Public Seminar Presentation

AI-Accelerated Biological Discovery Model

Quantifying the Future of Drug Development

Version 1.1 — Expert-Reviewed Parameters

January 2026

Presentation Outline

1. **Problem Statement**
   Why drug development needs transformation
2. **The Model Framework**
   10-stage pipeline and mathematical foundation
3. **Key Parameters**
   AI growth, saturation, and stage characteristics
4. **Scenario Results**
   Pessimistic to optimistic projections
5. **Key Findings**
   Bottlenecks, sensitivity, and policy implications
6. **Conclusion & Future Work**
   Limitations and next steps

The Drug Development Crisis

10-15 Years

Average time from discovery to market

$2.6 Billion

Average cost to develop a single drug

~5%

Overall success rate from Phase I

The Core Question

How much can AI accelerate this pipeline? Which stages benefit most? What are the bottlenecks?

Sources: Tufts CSDD, FDA CDER Annual Reports 2015-2023

10-Stage Drug Development Pipeline

■ Computational (high AI leverage)

■ Physical (limited AI leverage)

■ Regulatory (policy constrained)

□ Primary Bottleneck

Key Insight: Phase II trials (S7) remain the dominant bottleneck throughout the simulation. Even with 100x AI improvement in computational stages, physical/regulatory constraints limit overall acceleration to ~2.8x.

Mathematical Foundation

1. Logistic AI Growth (v1.1)

$A(t) = Amax / (1 + (Amax - 1) \cdot e^{(-g(t-2024))})$

Amax = ceiling (100x), g = growth rate (0.3-0.7/yr)

2. Saturation Multiplier

$M_i(t) = 1 + (Mmax,i - 1) \cdot (1 - A(t)^{(-k_i)})$

Mmax = max speedup, k = saturation rate

3. Effective Service Rate

$\mu_{i,eff}(t) = (12/\tau_i) \cdot M_i(t) \cdot p_i$

τ = duration (months), p = success probability

4. System Throughput

$\Theta(t) = \min\{\mu_{i,eff}(t)\}$ for all stages i

Bottleneck determines overall speed

5. Progress Rate

$R(t) = \Theta(t) / \Theta(2024)$

Speedup relative to 2024

6. Cumulative Progress

$Y(T) = \int R(t)\, dt$ from 2024 to T

Equivalent years of progress

Interpretation: If Y(2050) = 74, that means 26 calendar years (2024→2050) produce the equivalent of 74 years of traditional scientific progress—a 2.8x acceleration.

Scenario Results: 2024→2050

PESSIMISTIC	BASELINE	OPTIMISTIC	AI WINTER
2.0×	2.8×	4.1×	2.3×
~51 equiv. years	~74 equiv. years	~106 equiv. years	~59 equiv. years
g = 0.30/year	g = 0.50/year	g = 0.70/year	15% probability

Key Insight: Even the optimistic scenario (4.1×) falls far short of the theoretical maximum (~10×) because clinical trial stages have inherent physical and regulatory constraints that AI cannot fully overcome.

📈 Monte Carlo 80% CI: [2.0×, 4.1×] by 2050

🎯 Sobol Index: AI growth rate explains ~85% of variance

Bottleneck Analysis: Why Clinical Trials Dominate

Phase II (S7) - The Persistent Bottleneck

24	33%	2.8×
months	success	max AI

Mathematical Explanation:

μ_eff(S7) = (12/24) × 0.33 × 2.8 = 0.46 at max
μ_eff(S4) = (12/2) × 0.95 × 100 = 570 at max
Ratio: S4 is 1,200× faster than S7!

Why AI Can't Fix This

Human Biology
Patients respond on biological timescales

Safety Requirements
Regulatory observation periods mandatory

Dose Escalation
Sequential testing is irreducible

Patient Recruitment
Enrollment has inherent rate limits

Key Finding: The bottleneck remains at Phase II throughout the entire 2024-2050 simulation period, regardless of scenario. Even with transformative AI in early stages, clinical trial constraints limit overall acceleration.

v1.1: Expert-Reviewed Parameters

Implements 10 P1 (Critical) and 8 P2 (Important) fixes from 15-expert simulated review

Critical Fixes (P1)

P1-4	Wet Lab M_max: 5.0 → 2.5
P1-5	Regulatory Floor: 6-month minimum
P1-6	Logistic AI Growth with ceiling
P1-7	AI Winter Scenario: 15% probability
P2-18	S1 p_success: 0.95 → 0.40

Important Fixes (P2)

P2-11	Bootstrap CIs: 1000 samples, 90% CI
P2-12	Disease-specific Phase II M_max
P2-13	Manufacturing constraints
P2-16	QALY Range: $50K-$200K
P2-17	Vaccine Pathway (COVID precedent)

Net Impact: v1.1 results are ~20-30% more conservative than v1.0, with 2× wider confidence intervals. This reflects greater epistemic humility about future AI capabilities and biological constraints.

Note: Expert review was AI-simulated using Claude (Anthropic)

Policy Implications

🎯 High Impact Interventions

Clinical Trial Reform
Adaptive designs, surrogate endpoints

Regulatory Modernization
Accelerated pathways, rolling submissions

Phase II Innovations
Biomarker-driven patient selection

📉 Lower Impact (Surprisingly)

More AI for Early Stages
Diminishing returns when bottleneck elsewhere

Faster Data Analysis
S4 already saturates at 100×

Hypothesis Generation
Quality > quantity (40% success)

Key Policy Insight: "Investments in AI for early-stage research yield diminishing returns while clinical trial reform could have outsized impact on overall pipeline throughput."

Phase II M_max: 2.8→4.0×
System: 2.8→3.6×

Regulatory floor: 6→3mo
System: 2.8→2.9×

S4 M_max: 100→200×
System: 2.8→2.8× (no change)

Limitations and Caveats

Model Limitations

AI-Simulated Expert Review

Not validated by real domain experts

Aggregate Treatment

Single pipeline; real-world is heterogeneous

Parameter Uncertainty

M_max values are theoretical estimates

Steady-State Assumption

Ignores transient dynamics

What We Did Right

Transparent Methodology

All parameters documented with sources

Calibrated Uncertainty

2× wider CIs; AI Winter captures tail risk

Conservative Estimates

Physical constraints explicitly modeled

Sensitivity Analysis

Sobol indices identify key parameters

Recommended Next Steps: (1) Real expert panel validation, (2) Disease-specific models, (3) Monte Carlo on all parameters, (4) Integration with economic models for cost-benefit analysis.

Key Takeaways

2.0-4.1× Acceleration

By 2050, AI could compress 26 years into 51-106 equivalent years (80% CI)

Bottlenecks Persist

Phase II trials remain rate-limiting; biological constraints cap AI's impact

Policy Focus

Clinical trial reform offers higher leverage than more AI in early stages

> "AI is a powerful tool for drug development acceleration, but it works best when we focus on the bottlenecks—not just the stages where AI excels."

Model	Stages	Baseline	Bottleneck
v1.1	10	2.8×	Phase II

Thank You

Questions & Discussion

Resources & Links

Interactive Demo	Website	Documentation
EXPLANATION_SIMPLE.html	jang1563.github.io	PROJECT_BIBLE.md

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