GreenNano Analytics – User Guide

Scope of This Guide

This document explains **how to use GreenNano Analytics**, focusing exclusively on:

- required **input files**
- **user-controlled parameters** in the interface
- **output plots and tables**, with guidance on interpretation

This guide is intended for end users (researchers, engineers, analysts) and deliberately avoids implementation details.

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1. Input Data

1.1 AF_vectors.csv (Material-Level Data)

This file defines the materials under investigation.

Required content:

- **Material identifier**: either Original_Index or Material_Name
- **Atomic fractions**: AF_1 … AF_118, representing stoichiometry in element space
- **Performance indicators**:
  - P1 (e.g. temperature stability)
  - P2 (e.g. magnetization)
  - P3 (e.g. coercivity)

Atomic fractions must sum to 1 for each material.

1.2 Materials Database 1.csv (Element-Level Data)

This file contains global information about chemical elements.

Required columns:

- Z (atomic number)
- Annual production (tons/year)
- Global reserves (tons)

Optional columns (if present, they will be used automatically):

- HHI (Herfindahl–Hirschman Index)
- ESG score
- Supply risk
- Companionality (%)

Missing values are handled conservatively and shown explicitly in the outputs.

1.3 MF_sustainability_rank.csv (Sustainability Indicators)

This file provides material-level sustainability scores.

Required columns:

- S1 … S10 (dimensionless scores in the range [0, 1])

These scores represent different sustainability dimensions (environmental, social, economic, geopolitical, etc.).

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2. Sidebar Controls

2.1 Performance Tiers

For each performance indicator (P1, P2, P3), the user defines:

- the number of discrete tiers
- threshold values separating tiers

Raw values are mapped to normalized scores between 0 and 1. This allows heterogeneous performance metrics to be combined consistently.

2.2 Performance Weights

Users assign weights to P1, P2, and P3.

- The sum of the weights is automatically enforced to be 1.
- The resulting **OPS (Overall Performance Score)** is a weighted geometric mean.

Interpretation:

- Higher OPS → better overall performance according to user priorities.

2.3 Sustainability Weights

Users assign weights to S1…S10.

- The sum of the weights **must be exactly 1**.
- If the condition is violated, the app stops and requests correction.

The resulting **SS (Sustainability Score)** is computed as a weighted geometric mean.

Interpretation:

- Low values in any S_i strongly penalize SS.
- Weight choices directly encode sustainability priorities.

2.4 Soft Pareto Tolerances (ε)

Two tolerances define a **soft Pareto set**:

- ε_OPS: allowed degradation in performance
- ε_SS: allowed degradation in sustainability

Asymmetric choices (e.g. stricter ε_SS) express stronger sustainability constraints.

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3. Output Tabs

3.1 Pareto Ranking (OPS vs SS)

What you see:

- Scatter plot of OPS (x-axis) vs SS (y-axis)
- Points classified as:
    - *Optimal Choice* (Pareto or ε-Pareto set)
    - *Standard*

How to read it:

- Top-right region contains the best trade-offs
- A small Pareto set indicates strict constraints
- A large Pareto set indicates relaxed constraints

A table lists the materials belonging to the Pareto set.

3.2 Scalability Map (Weakest-Link Analysis)

What you see:

- x-axis: Long-term scalability (Plong)
- y-axis: Maximum yearly production (Pmax)
- Log–log scale
- Points colored by a selectable metric (SS, HHI, ESG, etc.)

Interpretation:

- Moving top-right corresponds to better scalability
- Grey points indicate missing data for the selected metric
- Colors reveal correlations or tensions between scalability and sustainability

This plot directly visualizes scaling feasibility.

3.3 Production Bottlenecks (Pareto Set)

What you see:

- A ranked list of elements
- Each entry shows how many Pareto materials are limited by that element

Interpretation:

- Frequently occurring elements are structural bottlenecks
- These elements deserve special attention for substitution, recycling, or policy measures

This output connects materials design to supply-chain strategy.

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4. Practical Usage Guidelines

- Start with default weights and ε values
- Adjust sustainability weights first
- Then relax ε_{OPS} before ε_{SS}
- Inspect bottlenecks before selecting candidates

The tool is best used iteratively.

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5. Key Takeaways

- GreenNano Analytics does not provide a single answer
- It reveals constraints, trade-offs, and leverage points
- Interpretability and transparency are core design principles

The outputs should guide informed decision-making, not replace expert judgment.