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AI-Optimized Pyrolysis: A Machine Learning Framework for Predictive Waste-to-Energy Conversion

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1. INTRODUCTION & AIM

THE DUAL CRISIS

- Global MSW generation projected to reach 3.4 billion tons/year by 2050
- Over 60% of waste ends up in landfills, generating methane and contaminating groundwater
- Fossil fuels represent ~80% of global energy; urgent need for sustainable alternatives
- Pyrolysis converts waste into bio-oil, syngas & biochar in a zero-oxygen environment

RESEARCH GAPS ADDRESSED

- Existing studies focus on single feedstocks with limited generalizability
- No standardized predictive yield-optimization tools exist in the literature
- **This study addresses all three gaps with one unified physics-informed framework**

2. RESULTS & DISCUSSION

0.78	0.76	0.59
SYNGAS R^2	BIO-OIL R^2	BIOCHAR R^2

- ✔ XGBoost outperforms RF, SVR, and MLP for pyrolysis data
- ✔ MAE of 2.8–4.3 percentage points across all three outputs
- ✔ Physics constraints enforce mass balance: bio-oil + syngas + biochar ≈ 100%
- ✔ Residual plots confirm unbiased predictions across all phases (Fig. 4)

3. METHODOLOGY

DATASET

- 619 validated experimental scenarios
- 75 biomass feedstock types
- 12 input features (proximate + ultimate composition, process params)

MODEL BENCHMARKING

- XGBoost vs. RF, SVR, MLP
- XGBoost selected for superior non-linear performance
- Multi-output normalization to stabilize gradient behavior

VALIDATION

- 80/20 stratified train-test split
- Stratified 5-fold cross-validation
- Stratified by temperature and feedstock class

PHYSICS CONSTRAINTS

- Mass balance enforced post-processing
- Monotonicity: char yield decreases as T increases
- Thermochemical consistency maintained throughout

Fig. 3 — Feature Importance Rankings (All Phases)

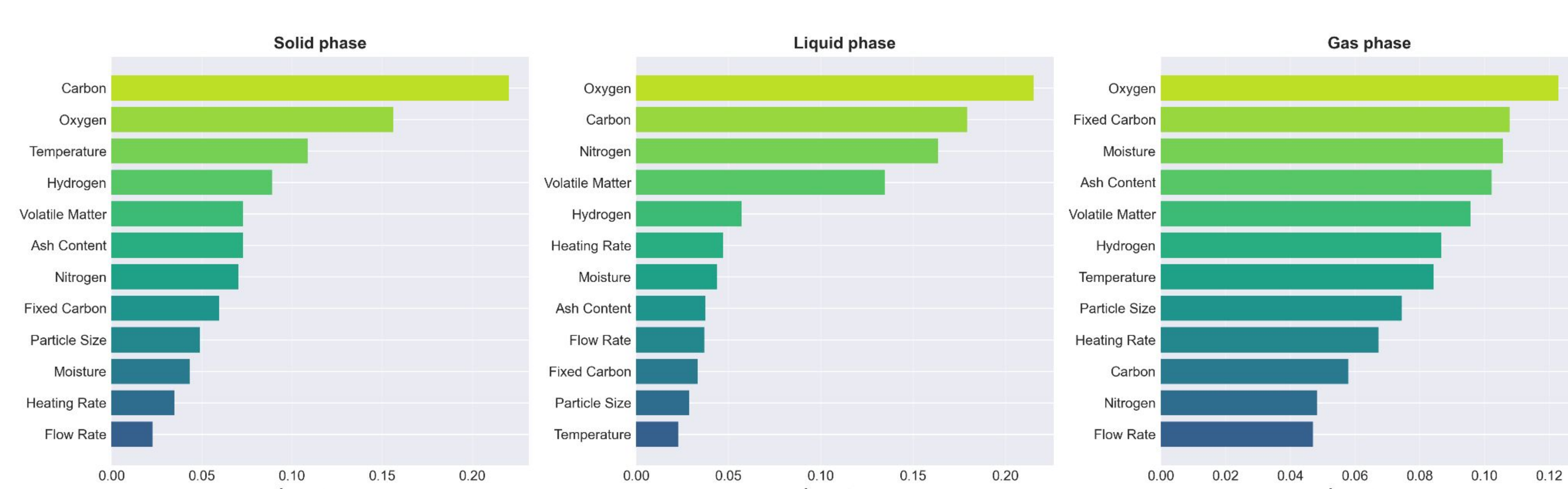
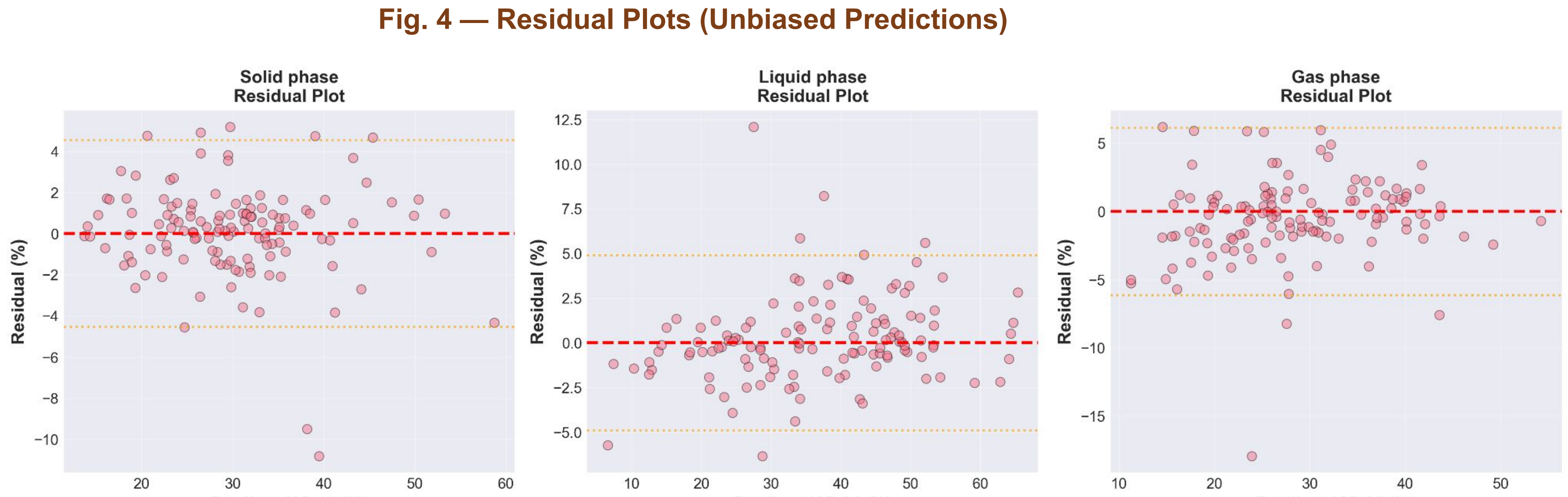


Fig. 4 — Residual Plots (Unbiased Predictions)



4. KEY FINDINGS & FIGURES

Fig. 1 — Model Performance: Predicted vs. Actual Yields

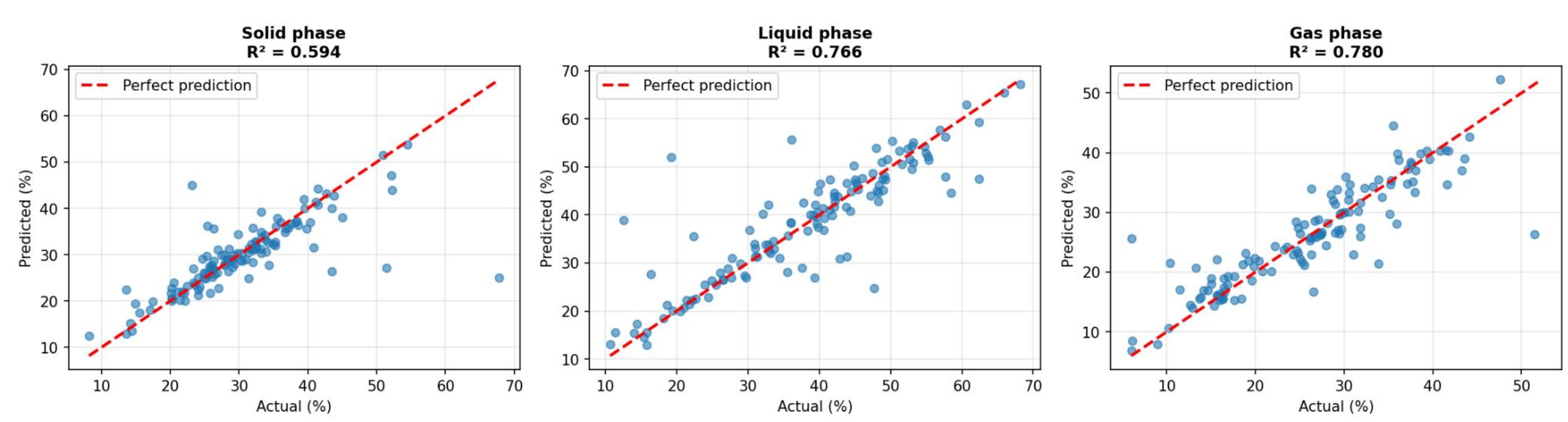


Fig. 2 — Temperature Effect on Product Distribution

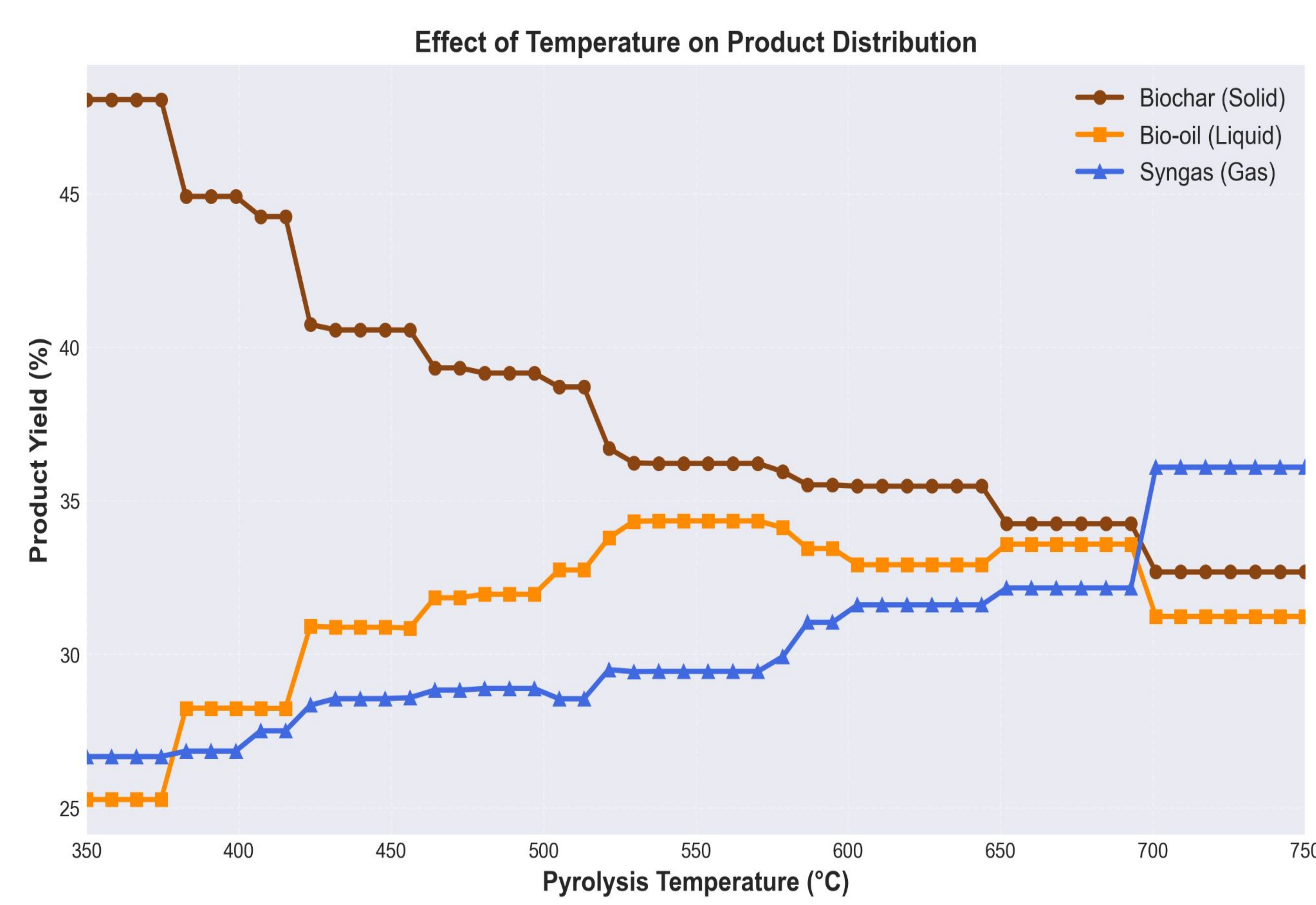
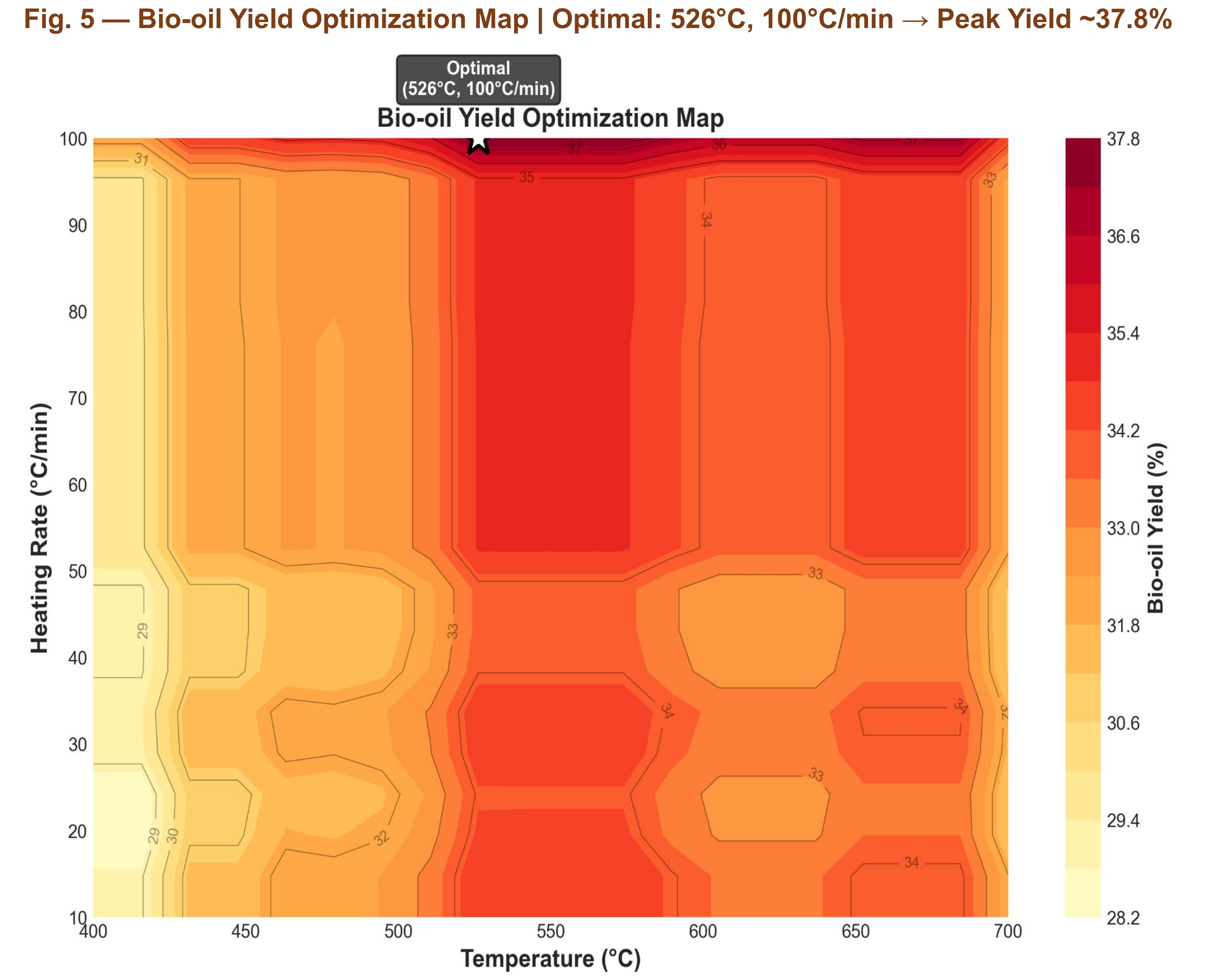


Fig. 5 — Bio-oil Yield Optimization Map | Optimal: 526°C, 100°C/min → Peak Yield ~37.8%



5. CONCLUSIONS

- ✔ First physics-informed ML framework combining multi-feedstock benchmarking with thermodynamic constraints
- ✔ XGBoost outperforms RF, SVR, MLP for high-dimensional chemical pyrolysis data
- ✔ **Optimal bio-oil at 526°C and 100°C/min — peak yield ~37.8%**
- ✔ 50–70% fewer GHG emissions vs. incineration; biochar sequesters C for 500+ years
- ✔ Plant payback 3–6 years; capital ~$5–10M for a mid-size facility

6. FUTURE WORK

- → Expand dataset to co-pyrolysis (plastic-biomass blends) and catalytic cases
- → Integrate real-time sensor data for closed-loop reactor control
- → Apply reinforcement learning for fully autonomous process optimization
- → Develop hybrid physics-ML architectures with uncertainty quantification
- → Link framework to urban circular economy deployment strategies