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New Trends in Parameter Identification in Mathematical Model

Approximate Bayesian Computation - ABC

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OUTLINE

1. INTRODUCTION

2. APROXIMATION BAYESIAN COMPUTATION - ABC

3. CASE OF STUDY - RESIDENCE TIME

3.1 RESULTS

3.2 SIMULATED MEASUREMENTS

3.3 ACTUAL MEASUREMENTS

1. INTRODUCTION

Why use algorithms of model selection?

Many hypotheses

Many models

Verify all models simultaneously

1. INTRODUCTION

AKAIKE

$$AIC = -2\log\left[L\left(\hat{\theta}\right)\right] + 2(Np)$$

Where:

$L(.)$ is the likelihood

Np is the number of parameters

AKAIKE

$$AICc = -2\log\left[L\left(\hat{\theta}\right)\right] + 2Np\frac{2Np+1}{N_m - Np - 1}$$

Where:

N_m is the number of measurements

The best model imply the lowest values of AIC and AICc

1. INTRODUCTION

AKAIKE

$$AIC = -2\log\left[L(\hat{\theta})\right] + 2(Np)$$

Where:

$L(.)$ is the likelihood

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AKAIKE

$$AICc = -2\log\left[L(\hat{\theta})\right] + 2Np \frac{2Np + 1}{N_m - Np - 1}$$

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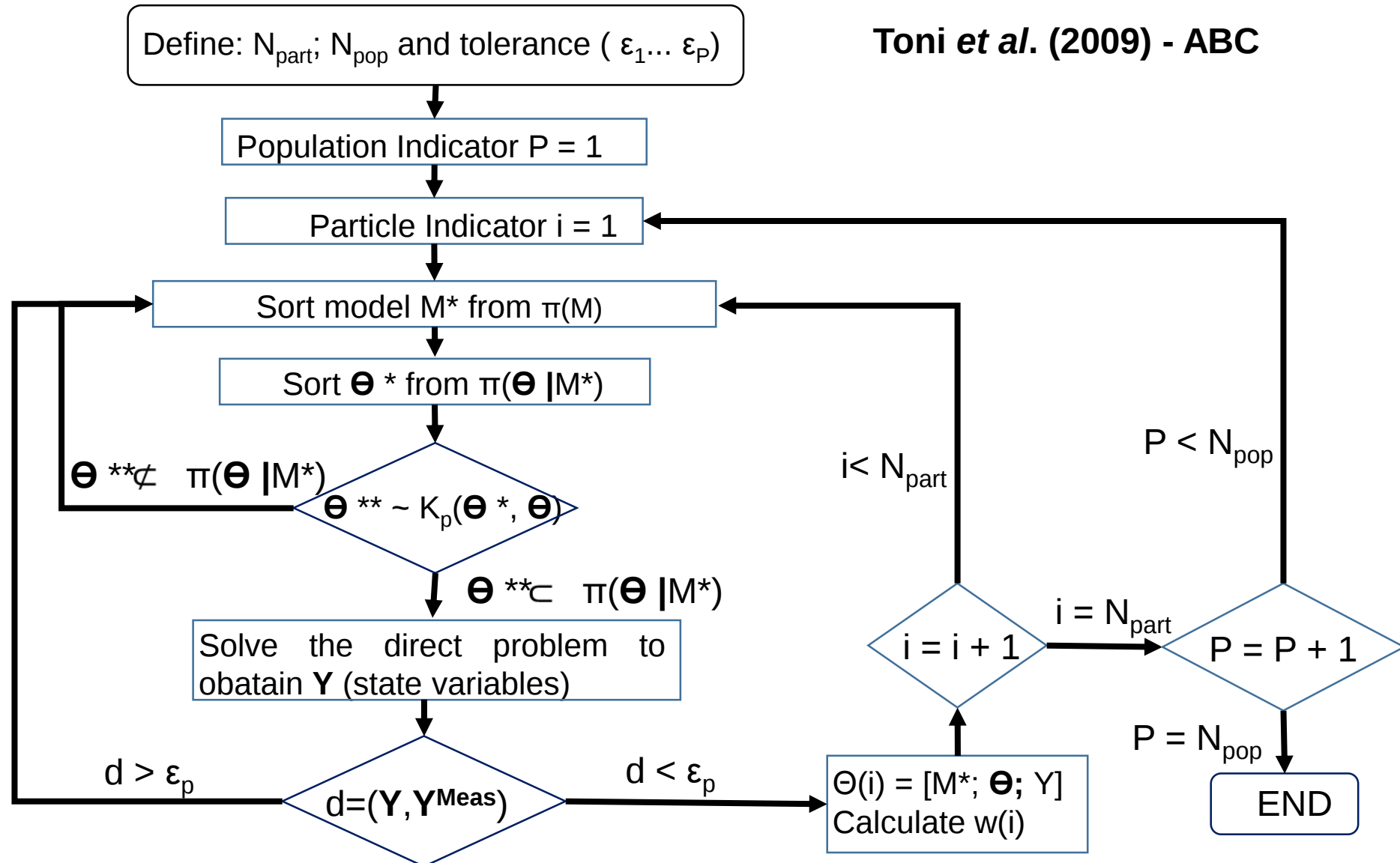
What to do when it is difficult to model the likelihood?



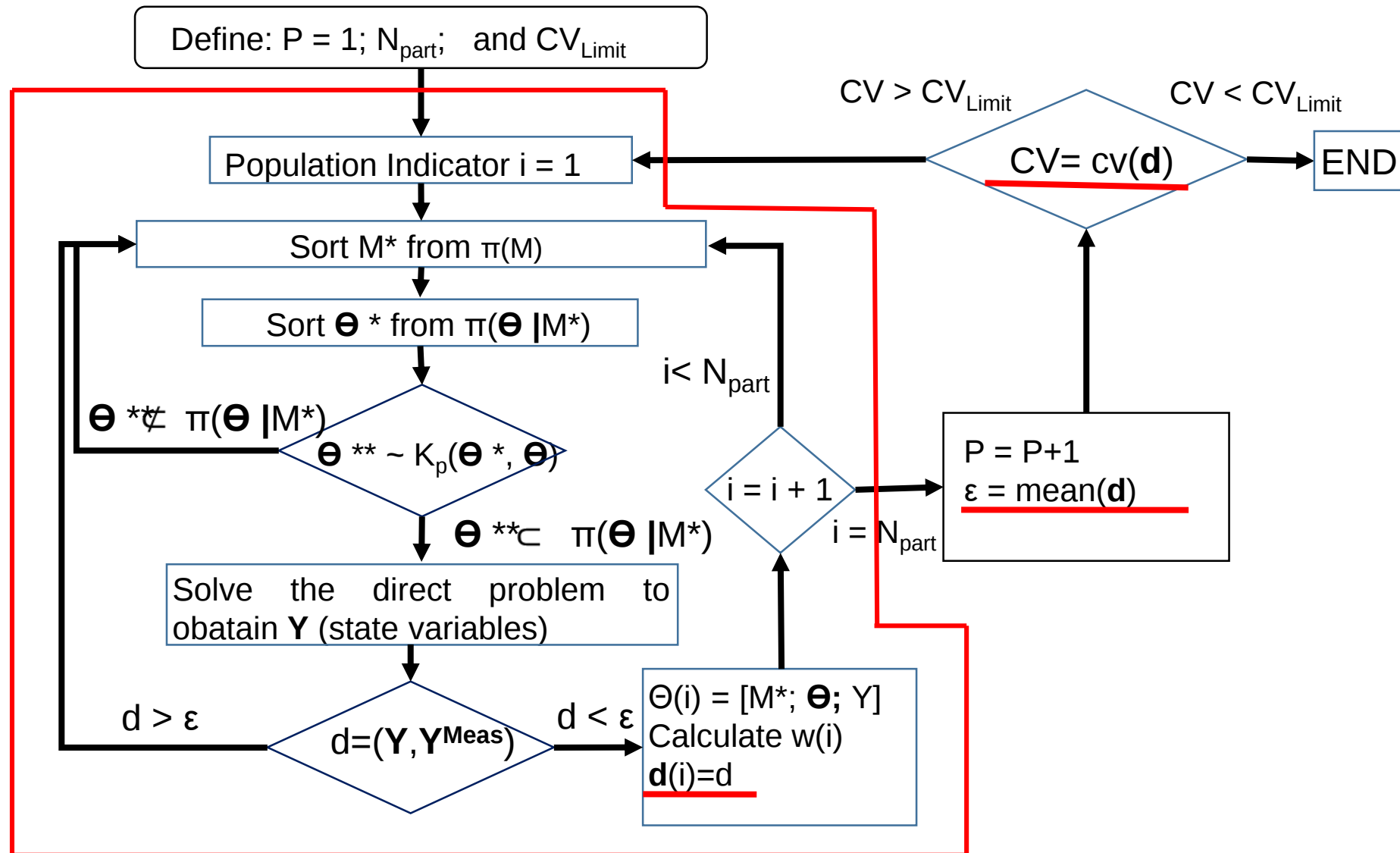
Use the Approximation Bayesian Computation because this technique does not require to model the likelihood

2. APROXIMATION BAYESIAN COMPUTATION - ABC

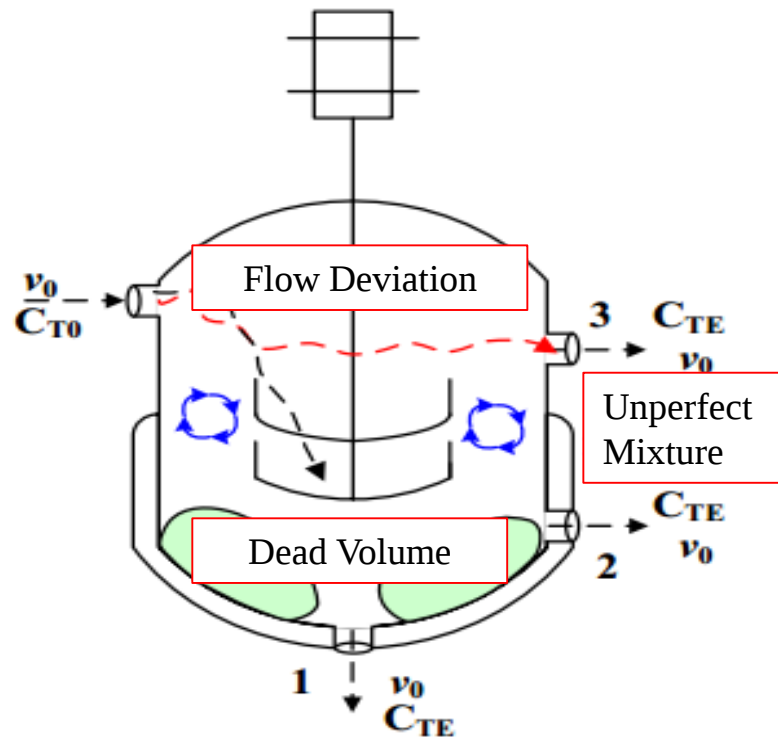
Toni *et al.* (2009) - ABC



2. APROXIMATION BAYESIAN COMPUTATION - ABC



Case of Study 1 – Residence Time



Flow Deviation

β

Dead Volume

α

Models to Distribution Time Residence (RTD)

Model 1

$$C_{TE}(t) = C_{T_0} \left[1 - e^{-\left(\frac{t}{\alpha\tau}\right)} \right]$$

$$F(t) = 1 - e^{-\left(\frac{t}{\alpha\tau}\right)}$$

$$E(t) = \frac{1}{\alpha\tau} e^{-\left(\frac{t}{\alpha\tau}\right)}$$

Model 2

$$C_{TE}(t) = C_{T_0} \left[1 - (1 - \beta) e^{\left(\frac{(1-\beta)t}{\tau}\right)} \right]$$

$$F(t) = 1 - (1 - \beta) e^{\left(\frac{(1-\beta)t}{\tau}\right)}$$

$$E(t) = \frac{(1 - \beta)^2}{\tau} e^{\frac{(1-\beta)t}{\tau}}$$

Model 3

$$\alpha\tau \frac{dC_{T_1}(t)}{dt} = C_{T_0} + (1 - \beta)C_{T_2} - (1 + \beta)C_{T_1}$$

$$(1 - \alpha)\tau \frac{dC_{T_2}(t)}{dt} = \beta C_{T_1} - (1 - \beta)C_{T_2}$$



Specific Cases

Model 3 converges to model 1 when:

$$\beta = 0$$

Model 3 converges to model 2 when:

$$\alpha = 0$$



VERIFICATION

Simulated Data from:

Model 1

Model 2

Model 3

Models 1 and 2

VALIDATION

Experimental Data

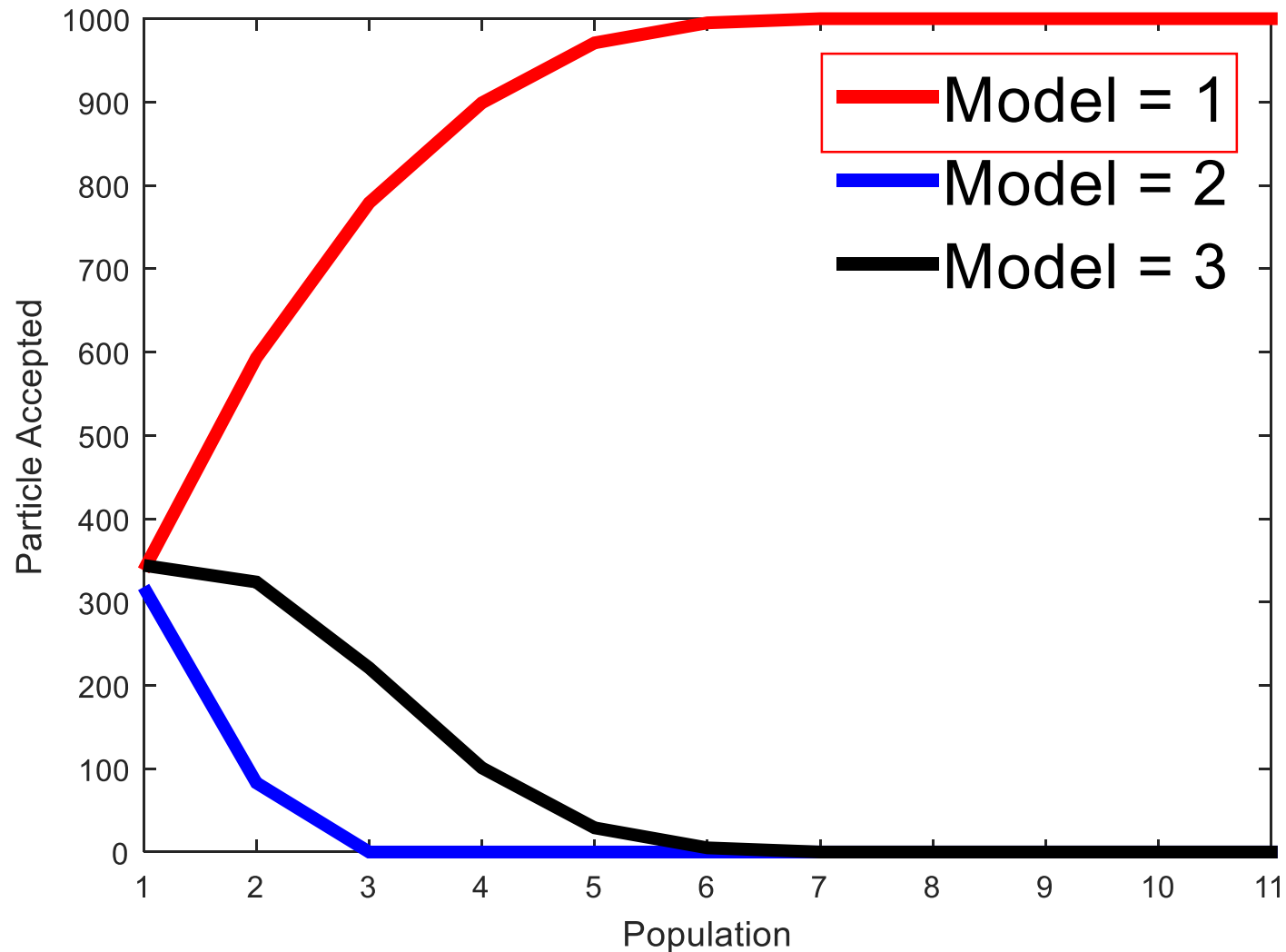
Parameters Reference $\alpha = 0.5$ $\beta = 0.5$

$$C^{Meas} = N(C^{exact}, 0.01C^{exact})$$

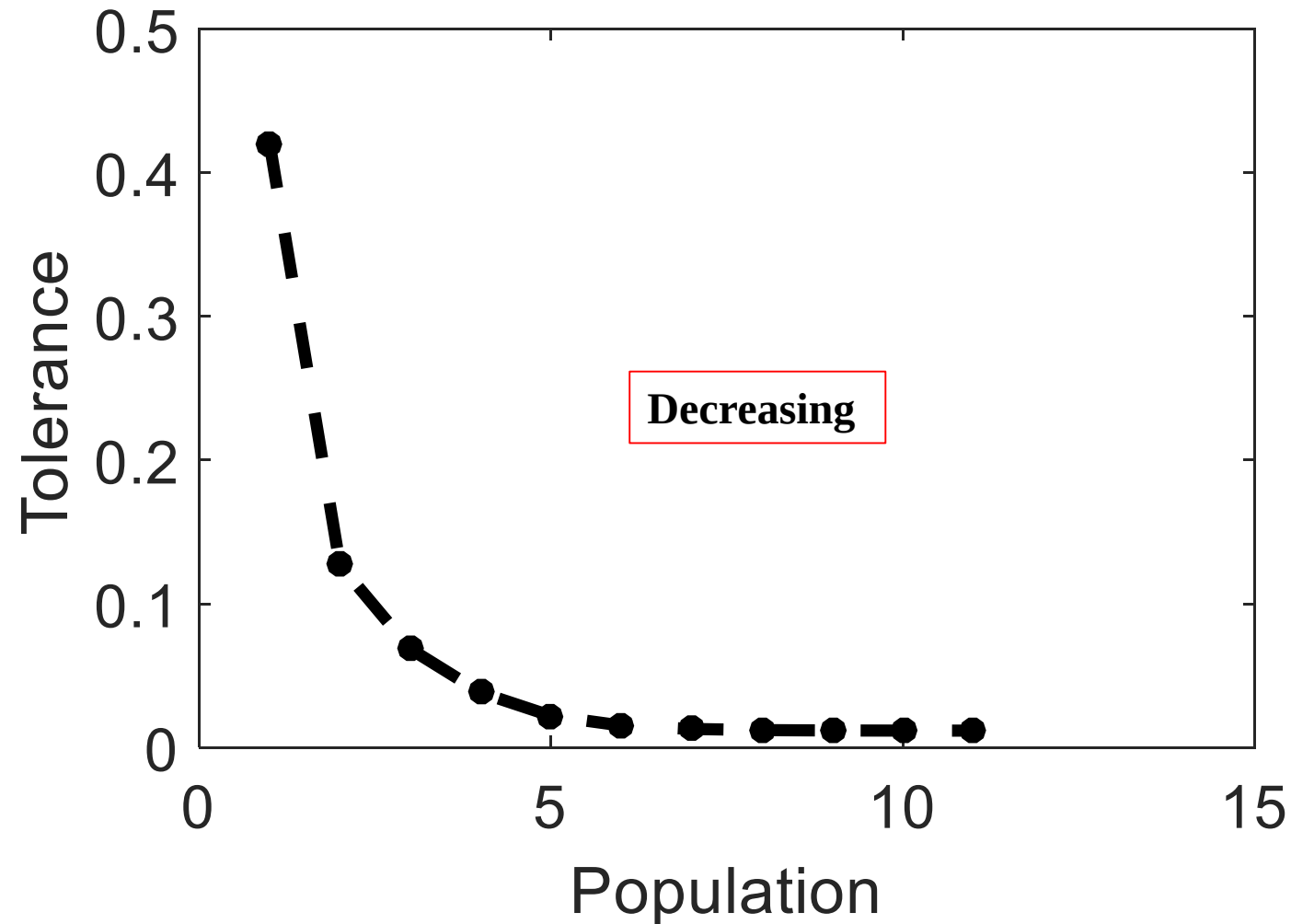
Prior distribution $Uniform[0 \ 1]$

1000 particles

Simulated Data Generated from Model 1

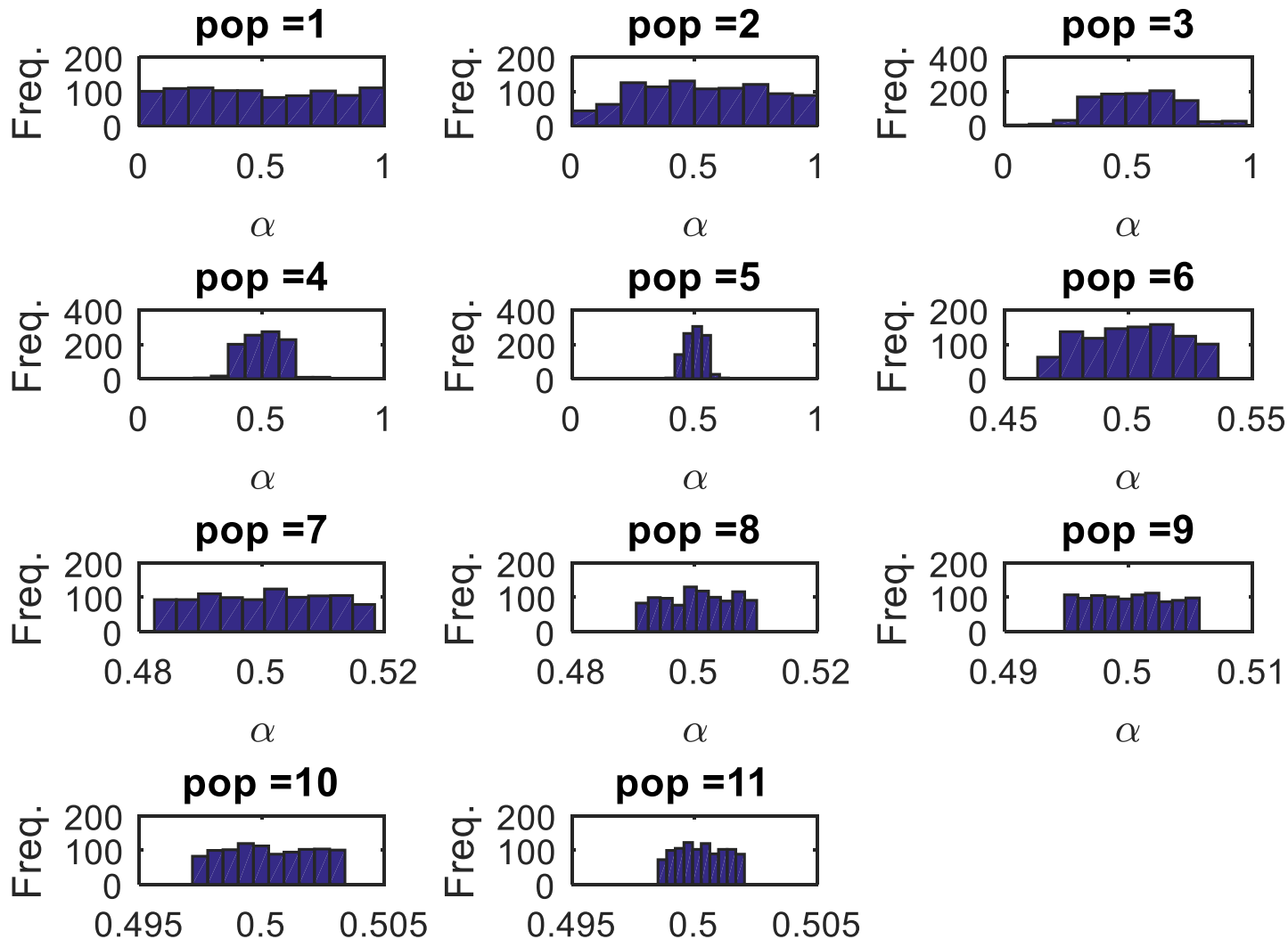


Simulated Data Generated from Model 1



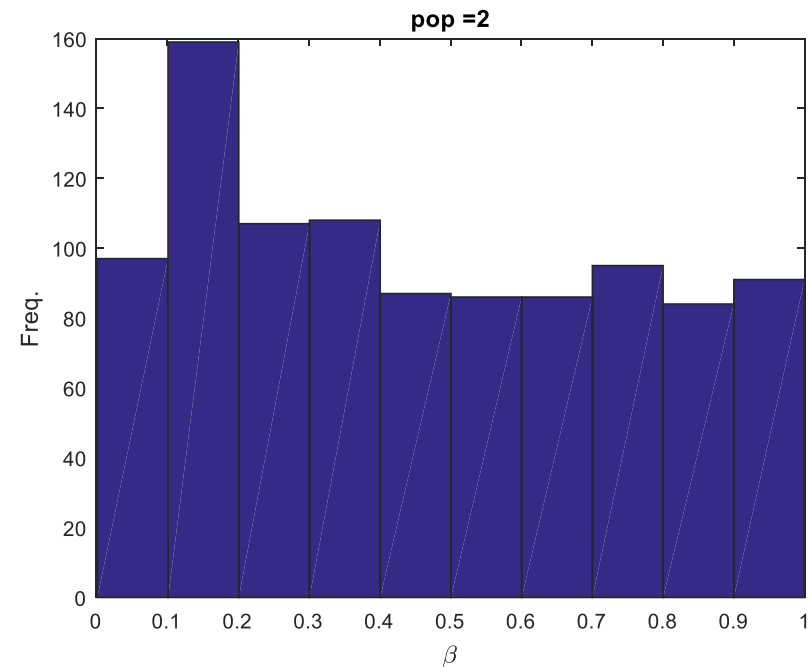
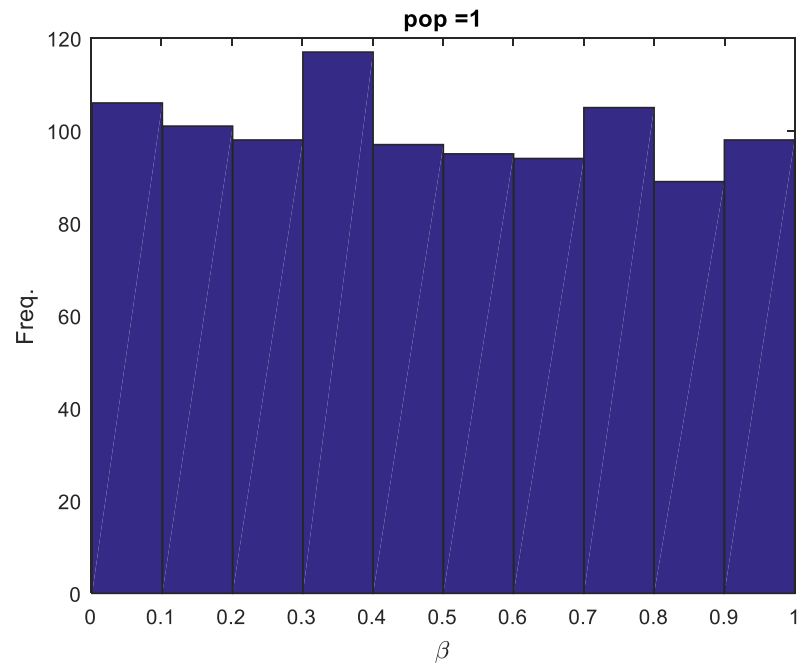
Simulated Data Generated from Model 1 - Modelo 1 (Selected)

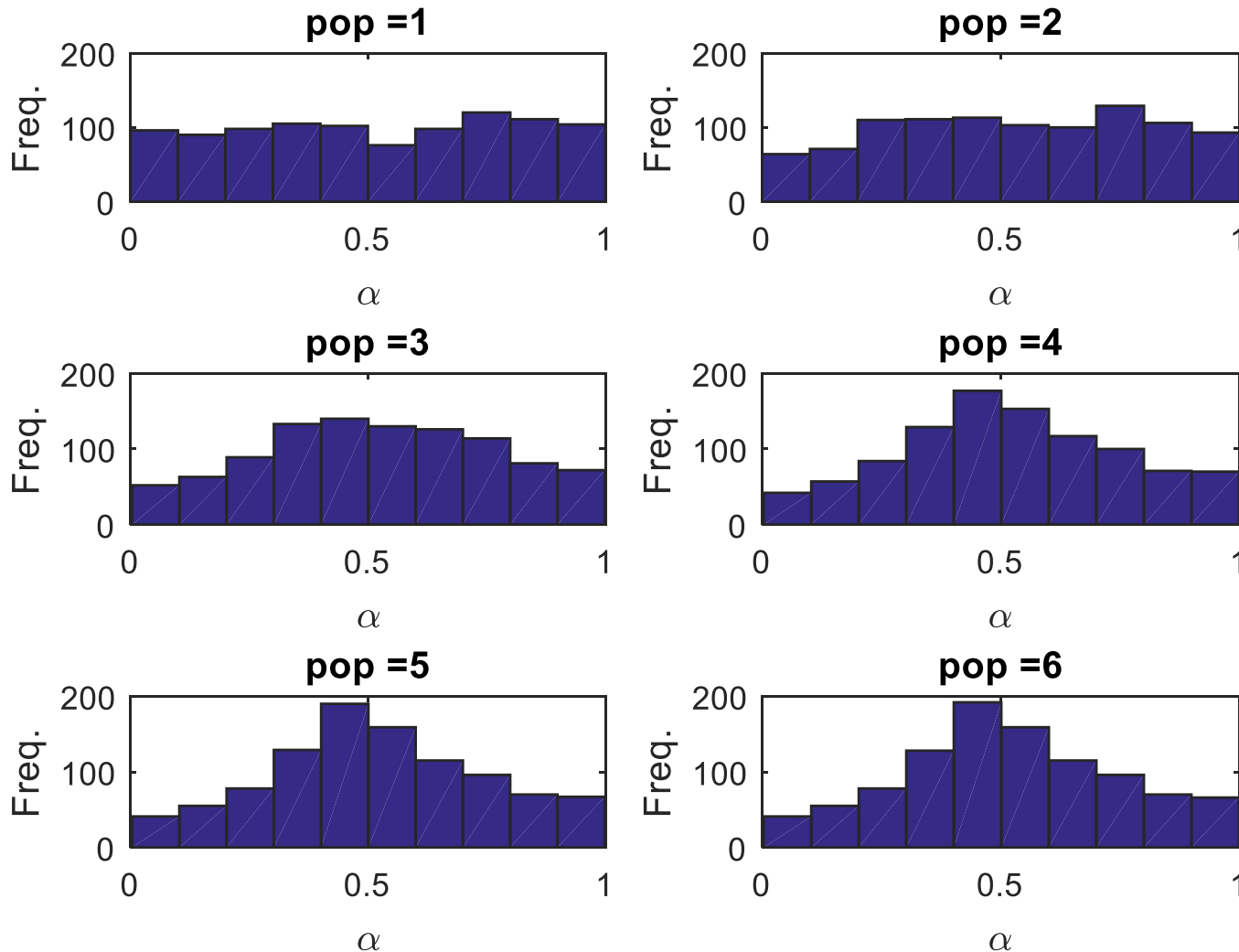
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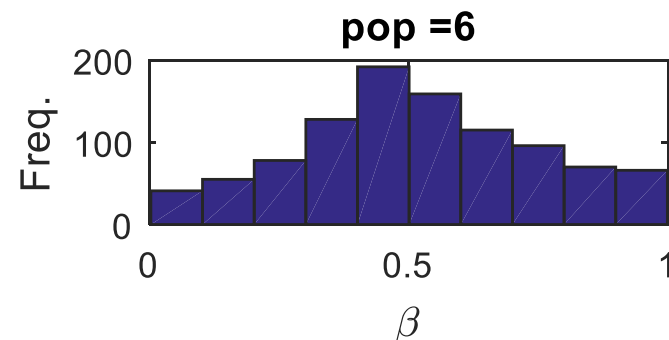
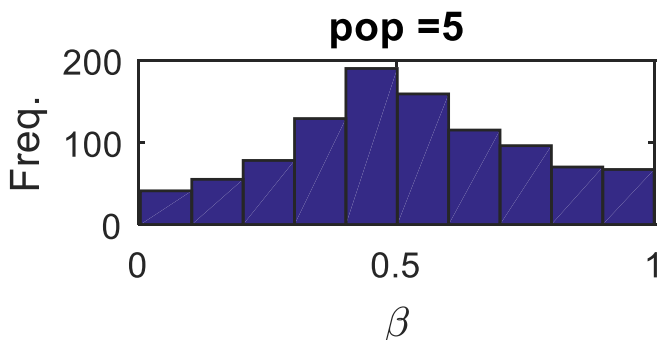
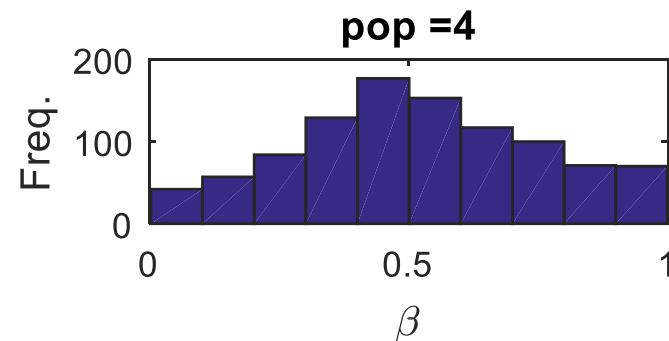
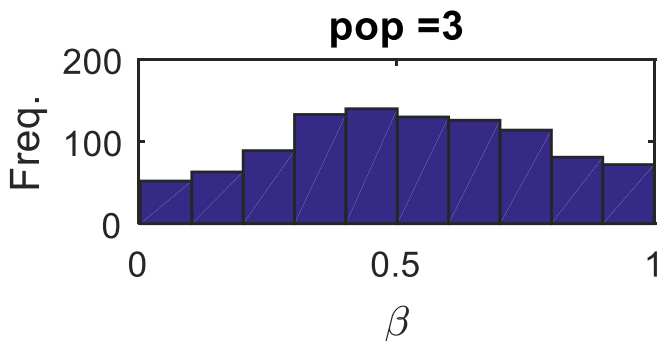
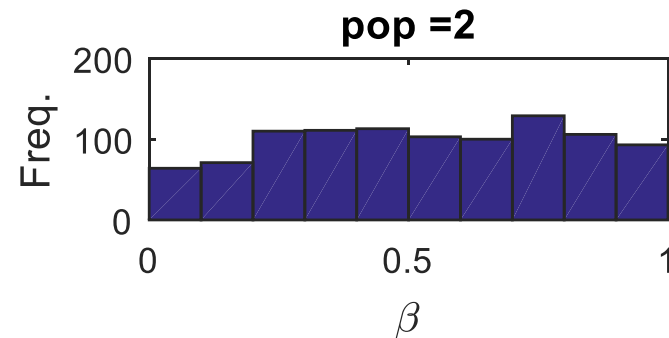
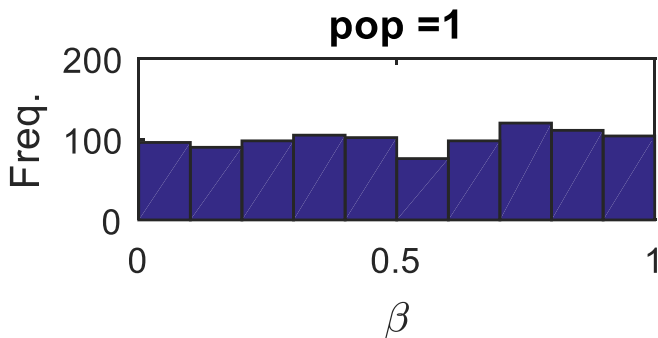


Simulated Data Generated from Model 1 - Model 2 (not selected)

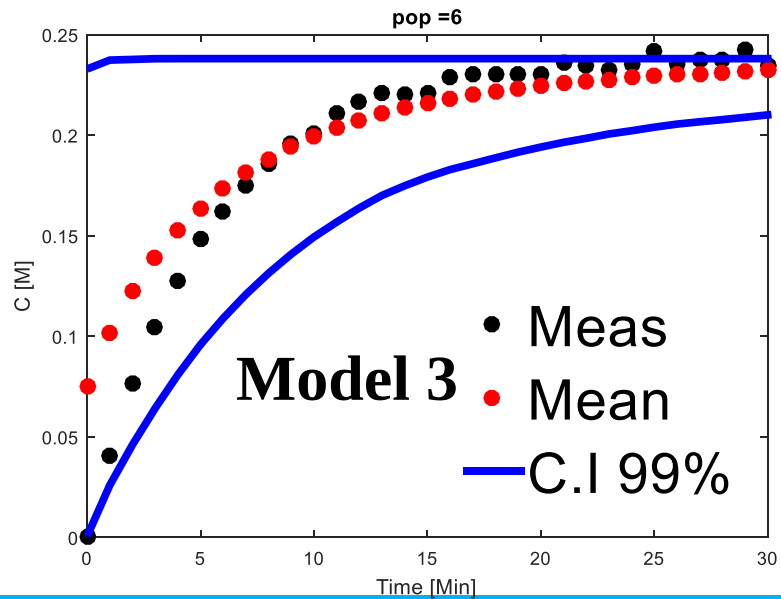
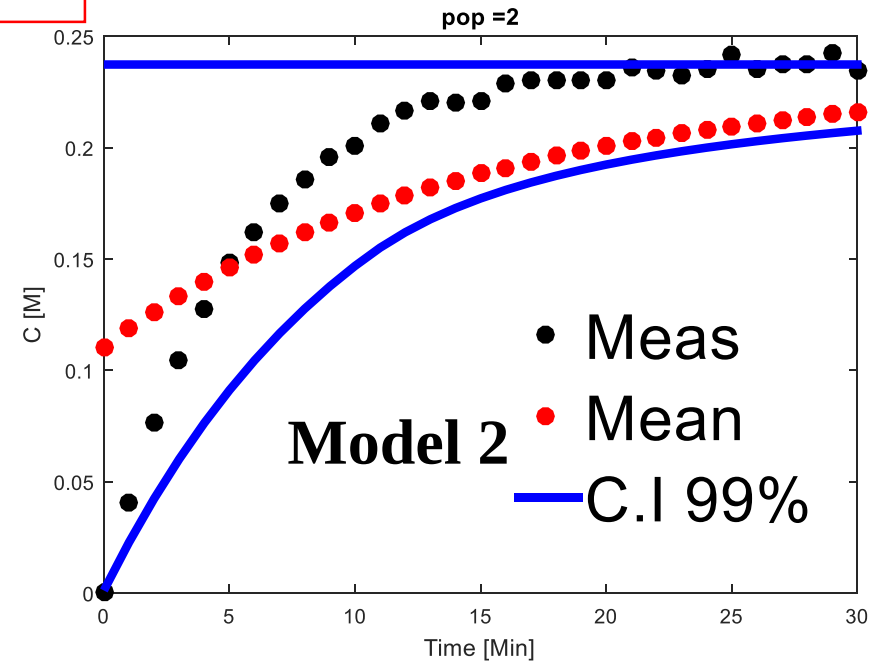
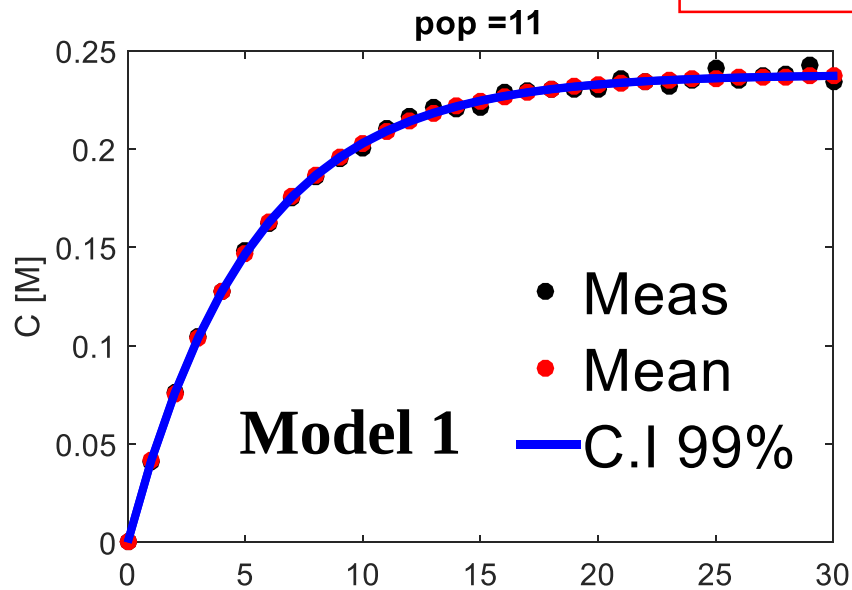
Parameters Reference $\alpha = 0.5$ $\beta = 0.5$



Simulated Data Generated from Model 1 – Model 3(not selected)Parameters Reference $\alpha = 0.5$ $\beta = 0.5$ 

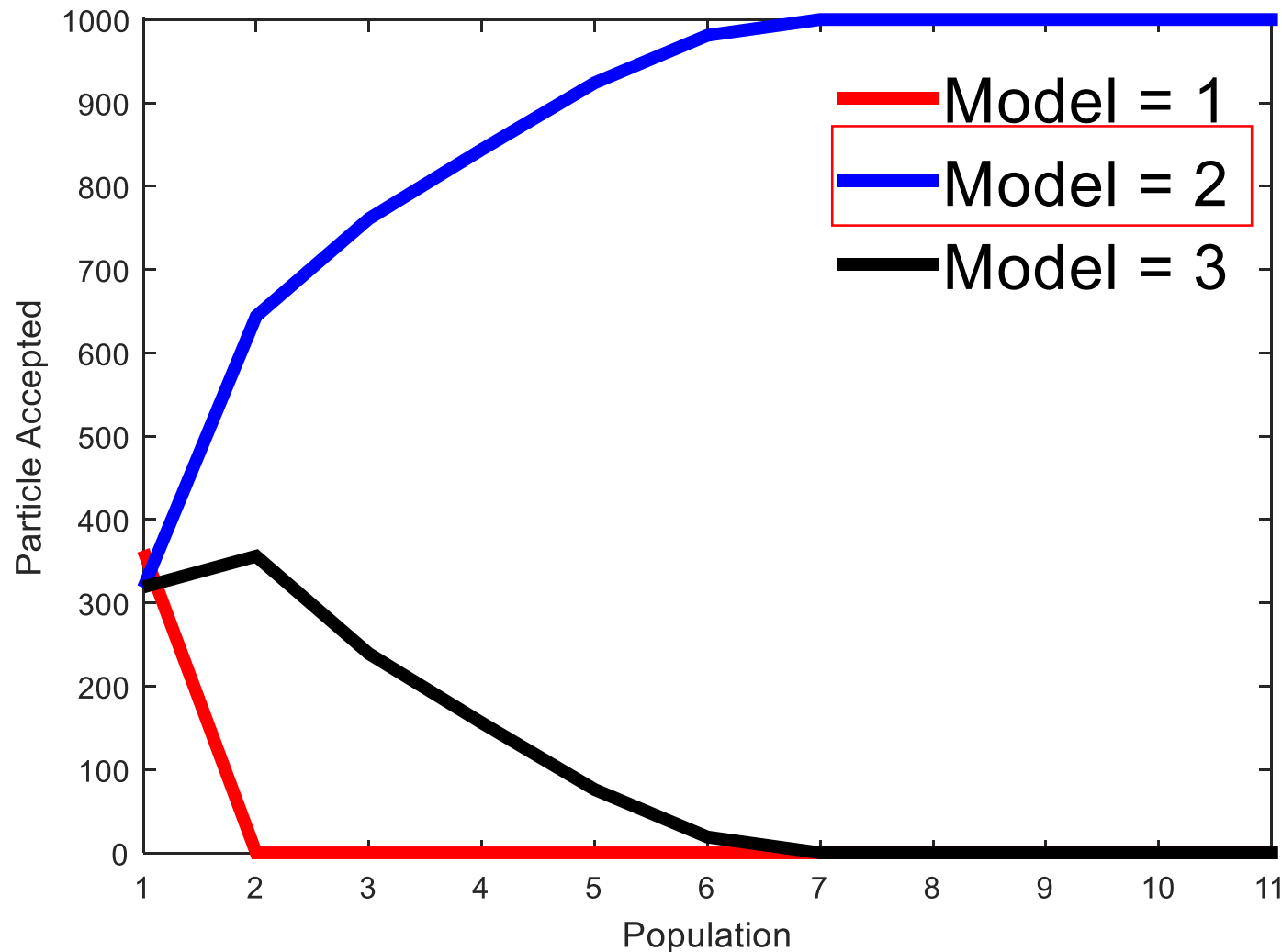
Simulated Data Generated from Model 1 – Model 3 (not selected)Parameters Reference $\alpha = 0.5$ $\beta = 0.5$ 

Simulated Data Generated from Model 1

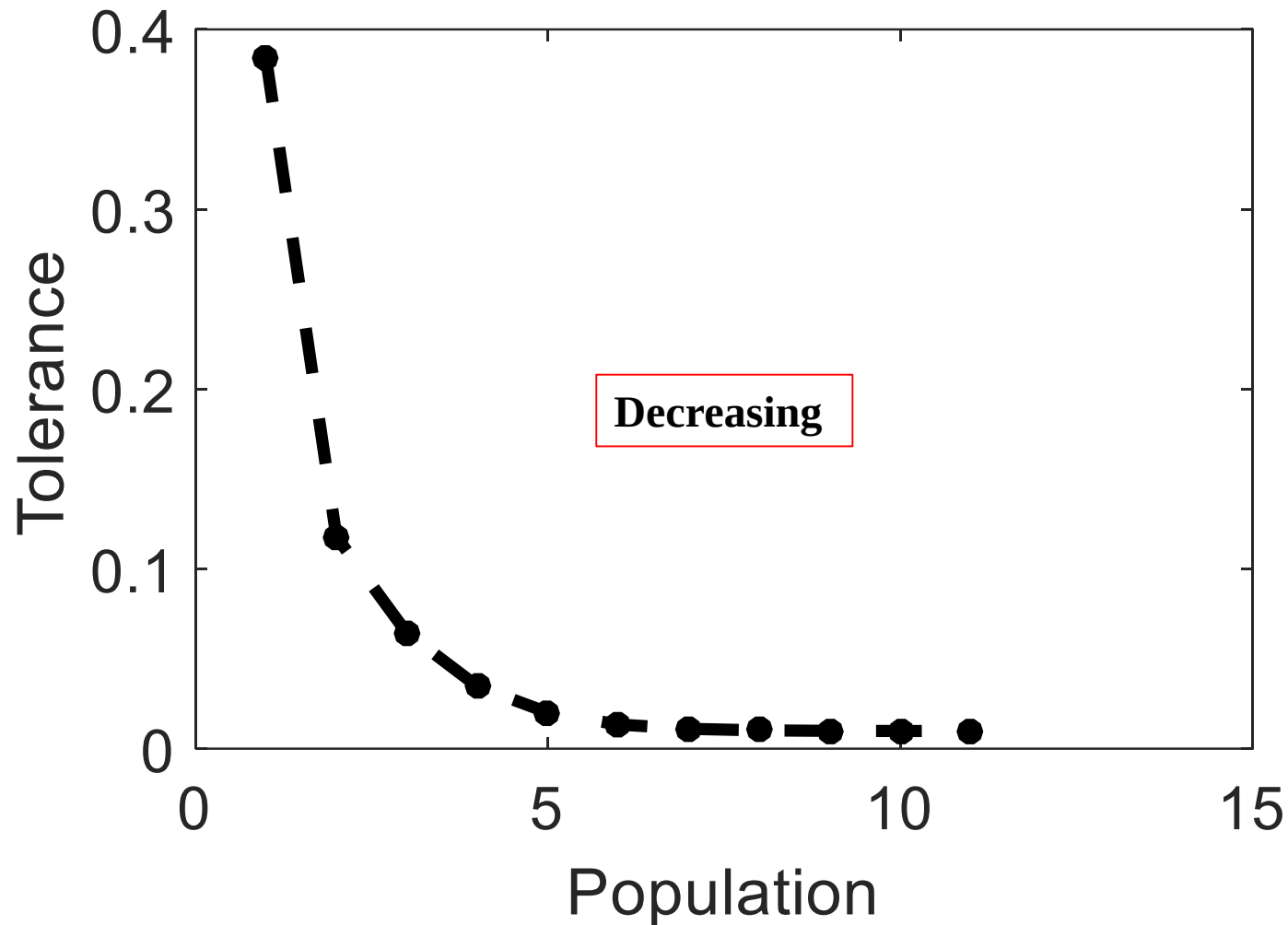


Nice !!

Simulated Data Generated from Model 2

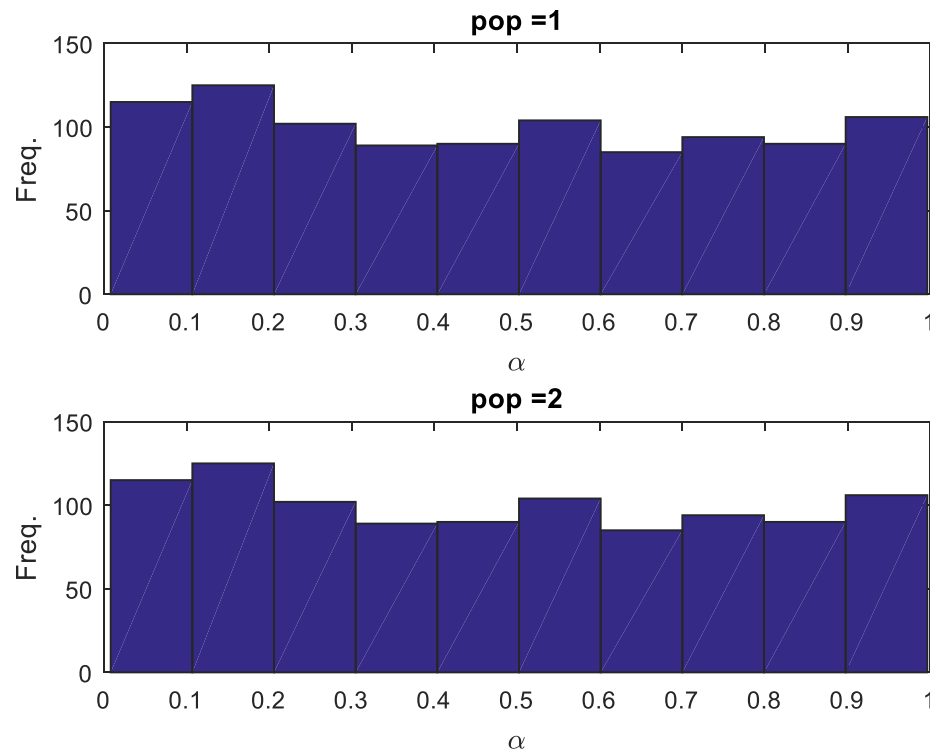


Simulated Data Generated from Model 2



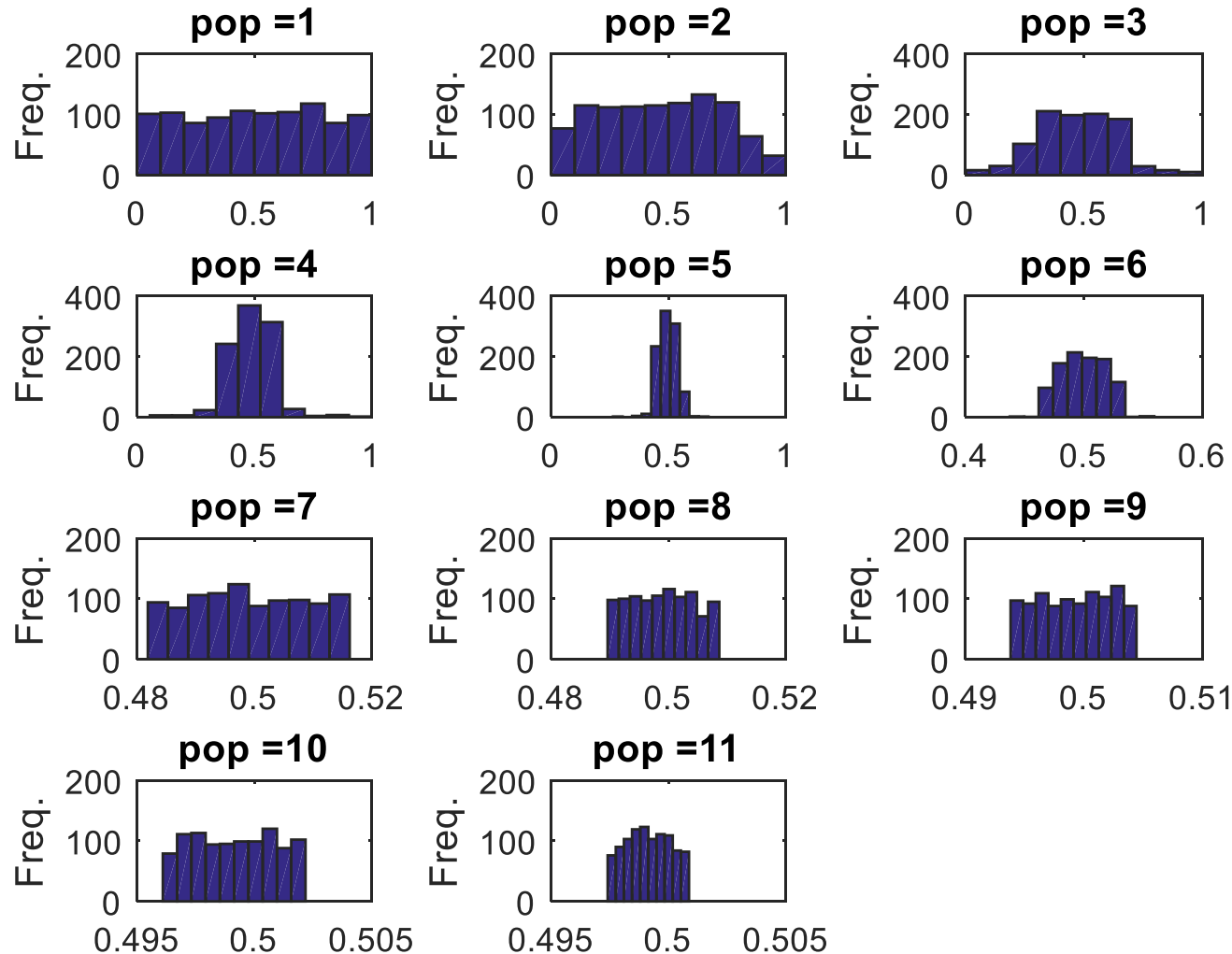
Simulated Data Generated from Model 2 – Model 1 (not selected)

Parameters Reference $\alpha = 0.5$ $\beta = 0.5$



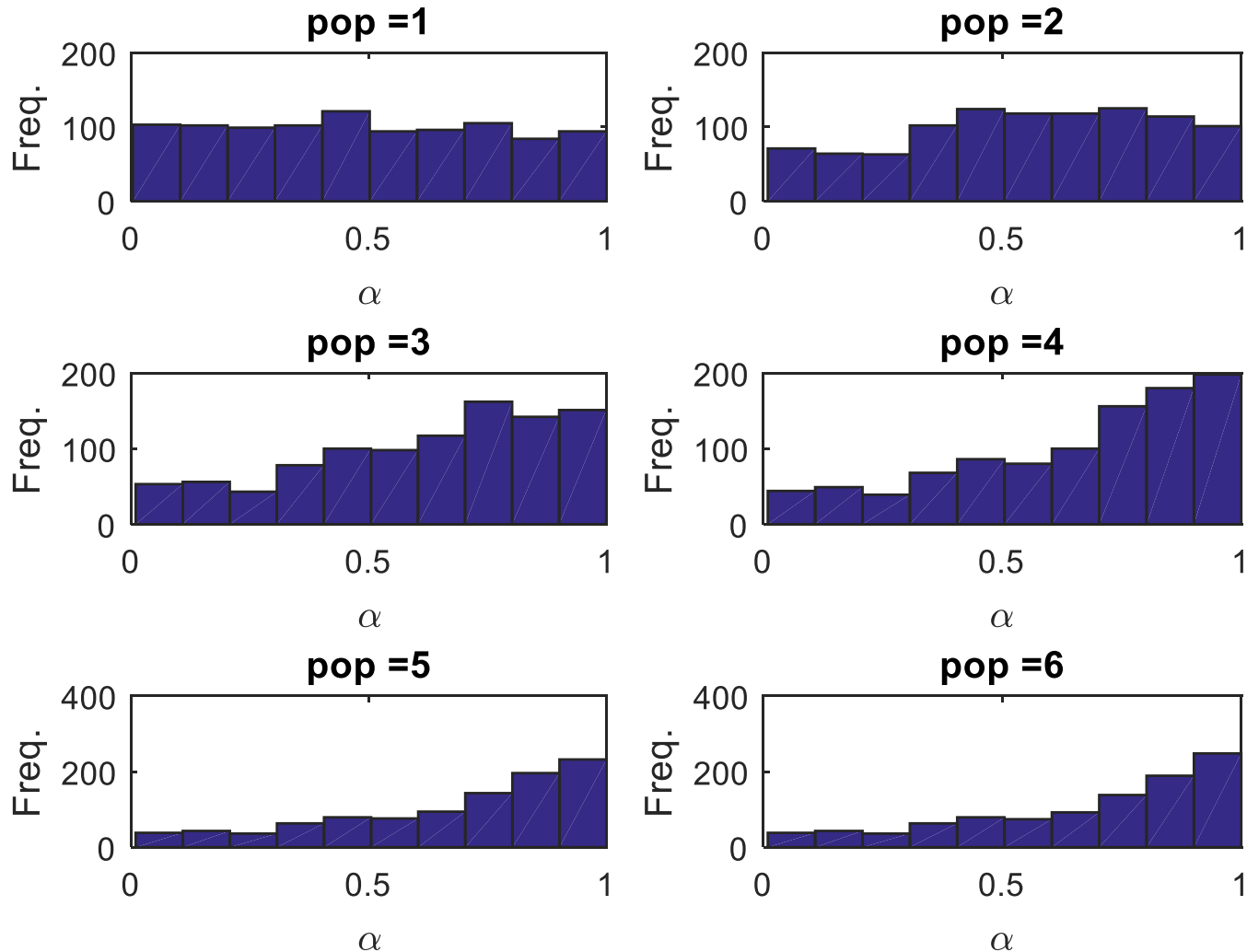
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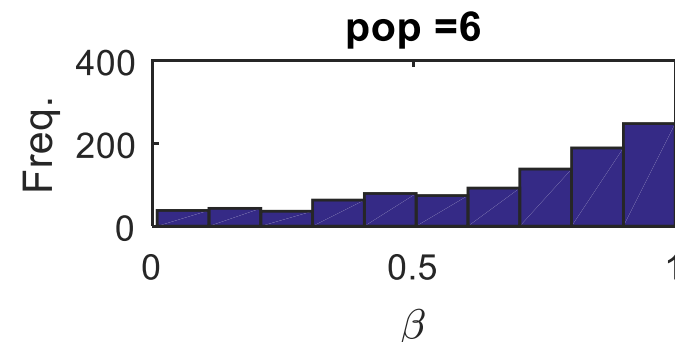
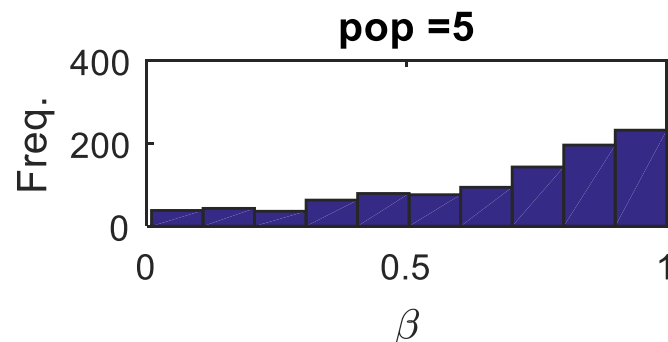
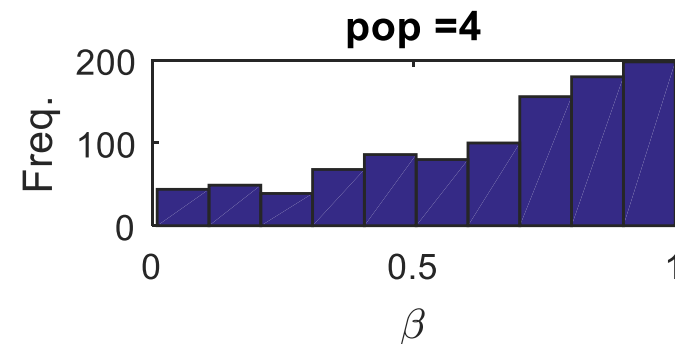
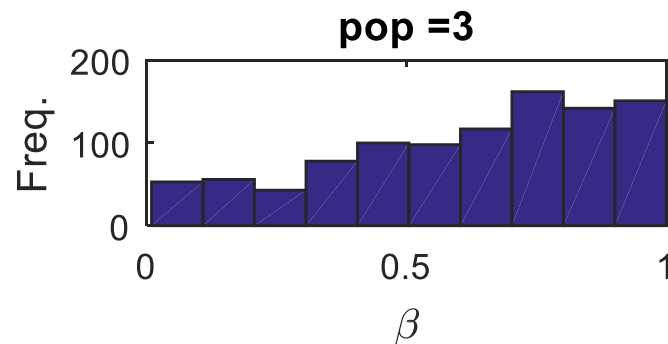
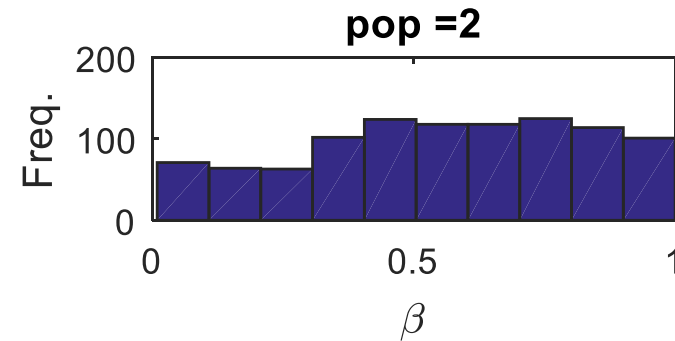
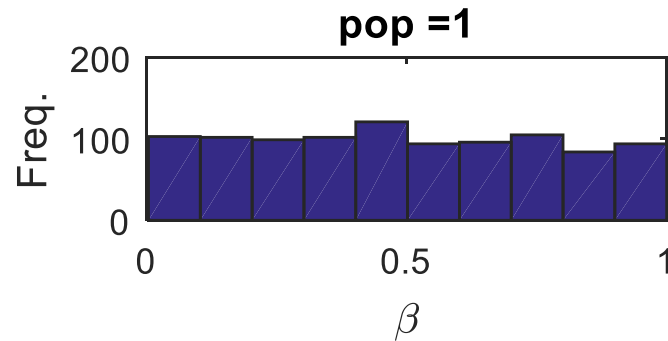
Parameters Reference $\alpha = 0.5$ $\beta = 0.5$



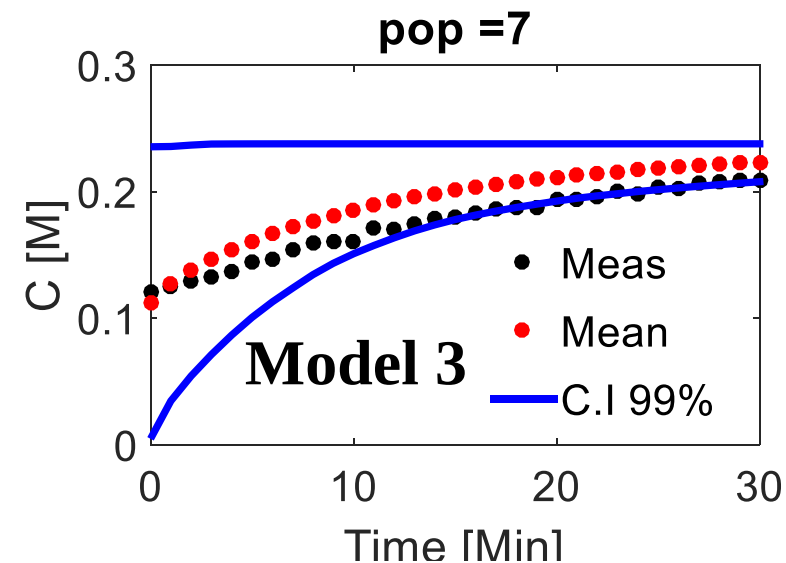
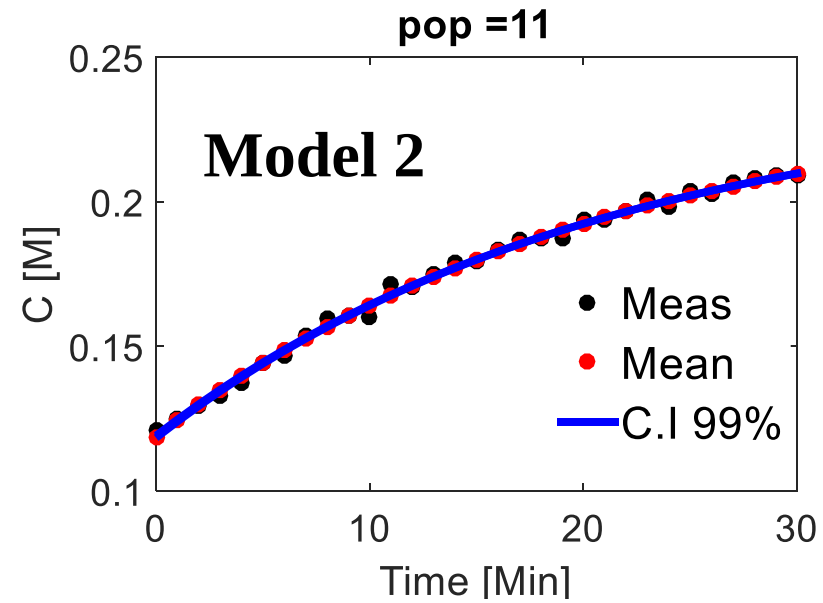
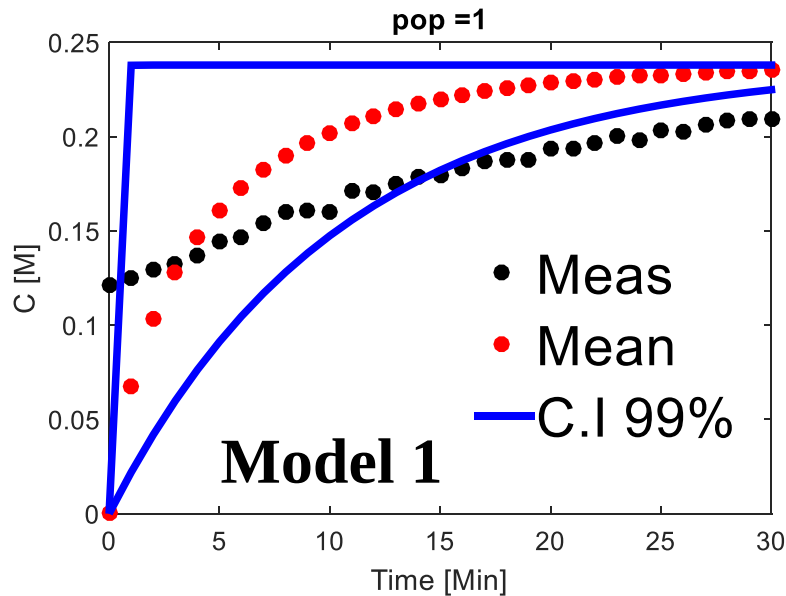
Simulated Data Generated from Model 2 – Model 3 (not selected)

Parameters Reference $\alpha = 0.5$ $\beta = 0.5$



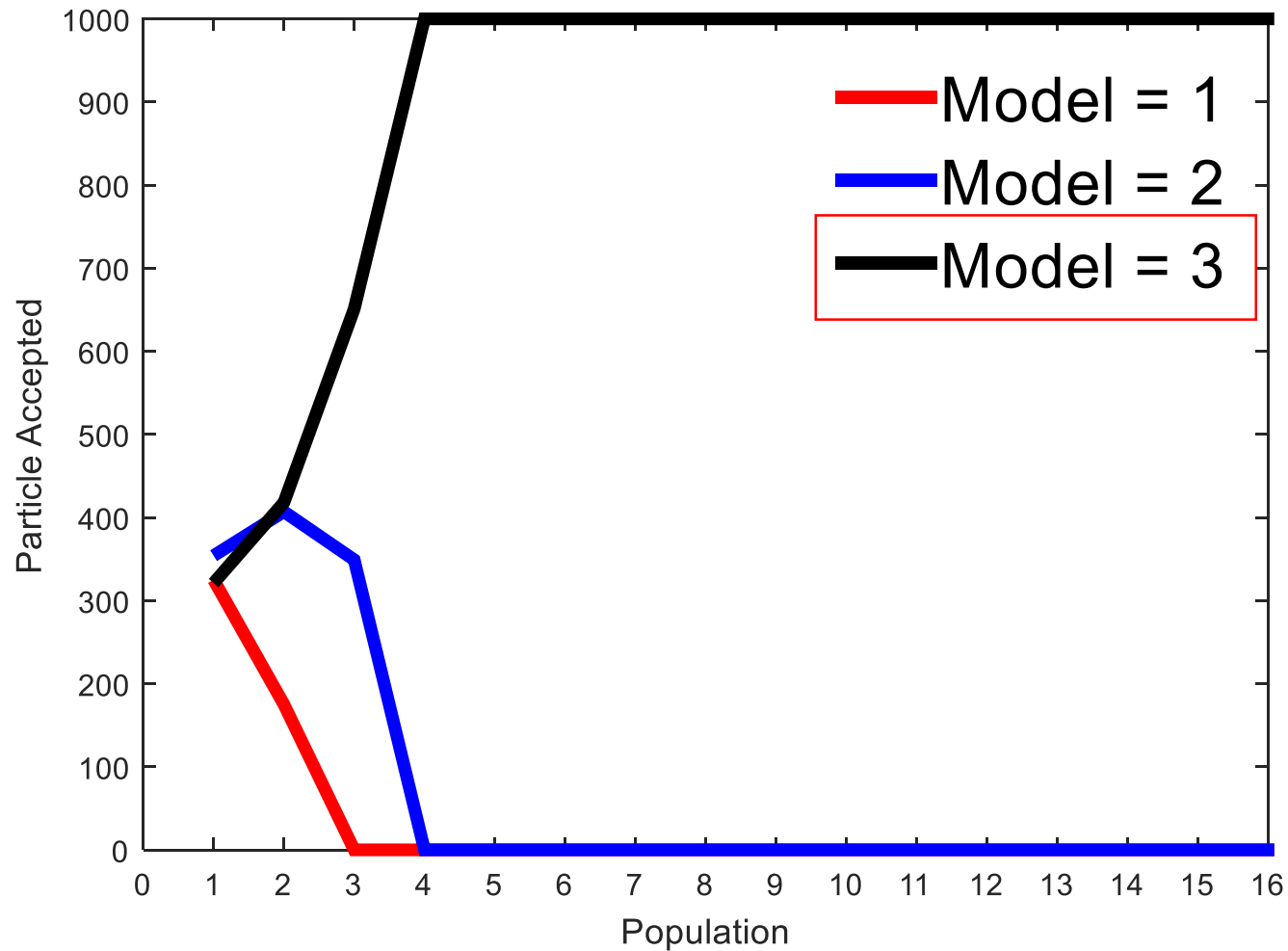
Simulated Data Generated from Model 2 – Model 3 (not selected)Parameters Reference $\alpha = 0.5$ $\beta = 0.5$ 

Simulated Data Generated from Model 2

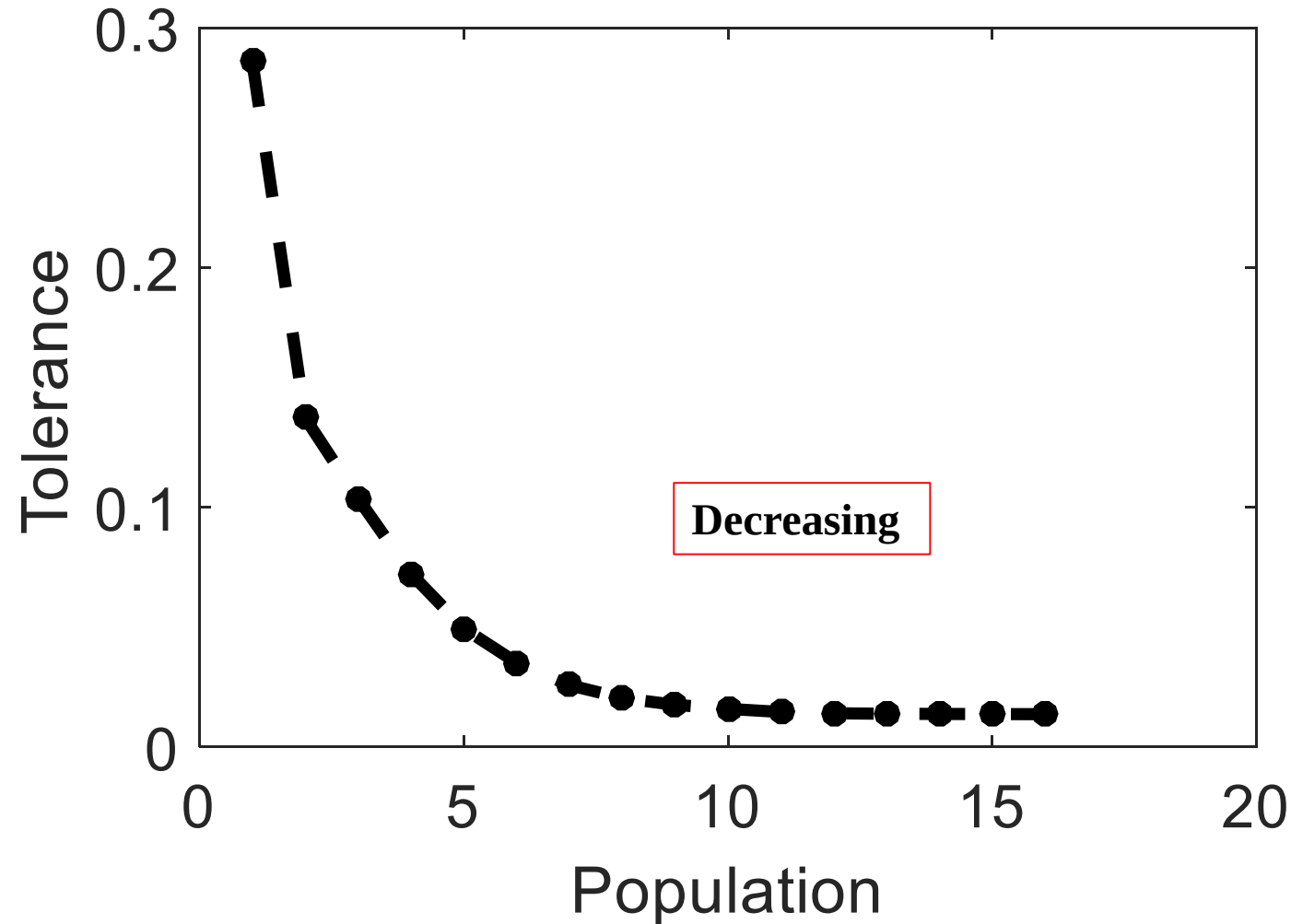


Nice !!

Simulated Data Generated from Model 3

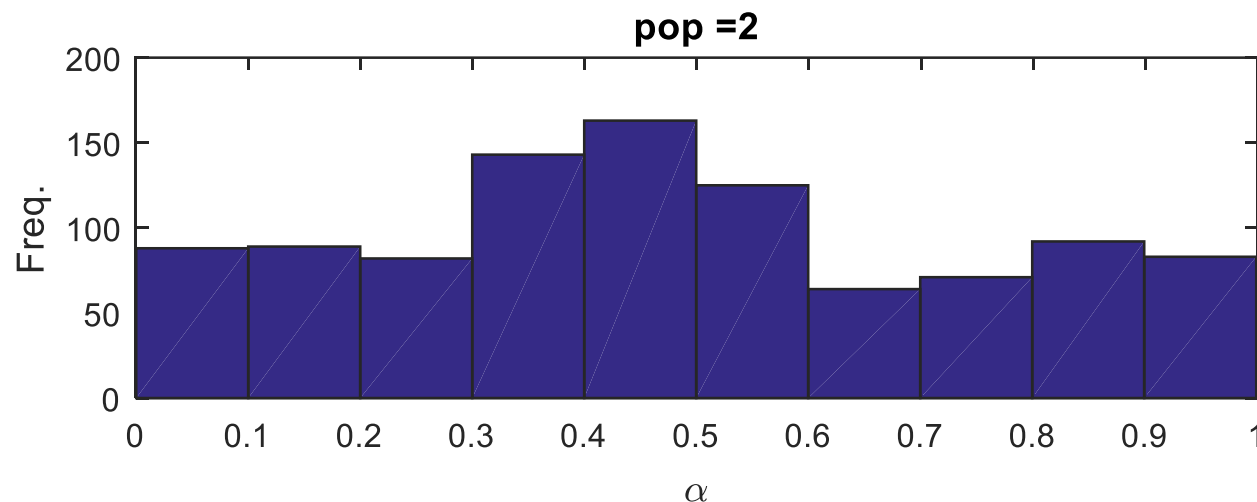
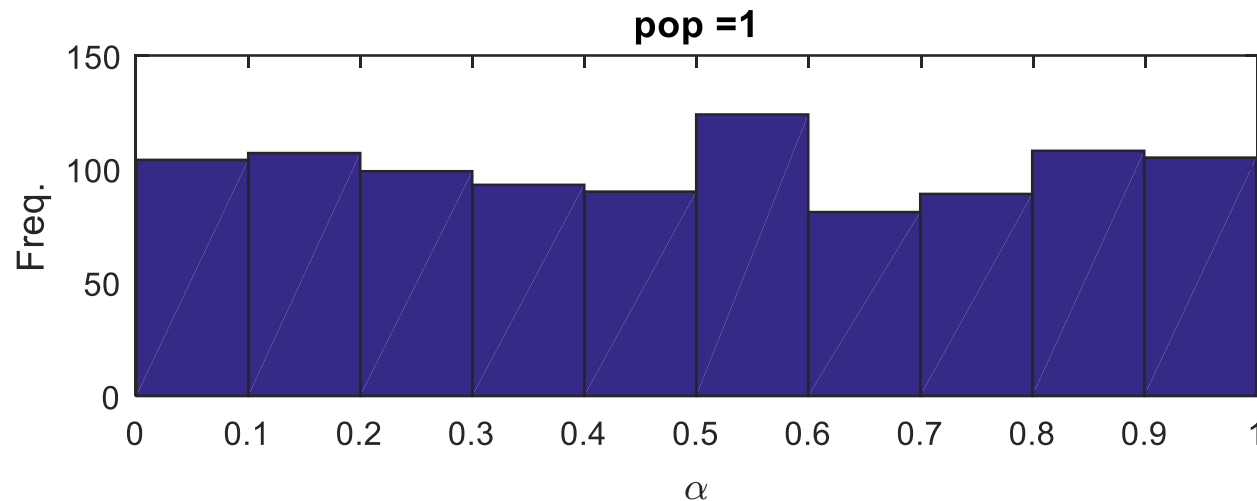


Simulated Data Generated from Model 3



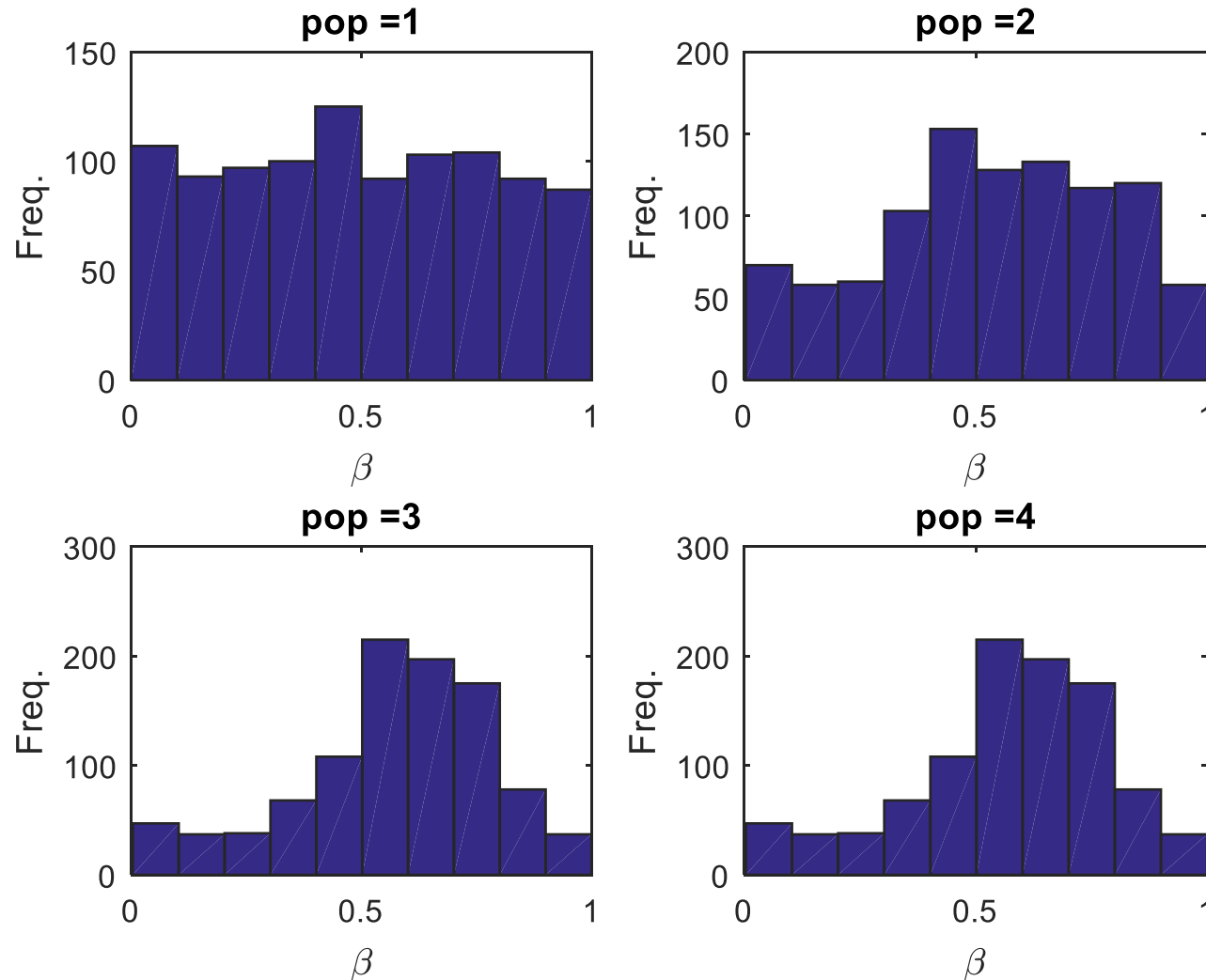
Simulated Data Generated from Model 3 – Model 1 (not selected)

Parameters Reference $\alpha = 0.5$ $\beta = 0.5$



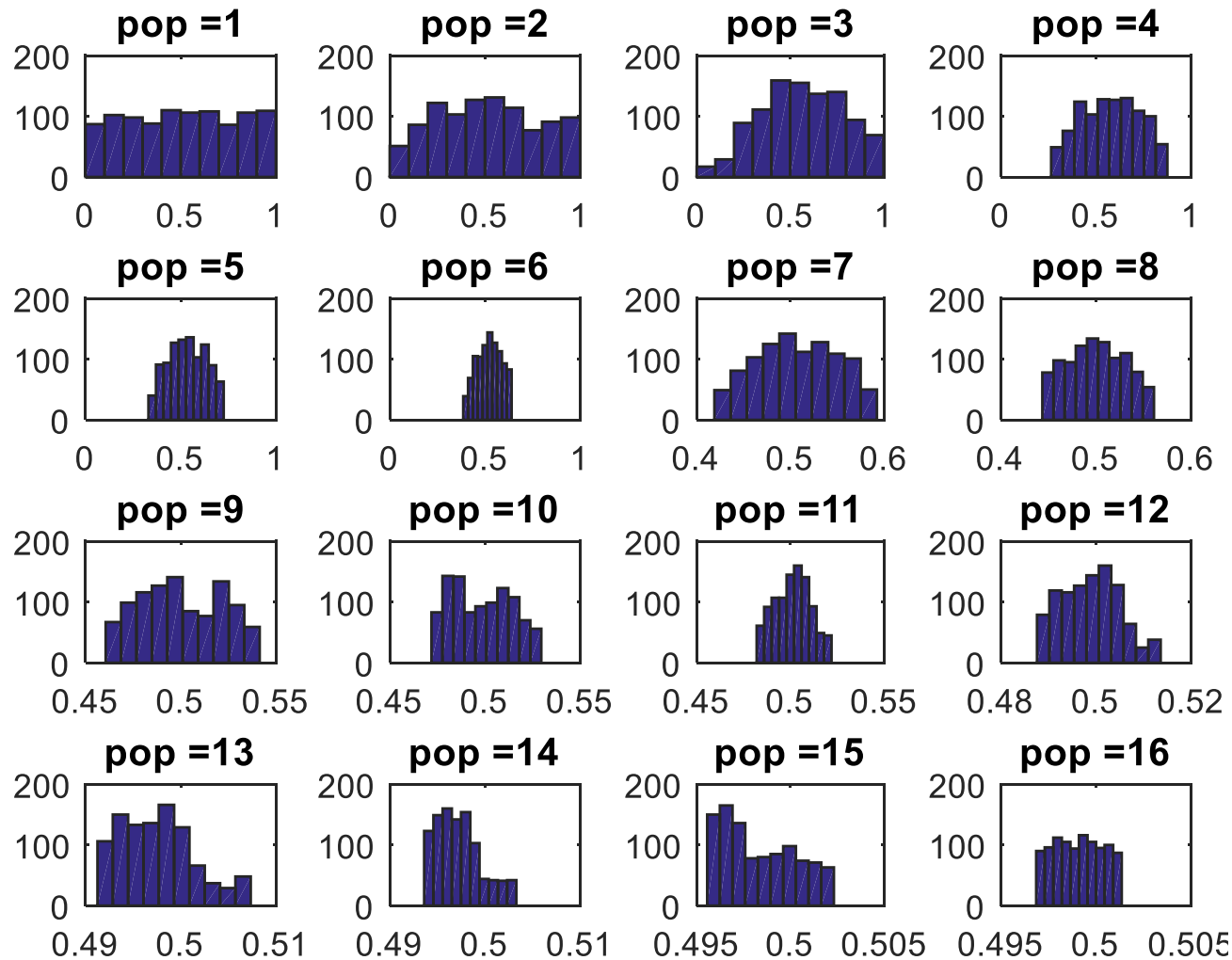
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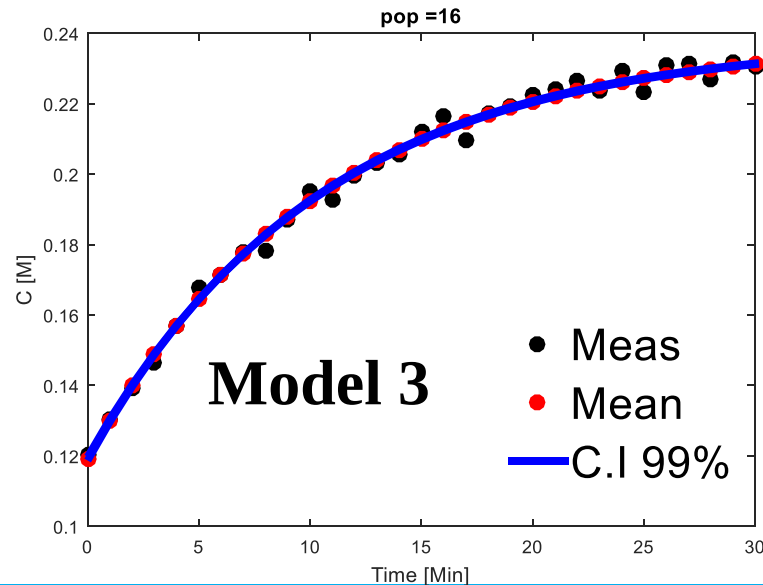
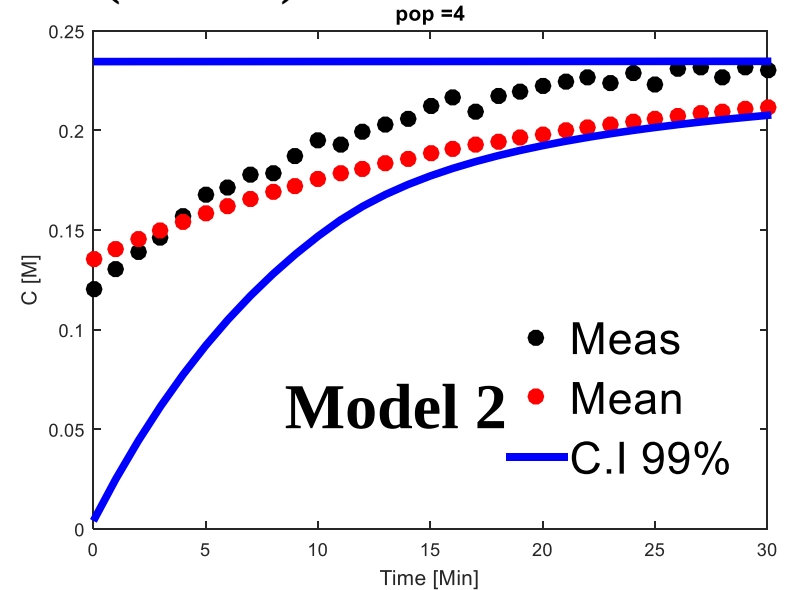
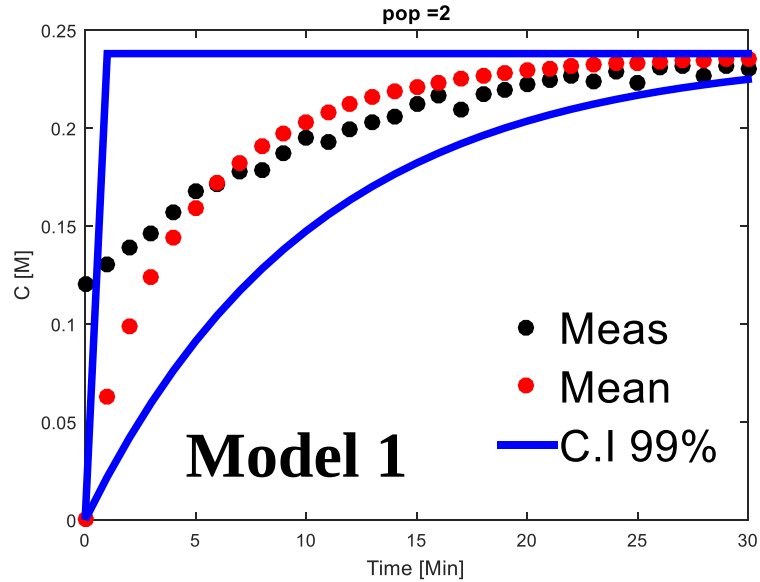


Simulated Data Generated from Model 3 – Model 3 (selected)

Parameters Reference $\alpha = 0.5$ $\beta = 0.5$

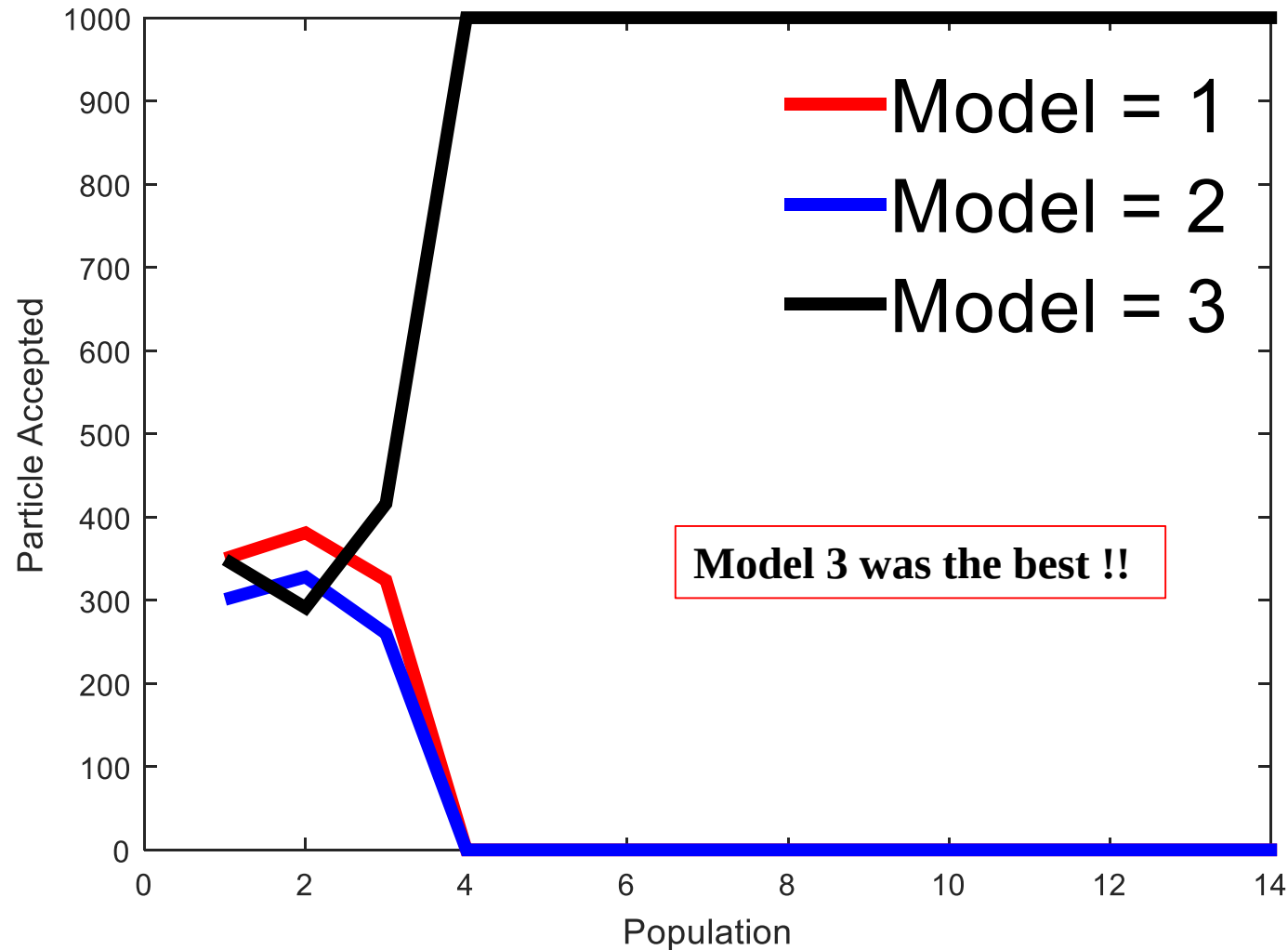


Simulated Data Generated from Model 3 – Model 3 (selected)

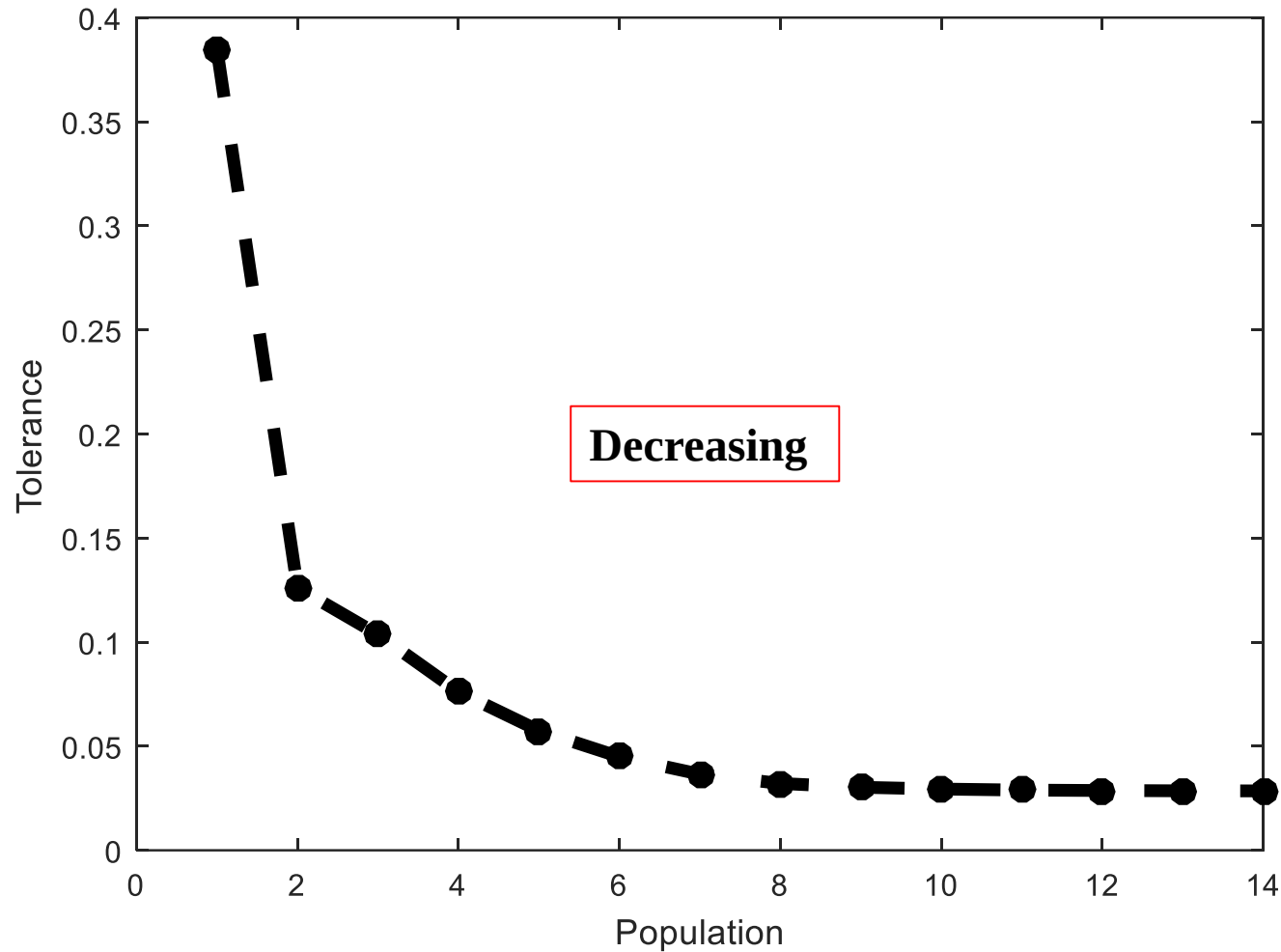


Nice !!

Simulated Data Generated from Models 1 and 2

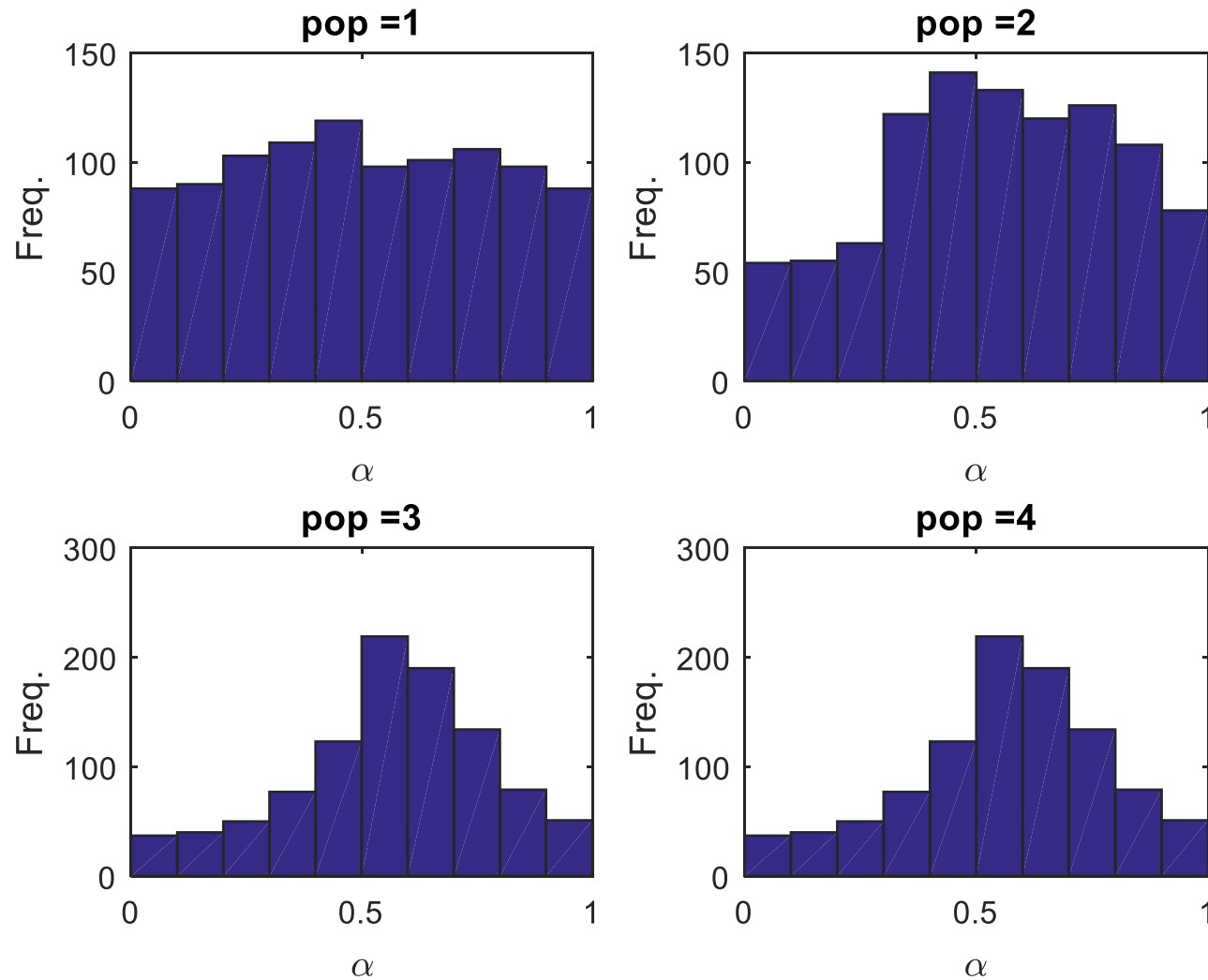


Simulated Data Generated from Models 1 and 2



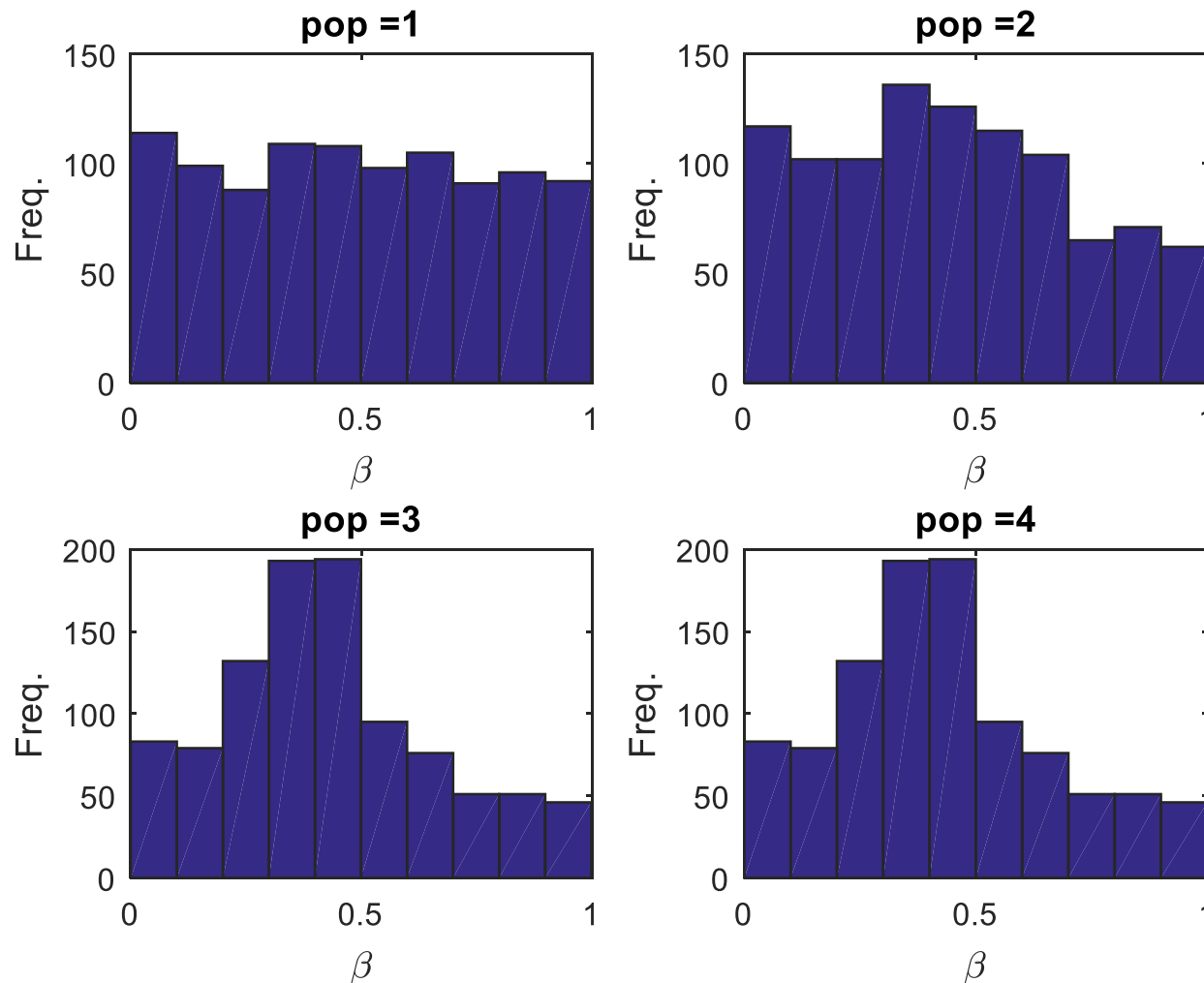
Simulated Data Generated from Models 1 and 2

Model 1 (not selected)



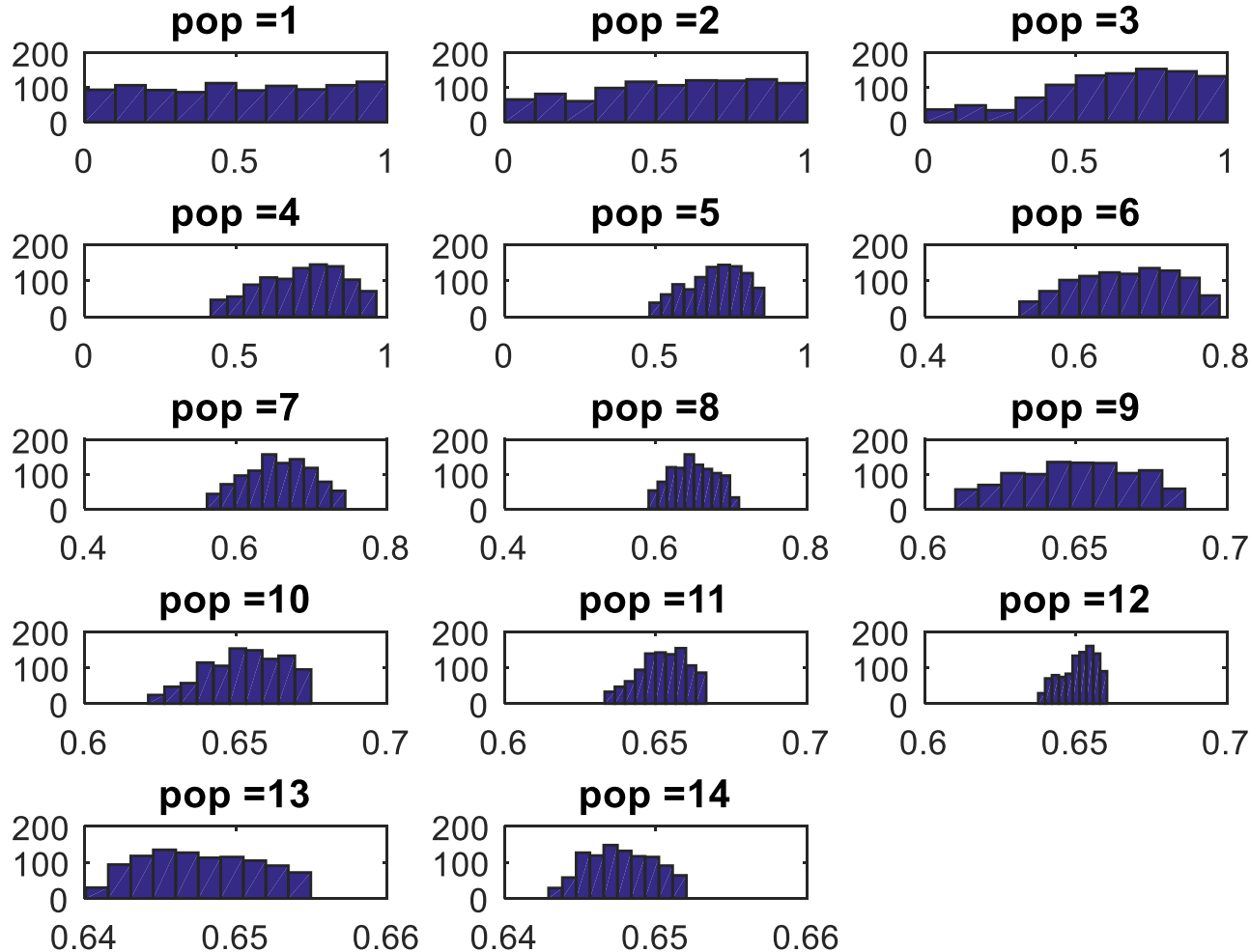
Simulated Data Generated from Models 1 and 2

Model 2 (not selected)



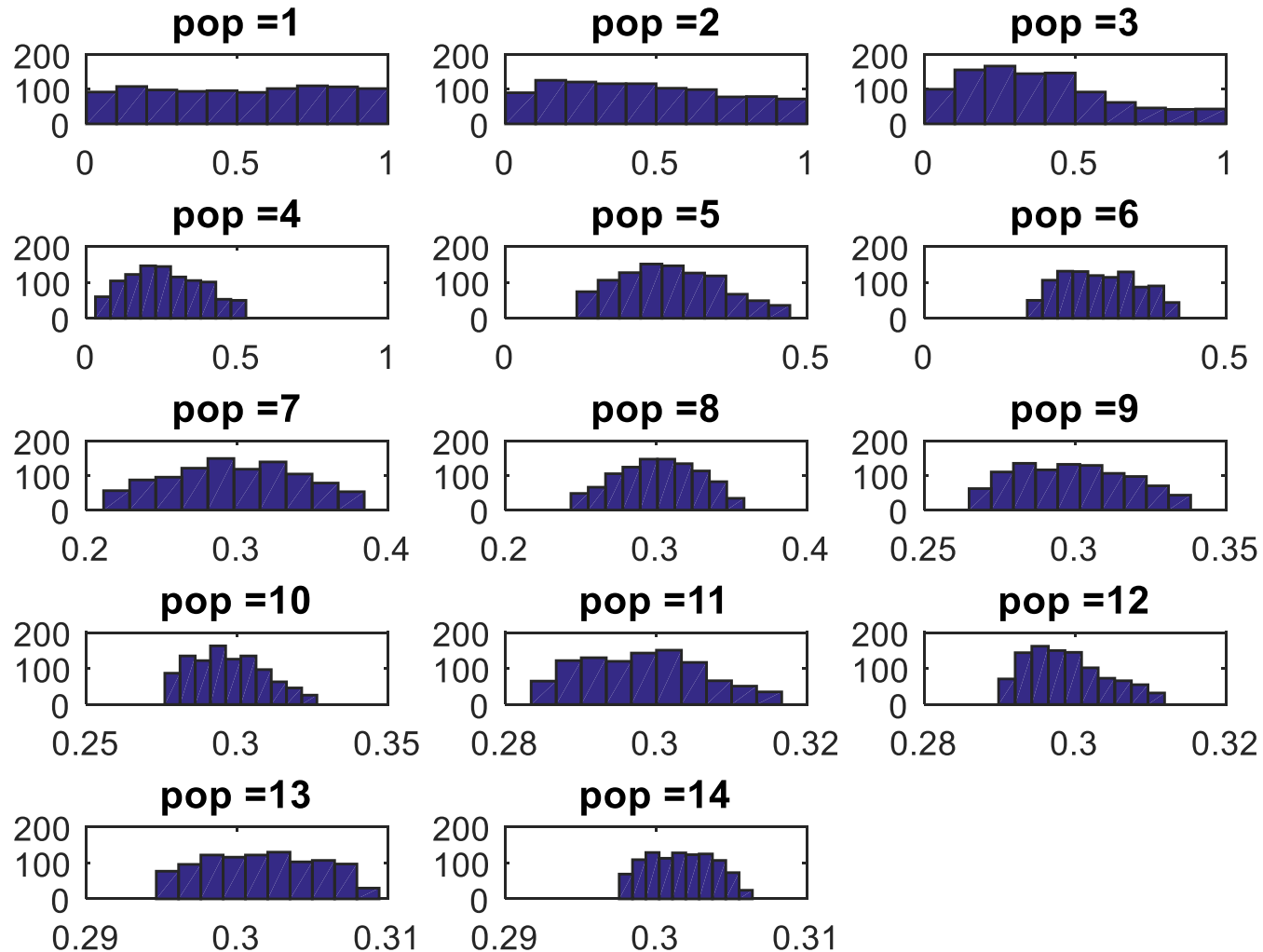
Simulated Data Generated from Models 1 and 2

Model 3 (selected)

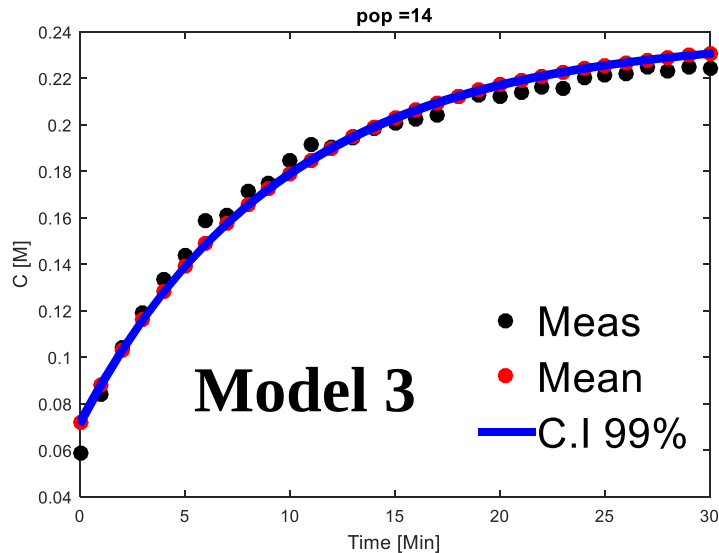
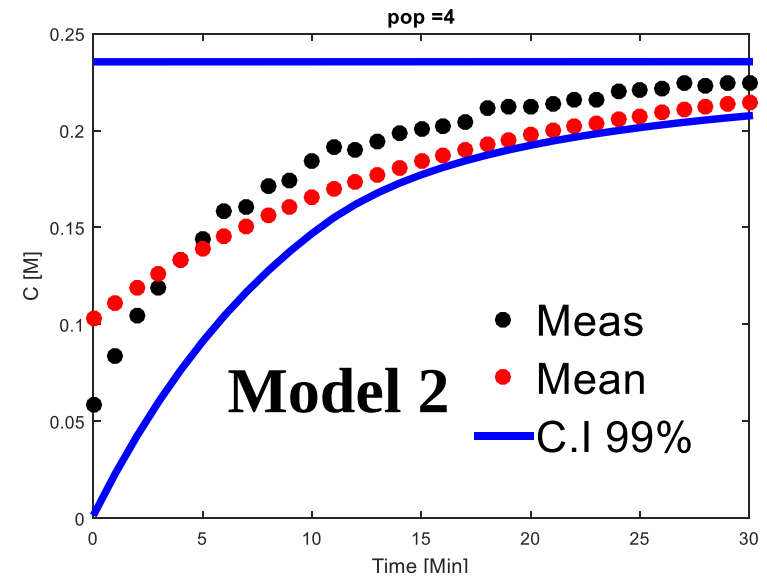
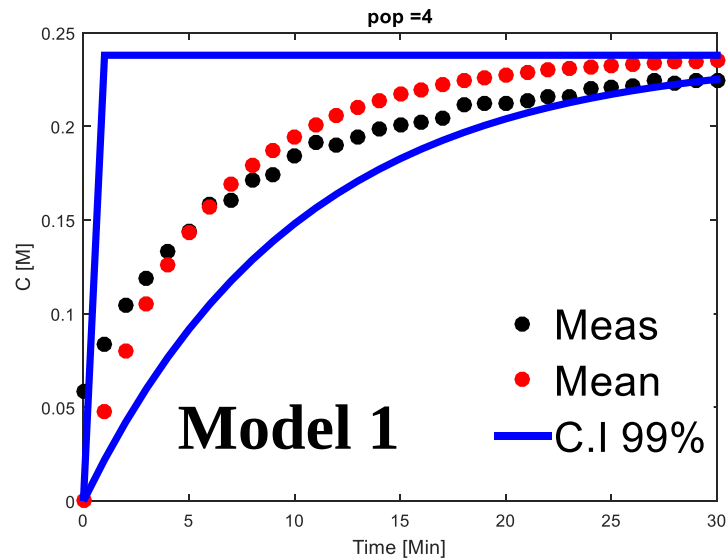


Simulated Data Generated from Models 1 and 2

Model 3 (selected)



Simulated Data Generated from Models 1 and 2



Nice !!

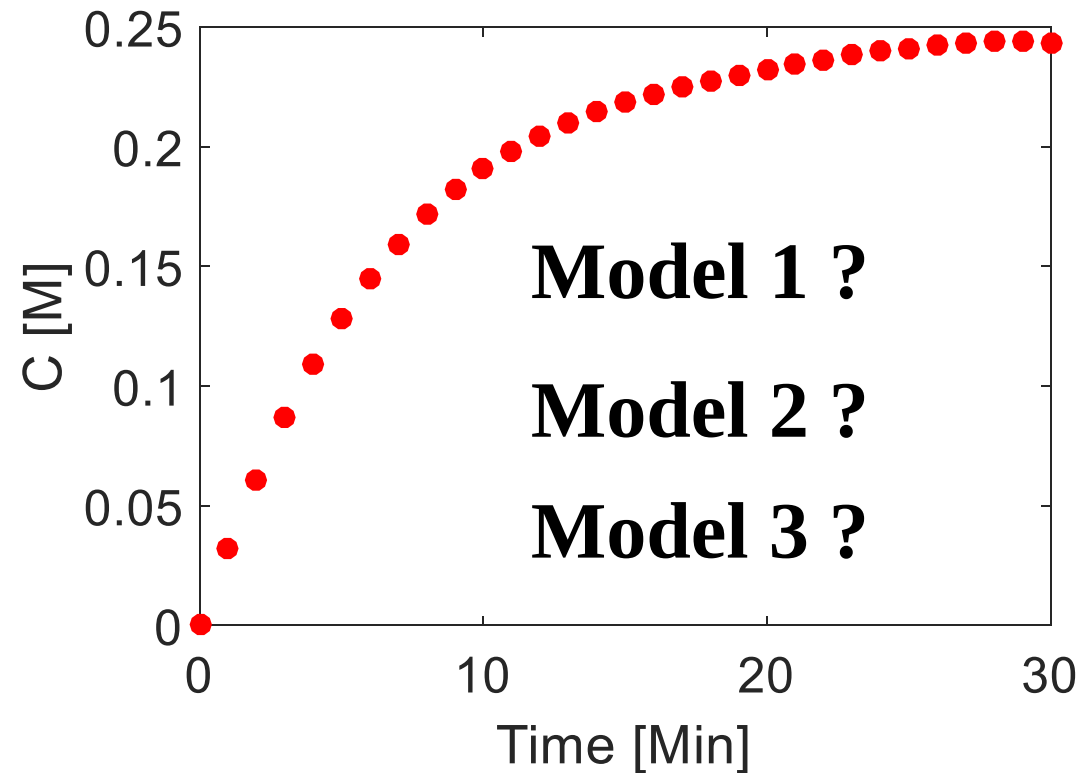
3. Experimental Data

Experimental Setup

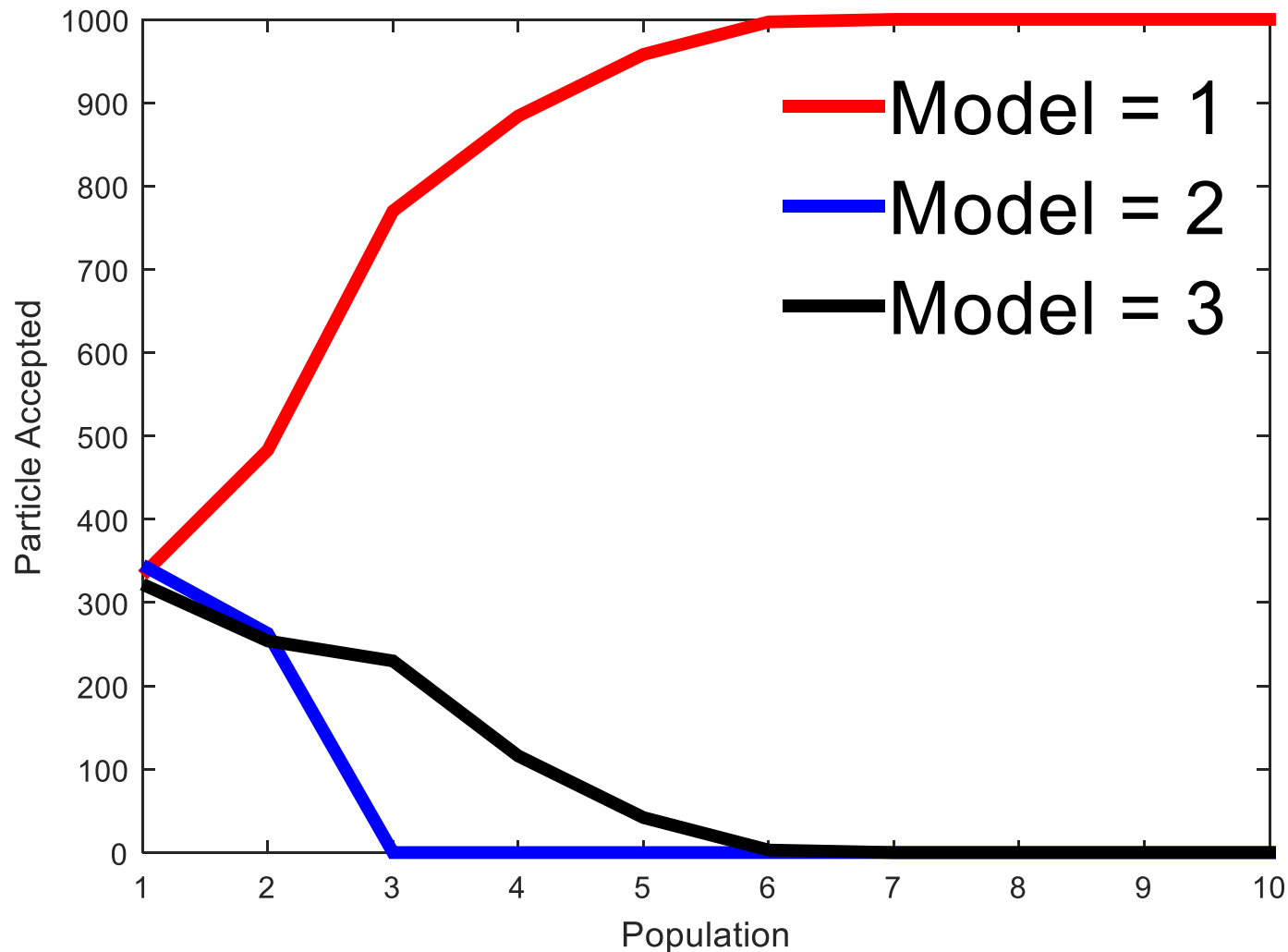


Frequency: 150 rpm

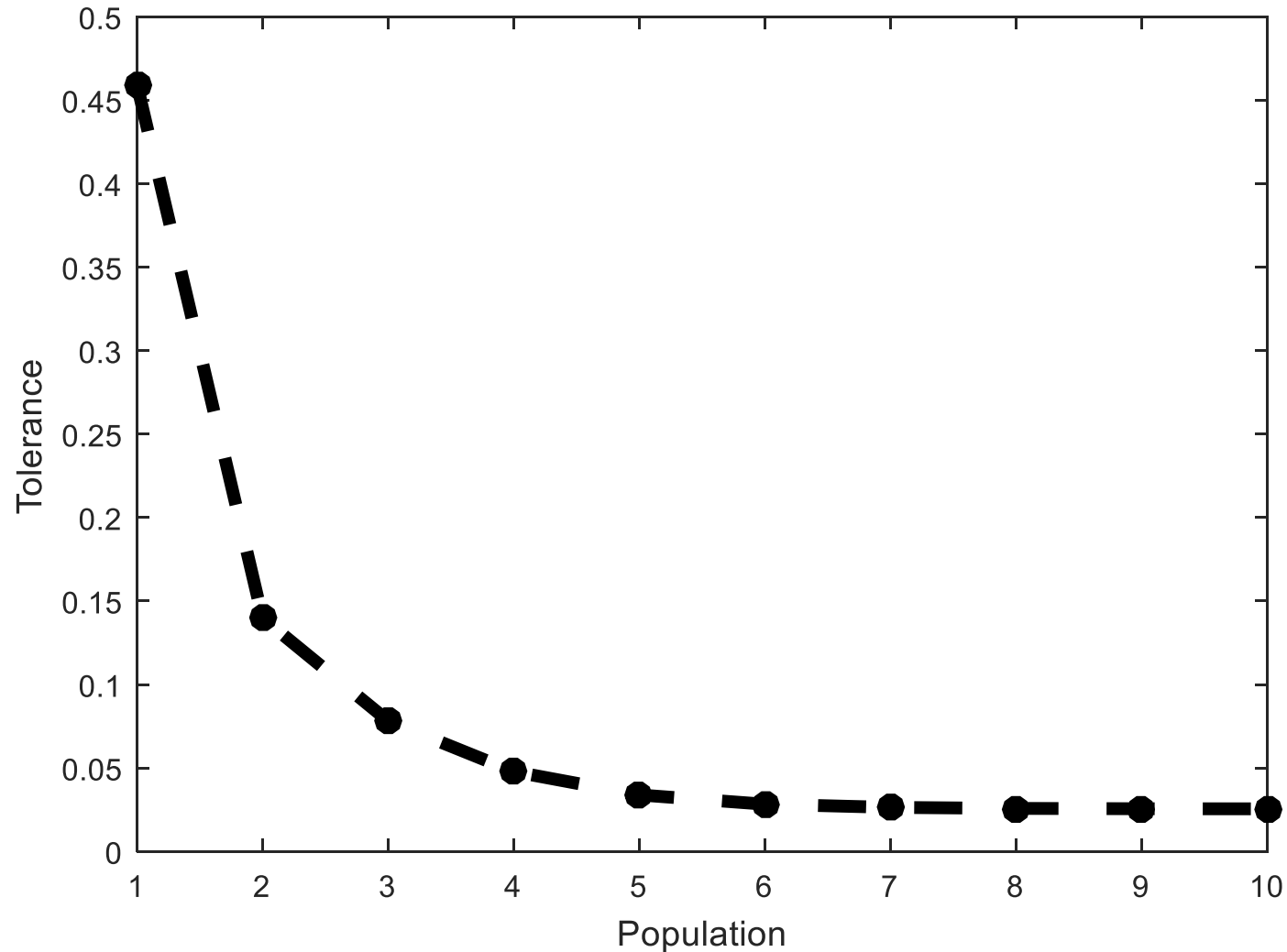
Spectroscopy



Experimental Data

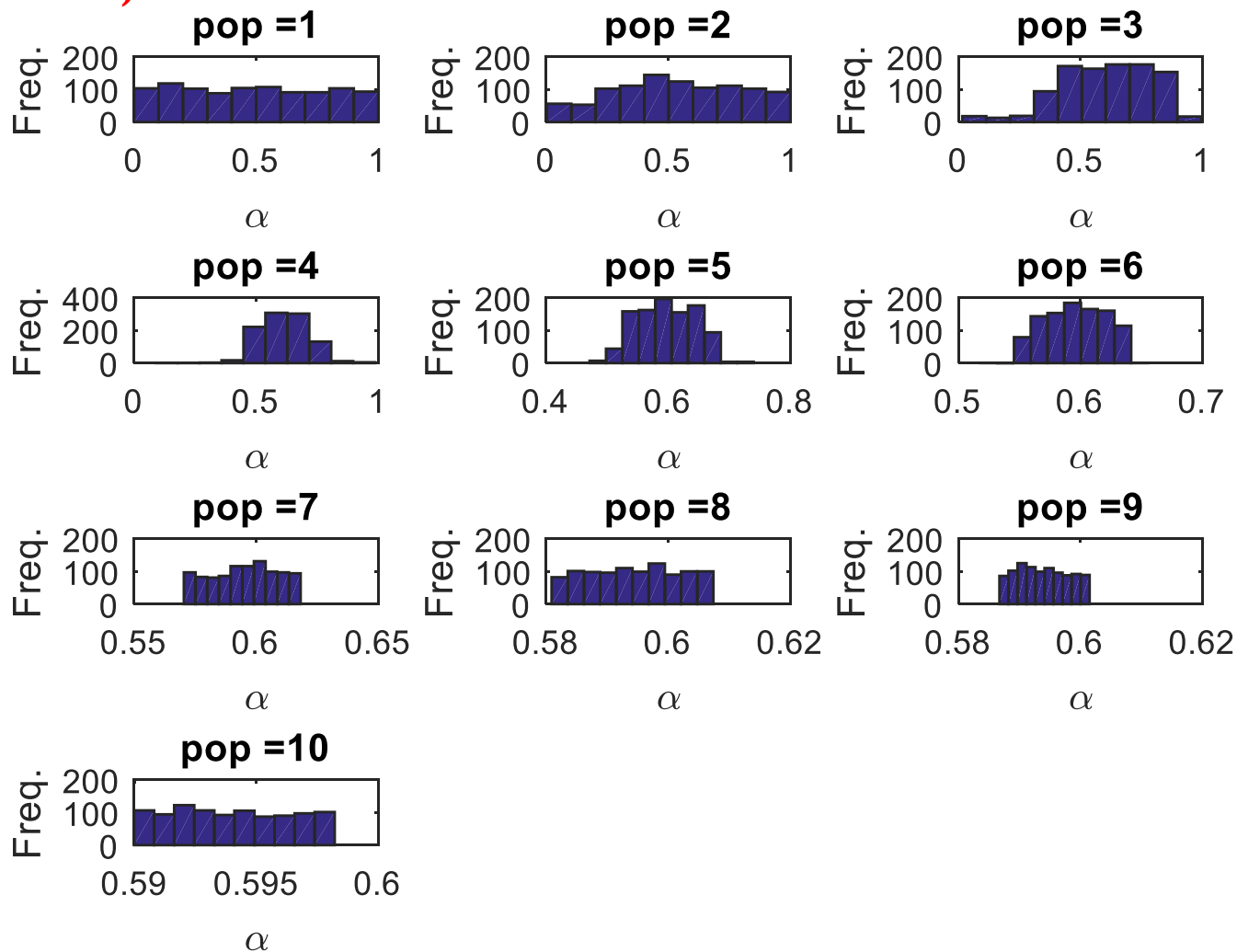


Experimental Data



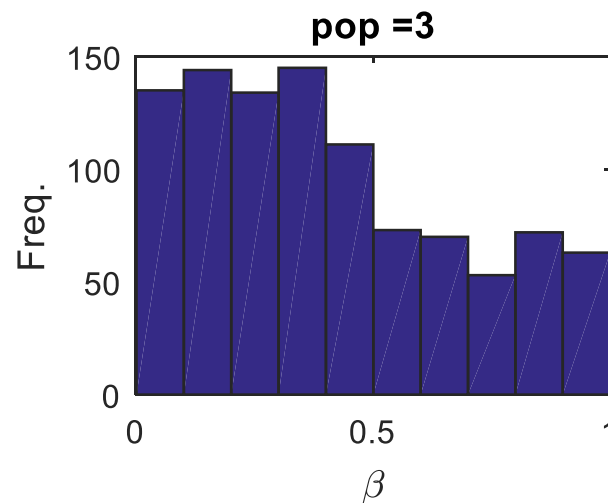
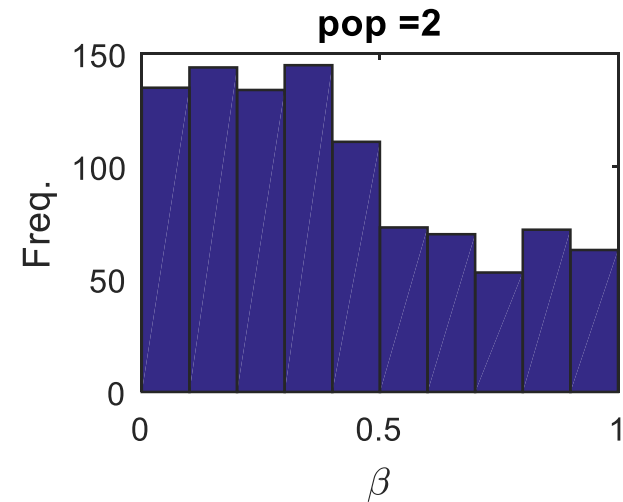
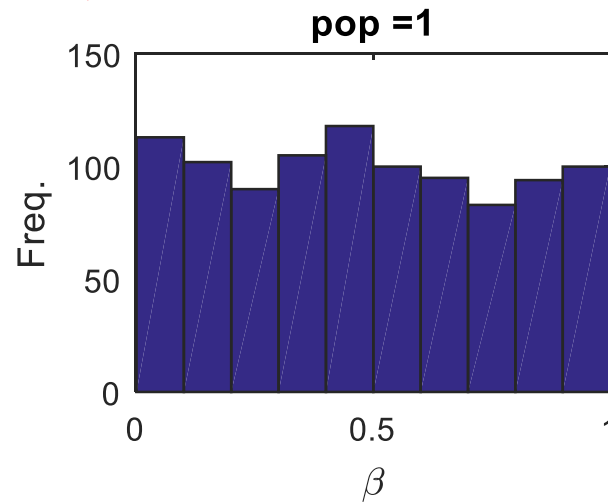
Experimental Data

Model 1 (selected)



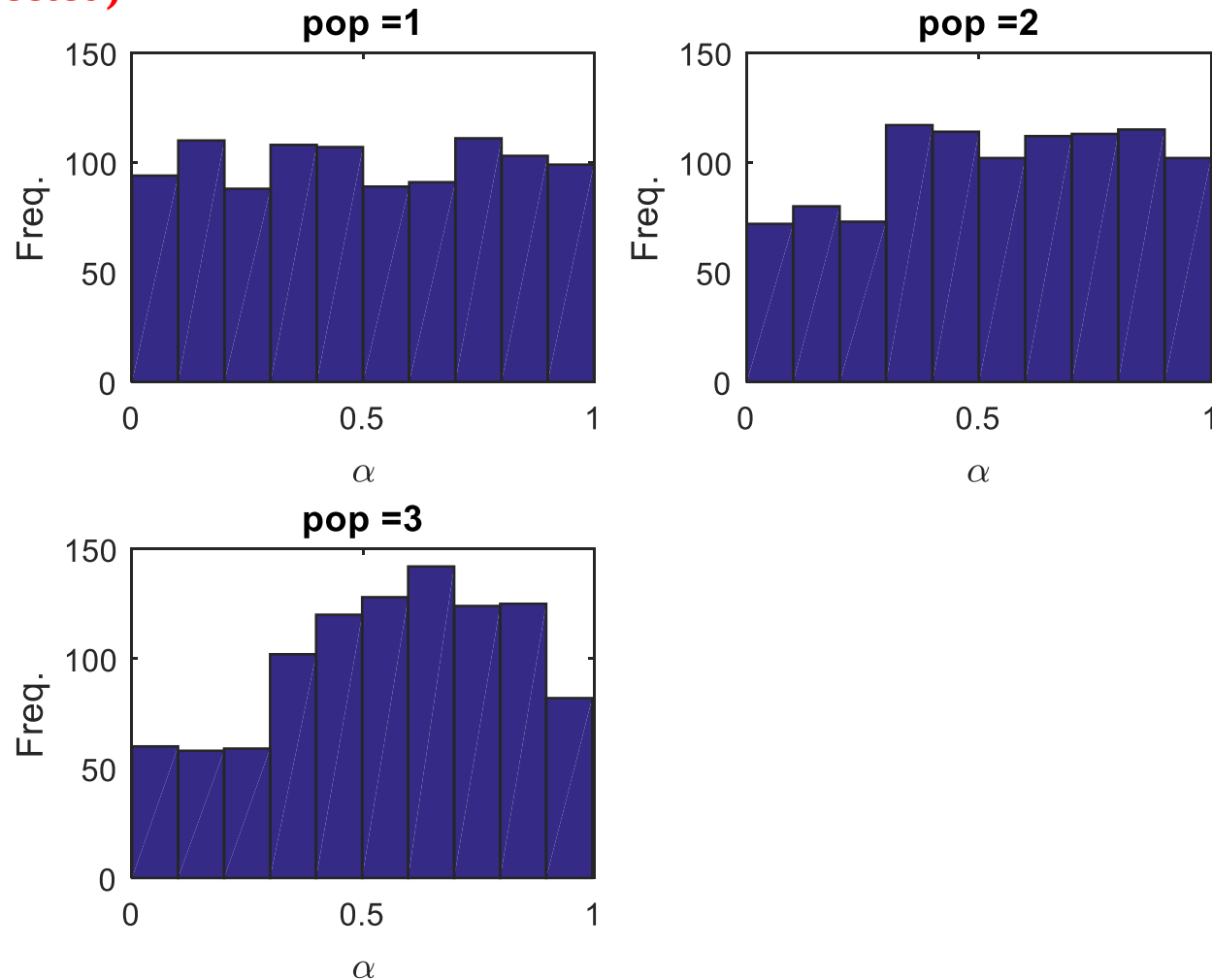
Experimental Data

Model 2 (not selected)



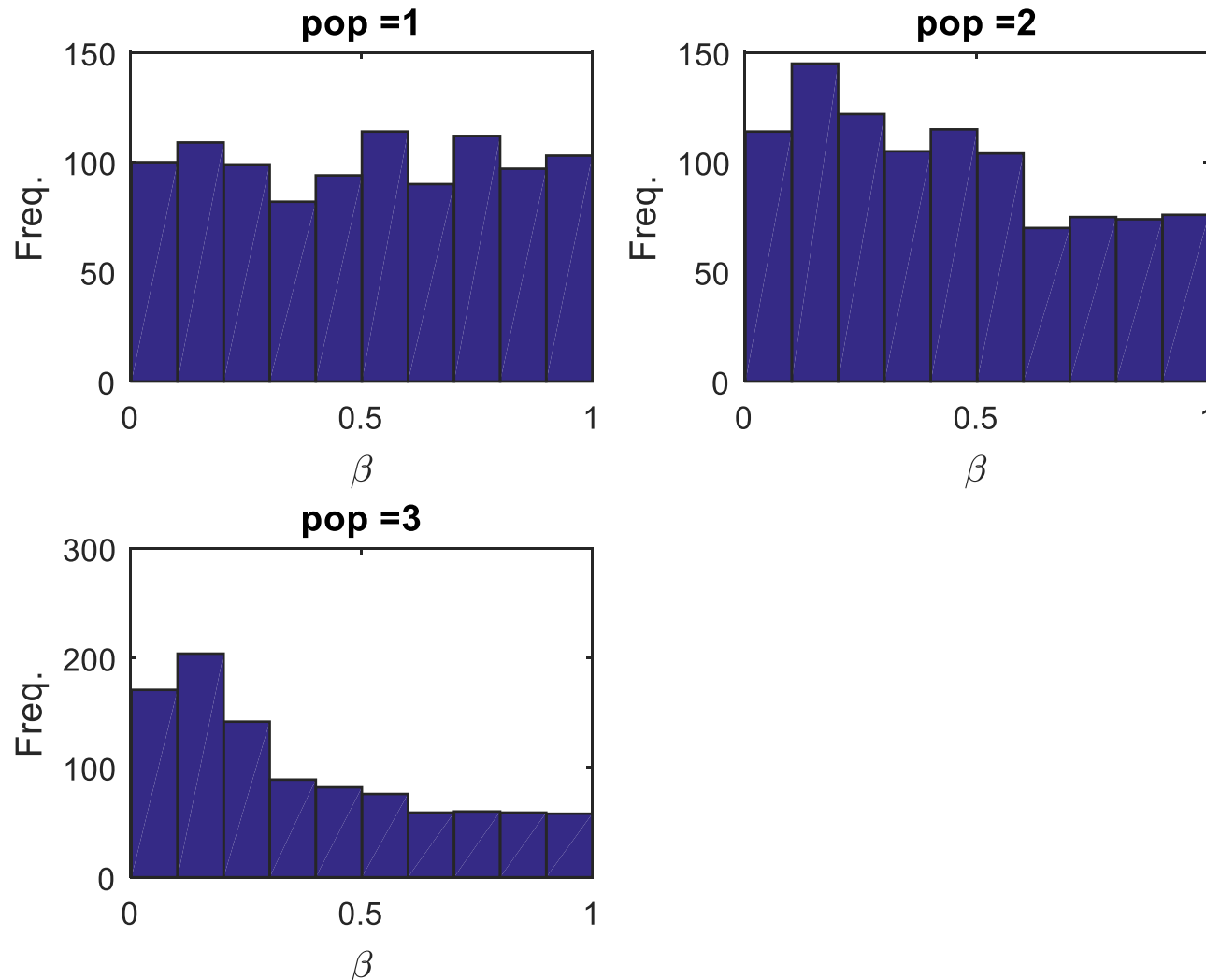
Experimental Data

Model 3 (not selected)

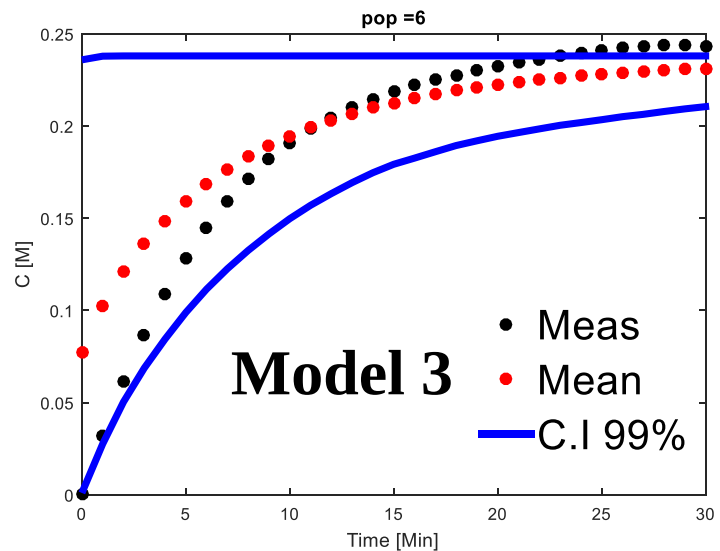
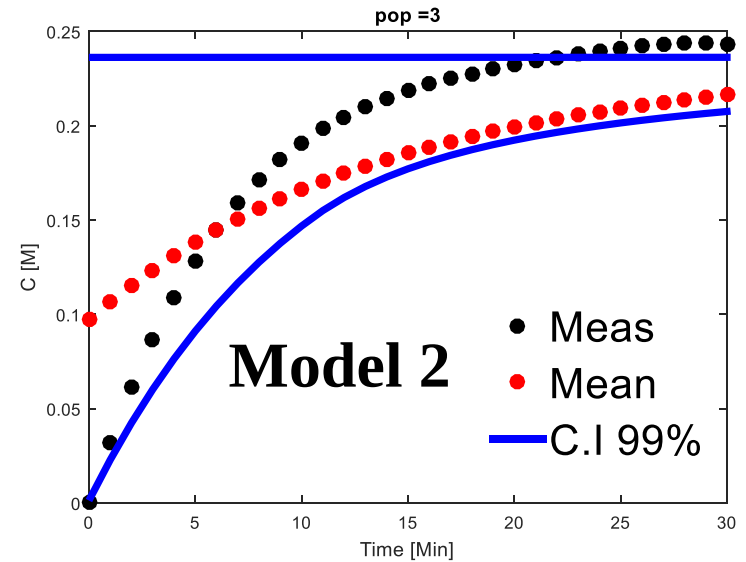
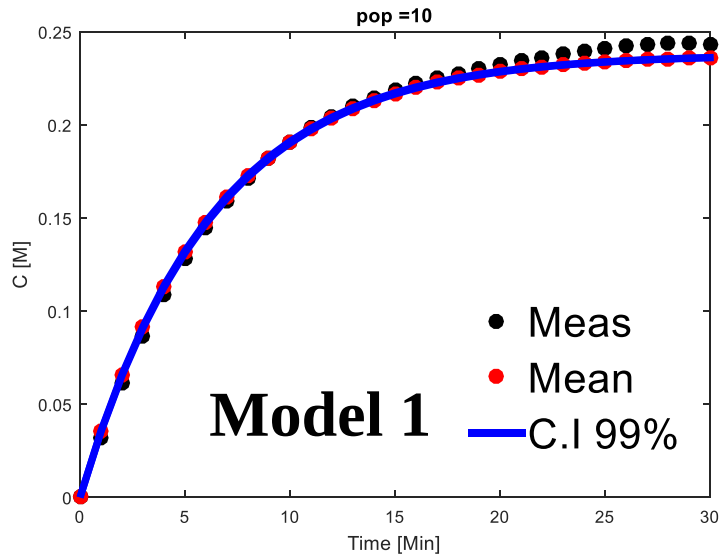


Experimental Data

Model 3 (not selected)



Experimental Data



Why model 3 was not selected?

ISSUES

Model 3 converges to model 1 when:

$$\beta = 0$$

Model 3 converges to model 2 when:

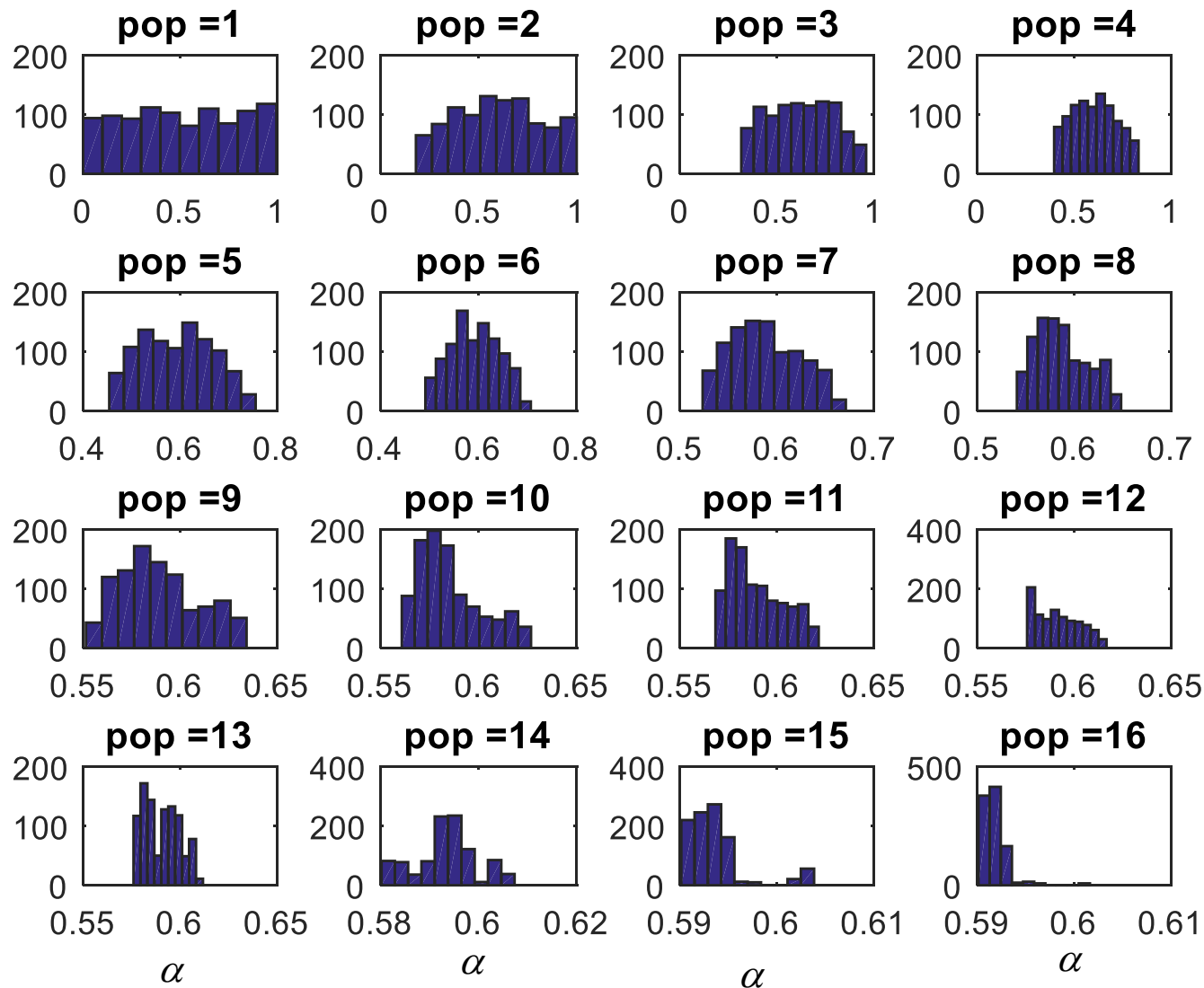
$$\alpha = 0$$

Since model 1 is the best, it is expected that model 3 be also appropriate with $\beta = 0$.

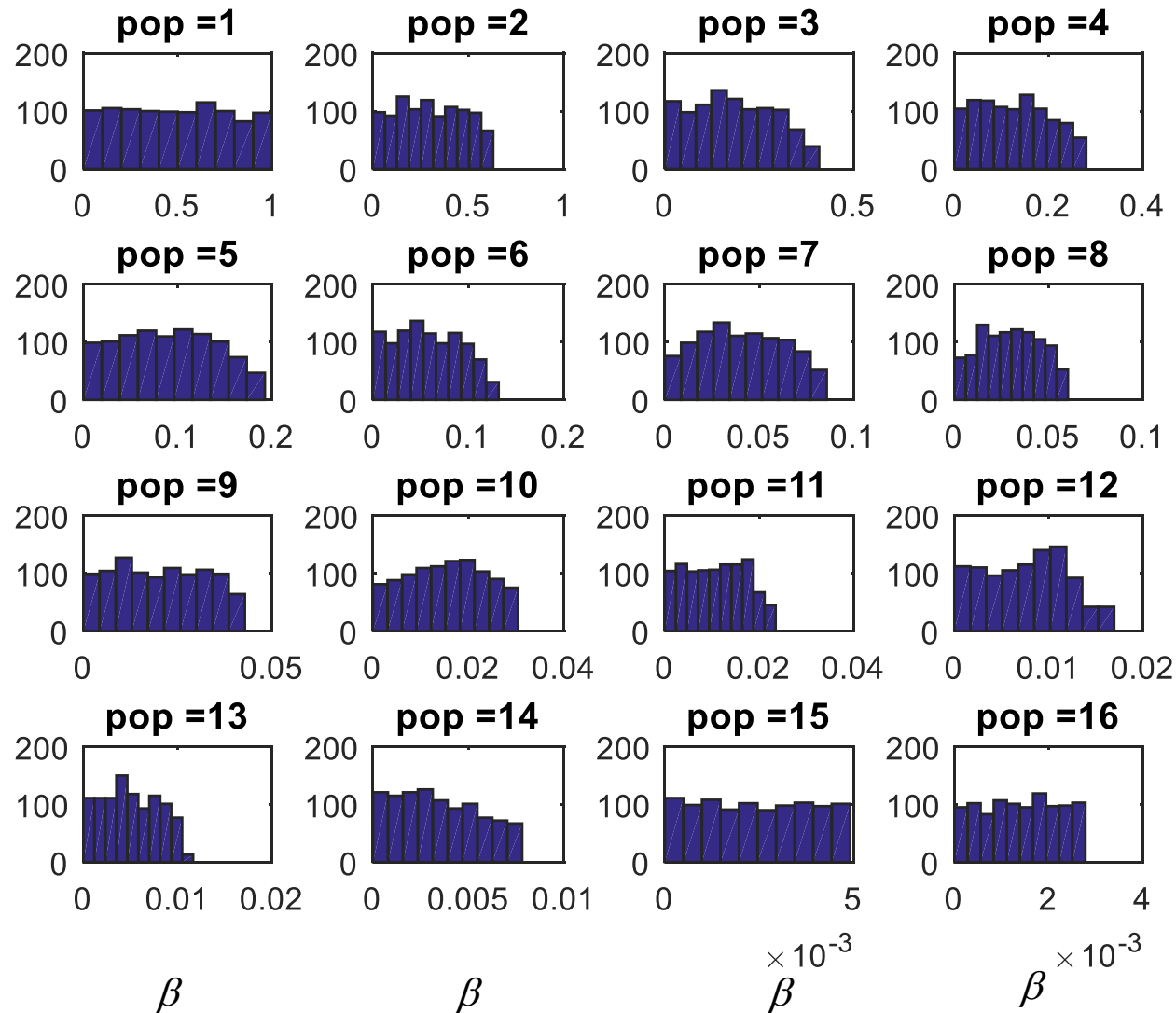


**Test: Estimate parameters
for model 3**

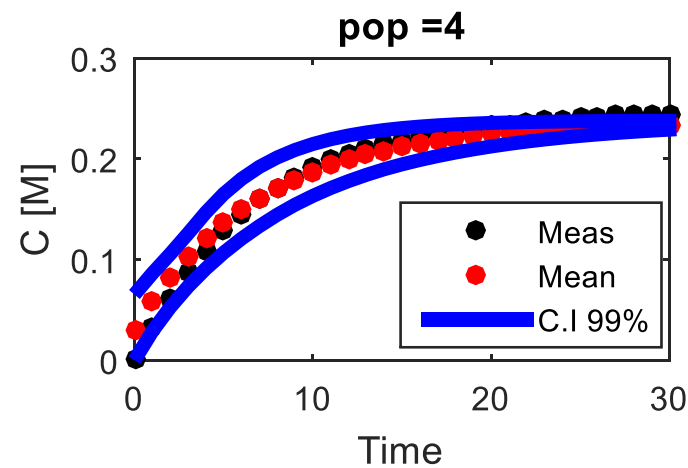
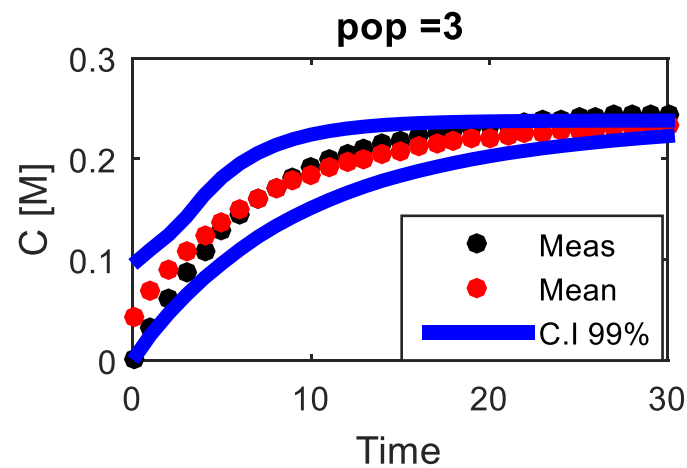
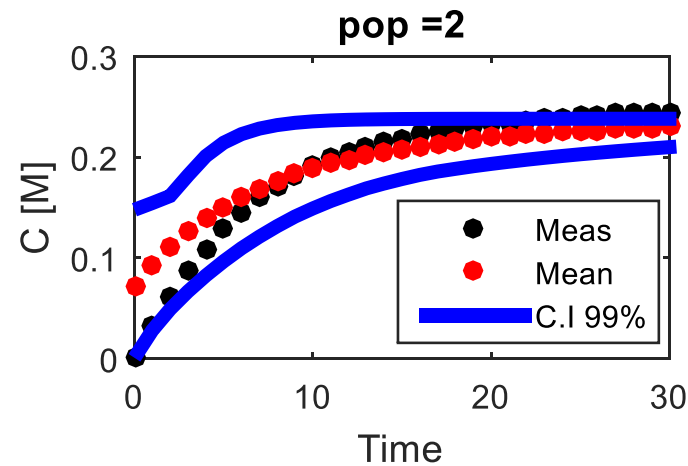
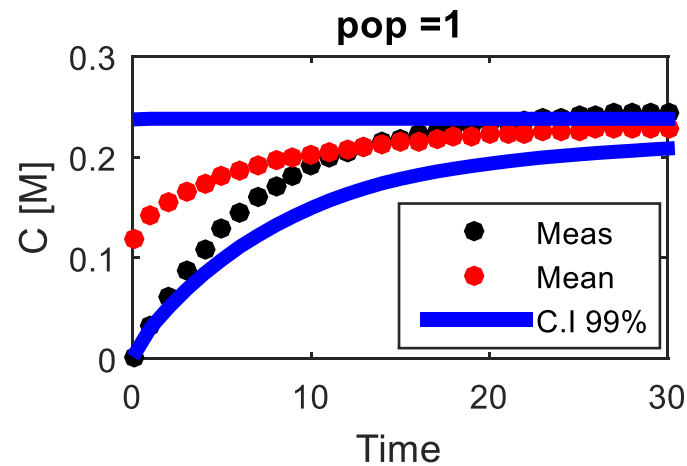
Using only Model 3



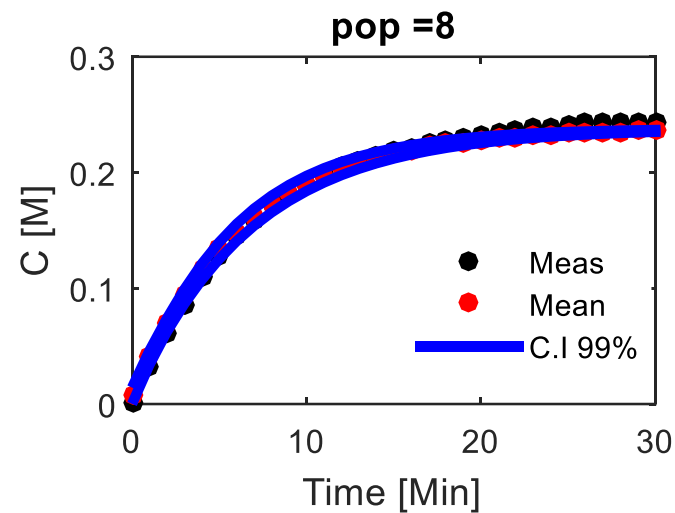
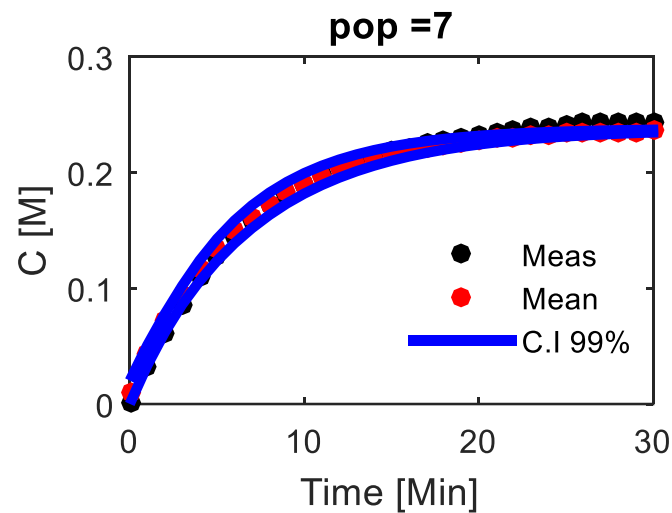
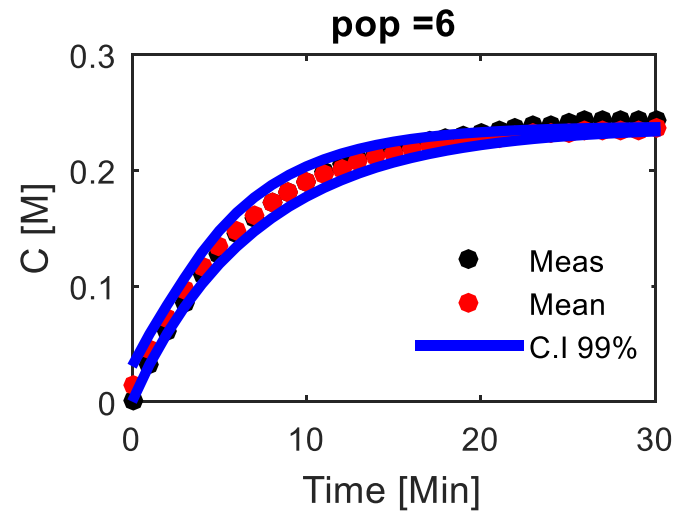
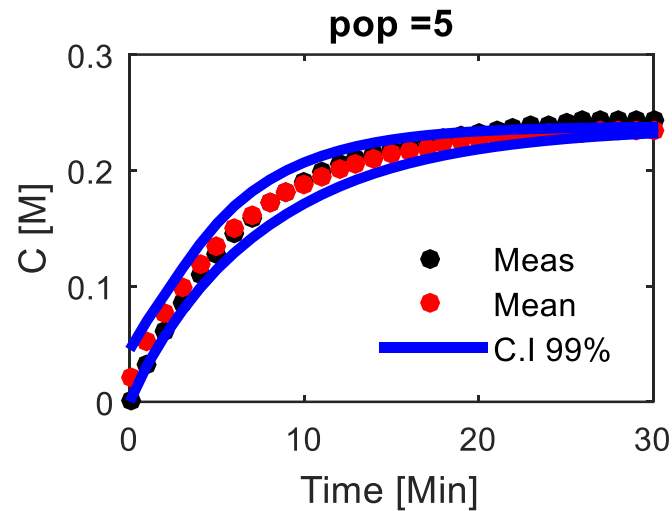
Using only Model 3



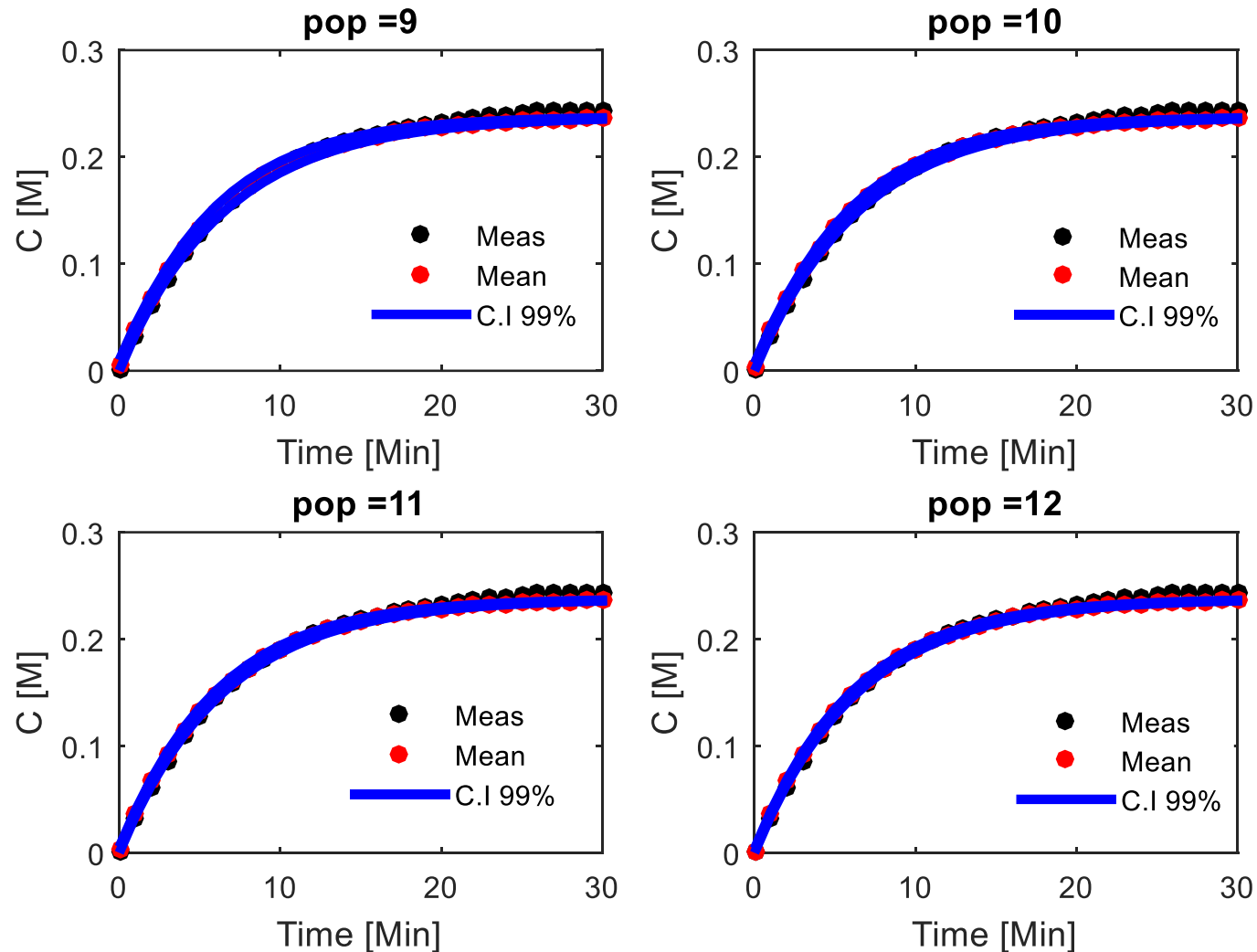
Using only Model 3



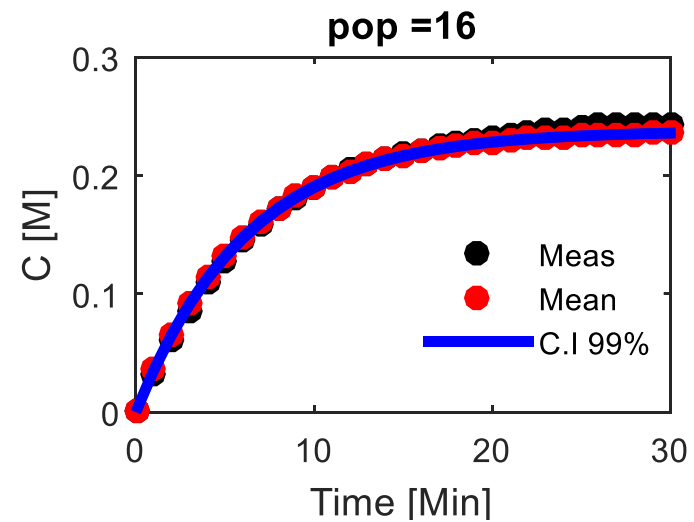
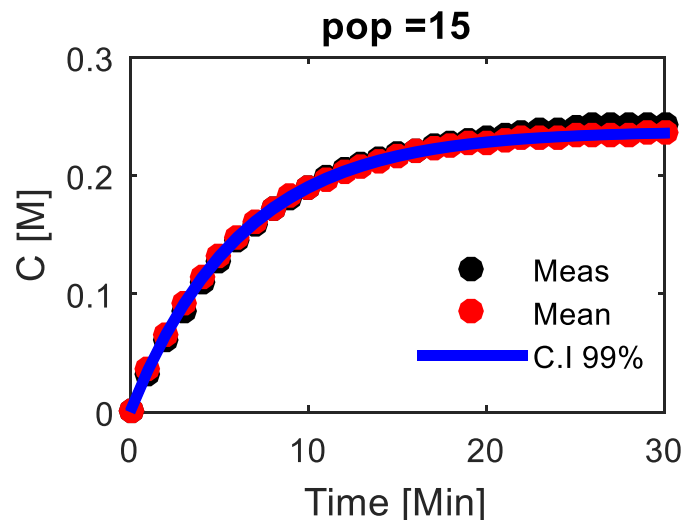
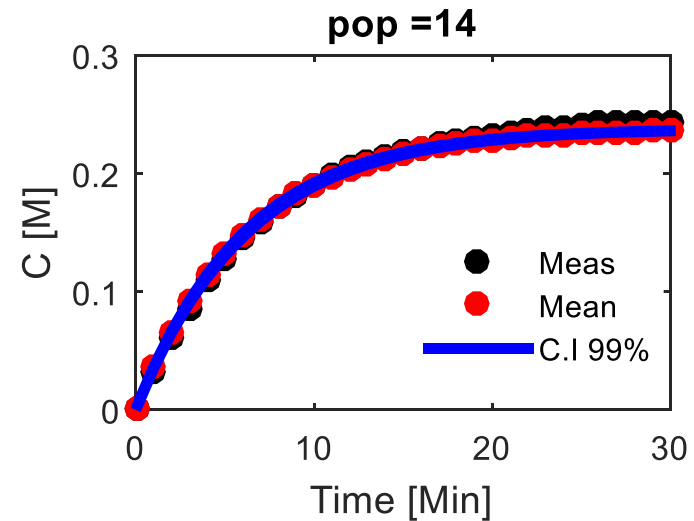
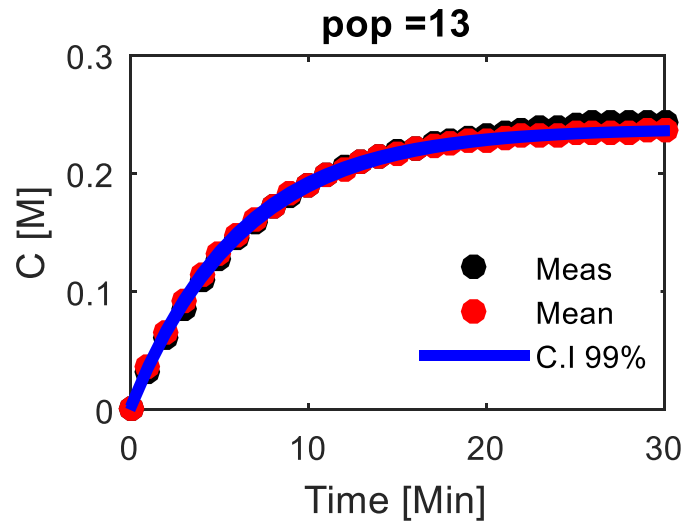
Using only Model 3



Using only Model 3



Using only Model 3





THANKS!

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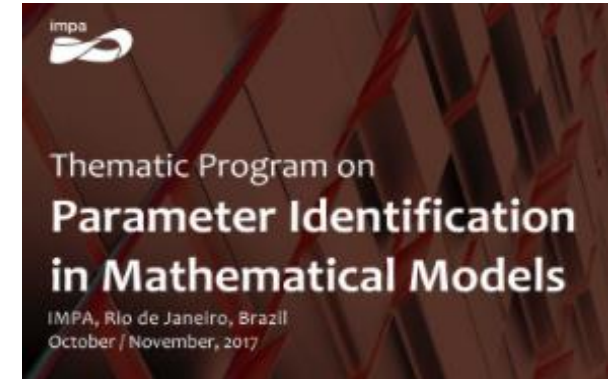
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