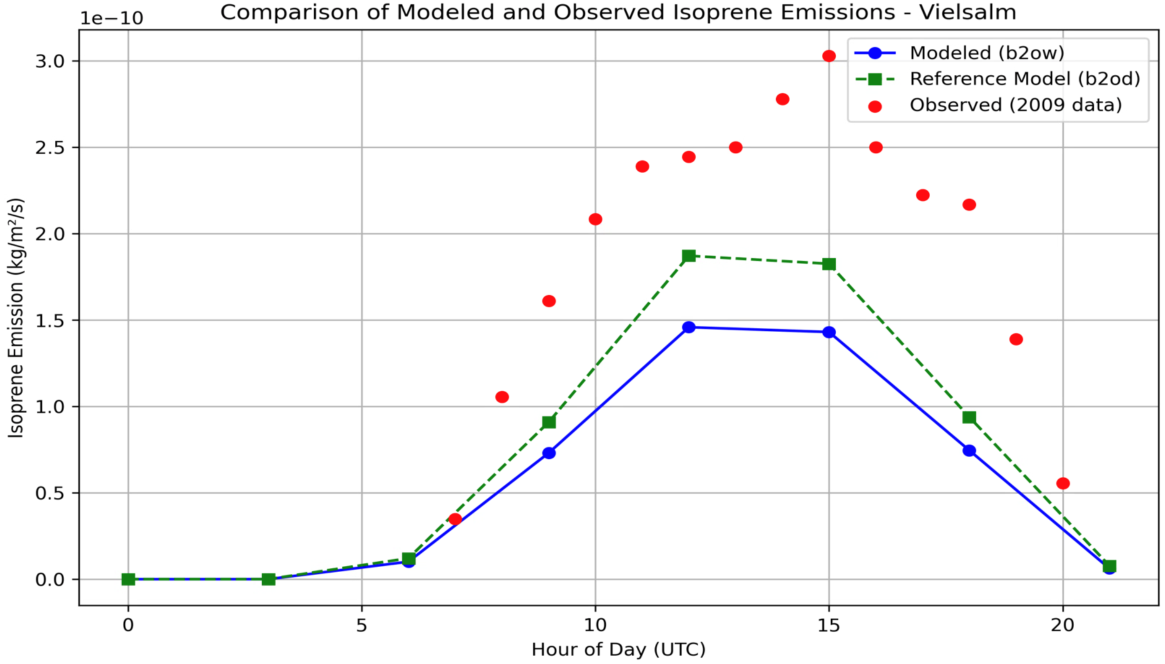




Offline box-model set up

Study Site: Vielsalm eddy-covariance tower (50.30 °N, 5.90 °E) in a temperate forest canopy of the Belgian Ardennes.

Well-Mixed Canopy Layer:

- Height varies hourly with ERA5 PBL: ~500 m at night → ~2000 m by midday.

Forcing (MEGAN v2.1 online):

- **LAI:** fixed at 3.0 $m^2\ m^{-2}$, **Temperatures:** soil = 290 K; skin = 295 K , **CO_2:** 410 ppm
- Emission potential : 2.88 $mgm^{-2}\ hr^{-1}$

Campaign: May 1 – Oct 1, 2009 & 2010
Flux Characteristics:

- **Observed Peak**: ≈ 5 mg $m^{-2}\ h^{-1}$ (daily mean)
- **Model Comparison** (H3, SEF = 2.88 mg $m^{-2}\ h^{-1}$):
- 2009 bias = –8.5 % (r = 0.92)
- 2010 bias = –1.0 % (r = 0.91)

Purpose:
Isolate the MEGAN emission formulation under controlled meteorology, chemistry, and transport for direct comparison to Vielsalm observations.

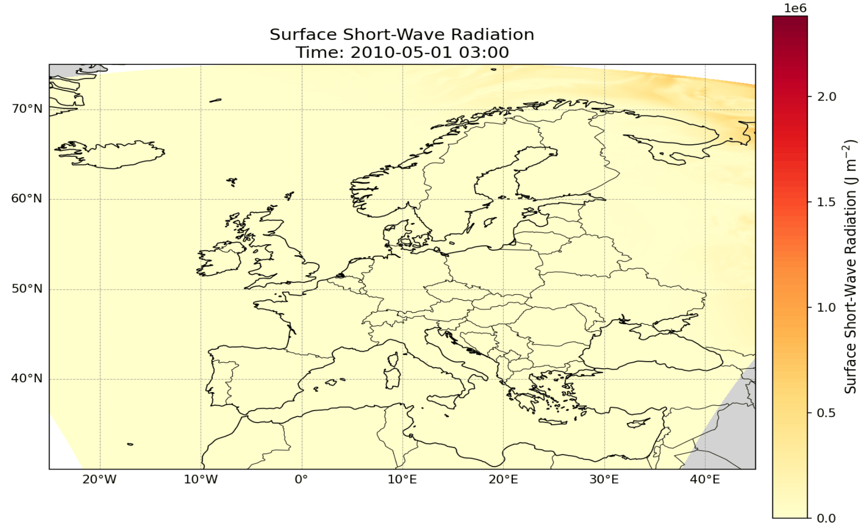
Observational and meteorological data

VOC Flux Observations

- **Instrument & File:** PTR-MS eddy-covariance flux (Flux_M69)
- **Units:** $\mu g\ m^{-2}\ s^{-1}$ → converted to $mg\ m^{-2}\ h^{-1}$
- **Time Info:** Local timestamp → extract hour, day, month for diurnal/seasonal analysis

Meteorological Forcing

- **Air Temperature:** 2 m $T_{2}m$ from ERA5
- **Radiation:** SSRD ($J\ m^{-2}$ per 3 h) → PPFD ($\mu mol\ m^{-2}\ s^{-1}$) via × 4.6 conversion
- **Boundary-Layer Dynamics:** Wind speed → ERA5 PBL height (500–2000 m) for entrainment



The observed surface-downward shortwave radiation across Europe from May through October 2010, highlighting the seasonal increase in solar input that drives isoprene emission variability.

Box model : detailed description

1. Base emission factor : 2.88 $mgm^{-2}h^{-1}$ **(Bauwens et al , 2018)**
2. Temperature response :

$$\gamma_T = \frac{Z_E\, Z_{C2}\, \exp\left(Z_{C1}\, X\right)}{Z_{C2} - Z_{C1}\left[1 - \exp\left(Z_{C2}\, X\right)\right]},$$

$$X = \frac{\frac{1}{T_{\text{opt}}} - \frac{1}{T_H}}{0.00831}, \quad Z_E = 1.75\, \exp\left(0.08\,(T_{\text{daily}} - 297\,\text{K})\right).$$

- $\mathbf{Z_E}$ is the activation-energy term that sets the maximum value of the γ_T curve.
- T_{opt} : optimum temperature where the emission gets its peak.
- z_{C1} and Z_{C2}: two parameters controls the γ_T slope.

3. Light (PPFD) Response:

$$\Phi' = \frac{\Phi}{3000}, \quad \gamma_P = \max\left(0,\ 2.46\,\Phi'\,[1 + 0.0005(\Phi_{\text{daily}} - 400)] - 0.9\,\Phi'^2\right)$$

- Φ' shows how bright it is now.
- Φ : PPFD at a given hour.
- Equation is derived so that if the day as a whole was especially sunny

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Box model

4. LAI response :

$$\gamma_{\text{LAI}} = 1 \times \frac{0.49\,\text{LAI}}{\sqrt{1 + 0.2\,\text{LAI}^2}} \quad (\text{for LAI} = 3.0)$$

5. CO2 inhibition:

$$\gamma_{CO_2} = 1.344 - \frac{1.344\,(0.7\,C_a)^{1.4614}}{585^{1.4614} + (0.7\,C_a)^{1.4614}}, \quad C_a = 410 \text{ ppm}$$

- CO_2 is very low, leaves produce isoprene at their “full” rate 1.344,
- Higher CO_2 → Less isoprene per leaf area.

6. Canopy emission factor :

$$\gamma_{CE} = \gamma_{LAI}\,\gamma_T \left[(1 - LDF) + \gamma_P\,LDF\right], \quad LDF = 1.0$$

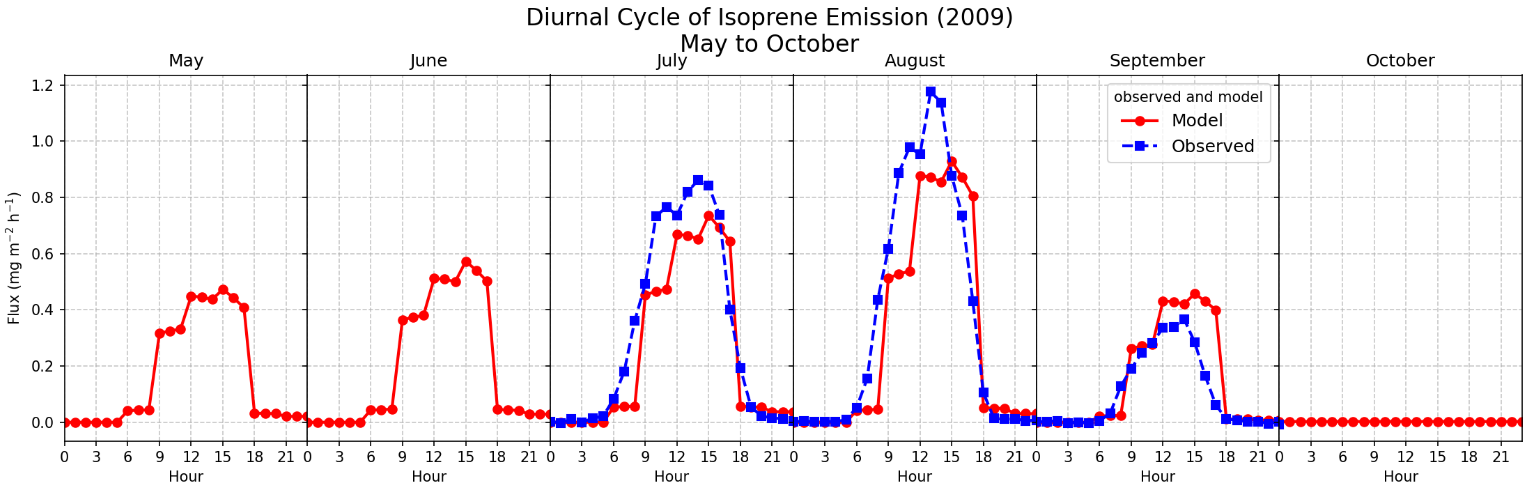
7. Final Flux :

$$\boxed{F = EF_0 \times \gamma_{CE} \times \gamma_{CO_2} \quad \left[\text{mg}\,\text{m}^{-2}\,\text{h}^{-1}\right]}$$

Diurnal Cycle of Isoprene Emissions : Model vs. Observations at Vielsalm

- Both model (red) and observations (blue) show near-zero night flux, rapid sunrise ramp, and afternoon decline.
- Morning ramp and fall-off timing are well captured across all months. Model underestimates peak midday flux by ~10–20 % in midsummer (July–August).

- Seasonal Trend:
  - Peak amplitude rises from May (~0.56 mg m^{-2} h^{-1}) to August (~1.18 mg m^{-2} h^{-1}), then declines into autumn.
  - Model follows the seasonal shape but with muted maxima.



Diurnal and Seasonal model-observation comaparison

Diurnal cycles (May–Oct):

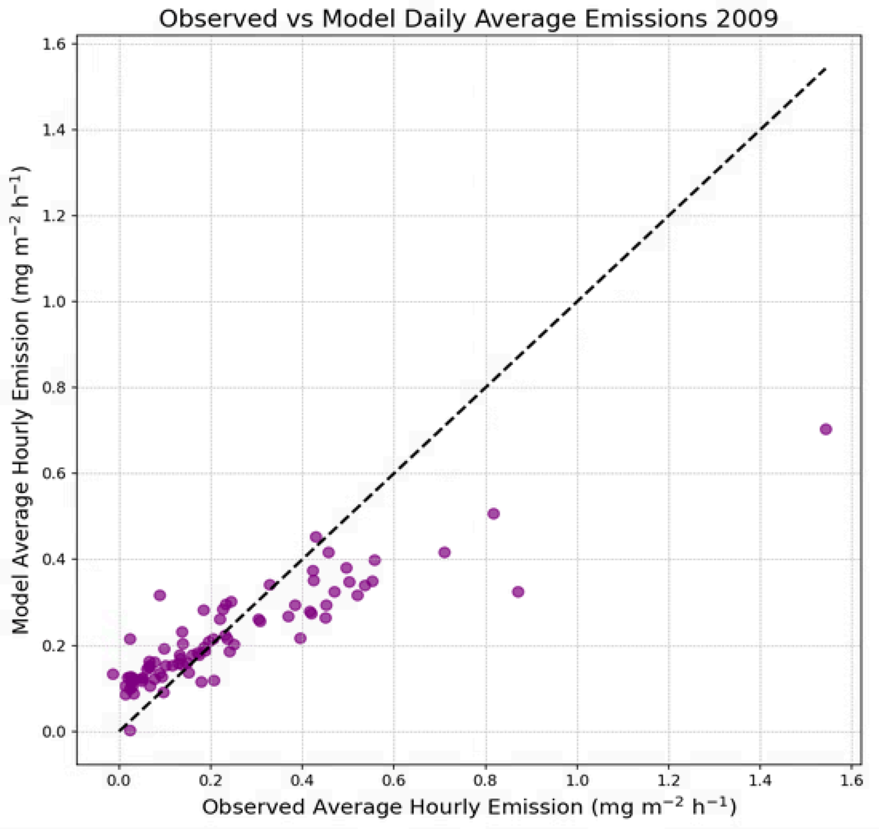
- Model captures sunrise ramp & afternoon decline
- Systematically underestimates midday peak by 10–15 % in midsummer

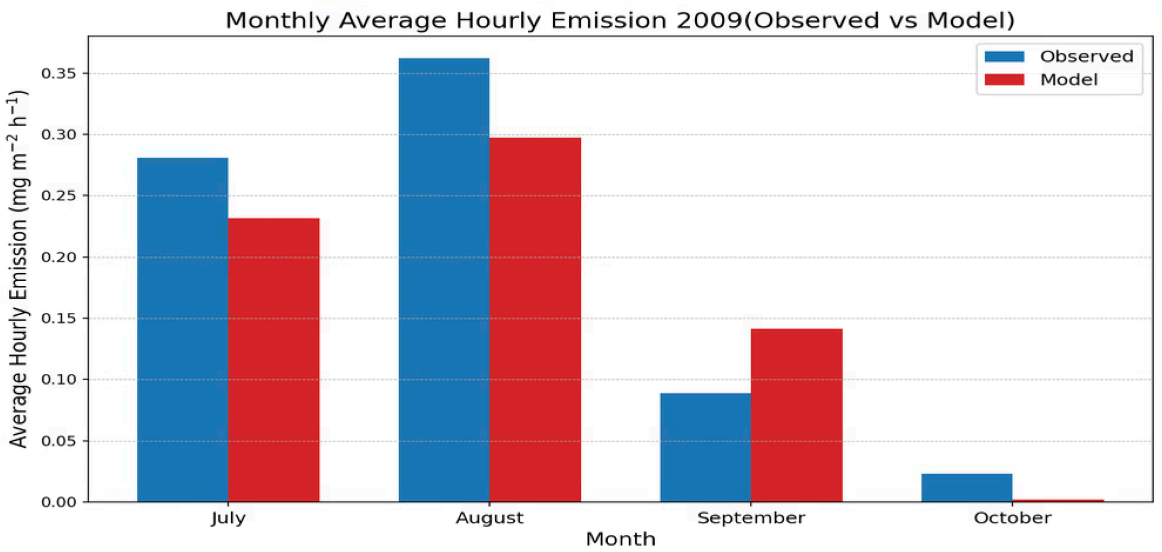
Daily-mean scatter :

- Generally linear (r≈0.9), but model underpredicts high-flux days

Monthly average hourly emissions :

- Seasonal decline from July (0.28 mg m^{-2} h^{-1} obs) to October (~0.02 mg m^{-2} h^{-1})
- Model follows trend but low by ~10–15 % in July/August





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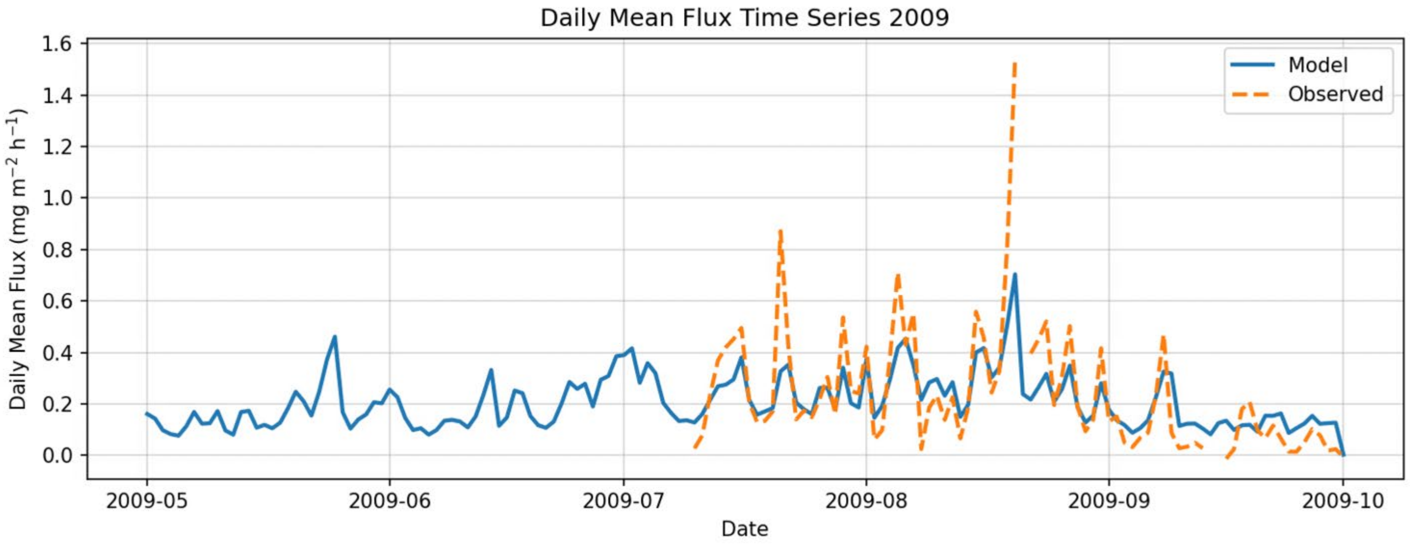
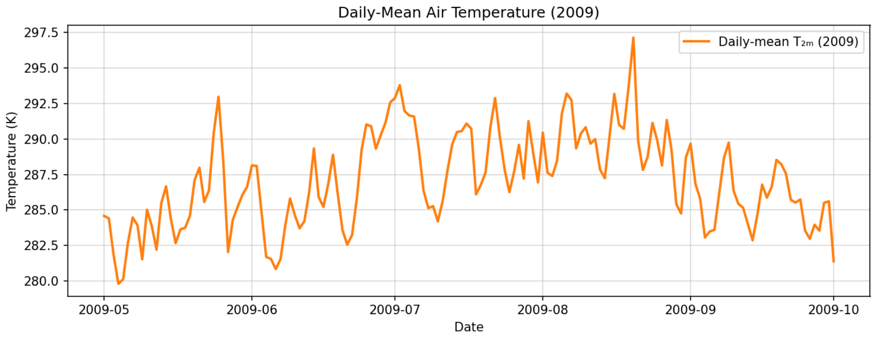
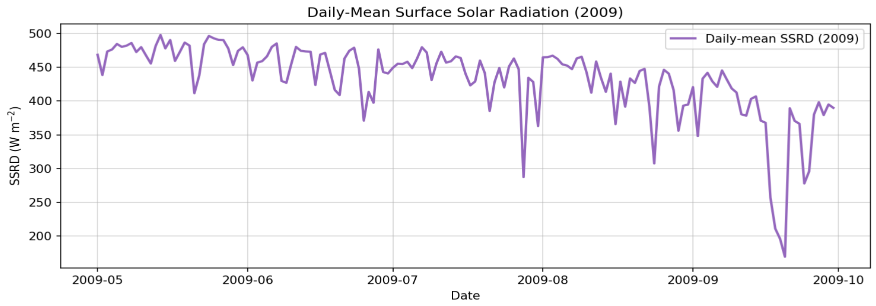
Daily Mean Flux Time Series (May–Oct 2009)

- **Synoptic Variability:** Model captures week-to-week trends and seasonal rise/fall.
- **High-Emission Events:** Observed spikes (e.g., late July, mid-August) exceed model peaks by up to ~0.8 mg m^{-2} h^{-1}.
- **Overall Bias:** Model slightly underestimates extreme flux days, though mean behavior is well represented ($r \approx 0.9$).
- **Data Note:** Observations from July onward; pre-July data pending integration.







Parameter tuning of γ_T

Midday peak misfit: The default temperature-response underestimates 12:00–15:00 UTC emissions.

Sensitivity control:
•$T_{opt,0}$ shifts the temperature at which emissions peak.
•α controls how sharply E_{opt} (the activation energy) grows with T_{opt}.

$$\gamma_T = \frac{E_{opt}\, C_2\, \exp(C_1 X)}{C_2 - C_1\left[1 - e^{C_2 X}\right]} \quad , \quad X = \frac{\frac{1}{T_{opt}} - \frac{1}{T_{air}}}{R_g}$$

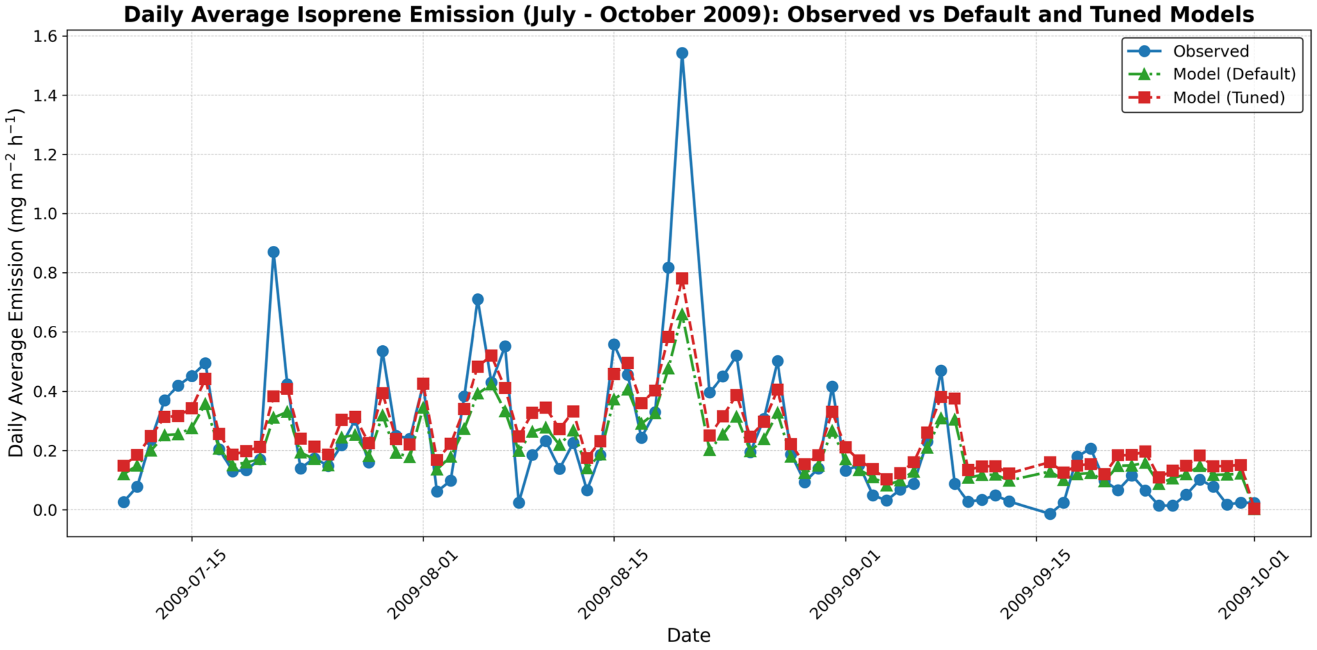
$$T_{opt} = T_{opt,0} + \beta\,(T_{air} - T_0) \quad , \quad E_{opt} = D_0\, \exp\left[\alpha\,(T_{opt} - T_0)\right]$$

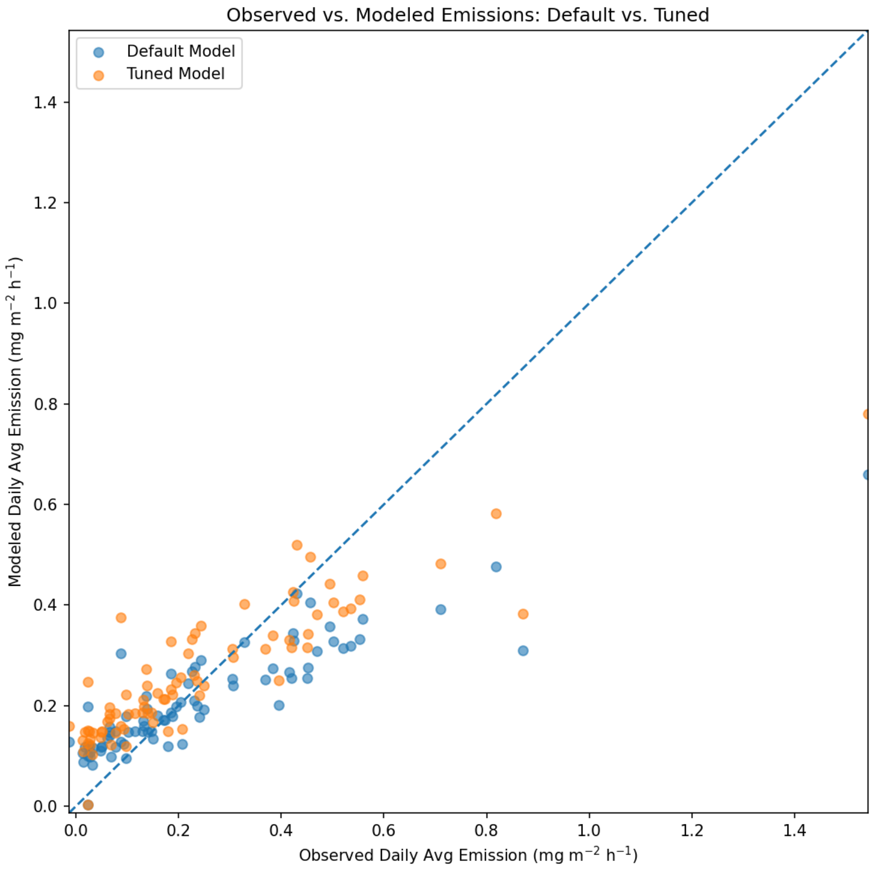
Which parameters were varied?
• $\mathbf{T_{opt,0}}$: 310 → 320 K (Δ = 1 K)
• **α** : 0.07 → 0.09 K^{-1} (Δ = 0.002 K^{-1})

Fit Metric :

$$\text{RMSE} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(F_{\text{model,i}} - F_{\text{obs,i}}\right)^2}$$

Parameter tuning of γ_T



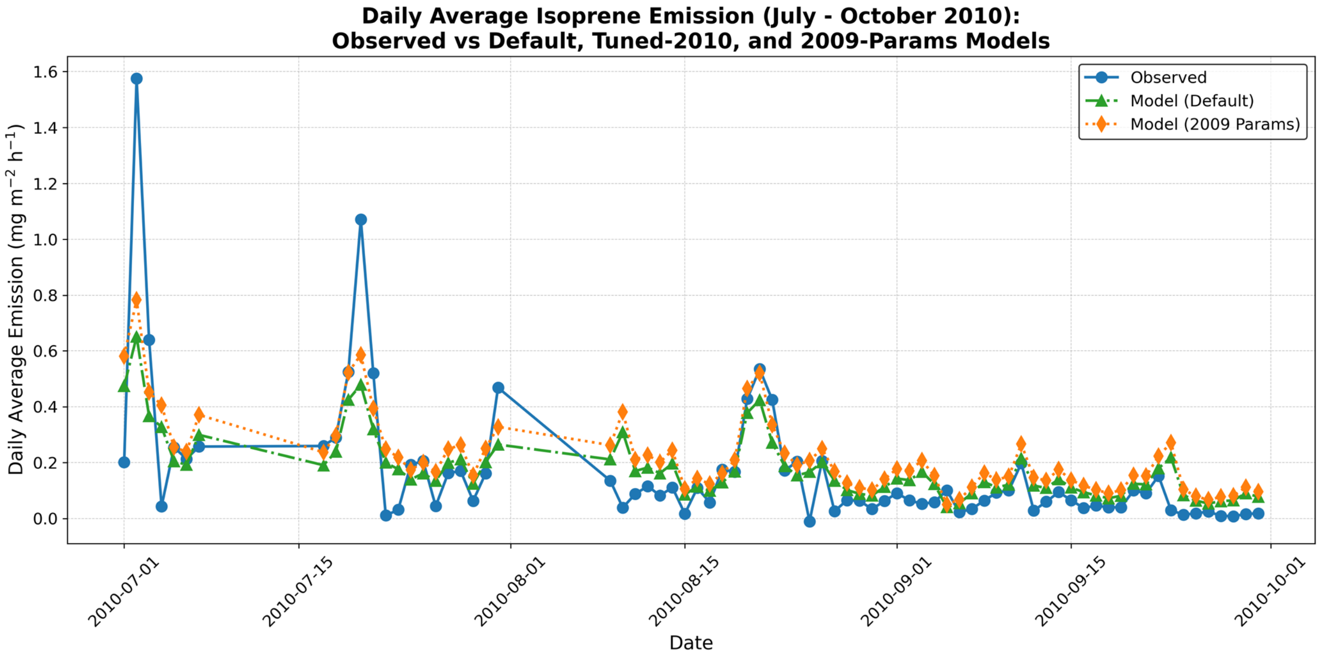


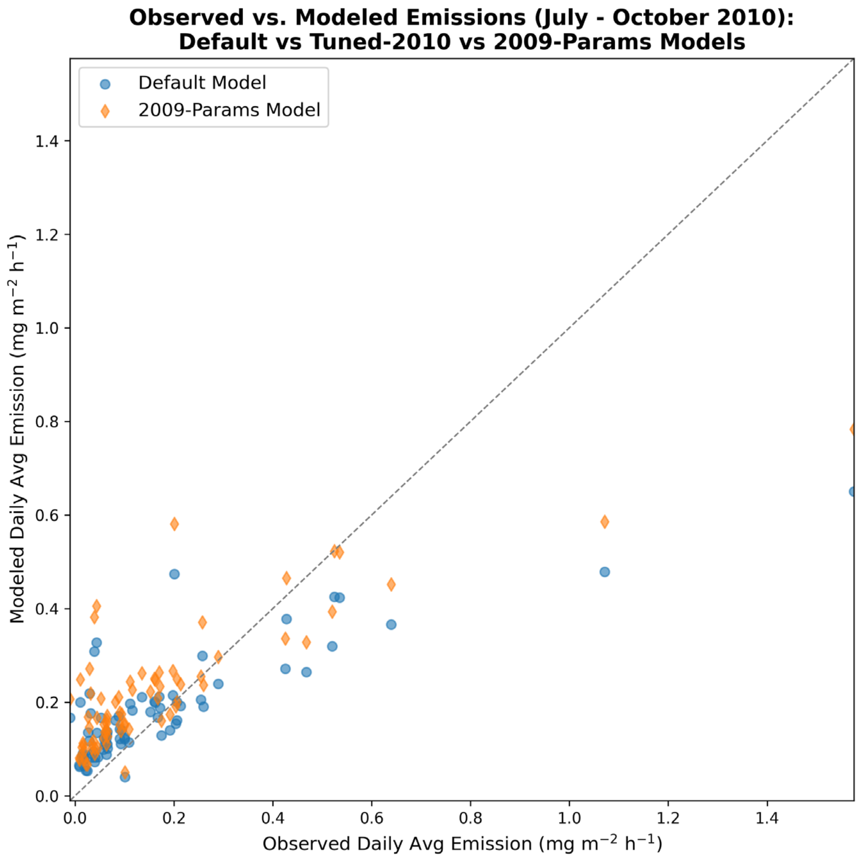
Best-fit parameters & performance

- $T_{opt,0}$=311.0 K
- α=0.07 K^{-1}
- **RMSE** = 0.143 mg m^{-2} h^{-1}

(~15% improvement over default)

Parameter tuning of γ_T





- Applying 2009 γ_t parameters to 2010 data captures mid-July/mid-August peaks more accurately than other runs.
- The 2009-parameter time series aligns closely with the highest observed days, showing how small T_{opt} and α shifts drive peak-day emissions.
- In the scatter plot, high-emission points using 2009 parameters lie nearest the 1:1 line, improving peak-day agreement without skewing lower-emission values.

Conclusion and Future Work

Conclusions

- The MEGAN framework reproduces the seasonal and diurnal timing of isoprene emissions ($r \approx 0.9$) but underestimates midsummer peak fluxes by ~15 %.
- Retuning the temperature response (γ_T) to T_{opt} = 311 K and α = 0.07 K^{-1} reduces daily-mean RMSE by ~15 % and more accurately captures high-emission days.
- The optimal γ_T parameters remained stable between 2009 and 2010, indicating a robust biochemical temperature response across varying meteorological conditions.

Future Work

- Integrate full-season flux data and hourly radiation, LAI, and soil/skin temperatures.
- Tune the γ_p (light-response) parameters—optimizing how the model scales isoprene emissions with varying solar radiation—to further enhance agreement between modeled and observed fluxes..
- Apply tuned γ_T in regional/global BVOC models to assess air-quality impacts.