

# p-pd\_optim

July 28, 2025

## 1 This notebook compares all populations to the ground truth data collected

```
[1646]: import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
import numpy as np
from sklearn.metrics import mean_squared_error, r2_score, \
    root_mean_squared_error, mean_absolute_percentage_error, \
    median_absolute_error, mean_absolute_error
from datetime import datetime
import os
from collections import defaultdict

from garisom_tools import GarisomModel
from garisom_tools.montecarlo.config import GarisomMonteCarloConfig
from garisom_tools.utils.metric import normalized_nash_sutcliffe_efficiency

[1647]: data = {
    "ccr": {
        "pop": 1,
        "ground": {
            "hourly": "data/ground/ccr_hourly_data.csv",
            "leaf": "data/ground/ccr_leaftemp.csv",
            "stderr": "data/ground/ccr_std_error.csv",
            "gw_treatment_averages": "data/ground/ccr_gw_treatment_averages_pm.
↪csv",
            "leaf_treatment_averages": "data/ground/
↪ccr_leaftemp_treatment_averages_pm.csv",
            "leaf-air_treatment_averages": "data/ground/
↪ccr_leaf-air_treatment_averages_pm.csv"
        },
        "pred": {
            "GW": {
                "low": "montecarlo/output/ccr/gw/20250728_111938/ci_low.csv",
                "high": "montecarlo/output/ccr/gw/20250728_111938/ci_high.csv",
                "main": "montecarlo/output/ccr/gw/20250728_111938/config.json",
```

```

    },
    "leaftemp": {
        "low": "montecarlo/output/ccr/leaftemp/20250728_111936/ci_low.
↪CSV",
        "high": "montecarlo/output/ccr/leaftemp/20250728_111936/ci_high.
↪CSV",
        "main": "montecarlo/output/ccr/leaftemp/20250728_111936/config.
↪json",
    },
    "P-PD": {
        "low": "montecarlo/output/ccr/pd/20250728_115558/ci_low.csv",
        "high": "montecarlo/output/ccr/pd/20250728_115558/ci_high.csv",
        "main": "montecarlo/output/ccr/pd/20250728_115558/config.json",
    },
    "P-MD": {
        "low": "montecarlo/output/ccr/md/20250728_115833/ci_low.csv",
        "high": "montecarlo/output/ccr/md/20250728_115833/ci_high.csv",
        "main": "montecarlo/output/ccr/md/20250728_115833/config.json",
    },
    }
},
"nrv": {
    "pop": 3,
    "ground": {
        "hourly": "data/ground/nrv_hourly_data.csv",
        "leaft": "data/ground/nrv_leaftemp.csv",
        "stderr": "data/ground/nrv_std_error.csv",
        "gw_treatment_averages": "data/ground/nrv_gw_treatment_averages_pm.
↪CSV",
        "leaft_treatment_averages": "data/ground/
↪nrv_leaftemp_treatment_averages_pm.csv",
        "leaf-air_treatment_averages": "data/ground/
↪nrv_leaf-air_treatment_averages_pm.csv"
    },
    "pred": {
        "GW": {
            "low": "montecarlo/output/nrv/gw/20250728_133549/ci_low.csv",
            "high": "montecarlo/output/nrv/gw/20250728_133549/ci_high.csv",
            "main": "montecarlo/output/nrv/gw/20250728_133549/config.json",
        },
        "leaftemp": {
            "low": "montecarlo/output/nrv/leaftemp/20250728_140103/ci_low.
↪CSV",
            "high": "montecarlo/output/nrv/leaftemp/20250728_140103/ci_high.
↪CSV",

```

```

        "main": "montecarlo/output/nrv/leaftemp/20250728_140103/config.
↪json",
    },
    "P-PD": {
        "low": "montecarlo/output/nrv/pd/20250728_141320/ci_low.csv",
        "high": "montecarlo/output/nrv/pd/20250728_141320/ci_high.csv",
        "main": "montecarlo/output/nrv/pd/20250728_141320/config.json",
    },
    "P-MD": {
        "low": "montecarlo/output/nrv/md/20250728_144204/ci_low.csv",
        "high": "montecarlo/output/nrv/md/20250728_144204/ci_high.csv",
        "main": "montecarlo/output/nrv/md/20250728_144204/config.json",
    },
    },
    },
    "tsz": {
        "pop": 4,
        "ground": {
            "hourly": "data/ground/tsz_hourly_data.csv",
            "leaft": "data/ground/tsz_leaftemp.csv",
            "stderr": "data/ground/tsz_std_error.csv",
            "gw_treatment_averages": "data/ground/tsz_gw_treatment_averages_pm.
↪csv",
            "leaft_treatment_averages": "data/ground/
↪tsz_leaftemp_treatment_averages_pm.csv",
            "leaf-air_treatment_averages": "data/ground/
↪tsz_leaf-air_treatment_averages_pm.csv"
        },
        "pred": {
            "GW": {
                "low": "montecarlo/output/tsz/gw/20250728_144831/ci_low.csv",
                "high": "montecarlo/output/tsz/gw/20250728_144831/ci_high.csv",
                "main": "montecarlo/output/tsz/gw/20250728_144831/config.json",
            },
            "leaftemp": {
                "low": "montecarlo/output/tsz/leaftemp/20250728_152453/ci_low.
↪csv",
                "high": "montecarlo/output/tsz/leaftemp/20250728_152453/ci_high.
↪csv",
                "main": "montecarlo/output/tsz/leaftemp/20250728_152453/config.
↪json",
            },
        },
        "P-PD": {
            "low": "montecarlo/output/tsz/pd/20250728_152530/ci_low.csv",
            "high": "montecarlo/output/tsz/pd/20250728_152530/ci_high.csv",
            "main": "montecarlo/output/tsz/pd/20250728_152530/config.json",
        },
    },

```

```

    },
    "P-MD": {
      "low": "montecarlo/output/tsz/md/20250728_160227/ci_low.csv",
      "high": "montecarlo/output/tsz/md/20250728_160227/ci_high.csv",
      "main": "montecarlo/output/tsz/md/20250728_160227/config.json",
    },
  },
  "jla": {
    "pop": 2,
    "ground": {
      "hourly": "data/ground/jla_hourly_data.csv",
      "left": "data/ground/jla_leftemp.csv",
      "stderr": "data/ground/jla_std_error.csv",
      "gw_treatment_averages": "data/ground/jla_gw_treatment_averages_pm.
↪csv",
      "left_treatment_averages": "data/ground/
↪jla_leftemp_treatment_averages_pm.csv",
      "leaf-air_treatment_averages": "data/ground/
↪jla_leaf-air_treatment_averages_pm.csv"
    },
    "pred": {
      "GW": {
        "low": "montecarlo/output/jla/gw/20250728_122802/ci_low.csv",
        "high": "montecarlo/output/jla/gw/20250728_122802/ci_high.csv",
        "main": "montecarlo/output/jla/gw/20250728_122802/config.json",
      },
      "leftemp": {
        "low": "montecarlo/output/jla/leftemp/20250728_123033/ci_low.
↪csv",
        "high": "montecarlo/output/jla/leftemp/20250728_123033/ci_high.
↪csv",
        "main": "montecarlo/output/jla/leftemp/20250728_123033/config.
↪json",
      },
    },
    "P-PD": {
      "low": "montecarlo/output/jla/pd/20250728_130549/ci_low.csv",
      "high": "montecarlo/output/jla/pd/20250728_130549/ci_high.csv",
      "main": "montecarlo/output/jla/pd/20250728_130549/config.json",
    },
    "P-MD": {
      "low": "montecarlo/output/jla/md/20250728_131702/ci_low.csv",
      "high": "montecarlo/output/jla/md/20250728_131702/ci_high.csv",
      "main": "montecarlo/output/jla/md/20250728_131702/config.json",
    },
  },
}

```

```

    },
}

```

```

[1648]: def get_output_from_space_parallel(pop: int, results_files: list[str], params,
      ↪model_dir, config_file) -> list[pd.DataFrame | None]:

    Xs = []

    for result in results_files:
        config = GarisomMonteCarloConfig.from_json(result)
        Xs.append(config.parameters)

    outputs = GarisomModel.run_parallel(
        X=Xs,
        params=params,
        population=pop,
        config_file=config_file,
        model_dir=model_dir,
        workers=12
    )

    return outputs

```

```

[1649]: def get_output_from_space(pop: int, result: str, params, model_dir,
      ↪config_file) -> pd.DataFrame | None:

    config = GarisomMonteCarloConfig.from_json(result)

    outputs = GarisomModel.run(
        X=config.parameters,
        params=params,
        population=pop,
        config_file=config_file,
        model_dir=model_dir,
    )

    return outputs

```

```

[1650]: params = pd.read_csv("./DBG/parameters.csv")
model_dir = './garisom/02_program_code'
config_file = os.path.abspath("./DBG/configuration.csv")

```

```

[1651]: for pop in data.keys():
    num = data[pop]["pop"]
    for grd in data[pop]["ground"].keys():
        data[pop]["ground"][grd] = pd.read_csv(data[pop]["ground"][grd])

```

```

main_res = []
for var in data[pop]["pred"].keys():
    for prd in data[pop]["pred"][var].keys():
        if prd == "main" and data[pop]["pred"][var][prd]:
            main_res.append(data[pop]["pred"][var][prd]) # Get main result
↪file to run batch
            # data[pop]["pred"][var][prd] = get_output_from_space(
            #     num,
            #     data[pop]["pred"][var][prd],
            #     params,
            #     model_dir,
            #     config_file
            # )
        elif data[pop]["pred"][var][prd]:
            data[pop]["pred"][var][prd] = pd.
↪read_csv(data[pop]["pred"][var][prd])

main_out = get_output_from_space_parallel(
    num,
    main_res,
    params,
    model_dir,
    config_file
)

for i, var in enumerate(data[pop]["pred"].keys()):
    for prd in data[pop]["pred"][var].keys():
        if prd == "main" and data[pop]["pred"][var][prd]:
            data[pop]["pred"][var][prd] = main_out[i] # Take batched
↪output and add accordingly

```

```

100%|      | 4/4 [00:04<00:00,  1.08s/it]
100%|      | 4/4 [00:04<00:00,  1.14s/it]
100%|      | 4/4 [00:04<00:00,  1.17s/it]
100%|      | 4/4 [00:04<00:00,  1.21s/it]

```

```
[2073]: optim_var="P-PD" # GW/leaftemp/P-PD/P-MD
```

## 1.1 Metrics across populations

```

[2074]: def cmp_pred_to_ground_metrics(columns, ground, pred, start, end, show=True):

    fit = {}

    for col in columns:

```

```

col_ground = ground[ground['julian-day'].between(start, end)][col].
↳dropna()
col_pred = pred[col]

col_pred = col_pred.loc[col_ground.index]

mse = mean_squared_error(col_ground, col_pred)
rmse = root_mean_squared_error(col_ground, col_pred)
mape = mean_absolute_percentage_error(col_ground, col_pred)
made = median_absolute_error(col_ground, col_pred)
mae = mean_absolute_error(col_ground, col_pred)
r2 = r2_score(col_ground, col_pred)
r2 = 0 if r2 < 0 else r2
nnse = normalized_nash_sutcliffe_efficiency(col_ground, col_pred)

fit[col] = {
    'mse' : mse,
    'rmse' : rmse,
    'mape' : mape,
    'made' : made,
    'mae' : mae,
    'r2' : r2,
    'nnse' : nnse
}

if show:

    # Plot ground vs pred with fitted line and 1:1 correspondence
    plt.figure(figsize=(8, 6))
    plt.scatter(col_ground, col_pred, label='Data Points', alpha=0.7)
    plt.plot([col_ground.min(), col_ground.max()], [col_ground.min(),
↳col_ground.max()], 'r--', label='1:1 Line')

    # Fit a line to the data
    fit_coeff = np.polyfit(col_ground, col_pred, 1)
    fit_line = np.poly1d(fit_coeff)
    plt.plot(col_ground, fit_line(col_ground), 'b-', label=f'Fitted_
↳Line: y={fit_coeff[0]:.2f}x+{fit_coeff[1]:.2f}')

    # Add metrics as text
    plt.text(0.05, 0.95, ''.join([f'{key}: {value:.2f}\n' for key,
↳value in fit[col].items()])),
        transform=plt.gca().transAxes, fontsize=10,
↳verticalalignment='top')

    plt.xlabel('Ground')
    plt.ylabel('Prediction')

```

```

plt.title(f'Ground vs Prediction: {col}')
plt.legend()
plt.grid(True)
plt.show()

return fit

```

```

[2075]: def get_overlap_perc(columns, ground, ground_stderr, pred_low, pred_high,
    ↪ start, end):

    fit = {}

    for col in columns:

        col_ground = ground[ground['julian-day'].between(start, end)][col].
    ↪ dropna()
        col_ground_stderr = ground_stderr[col].loc[col_ground.index]
        col_ground_low = col_ground - 1.96 * col_ground_stderr
        col_ground_high = col_ground + 1.96 * col_ground_stderr

        col_pred_low = pred_low[col]
        col_pred_low = col_pred_low.loc[col_ground.index]
        col_pred_high = pred_high[col]
        col_pred_high = col_pred_high.loc[col_ground.index]

        # Compute overlap: intervals [col_ground_low, col_ground_high] and
    ↪ [col_pred_low, col_pred_high]
        overlap_count = 0
        total = len(col_ground)
        for i in range(total):
            g_low = col_ground_low.iloc[i]
            g_high = col_ground_high.iloc[i]
            p_low = col_pred_low.iloc[i]
            p_high = col_pred_high.iloc[i]
            # Check if intervals overlap
            if (g_low <= p_high) and (p_low <= g_high):
                overlap_count += 1
        overlap_perc = overlap_count / total if total > 0 else np.nan

        fit[col] = overlap_perc

    return fit

```

```

[2076]: columns = ['P-PD', 'P-MD', 'GW', 'E-MD', 'leaftemp']
start_day = 201

```

```

stress_begin = 223
predrought_cutoff = 238
drought = 240          # drought measurement period, collected 3 days after
    ↪ initial drought began
post_drought = 242
leaft_data_start = 205
end_day = 266

```

```

[2077]: all_fits = {}
for pop in data.keys():
    ground = data[pop]["ground"]["hourly"]
    ground_stderr = data[pop]['ground']['stderr']
    pred = data[pop]["pred"][optim_var]["main"]
    pred_low = data[pop]["pred"][optim_var]["low"]
    pred_high = data[pop]["pred"][optim_var]["high"]

    print(f"Evaluating {pop} for {optim_var}")
    all_fits[pop] = cmp_pred_to_ground_metrics(columns, ground, pred,
    ↪ start_day, end_day, show=False)
    overlaps = get_overlap_perc(columns, ground, ground_stderr, pred_low,
    ↪ pred_high, start_day, end_day)
    for col in columns:
        all_fits[pop][col]['overlap'] = overlaps[col]

```

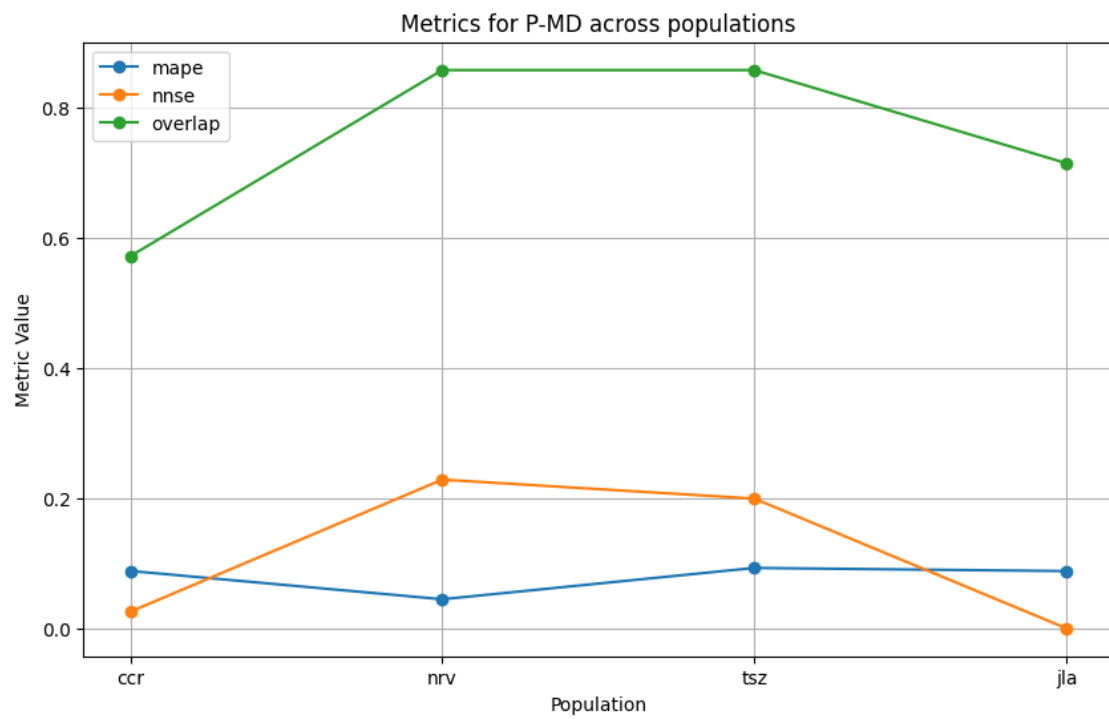
Evaluating ccr for P-PD  
 Evaluating nrv for P-PD  
 Evaluating tsz for P-PD  
 Evaluating jla for P-PD

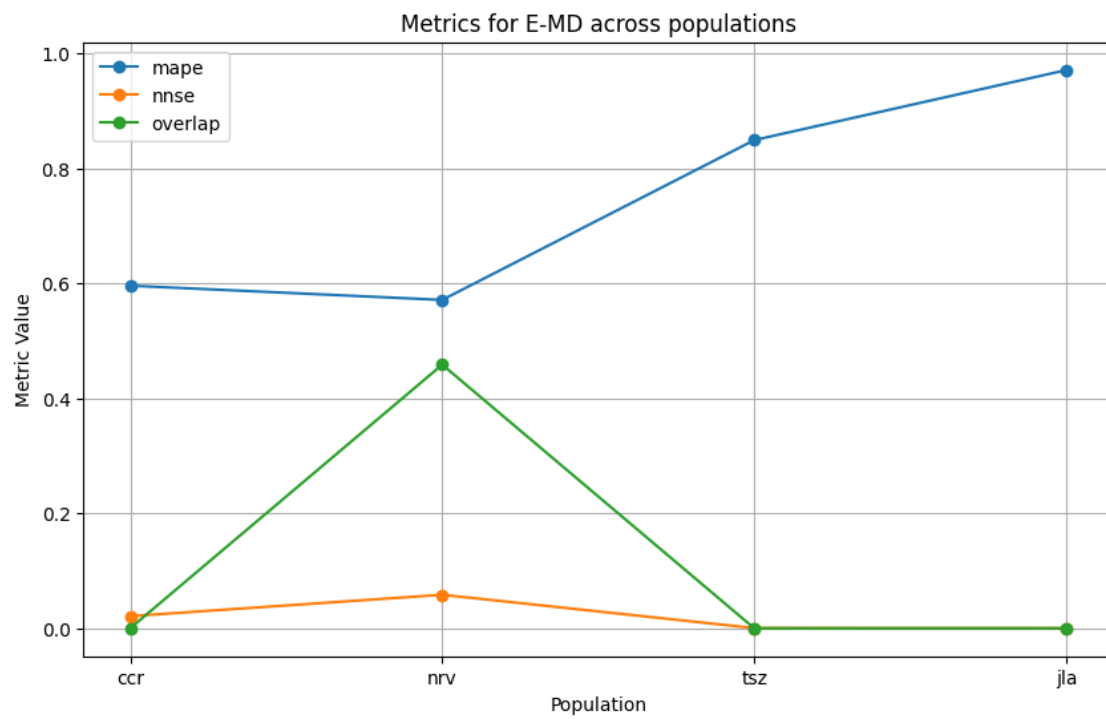
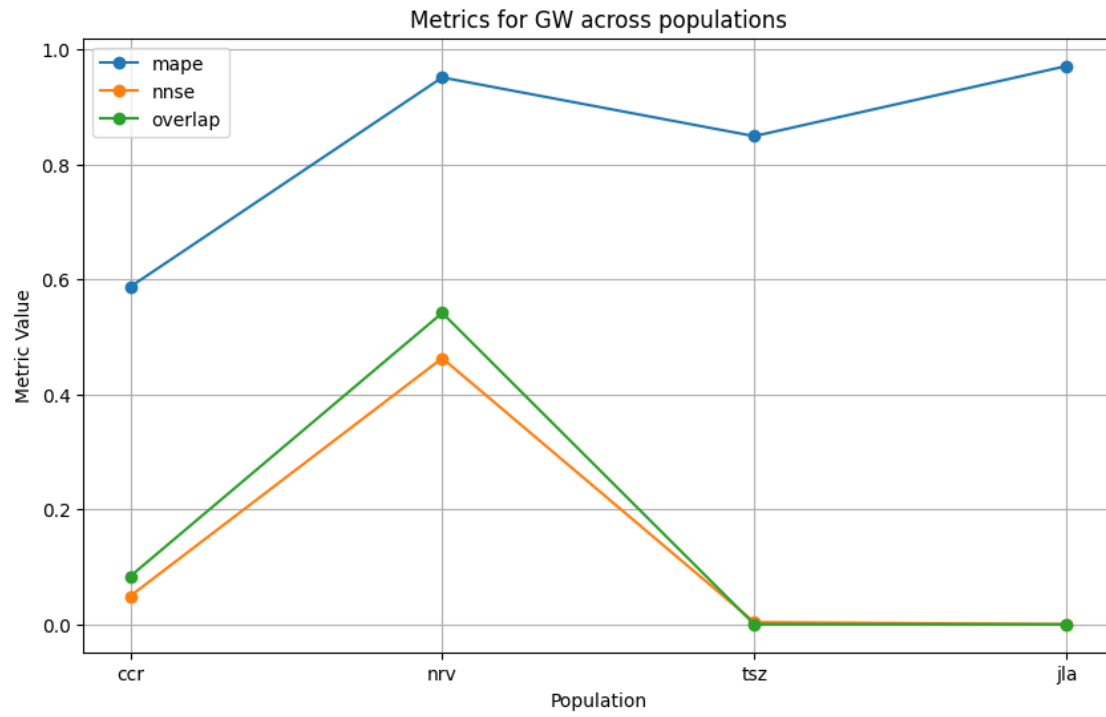
```

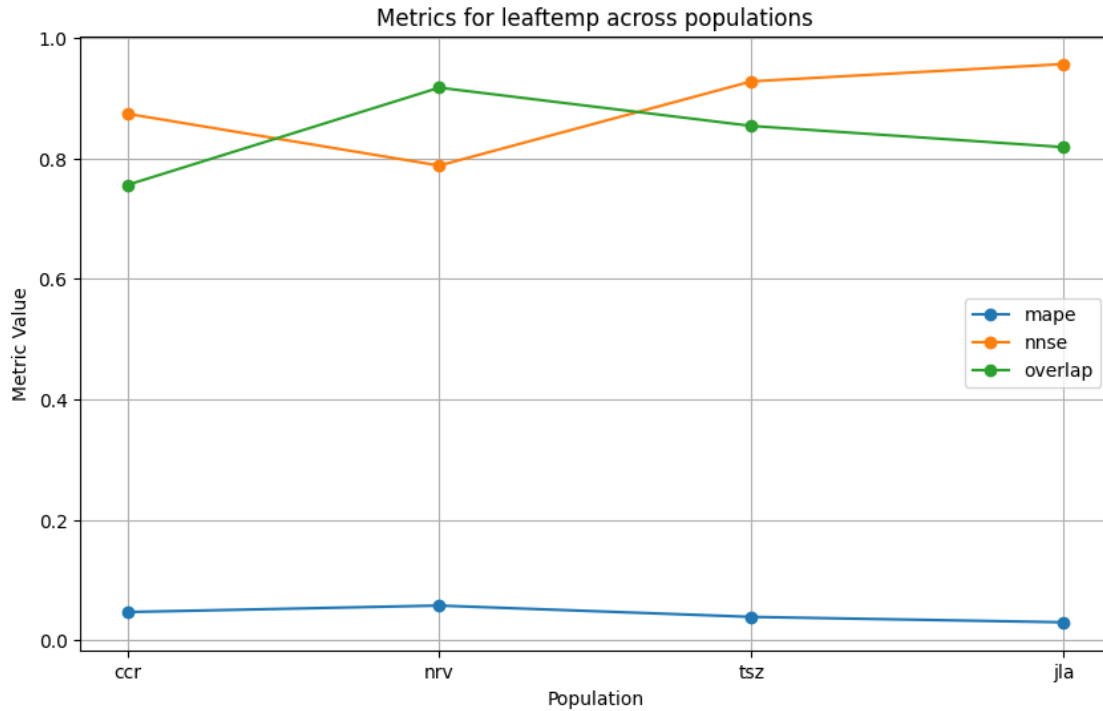
[2078]: metrics_to_plot = ['mape', 'nnse', 'overlap']
populations = list(all_fits.keys())

for col in columns:
    plt.figure(figsize=(10, 6))
    for metric in metrics_to_plot:
        values = [all_fits[pop][col][metric] if col in all_fits[pop] else np.
    ↪ nan for pop in populations]
        plt.plot(populations, values, marker='o', label=metric)
    plt.title(f"Metrics for {col} across populations")
    plt.xlabel("Population")
    plt.ylabel("Metric Value")
    plt.legend()
    plt.grid(True)
    # plt.savefig(f"{col}.png")

```







```
[2079]: def plot_errors(fits, metrics_to_plot, columns):
    populations = list(all_fits.keys())
    # Prepare data for seaborn catplot
    plot_data = []
    for metric in metrics_to_plot:
        for var in columns:
            for pop in populations:
                value = fits[pop][var][metric] if var in fits[pop] else np.nan
                plot_data.append({
                    "Metric": metric,
                    "Variable": var,
                    "Population": pop,
                    "Value": value
                })
    plot_df = pd.DataFrame(plot_data)

    colors = {
        'ccr': "#fa6363",      # light red
        'nrv': "#fbc454",      # light orange
        'tsz': "#658bff",      # light blue
        'jla': "#ae79ff"       # light purple
    }

    # Faceted barplot: one facet per metric, hue as population
```

```

g = sns.catplot(
    data=plot_df,
    x="Variable",
    y="Value",
    hue="Population",
    col="Metric",
    kind="bar",
    height=6,
    aspect=1,
    palette=colors
)

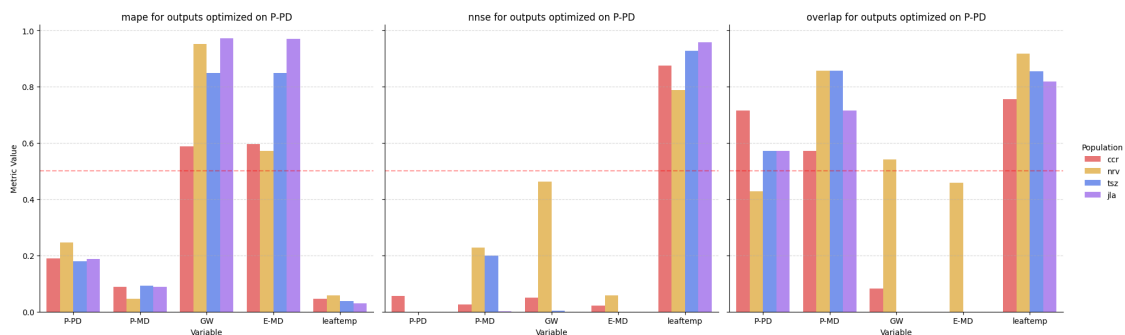
for ax in g.axes.flat:
    ax.yaxis.grid(True, linestyle='--', alpha=0.5)
    ax.axhline(y=0.5, color='red', linestyle='--', alpha=0.4)

# Set custom titles for each metric facet
metric_titles = {
    "mape": "Mean Absolute Percentage Error (MAPE)",
    "nnse": "Normalized Nash-Sutcliffe Efficiency (NNSE)",
    "overlap": "Prediction-Ground 95% CI Overlap"
}

for ax, metric in zip(g.axes.flat, g.col_names):
    ax.set_title(f"{metric} for outputs optimized on {optim_var}")
    g.set_axis_labels("Variable", "Metric Value")
    g.legend.set_bbox_to_anchor((1.0, 0.5))
    g.legend.set_loc("center left")
    plt.tight_layout()
    plt.show()

```

[2080]: `plot_errors(all_fits, metrics_to_plot, columns)`



## 1.2 Plots of prediction against ground truth

```
[2081]: def get_errors(ground, stderr):  
    # Get error bar  
    # col_ground_stderr has the same stderr across multiple timesteps, which  
    ↳ showcases the xerr  
    # Calculate xerr as the length of consecutive identical stderr values  
    ↳ divided by 2  
    stderr_values = stderr.values  
    xerr = np.zeros((2, len(ground)))  
    yerr = np.zeros_like(ground)  
    if len(stderr_values) > 0:  
        start_idx = 0  
        err_idx = 0  
  
        # Iterate through values  
        while start_idx < len(stderr_values):  
  
            # Get current val and set as yerr  
            current_val = stderr_values[start_idx]  
            yerr[err_idx] = current_val  
            run_length = 1  
  
            # Find the number of consecutive errors  
            while (start_idx + run_length < len(stderr_values)) and  
            ↳ (stderr_values[start_idx + run_length] == current_val):  
                run_length += 1  
  
            # Get the middle and determine left and right bounds from middle  
            ↳ and run_length  
            mid = (run_length + 1) / 2  
            xerr[:, err_idx] = np.array([max(0, mid - 1), max(0, run_length -  
            ↳ mid)])  
            start_idx += run_length  
  
            # Move to next stderr  
            err_idx += 1  
  
    return xerr, yerr
```

```
[2082]: unit = {  
    "P-PD" : "-MPa",  
    "P-MD" : "-MPa",  
    "GW" : "mmol s-1 m-2 (LA)",  
    "E-MD" : "mmol s-1 m-2 (LA)",  
    "K-plant" : "kg hr-1 m-2 (BA)",  
    'leaftemp' : "C"
```

```
}
```

```
[2083]: def plot_ground_pred(columns, stop, start=0):
        """
        Ground versus prediction graph with lines across all.

        stop and start are julian days!
        """

        for pop in data.keys():
            print(f"Population: {pop}")
            for col in columns:
                plt.figure(figsize=(12, 6))
                ground_df = data[pop]["ground"]["hourly"]
                stderr_df = data[pop]["ground"]["stderr"]
                pred_df = data[pop]["pred"][optim_var]["main"]
                low_df = data[pop]["pred"][optim_var]["low"]
                high_df = data[pop]["pred"][optim_var]["high"]

                # Filter for valid julian-day range

                ground_df = ground_df[ground_df['julian-day'].between(start, stop)]
                stderr_df = stderr_df[stderr_df['julian-day'].between(start, stop)]
                pred_df = pred_df[pred_df['julian-day'].between(start, stop)]
                low_df = low_df[low_df['julian-day'].between(start, stop)]
                high_df = high_df[high_df['julian-day'].between(start, stop)]

                # Filter ground and stderr for the current column, also align with
↪index
                col_ground = ground_df[col].dropna()
                col_ground_stderr = stderr_df[col].dropna()
                col_pred = pred_df[col]
                col_pred_low = low_df[col]
                col_pred_high = high_df[col]

                # Get error bars
                _, yerr = get_errors(col_ground, col_ground_stderr)

                # Plot ground with error bars
                plt.errorbar(
                    col_ground.index,
                    col_ground,
                    yerr=1.96 * yerr,
                    fmt='o',
                    alpha=0.6,
                    label=f'{pop} Ground 95% CI',
                    capsize=5,
```

```

        barsabove=True,
        color='navy'
    )

    # Plot prediction
    plt.plot(col_pred.index, col_pred, color="green", alpha=1,
    ↪label=f'Prediction')
    # plt.fill_between(col_pred.index, col_pred_low, col_pred_high,
    ↪color="green", alpha=0.4, label=f'Prediction 95%')

    plt.ylim(bottom=0)
    plt.title(f"Predicted vs Ground: {col}")
    plt.xlabel("Timestep")
    plt.ylabel(f"{col} {unit.get(col, '')}")
    plt.axvline(
        x=ground_df.index[(ground_df['julian-day'] == stress_begin) &
    ↪(ground_df['standard-time'] == 0)].item(),
        color='navy',
        linestyle='--',
        label='Pre-stress Cutoff',
        alpha=0.4
    )
    plt.axvline(
        x=ground_df.index[(ground_df['julian-day'] ==
    ↪predrought_cutoff) & (ground_df['standard-time'] == 0)].item(),
        color='navy',
        linestyle='--',
        label='Predrought Cutoff',
        alpha=0.4
    )
    plt.axvline(
        x=ground_df.index[(ground_df['julian-day'] == post_drought) &
    ↪(ground_df['standard-time'] == 0)].item(),
        color='navy',
        linestyle='--',
        label='Drought Cutoff',
        alpha=0.4
    )
    plt.legend()
    plt.grid(True)
    plt.show()

```

```

[2084]: def plot_ground_pred_two(columns, stop, start=0):
        """
        Ground versus prediction graph that only outputs for each timestep matching
        ↪to the ground truth data.

```

```

stop and start are julian days!
"""

for pop in data.keys():
    print(f"Population: {pop}")
    for col in columns:
        plt.figure(figsize=(12, 6))
        ground_df = data[pop]["ground"]["hourly"]
        stderr_df = data[pop]["ground"]["stderr"]
        pred_df = data[pop]["pred"][optim_var]["main"]
        low_df = data[pop]["pred"][optim_var]["low"]
        high_df = data[pop]["pred"][optim_var]["high"]

        # Filter for valid julian-day range
        ground_df = ground_df[ground_df['julian-day'].between(start, stop)]
        stderr_df = stderr_df[stderr_df['julian-day'].between(start, stop)]
        pred_df = pred_df[pred_df['julian-day'].between(start, stop)]
        low_df = low_df[low_df['julian-day'].between(start, stop)]
        high_df = high_df[high_df['julian-day'].between(start, stop)]

        # Filter ground and stderr for the current column
        col_ground = ground_df[col].dropna()
        col_ground_stderr = stderr_df[col].dropna()
        col_pred = pred_df[col].loc[col_ground.index]
        col_pred_low = low_df[col].loc[col_ground.index]
        col_pred_high = high_df[col].loc[col_ground.index]

        # Align prediction with ground index
        col_pred = col_pred.loc[col_ground.index]

        # Plot prediction
        # Calculate asymmetric yerr for prediction
        yerr_upper = col_pred_high - col_pred
        yerr_lower = col_pred - col_pred_low
        yerr_pred = [yerr_lower.values, yerr_upper.values]

        plt.errorbar(
            col_pred.index,
            col_pred,
            yerr=yerr_pred,
            fmt='^',
            alpha=1,
            label=f'{pop} Prediction',
            color="green",
            capsize=5
        )

```

```

# Get error bars
_, yerr = get_errors(col_ground, col_ground_stderr)

# Plot ground with error bars
plt.errorbar(
    col_ground.index,
    col_ground,
    yerr=1.96 * yerr,
    fmt='o',
    alpha=0.6,
    label=f'{pop} Ground',
    capsize=5,
    barsabove=True,
    color='navy'
)

plt.ylim(bottom=0)
plt.xlim(left=0, right=1600)
plt.title(f"Predicted vs Ground: {col}")
plt.xlabel("Timestep")
plt.ylabel(f"{col} {unit.get(col, '')}")

stress_idx = ground_df.index[(ground_df['julian-day'] ==
↳ stress_begin) & (ground_df['standard-time'] == 0)].item()
drought_idx = ground_df.index[(ground_df['julian-day'] ==
↳ predrought_cutoff) & (ground_df['standard-time'] == 0)].item()
post_idx = ground_df.index[(ground_df['julian-day'] ==
↳ post_drought) & (ground_df['standard-time'] == 0)].item()

# Shade pre-stress region
# plt.axvspan(
#     ground_df.index.min(),
#     stress_idx,
#     color='navy',
#     alpha=0.1,
#     label='Pre-stress Region'
# )
# Shade predrought region
plt.axvspan(
    stress_idx,
    drought_idx,
    color='orange',
    alpha=0.2,
    label='Predrought'
)
# Shade drought region
plt.axvspan(

```

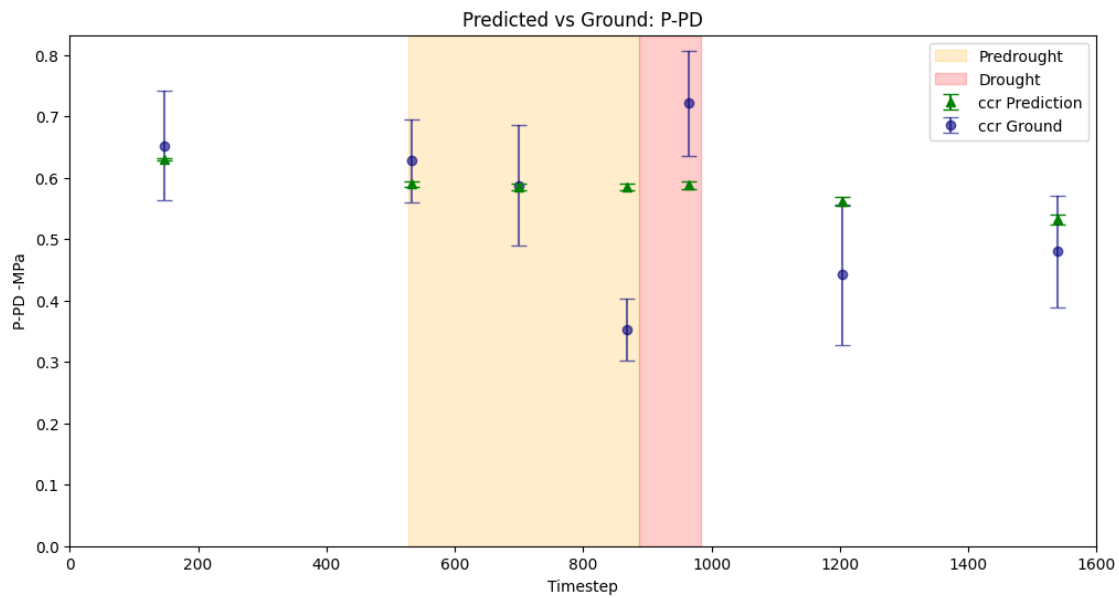
```

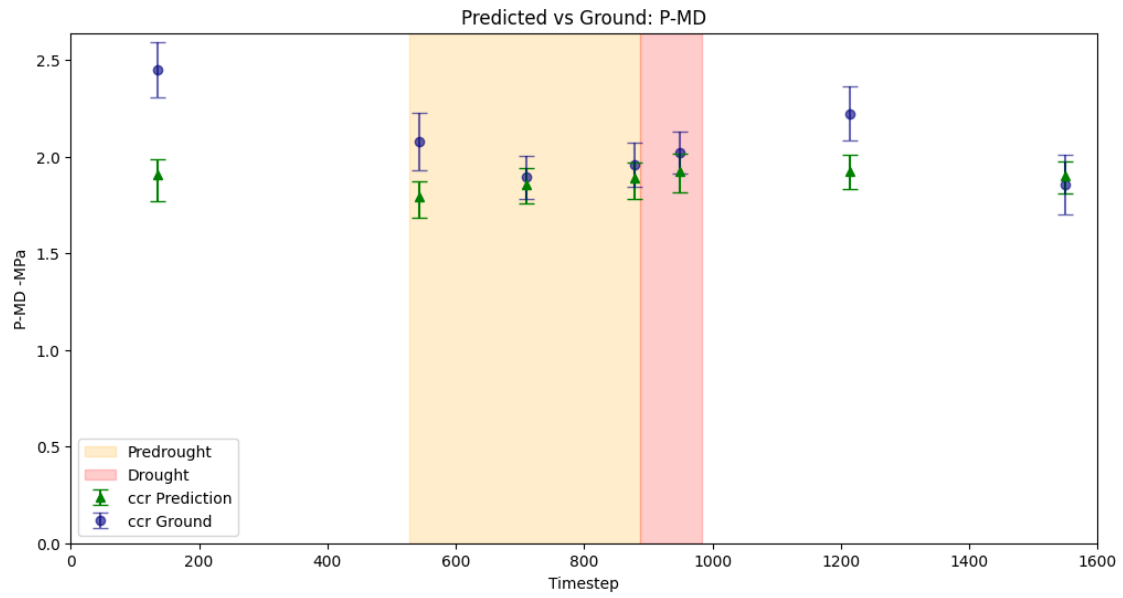
        drought_idx,
        post_idx,
        color='red',
        alpha=0.2,
        label='Drought'
    )
    # plt.axvspan(
    #     drought_idx,
    #     1600,
    #     color='navy',
    #     alpha=0.1,
    #     label='Post-drought Region'
    # )
    plt.legend()
    plt.show()
    # plt.savefig(f"{pop}_{col}.png")

```

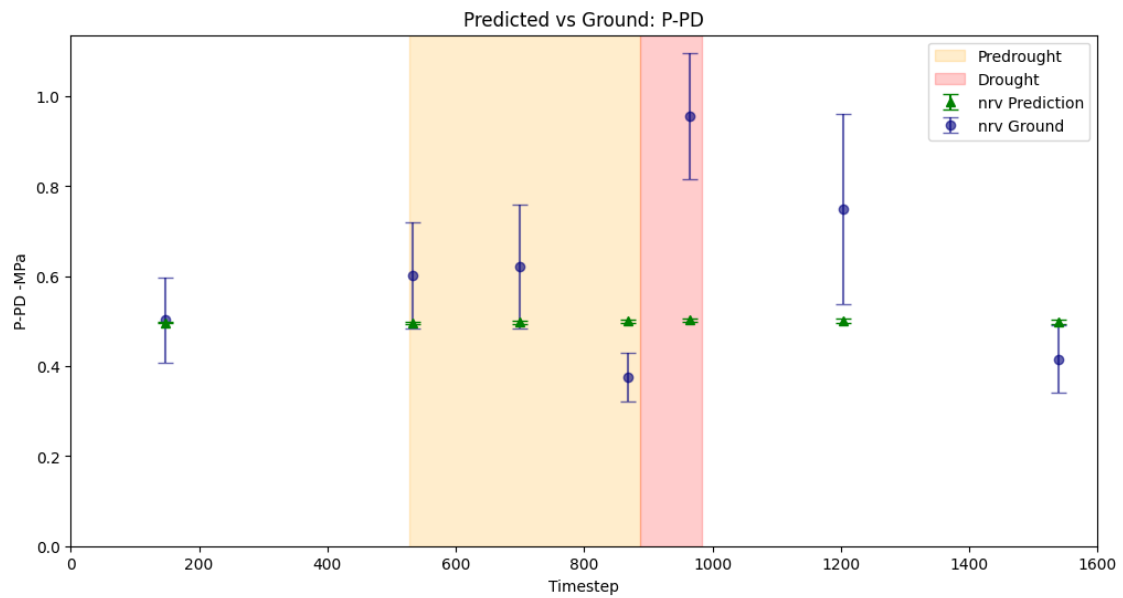
```
[2085]: plot_ground_pred_two(["P-PD", "P-MD"], stop=end_day)
```

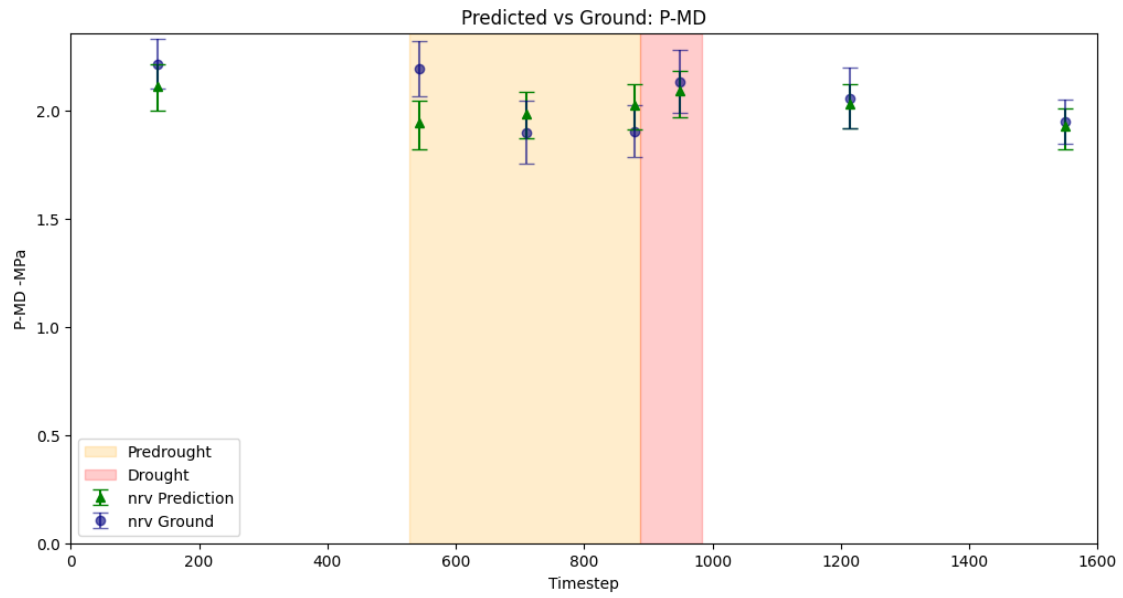
Population: ccr



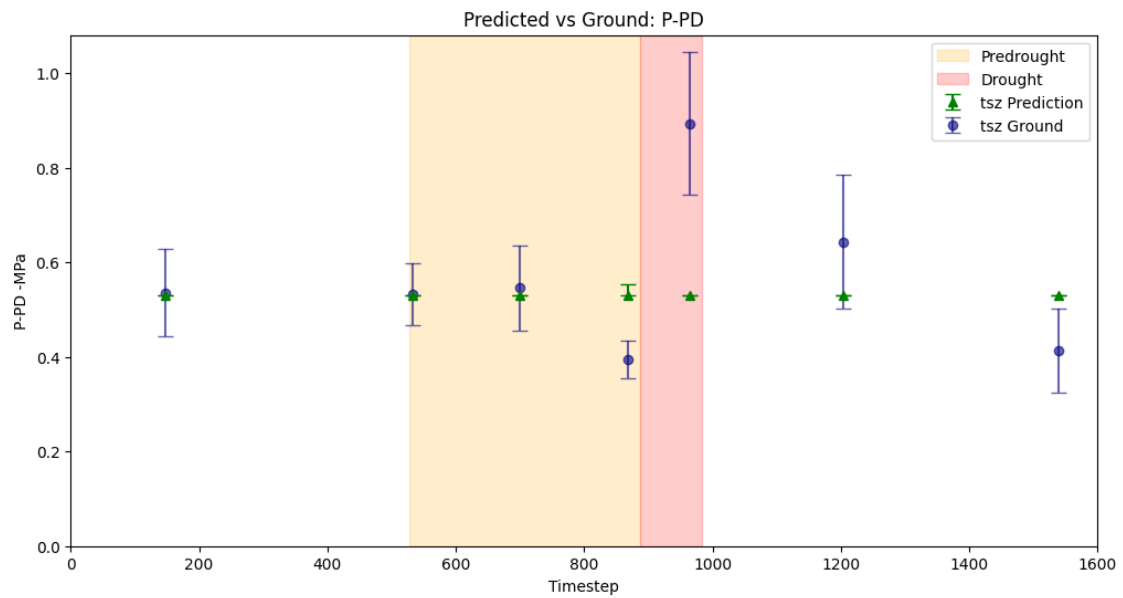


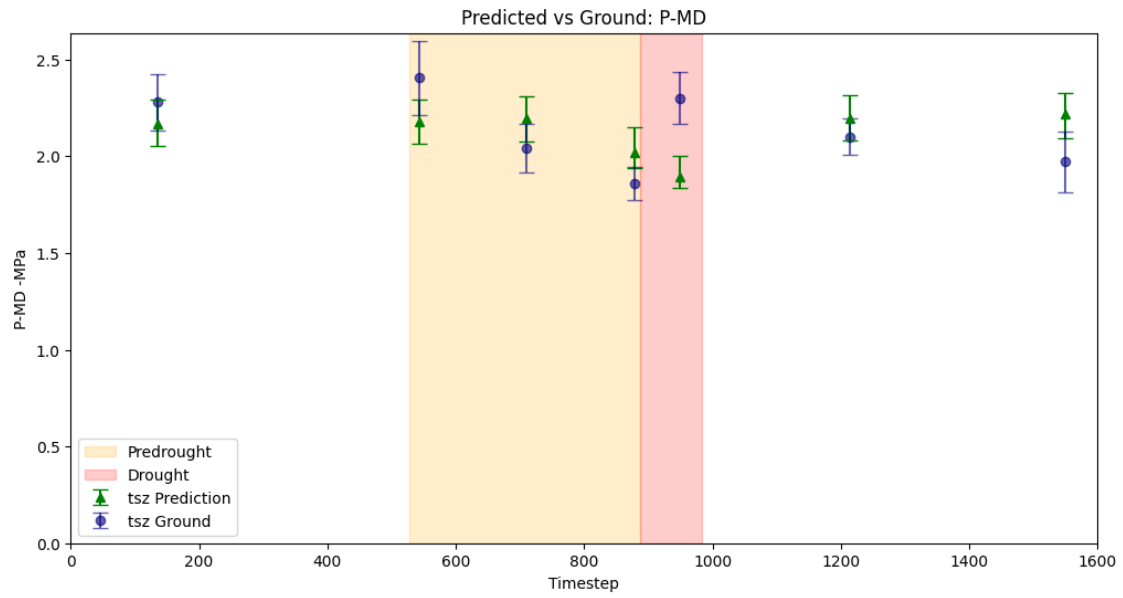
Population: nrv



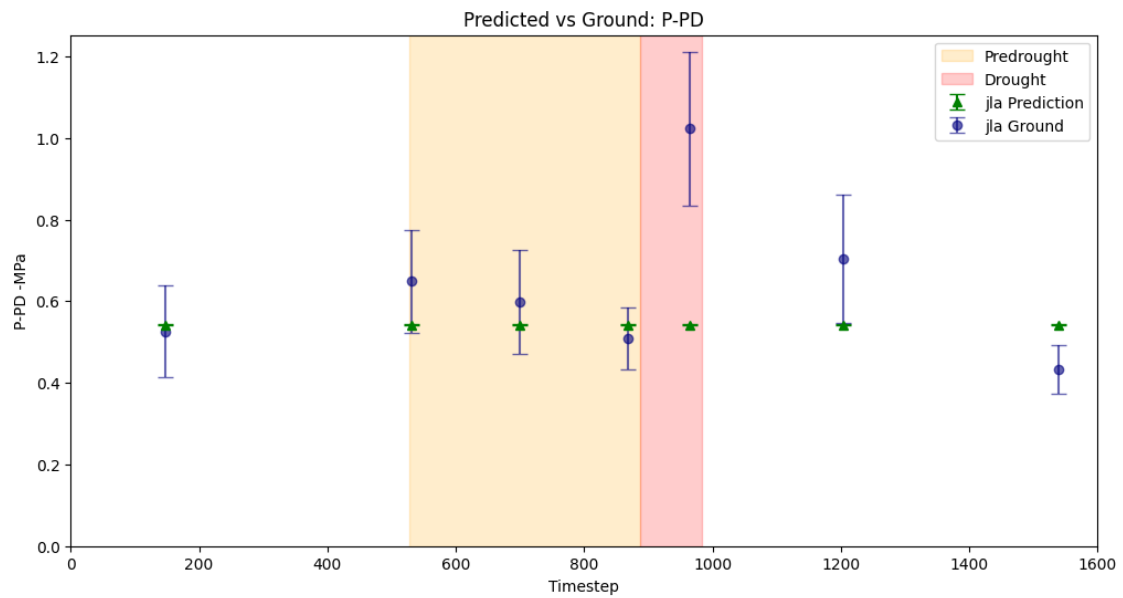


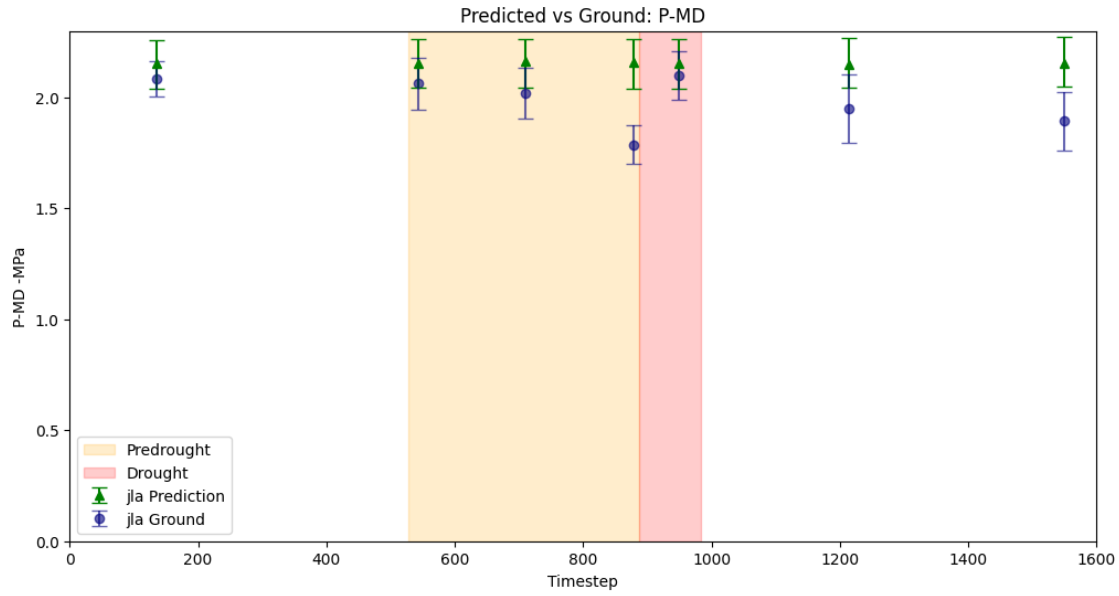
Population: tsz





Population: jla





```
[2086]: # plot_ground_pred(columns, stop=end_day)
```

### 1.3 Pred vs ground truth averaged across treatments

```
[2087]: # Treatments and their corresponding start and end julian-days
treatments = {
    "Pre-water stress": (201, 237),
    "Water stress": (238, 241),
    "Post-water stress": (242, 265),
}
```

```
[2088]: def plot_treatment_averages():
    """
    Create plots showing averaged ground truth and predictions for each
    ↪ treatment period
    across all populations, similar to the reference figure.
    """

    # Variables to plot
    variables = ["GW", "E-MD", "leaftemp", "leaf-air"]

    # Source elevations for each population (from the reference figure)
    source_elevations = {
        'ccr': 72,
        'nrv': 666,
        'tsz': 1212,
        'jla': 1521,
```

```

}

# Colors for each elevation (matching the reference figure)
pred_colors = {
    72: 'red',
    666: 'orange',
    1212: 'blue',
    1521: 'purple'
}

ground_colors = {
    72: '#ff9999',      # light red
    666: '#ffd580',     # light orange
    1212: '#99b3ff',    # light blue
    1521: '#c299ff'     # light purple
}

# Markers for each elevation
markers = {
    72: 'D',
    666: 's',
    1212: 'o',
    1521: '^'
}

for var in variables:

    plt.figure(figsize=(10, 6))

    treatment_names = list(treatments.keys())
    x_pos = np.arange(len(treatment_names))

    # For each population
    for pop in data.keys():
        elevation = source_elevations[pop]
        ground_color = ground_colors[elevation]
        pred_color = pred_colors[elevation]
        marker = markers[elevation]

        if var == 'GW' or var == 'E-MD':
            ground_df = data[pop]["ground"]["gw_treatment_averages"]
        elif var == 'leaf-temp':
            ground_df = data[pop]["ground"]["leaf_treatment_averages"]
        elif var == 'leaf-air':
            ground_df = data[pop]["ground"]["leaf-air_treatment_averages"]

        pred_df = data[pop]["pred"][optim_var]["main"]

```

```

pred_low_df = data[pop]["pred"][optim_var]["low"]
pred_high_df = data[pop]["pred"][optim_var]["high"]

pred_df['leaf-air'] = pred_df['leaftemp'] - pred_df['T-air']
pred_low_df['leaf-air'] = pred_low_df['leaftemp'] -
↳pred_low_df['T-air']
pred_high_df['leaf-air'] = pred_high_df['leaftemp'] -
↳pred_high_df['T-air']

ground_means = []
ground_errors = []
pred_means = []
yerr_pred_means = [[], []]

# Calculate means for each treatment period
for treatment, (start_day, end_day) in treatments.items():
    # Filter data for treatment period to be between 15:00 and 17:
    ↳00 like ground truth
    treatment_pred = pred_df[
        (pred_df['julian-day'].between(start_day, end_day)) &
        (pred_df['standard-time'] >= 15) &
        (pred_df['standard-time'] <= 17)
    ][var]
    treatment_pred_low = pred_low_df[
        (pred_low_df['julian-day'].between(start_day, end_day)) &
        (pred_low_df['standard-time'] >= 15) &
        (pred_low_df['standard-time'] <= 17)
    ][var]
    treatment_pred_high = pred_high_df[
        (pred_high_df['julian-day'].between(start_day, end_day)) &
        (pred_high_df['standard-time'] >= 15) &
        (pred_high_df['standard-time'] <= 17)
    ][var]

    yerr_upper = treatment_pred_high - treatment_pred
    yerr_lower = treatment_pred - treatment_pred_low
    yerr_pred_means[0].append(yerr_lower.mean())
    yerr_pred_means[1].append(yerr_upper.mean())

    pred_mean = treatment_pred.mean() if len(treatment_pred) > 0
↳else np.nan
    pred_means.append(pred_mean)

    # Select the average and stderr for the current treatment and
    ↳variable
    ground_mean = ground_df.loc[ground_df['treatment'] ==
↳treatment][f'{var}_avg'].values[0]

```

```

        ground_stderr = ground_df.loc[ground_df['treatment'] ==
↳treatment][f'{var}_stderr'].values[0]
        ground_means.append(ground_mean)
        ground_errors.append(ground_stderr)

    offset = 0.1 * (list(data.keys()).index(pop) - 1.5) # Center
↳around 0

    # Plot ground truth with error bars
    plt.errorbar(
        x_pos + offset,
        ground_means,
        yerr=[1.96 * err for err in ground_errors],
        fmt=marker,
        color=ground_color,
        markersize=8,
        capsize=10,
        capthick=1,
        label=f'{elevation}'
    )

    # Plot predictions
    plt.errorbar(
        x_pos + offset,
        pred_means,
        yerr=yerr_pred_means,
        fmt='x',
        color=pred_color,
        markersize=10,
        linewidth=2,
        capsize=10,
        label=None
    )

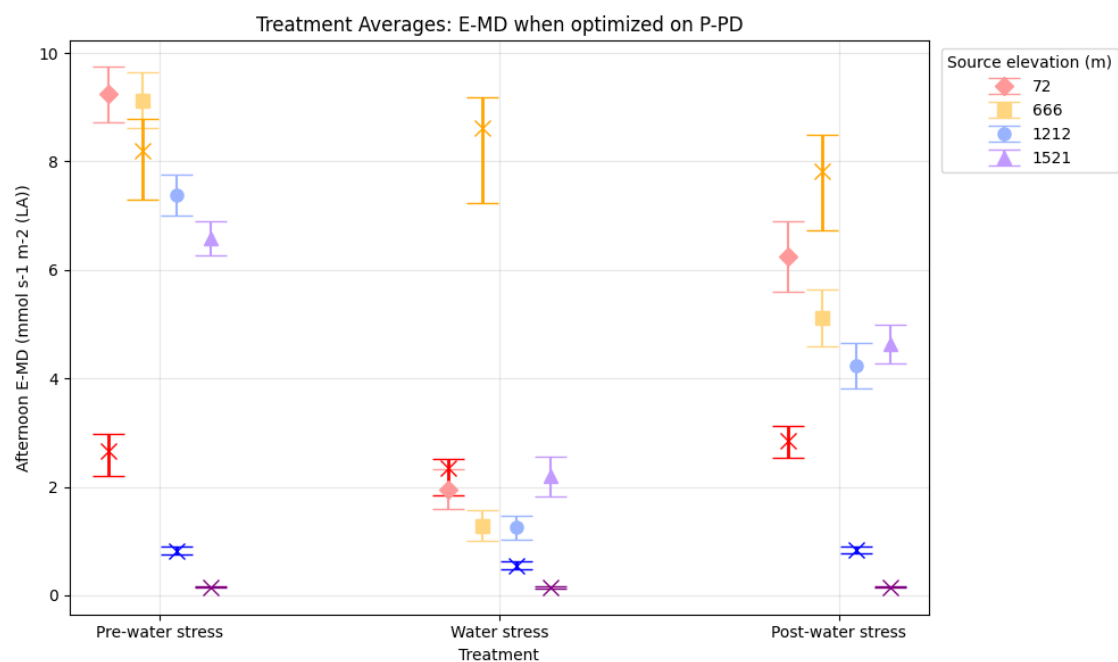
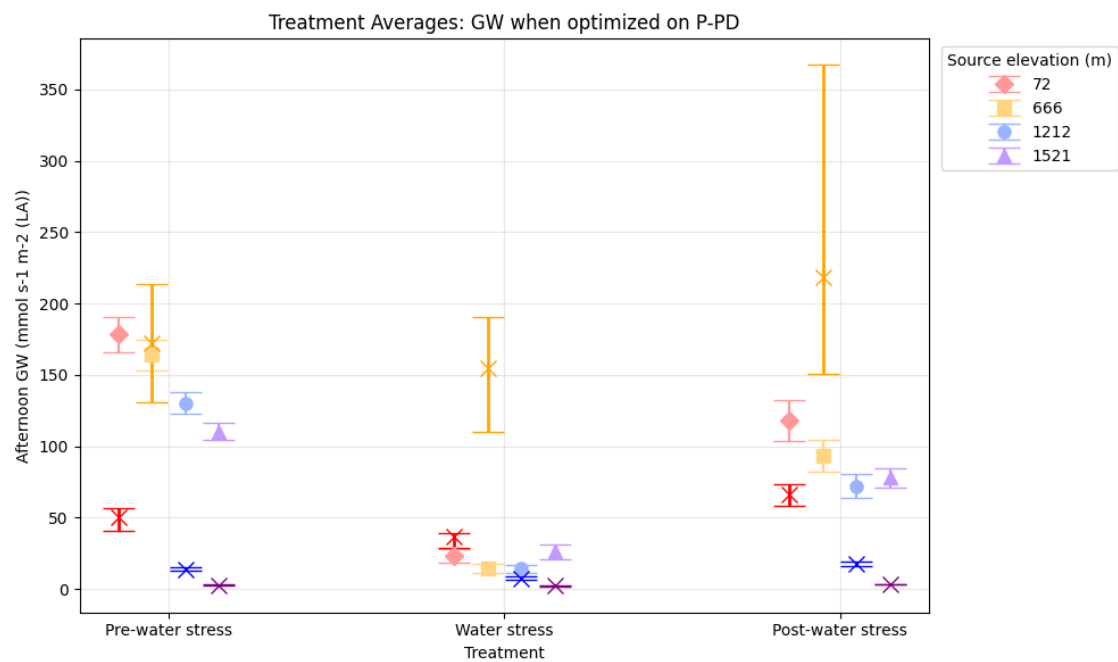
    # Customize plot
    plt.ylabel(f'Afternoon {var} ({unit.get(var, "")})')
    plt.xlabel('Treatment')
    plt.title(f'Treatment Averages: {var} when optimized on {optim_var}')
    plt.xticks(x_pos, treatment_names)
    plt.grid(True, alpha=0.3)

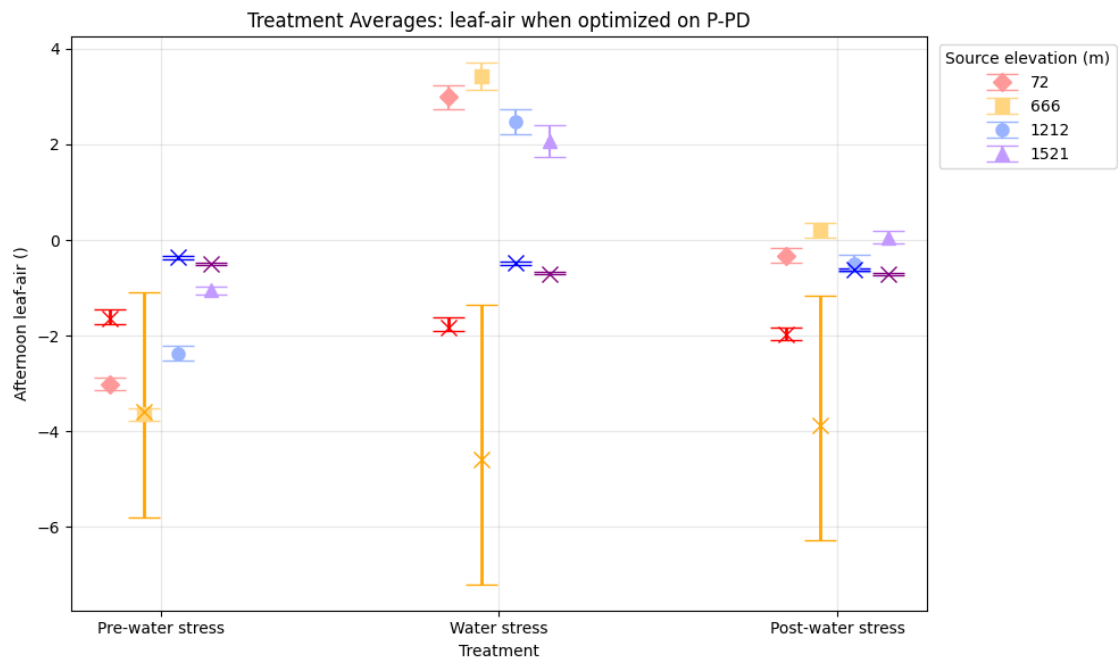
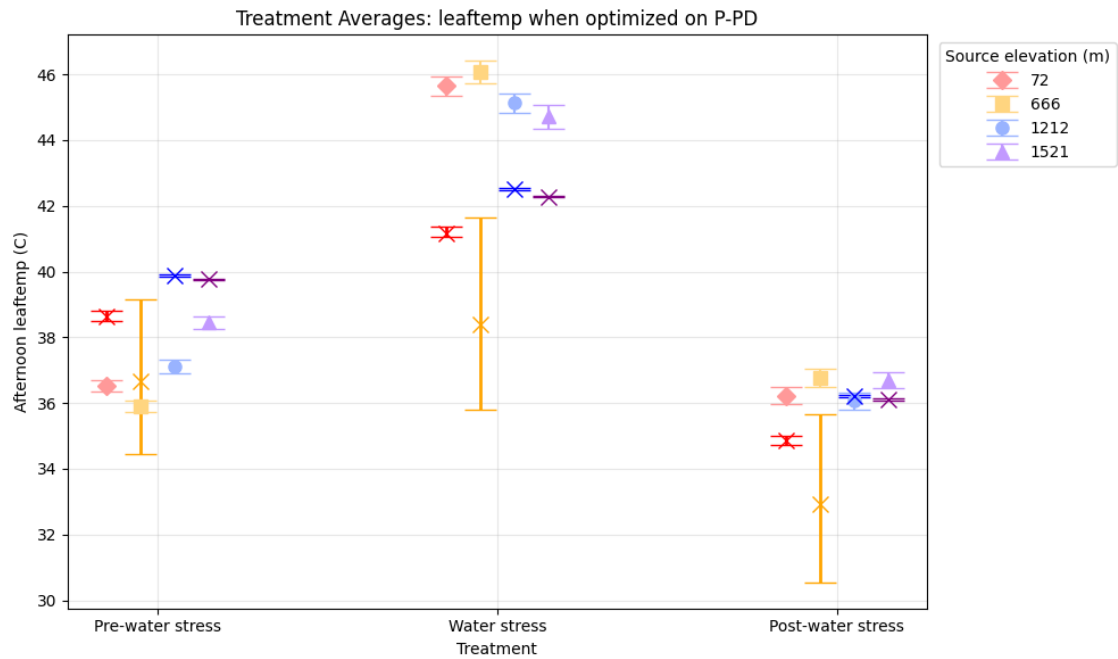
    # Add legend
    plt.legend(title='Source elevation (m)', bbox_to_anchor=(1.005, 1),
↳loc='upper left')

    plt.tight_layout()
    plt.show()

```

```
[2089] : plot_treatment_averages()
```





## 1.4 Leaf temperature

Averaged between 14:00 and 18:00

```
[2090]: def get_overlap_perc_leaft(ground, ground_stderr, pred, pred_stderr, start,
↳end):

    col_ground = ground.loc[start:end]
    col_ground_stderr = ground_stderr.loc[start:end]
    col_ground_low = col_ground - 1.96 * col_ground_stderr
    col_ground_high = col_ground + 1.96 * col_ground_stderr

    col_pred = pred.loc[start:end]
    col_pred_stderr = pred_stderr.loc[start:end]
    col_pred_low = col_pred - 1.96 * col_pred_stderr
    col_pred_high = col_pred + 1.96 * col_pred_stderr

    # Compute overlap: intervals [col_ground_low, col_ground_high] and
↳[col_pred_low, col_pred_high]
    overlap_count = 0
    total = len(col_ground)
    for i in range(total):
        g_low = col_ground_low.iloc[i]
        g_high = col_ground_high.iloc[i]
        p_low = col_pred_low.iloc[i]
        p_high = col_pred_high.iloc[i]
        # Check if intervals overlap
        if (g_low <= p_high) and (p_low <= g_high):
            overlap_count += 1
    overlap_perc = overlap_count / total if total > 0 else np.nan

    return overlap_perc
```

```
[2091]: def cmp_leaftemp_pred_to_ground_metrics(ground, ground_stderr, pred,
↳pred_stderr, start, end):

    col_ground = ground.loc[start:end]
    col_pred = pred.loc[start:end]

    mse = mean_squared_error(col_ground, col_pred)
    rmse = root_mean_squared_error(col_ground, col_pred)
    mape = mean_absolute_percentage_error(col_ground, col_pred)
    made = median_absolute_error(col_ground, col_pred)
    mae = mean_absolute_error(col_ground, col_pred)
    r2 = r2_score(col_ground, col_pred)
    r2 = 0 if r2 < 0 else r2
    nnse = normalized_nash_sutcliffe_efficiency(col_ground, col_pred)
    overlap = get_overlap_perc_leaft(ground, ground_stderr, pred, pred_stderr,
↳start, end)

    fit = {
```

```

        'mse' : mse,
        'rmse' : rmse,
        'mape' : mape,
        'made' : made,
        'mae' : mae,
        'r2' : r2,
        'nnse' : nnse,
        'overlap' : overlap
    }

    return fit

```

```

[2092]: leaft_fits = defaultdict(dict)

for pop in data.keys():
    print(f"Population: {pop}")
    leaft = data[pop]["ground"]["leaflet"]
    pred = data[pop]["pred"][optim_var]["main"]
    low = data[pop]["pred"][optim_var]["low"]
    high = data[pop]["pred"][optim_var]["high"]

    """ From Posch et al.
    Mean Tleaf calculated as average of Tleaf measured at 15 min intervals
    between 14:00 to 18:00
    each day in three pseudoreplicate leaves per tree, and three replicate
    trees per population. (B) The difference between Tleaf and air temperature
    (Tair) was also
    calculated for the same period.
    """

    daily_ground_leaflet_mean = leaft[(leaflet['standard-time'] >= 14) &
    (leaflet['standard-time'] <= 18)].groupby('julian-day')['leaflettemp'].mean()
    daily_pred_leaflet_mean = pred[(pred['standard-time'] >= 14) &
    (pred['standard-time'] <= 18)].groupby('julian-day')['leaflettemp'].mean()
    daily_low_leaflet_mean = low[(low['standard-time'] >= 14) &
    (low['standard-time'] <= 18)].groupby('julian-day')['leaflettemp'].mean()
    daily_high_leaflet_mean = high[(high['standard-time'] >= 14) &
    (high['standard-time'] <= 18)].groupby('julian-day')['leaflettemp'].mean()

    # Calculate daily mean of (leaflettemp - T-air) for ground and predictions, 14:
    00-18:00
    daily_ground_diff_mean = leaft[(leaflet['standard-time'] >= 14) &
    (leaflet['standard-time'] <= 18)].groupby('julian-day').apply(lambda df:
    (df['leaflettemp'] - df['Tair_C']).mean(), include_groups=False)

```

```

    daily_pred_diff_mean = pred[(pred['standard-time'] >= 14) &
    ↪(pred['standard-time'] <= 18)].groupby('julian-day').apply(lambda df:
    ↪(df['leaftemp'] - df['T-air']).mean(), include_groups=False)

    daily_low_diff_mean = low[(low['standard-time'] >= 14) &
    ↪(low['standard-time'] <= 18)].groupby('julian-day').apply(lambda df:
    ↪(df['leaftemp'] - df['T-air']).mean(), include_groups=False)

    daily_high_diff_mean = high[(high['standard-time'] >= 14) &
    ↪(high['standard-time'] <= 18)].groupby('julian-day').apply(lambda df:
    ↪(df['leaftemp'] - df['T-air']).mean(), include_groups=False)

    daily_pred_leaft_count = pred[(pred['standard-time'] >= 14) &
    ↪(pred['standard-time'] <= 18)].groupby('julian-day')['leaftemp'].count()
    daily_pred_leaft_std = pred[(pred['standard-time'] >= 14) &
    ↪(pred['standard-time'] <= 18)].groupby('julian-day')['leaftemp'].std()
    daily_pred_leaft_stderr = daily_pred_leaft_std / np.
    ↪sqrt(daily_pred_leaft_count)

    daily_ground_leaft_count = leaft[(leaft['standard-time'] >= 14) &
    ↪(leaft['standard-time'] <= 18)].groupby('julian-day')['leaftemp'].count()
    daily_ground_leaft_std = leaft[(leaft['standard-time'] >= 14) &
    ↪(leaft['standard-time'] <= 18)].groupby('julian-day')['leaftemp'].std()
    daily_ground_leaft_stderr = daily_ground_leaft_std / np.
    ↪sqrt(daily_ground_leaft_count)

    daily_pred_diff_count = pred[(pred['standard-time'] >= 14) &
    ↪(pred['standard-time'] <= 18)].groupby('julian-day').apply(lambda df:
    ↪df['leaftemp'].count(), include_groups=False)
    daily_pred_diff_std = pred[(pred['standard-time'] >= 14) &
    ↪(pred['standard-time'] <= 18)].groupby('julian-day').apply(lambda df:
    ↪(df['leaftemp'] - df['T-air']).std(), include_groups=False)
    daily_pred_diff_stderr = daily_pred_diff_std / np.
    ↪sqrt(daily_pred_diff_count)

    daily_ground_diff_count = leaft[(leaft['standard-time'] >= 14) &
    ↪(leaft['standard-time'] <= 18)].groupby('julian-day').apply(lambda df:
    ↪df['leaftemp'].count(), include_groups=False)
    daily_ground_diff_std = leaft[(leaft['standard-time'] >= 14) &
    ↪(leaft['standard-time'] <= 18)].groupby('julian-day').apply(lambda df:
    ↪(df['leaftemp'] - df['Tair_C']).std(), include_groups=False)
    daily_ground_diff_stderr = daily_ground_diff_std / np.
    ↪sqrt(daily_ground_diff_count)

    plt.figure(figsize=(12,4))

    plt.plot(daily_ground_leaft_mean.index, daily_ground_leaft_mean.values,
    ↪color="navy", alpha=1, label=f'Ground')

```

```

plt.fill_between(daily_ground_leafstderr.index, daily_ground_leafstderr.
↪values - 1.96 * daily_ground_leafstderr.values, daily_ground_leafstderr.
↪values + 1.96 * daily_ground_leafstderr.values, color='navy', alpha=0.4)

plt.plot(daily_pred_leafstderr.index, daily_pred_leafstderr.values,
↪color="green", alpha=1, label=f'Prediction')
plt.fill_between(daily_pred_leafstderr.index, daily_pred_leafstderr.
↪values - 1.96 * daily_pred_leafstderr.values, daily_pred_leafstderr.values
↪+ 1.96 * daily_pred_leafstderr.values, color='green', alpha=0.4)
# plt.fill_between(daily_high_leafstderr.index, daily_low_leafstderr.
↪values, daily_high_leafstderr.values, color='green', alpha=0.4, label="95%
↪Interval")

plt.xlabel("Timesteps")
plt.ylabel("Leaf temperature C")

# Generate date labels from July 24th to September 25th
start_date = datetime(2023, 7, 24)
end_date = datetime(2023, 9, 25)
date_range = pd.date_range(start=start_date, end=end_date, freq='D')

# Set x-ticks at the corresponding julian-day indices
julian_days = daily_ground_diff_mean.index
tick_indices = []
tick_labels = []
for i, date in enumerate(date_range):
    if i % 7 != 0:
        continue
    jd = date.timetuple().tm_yday
    if jd in julian_days:
        tick_indices.append(jd)
        tick_labels.append(date.strftime('%b %d'))

plt.ylim(bottom=25, top=50)
plt.xticks(tick_indices, tick_labels, rotation=45)
plt.title(f"Predicted leaf temperature for {pop}")
plt.legend()

# Shade pre-stress region
# plt.axvspan(
#     start_day,
#     stress_begin,
#     color='navy',
#     alpha=0.1,
#     label='Pre-stress Region'
# )
# Shade predrought region

```

```

plt.axvspan(
    stress_begin,
    predrought_cutoff,
    color='orange',
    alpha=0.2,
    label='Stress Begins'
)
# Shade drought region
plt.axvspan(
    predrought_cutoff,
    post_drought,
    color='red',
    alpha=0.2,
    label='Drought'
)
# plt.axvspan(
#
#
#
# ,
#     end_day,
#     color='navy',
#     alpha=0.1,
#     label='Post-drought Region'
# )

# plt.xlim(start_day, predrought_cutoff)
plt.show()

plt.figure(figsize=(12,4))
plt.plot(daily_ground_diff_mean.index, daily_ground_diff_mean.values,
↪color="navy", alpha=1, label=f'Ground')
plt.fill_between(daily_ground_diff_stderr.index, daily_ground_diff_mean.
↪values - 1.96 * daily_ground_diff_stderr.values, daily_ground_diff_mean.
↪values + 1.96 * daily_ground_diff_stderr.values, color='navy', alpha=0.4)

plt.plot(daily_pred_diff_mean.index, daily_pred_diff_mean.values,
↪color="green", alpha=1, label=f'Prediction')
plt.fill_between(daily_pred_diff_stderr.index, daily_pred_diff_mean.values
↪- 1.96 * daily_pred_diff_stderr.values, daily_pred_diff_mean.values + 1.96 *
↪daily_pred_diff_stderr.values, color='green', alpha=0.4)
# plt.fill_between(daily_high_diff_mean.index, daily_low_diff_mean.values,
↪daily_high_diff_mean.values, color='green', alpha=0.4, label="95% Interval")

plt.ylim(bottom=-6, top=4)
plt.xlabel("Timesteps")
plt.ylabel("Leaf temperature - Air temperature C")

```

```

# Generate date labels from July 24th to September 25th
start_date = datetime(2023, 7, 24)
end_date = datetime(2023, 9, 25)
date_range = pd.date_range(start=start_date, end=end_date, freq='D')

# Set x-ticks at the corresponding julian-day indices
julian_days = daily_ground_diff_mean.index
tick_indices = []
tick_labels = []
for i, date in enumerate(date_range):
    if i % 7 != 0:
        continue
    jd = date.timetuple().tm_yday
    if jd in julian_days:
        tick_indices.append(jd)
        tick_labels.append(date.strftime('%b %d'))

# Shade pre-stress region
# plt.axvspan(
#     start_day,
#     stress_begin,
#     color='navy',
#     alpha=0.1,
#     label='Pre-stress Region'
# )
# Shade predrought region
plt.axvspan(
    stress_begin,
    predrought_cutoff,
    color='orange',
    alpha=0.2,
    label='Stress Begins'
)
# Shade drought region
plt.axvspan(
    predrought_cutoff,
    post_drought,
    color='red',
    alpha=0.2,
    label='Drought'
)
# plt.axvspan(
#     post_drought,
#     end_day,
#     color='navy',
#     alpha=0.1,

```

```

#     label='Post-drought Region'
# )

plt.axhline(y=0, color='red', linestyle='--', alpha=0.4)

plt.xticks(tick_indices, tick_labels, rotation=45)
plt.title("Predicted difference in leaf temperature versus air temperature")
plt.legend()

plt.show()

leaft_fits[pop]['leaftemp-all'] = cmp_leaftemp_pred_to_ground_metrics(
    daily_ground_leaft_mean,
    daily_ground_leaft_stderr,
    daily_pred_leaft_mean,
    daily_pred_leaft_stderr,
    leaft_data_start,
    end_day
)

leaft_fits[pop]['leaftemp-predrought'] = _
↪cmp_leaftemp_pred_to_ground_metrics(
    daily_ground_leaft_mean,
    daily_ground_leaft_stderr,
    daily_pred_leaft_mean,
    daily_pred_leaft_stderr,
    leaft_data_start,
    predrought_cutoff - 1
)

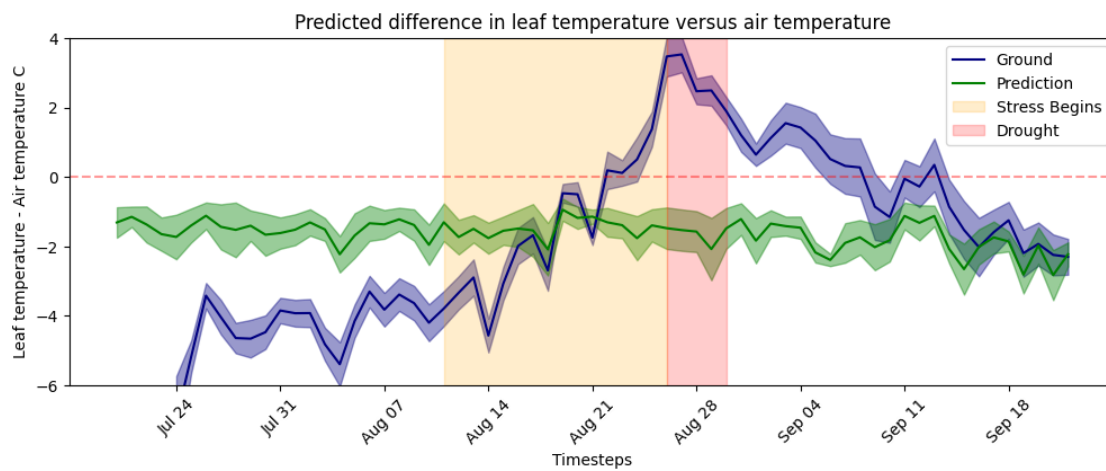
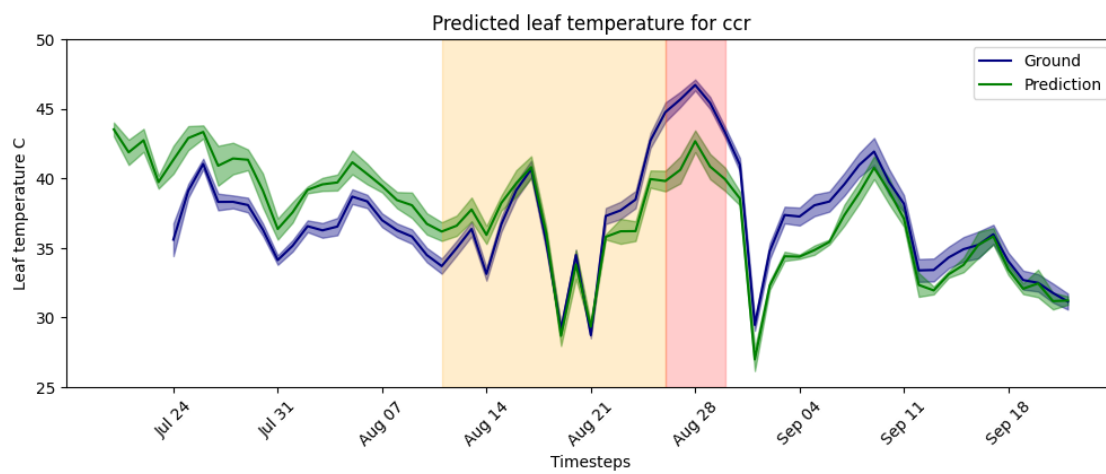
leaft_fits[pop]['leaftemp-drought'] = cmp_leaftemp_pred_to_ground_metrics(
    daily_ground_leaft_mean,
    daily_ground_leaft_stderr,
    daily_pred_leaft_mean,
    daily_pred_leaft_stderr,
    predrought_cutoff,
    post_drought - 1
)

leaft_fits[pop]['leaftemp-postdrought'] = _
↪cmp_leaftemp_pred_to_ground_metrics(
    daily_ground_leaft_mean,
    daily_ground_leaft_stderr,
    daily_pred_leaft_mean,
    daily_pred_leaft_stderr,
    post_drought,
    end_day
)

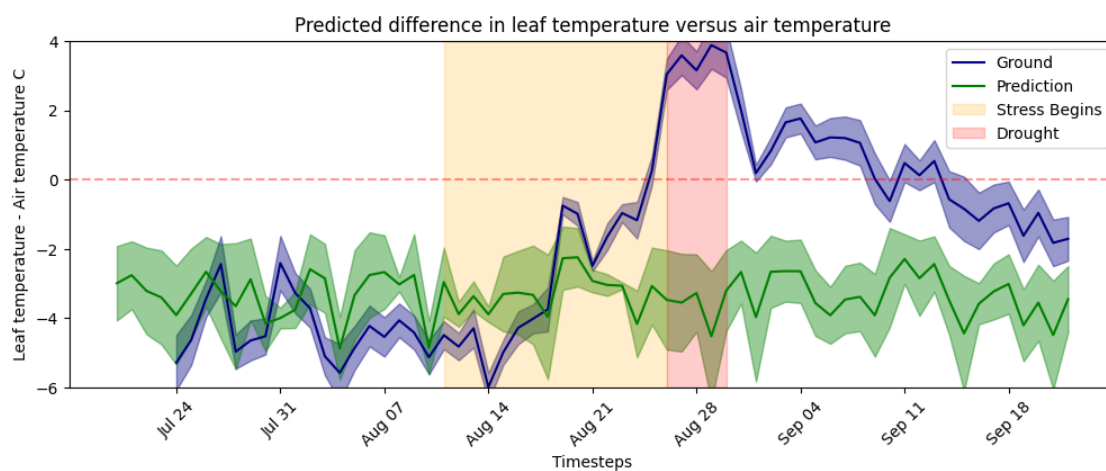
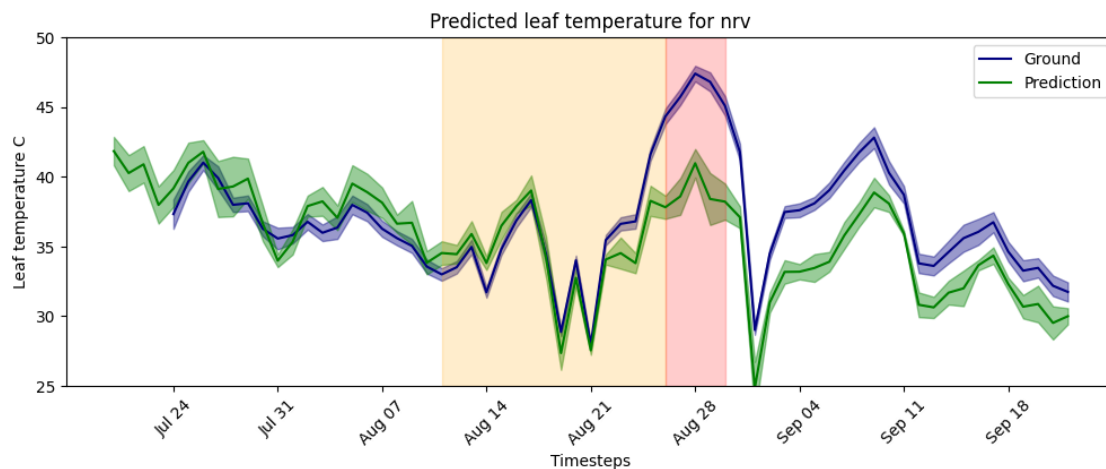
```

)

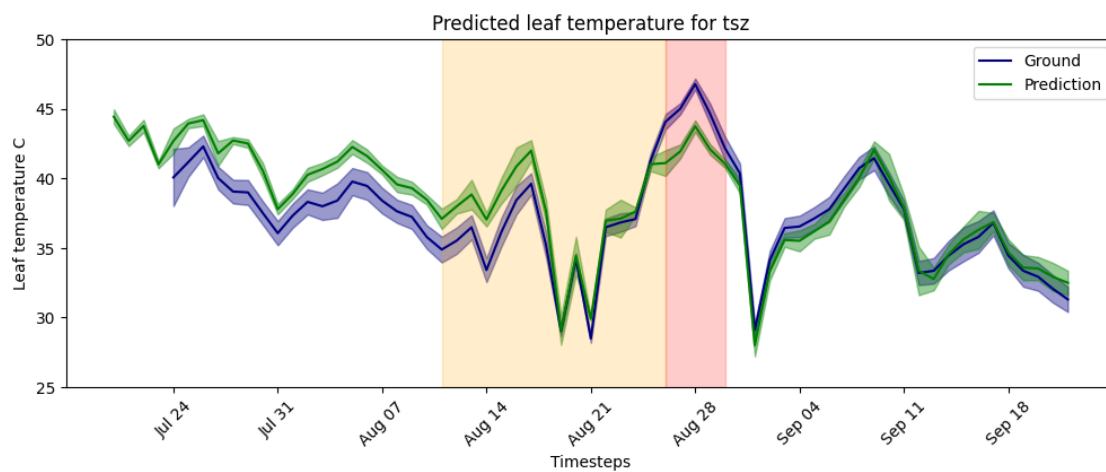
Population: ccr

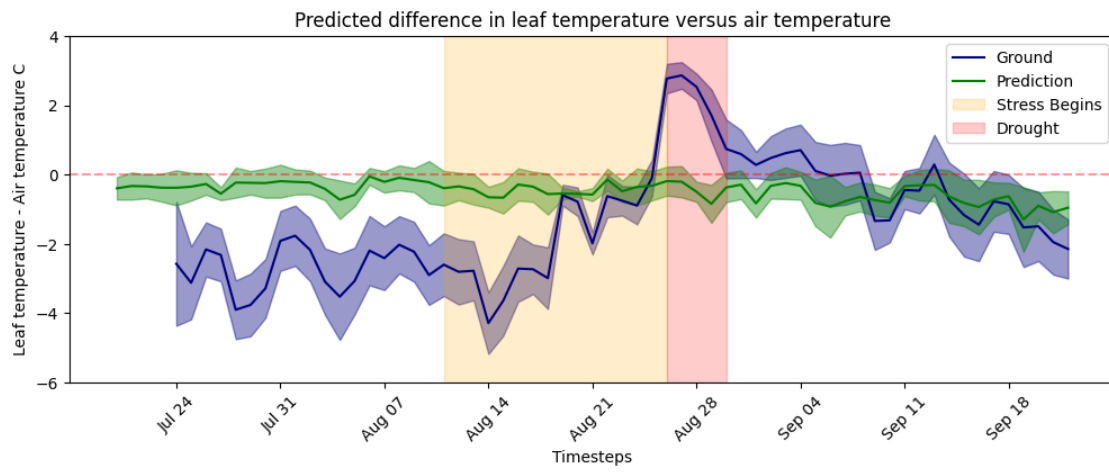


Population: nrv

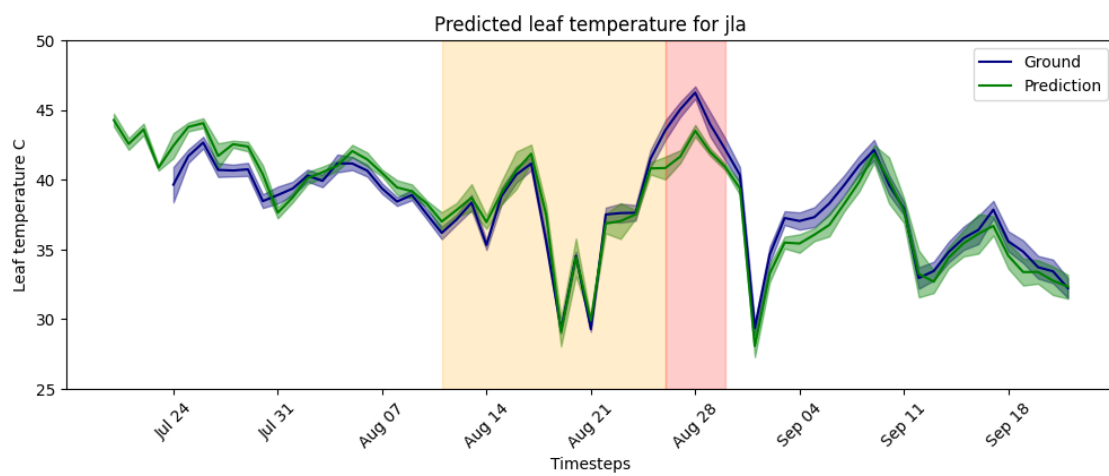


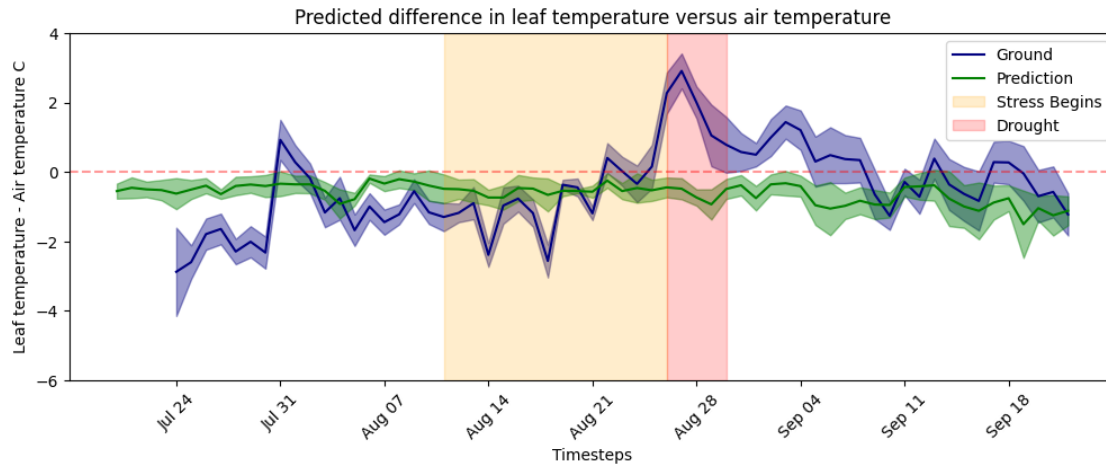
Population: tsz



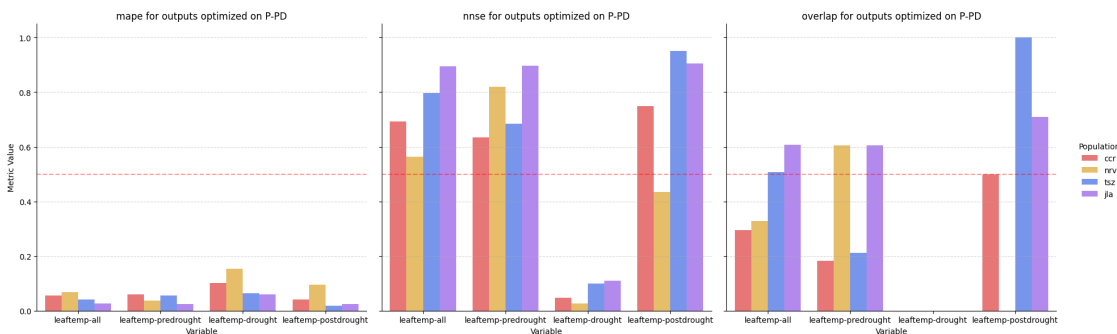


Population: jla





```
[2093]: plot_errors(leaft_fits, metrics_to_plot, ['leaftemp-all',
↳ 'leaftemp-predrought', 'leaftemp-drought', 'leaftemp-postdrought'])
```



## 1.5 Diurnal Plots

```
[2094]: def plot_diurnal(var, day, pred, stderr, ground, low, high):
    plt.figure(figsize=(10, 6))
    plt.plot(range(0, 24), pred.loc[pred['julian-day'] == day][var],
↳ label='Prediction', color='green')
    plt.fill_between(range(0, 24), low.loc[low['julian-day'] == day][var], high.
↳ loc[high['julian-day'] == day][var], color='green', alpha=0.4)
    col_ground = ground.loc[(ground['julian-day'] == day)][[var,
↳ 'standard-time']].dropna()
    plt.scatter(col_ground['standard-time'], col_ground[var], label='Ground
↳ Truth', color='navy')

    m_ground = ground.loc[(ground['julian-day'] == day)].
↳ set_index(['standard-time'])[var].dropna()
```

```

    m_stderr = stderr.loc[(ground['julian-day'] == day)].
    ↪set_index(['standard-time'])[var]].dropna()
    xerr, yerr = get_errors(m_ground, m_stderr)
    for i, (_, row) in enumerate(m_ground.iterrows()):
        plt.errorbar(
            row.name,
            row[var],
            yerr=1.96 * yerr[i],
            xerr=np.expand_dims(xerr[:, i], axis=1),
            color='navy'
        )

    plt.xticks(range(0, 24))
    plt.xlim(0, 23) # Ensure no gap on the left side of the origin
    plt.ylim(0, np.minimum(1000, np.maximum(np.max(pred[var]) + 0.1 * np.
    ↪max(pred[var]), np.max(ground[var]) + 0.1 * np.max(ground[var]))))
    plt.xlabel('Hour of Day')
    plt.ylabel(var)
    plt.title(f'Diurnal Plot of {var} on Julian Day {day}')
    plt.legend()
    plt.grid(False)
    plt.show()

```

```

[2095]: for pop in data.keys():
    print(f"Population: {pop}")

    # Get data for population
    ground = data[pop]['ground']['hourly']
    stderr = data[pop]['ground']['stderr']
    pred = data[pop]['pred'][optim_var]['main']
    low = data[pop]['pred'][optim_var]['low']
    high = data[pop]['pred'][optim_var]['high']

    day = 236
    plot_diurnal("GW", day, pred, stderr, ground, low, high)

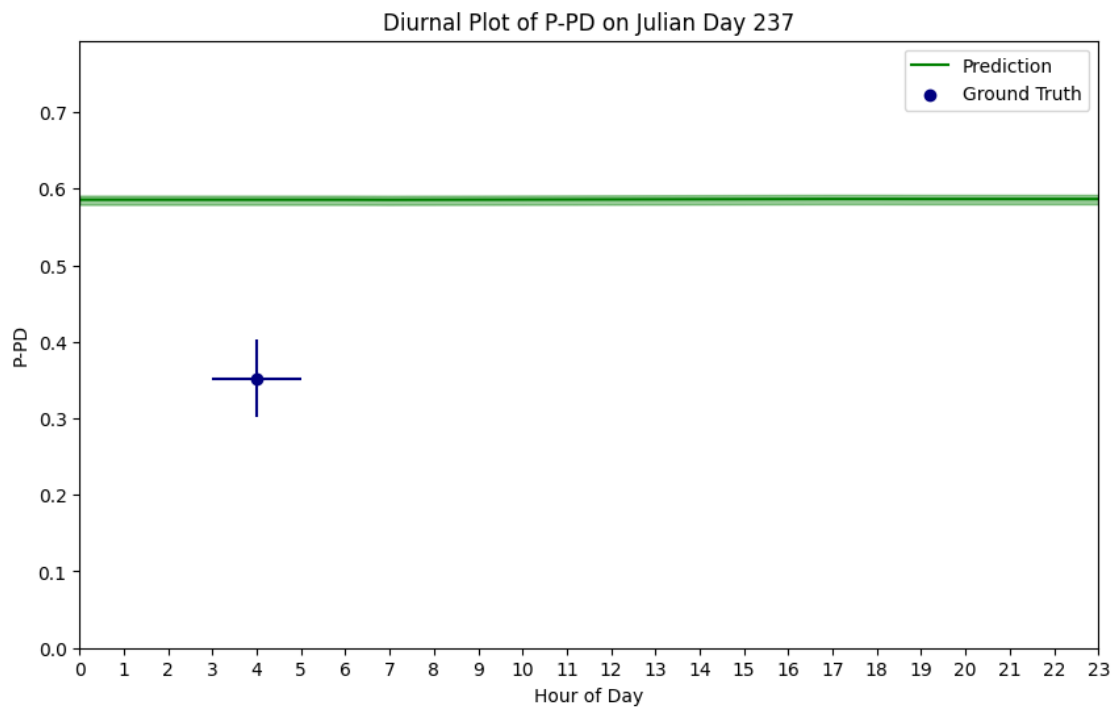
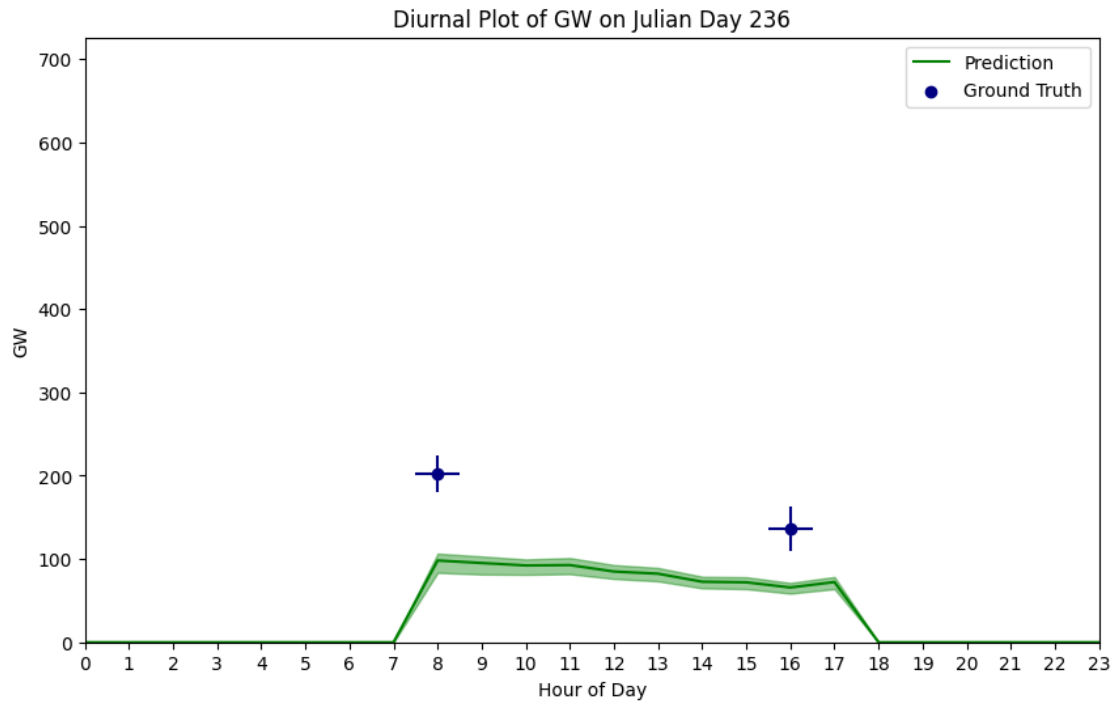
    day = 237
    plot_diurnal("P-PD", day, pred, stderr, ground, low, high)
    plot_diurnal("P-MD", day, pred, stderr, ground, low, high)

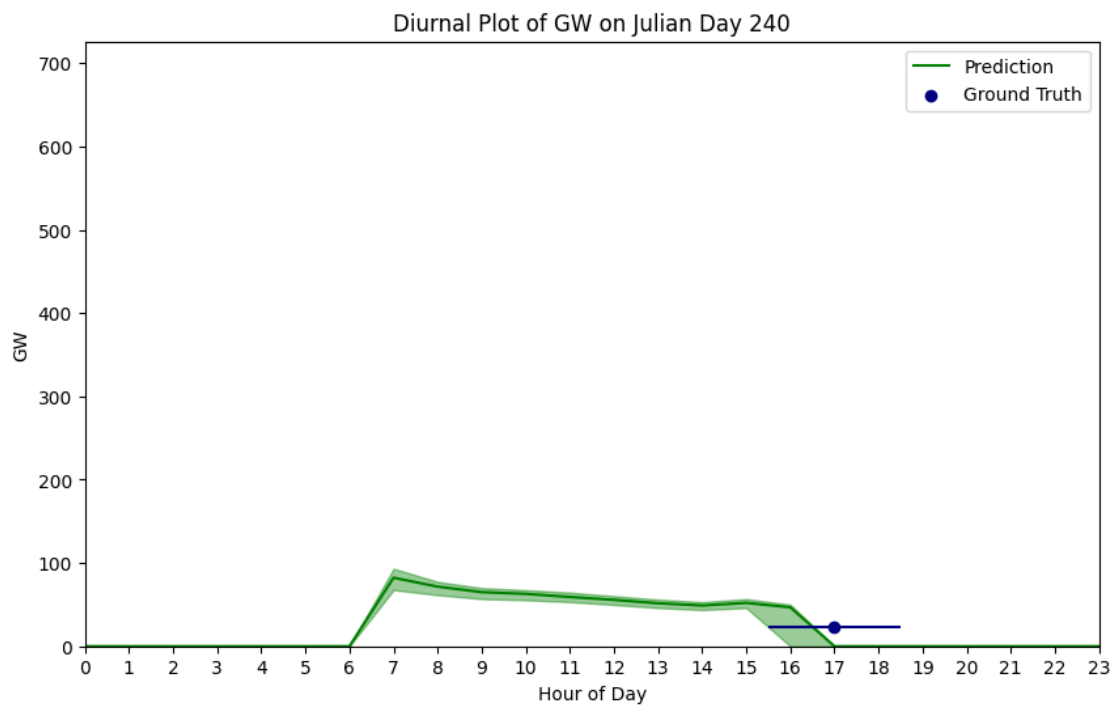
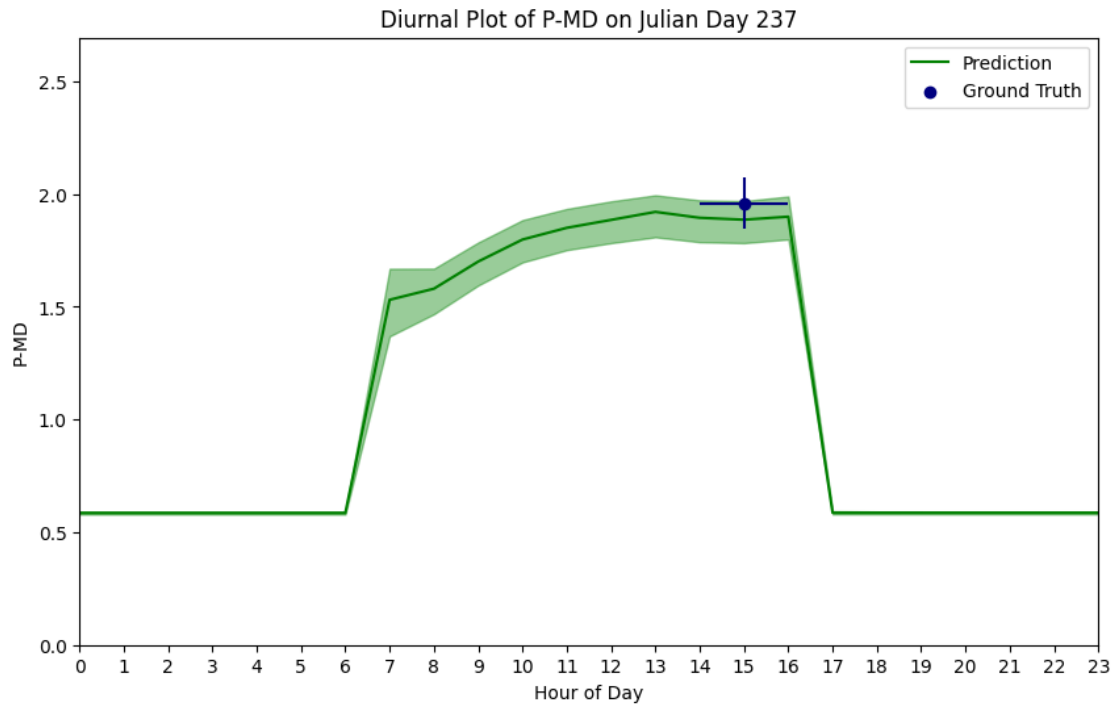
    day = 240
    plot_diurnal("GW", day, pred, stderr, ground, low, high)
    plot_diurnal("P-MD", day, pred, stderr, ground, low, high)

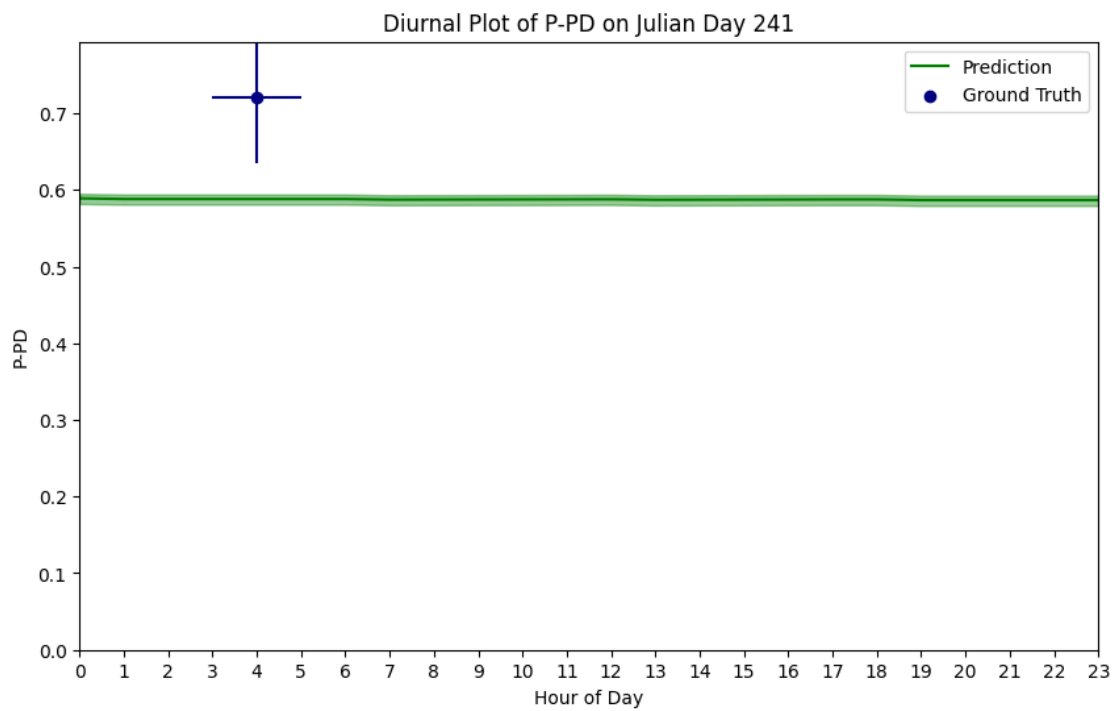
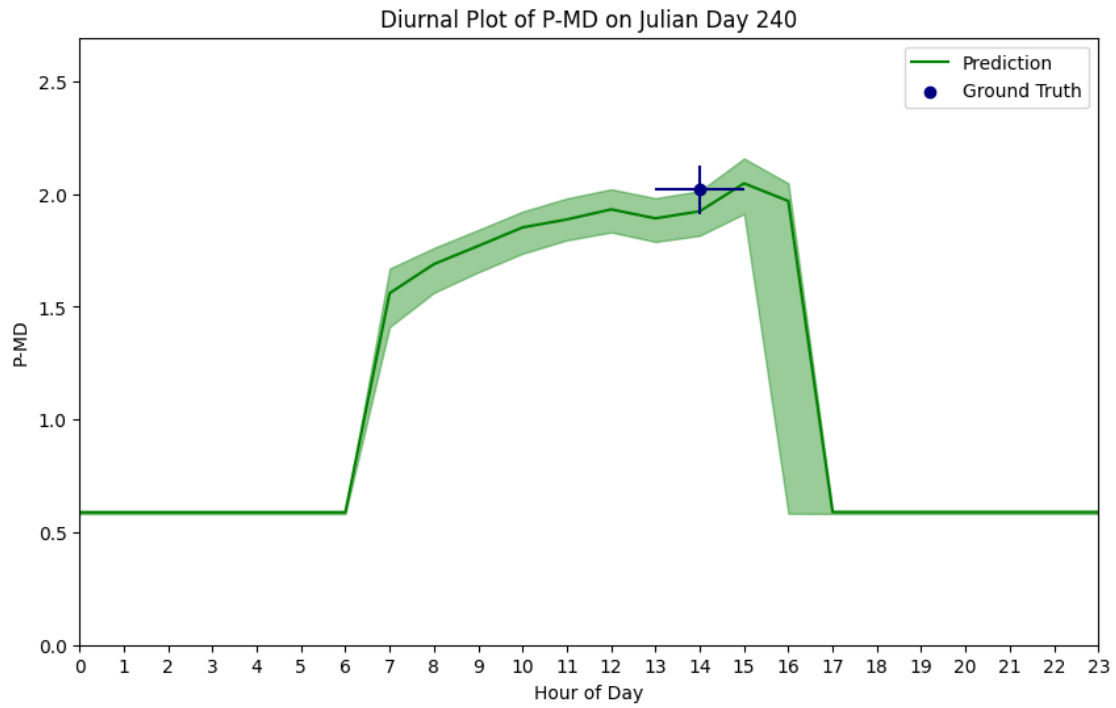
    day = 241
    plot_diurnal("P-PD", day, pred, stderr, ground, low, high)

```

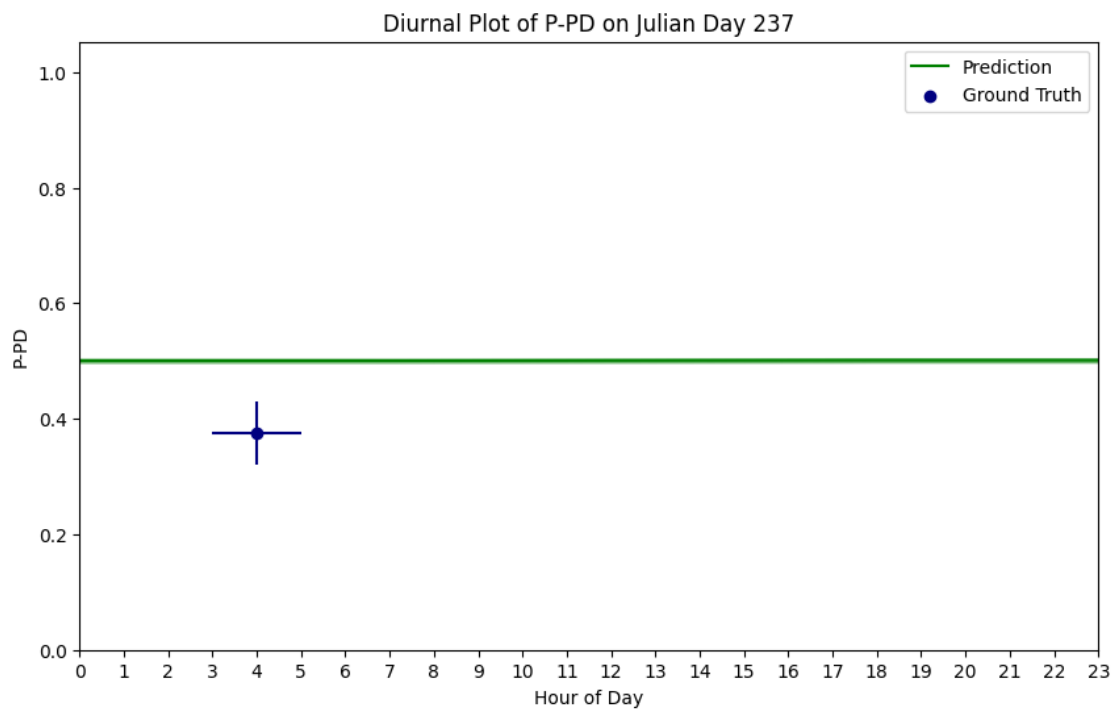
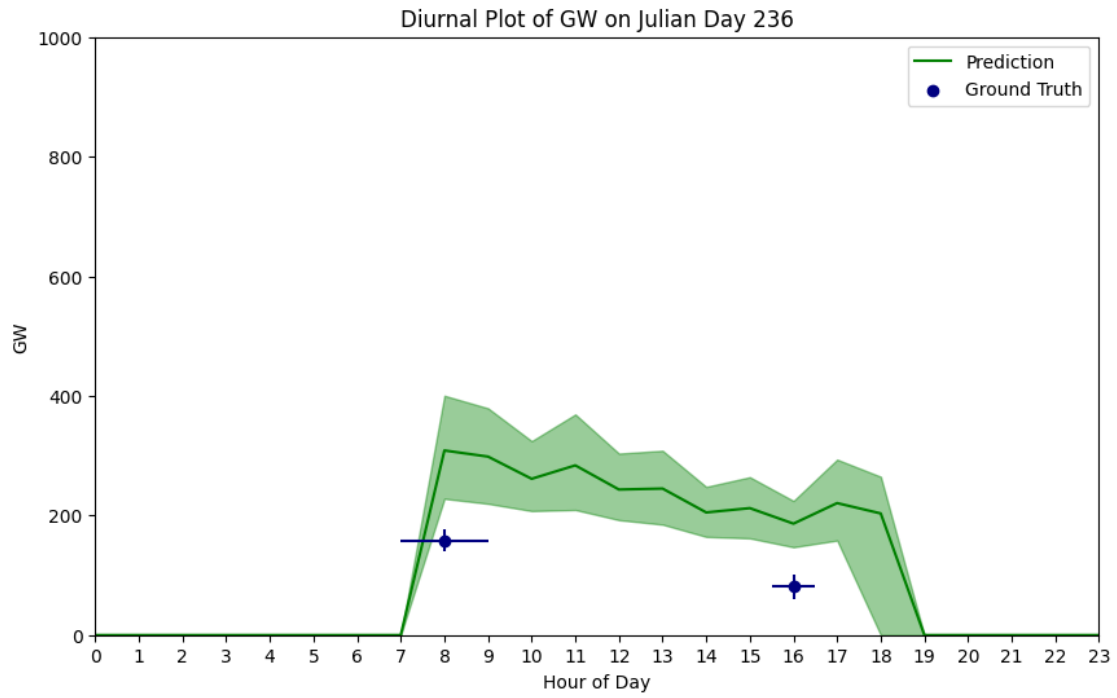
Population: ccr

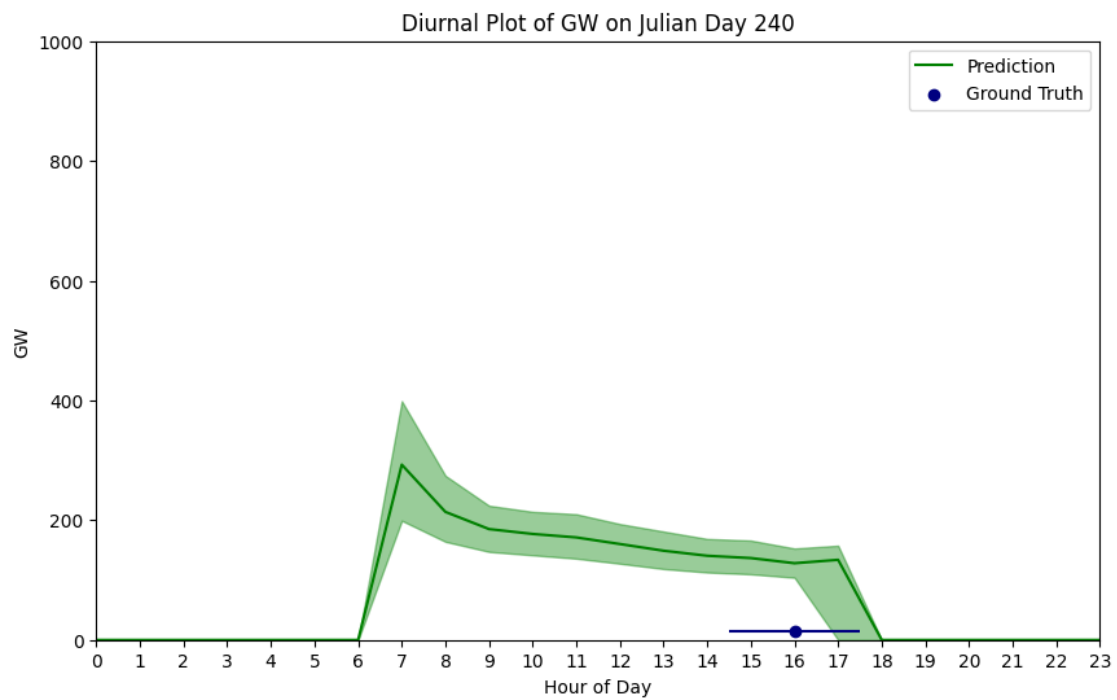
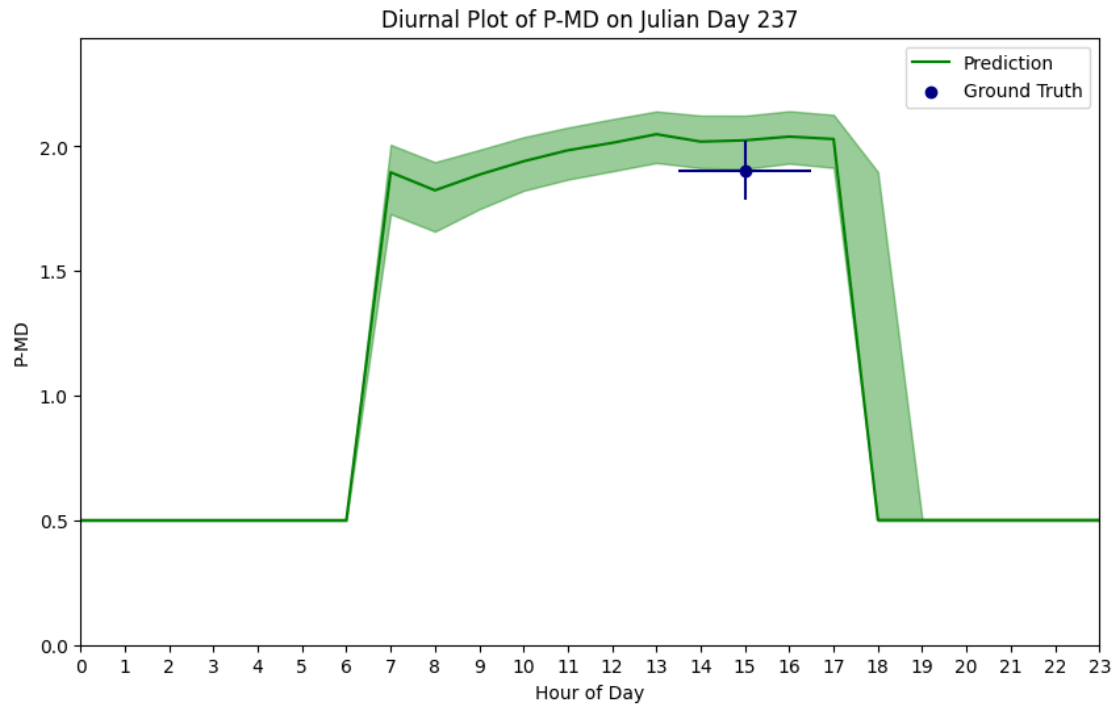


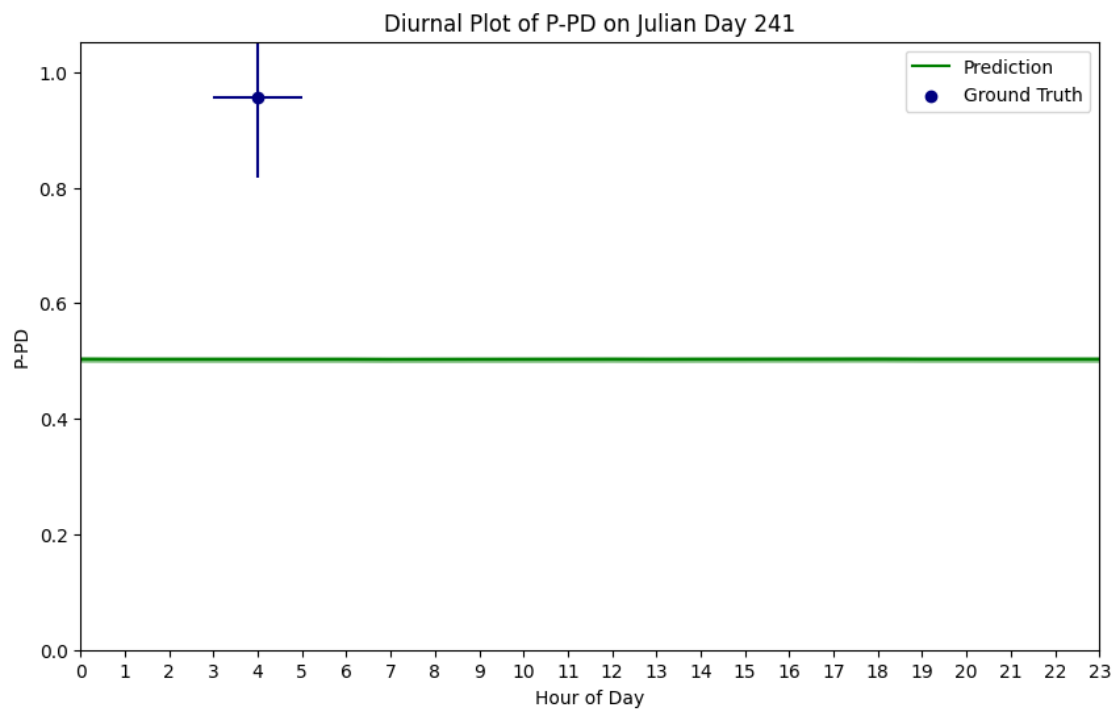
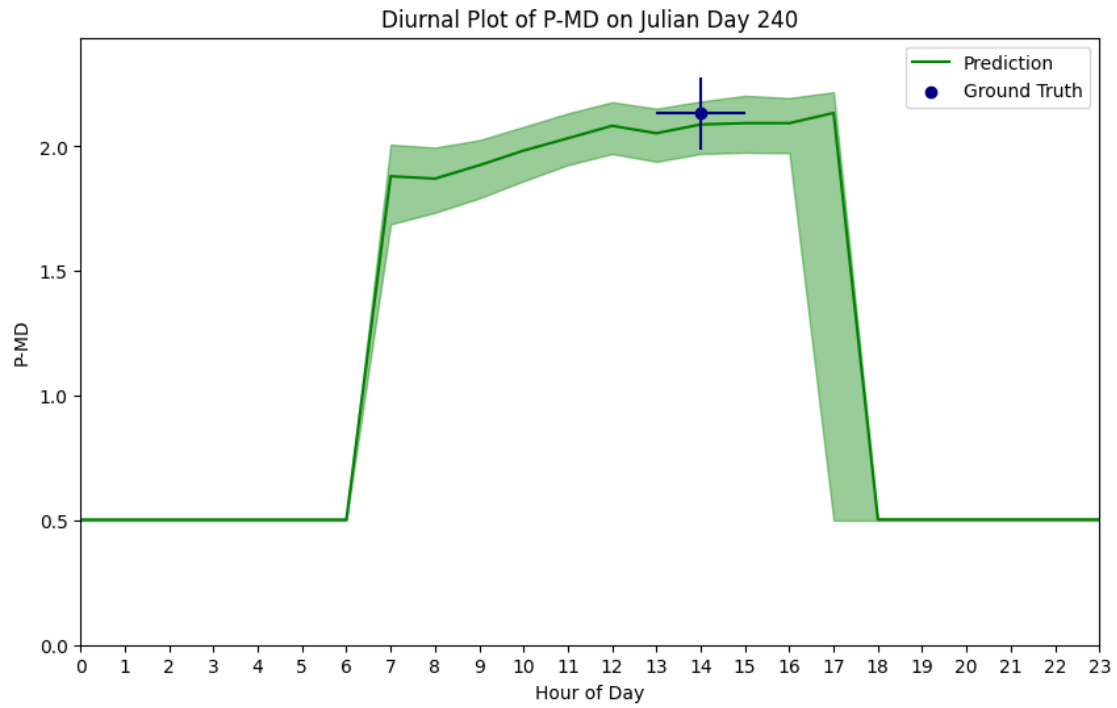




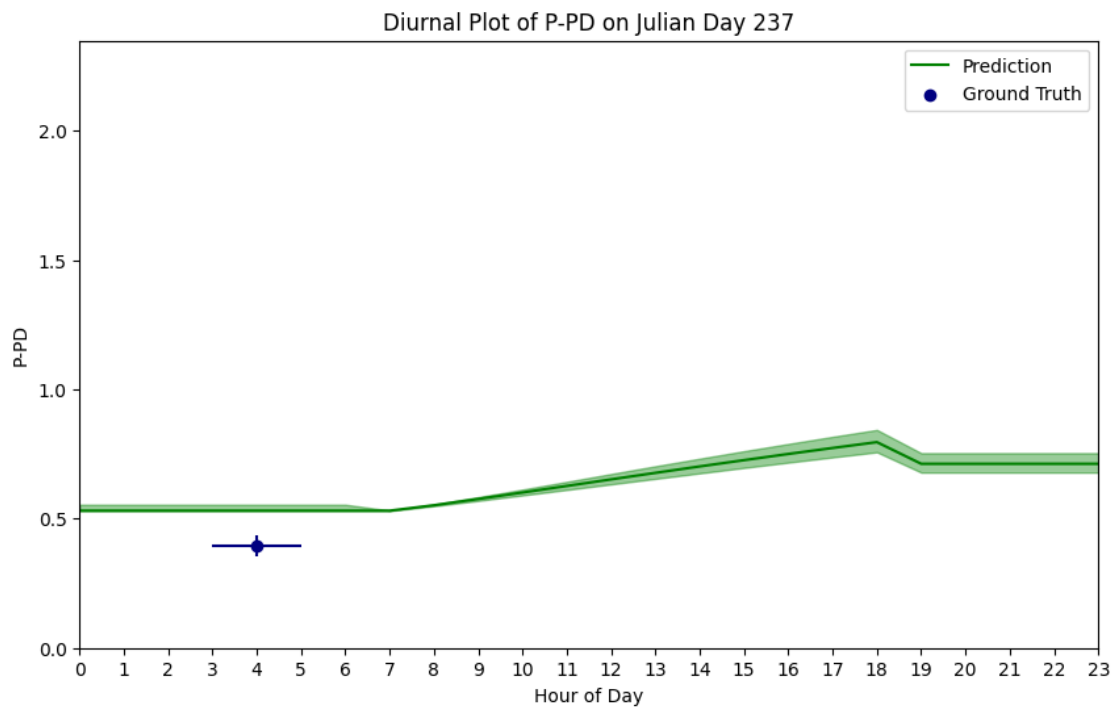
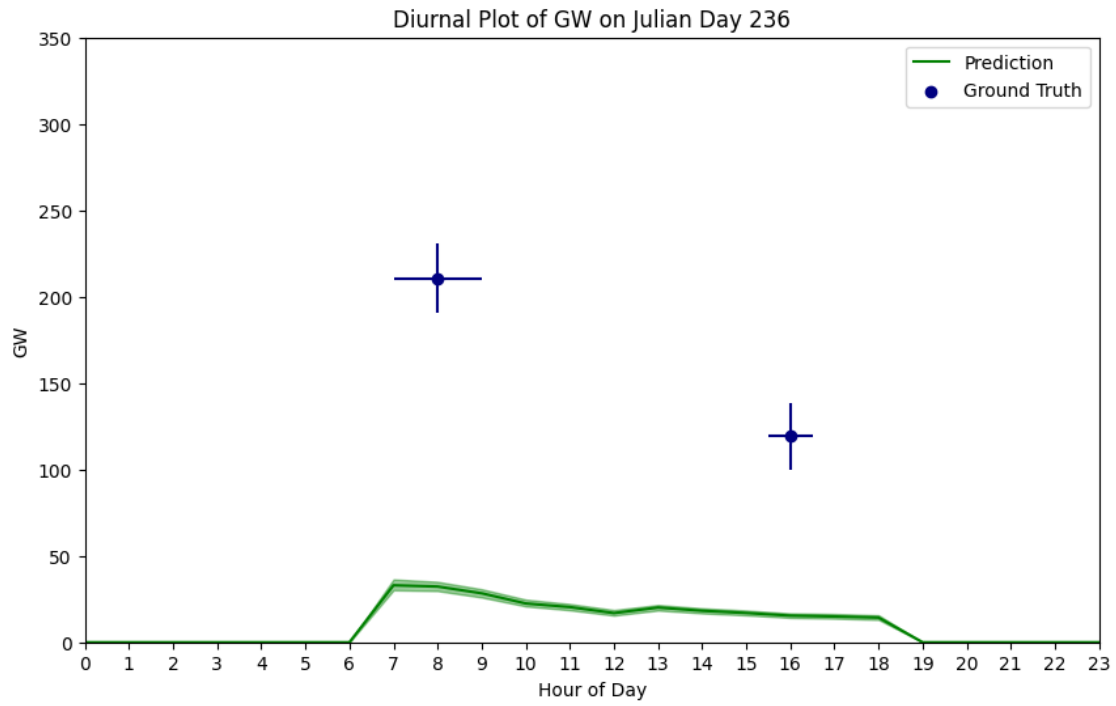
Population: nrv

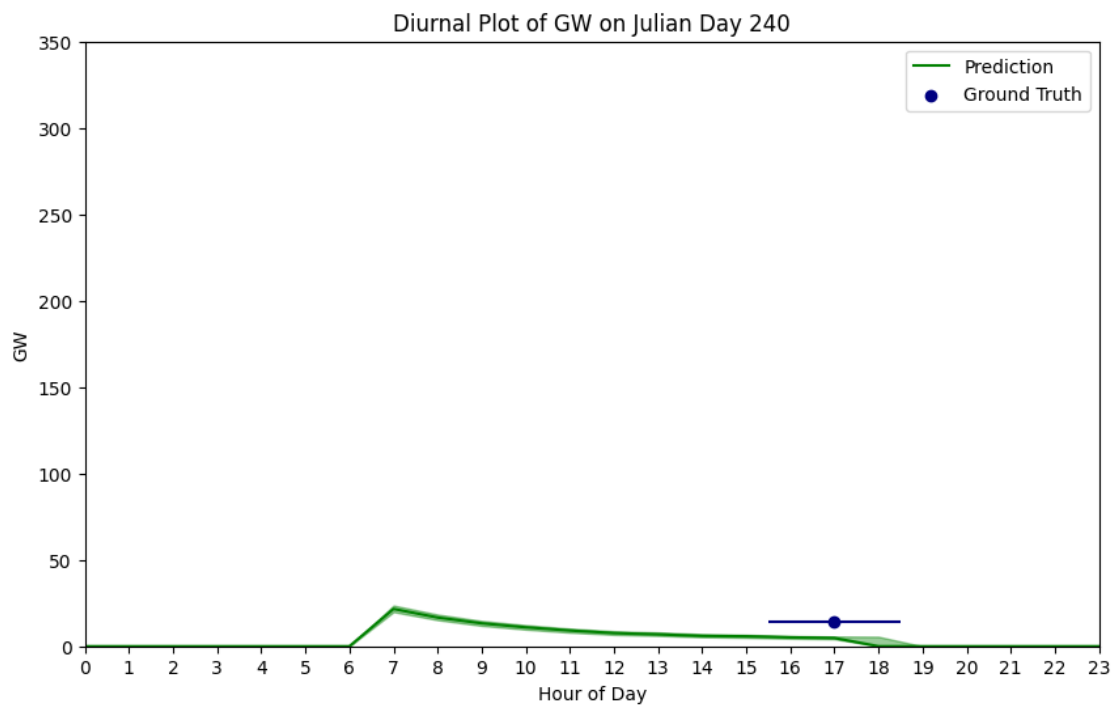
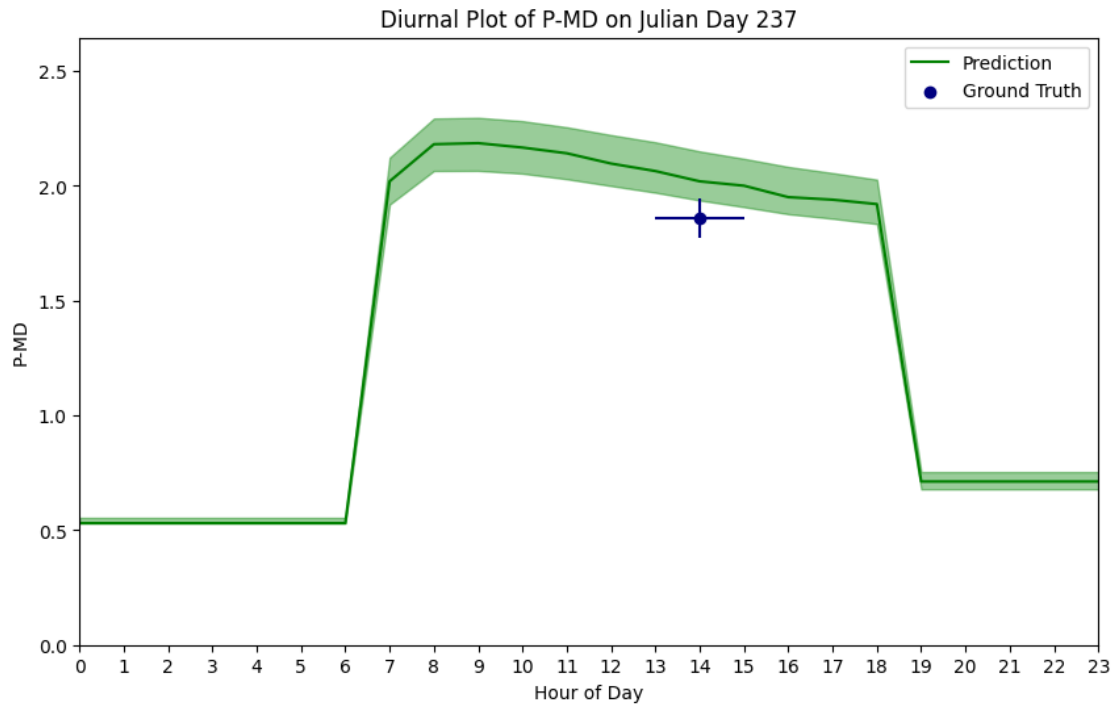


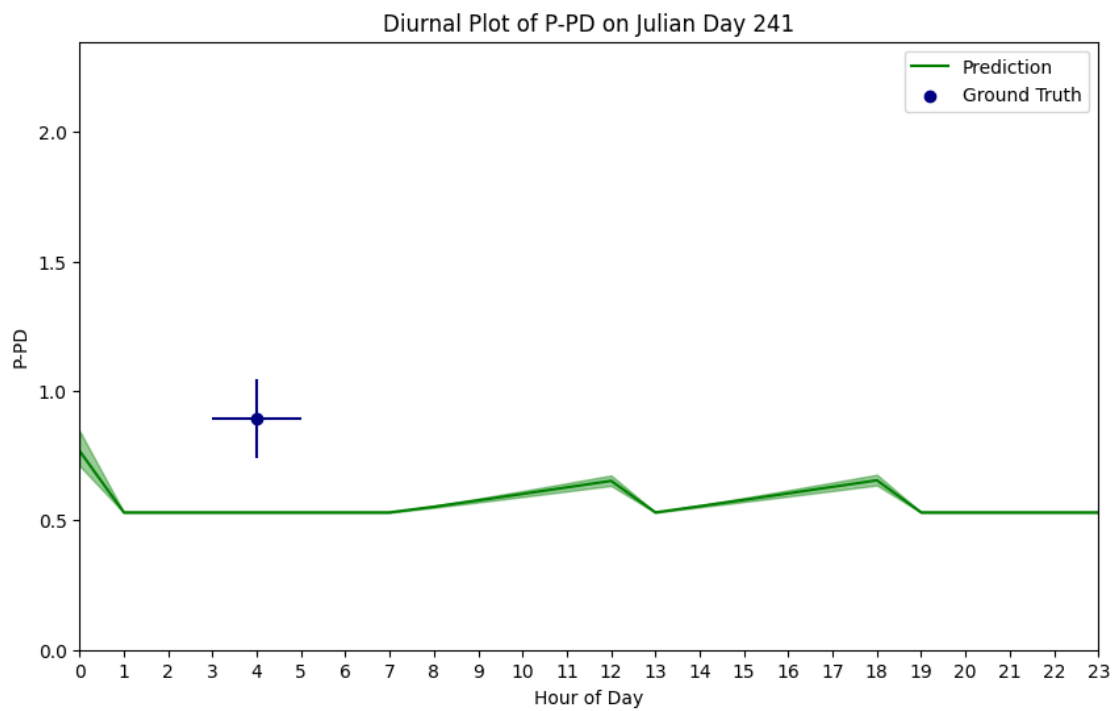
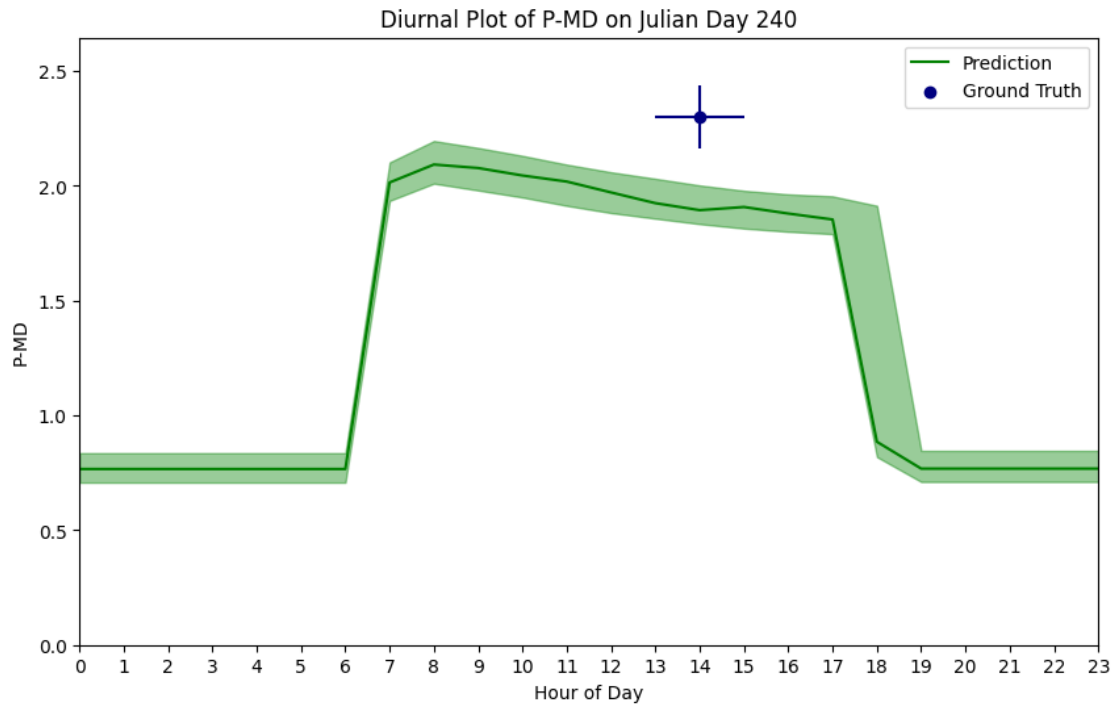




Population: tsz







Population: jla

