Model that works

January 12, 2022

Chemical Equation

$$\mathrm{CO} \underset{\mathrm{k_{AO}}}{\overset{\mathrm{k_{OA}}}{\rightleftharpoons}} \mathrm{CO^A} \underset{\mathrm{k_{BA}}}{\overset{\mathrm{k_{AB}}}{\rightleftharpoons}} \mathrm{CO^B} \underset{\mathrm{k_{OB}}}{\overset{\mathrm{k_{BO}}}{\rightleftharpoons}} \mathrm{CO} \tag{1}$$

Reaction Rate Equations

Region I

$$\frac{\partial \theta_\tau^B}{\partial \tau} = -k_{BO}\theta_\tau^B + k_{OB}P(M^B - \theta_\tau^B) \tag{2}$$

$$\frac{\partial \theta_\tau^A}{\partial \tau} = 0 \tag{3}$$

Region II

$$\frac{\partial \theta_\tau^B}{\partial \tau} = -k_{BA}P\theta_\tau^B + k_{AB}\theta_\tau^A(M - \theta_\tau^X) \tag{4}$$

$$\frac{\partial \theta_\tau^A}{\partial \tau} = k_{OA}P(M - \theta_\tau^X) - k_{AO}\theta_\tau^A - k_{AB}\theta_\tau^A(M - \theta_\tau^X) + k_{BA}P\theta_\tau^B \tag{5}$$

Region III

$$\frac{\partial \theta_\tau^B}{\partial \tau} = k_{AB}\theta_\tau^A(M - \theta_\tau^X) \tag{6}$$

$$\frac{\partial \theta_\tau^A}{\partial \tau} = -k_{AO}\theta_\tau^A - k_{AB}\theta_\tau^A(M - \theta_\tau^X) \tag{7}$$

Region IV

$$\frac{\partial \theta_\tau^B}{\partial \tau} = -k_{BO}\theta_\tau^B \tag{8}$$

$$\frac{\partial \theta_\tau^A}{\partial \tau} = 0 \tag{9}$$

Relations

$$\begin{aligned} &\theta_\tau^A + \theta_\tau^B = \theta_\tau^X \\ &0.5X_\tau^A + 0.33X_\tau^B = \theta_\tau^X \\ &X_\tau^A + X_\tau^B = 1. \end{aligned} \tag{10}$$

Equations used for fitting

Region I

Fitting B

$$\theta^B_{\tau+1} = [1 - k_{BO}\Delta\tau]\,\theta^B_\tau + k_{OB}P\Delta\tau(M - \theta^X_\tau) \tag{11}$$

Fitting A

$$\theta^A_{\tau+1} = 0 \tag{12}$$

Region II

Fitting B

$$\theta^B_{\tau+1} = [1 - k_{BA}P\Delta\tau]\,\theta^B_\tau + k_{AB}\Delta\tau\theta^A_\tau(M - \theta^X_\tau) \tag{13}$$

Fitting A

$$\theta^A_{\tau+1} = \left[1 - k_{AO}\Delta\tau - k_{AB}\Delta\tau(M - \theta^X_\tau)\right]\theta^A_\tau + k_{BA}P\Delta\tau\theta^B_\tau + k_{OA}\Delta\tau P(M - \theta^X_\tau) \tag{14}$$

Region III

Fitting B

$$\theta^B_{\tau+1} = \theta^B_\tau + k_{AB}\Delta\tau\theta^A_\tau(M - \theta^X_\tau) \tag{15}$$

Fitting A

$$\theta^A_{\tau+1} = \left[1 - k_{AO}\Delta\tau - k_{AB}\Delta\tau(M - \theta^X_\tau)\right]\theta^A_\tau \tag{16}$$

Region IV

Fitting B

$$\theta^B_{\tau+1} = [1 - k_{BO}\Delta\tau]\,\theta^B_\tau \tag{17}$$

Fitting A

$$\theta^A_{\tau+1} = 0 \tag{18}$$

Get k_{BO} from

$$ln(\frac{\theta_\tau^B}{\theta_0^B}) = -k_{BO}\tau \tag{19}$$

Get k_{OB} from

$$\theta_{\tau+1}^B - (1 - k_{BO})\theta_\tau^B = k_{OB}\Delta\tau P(M - \theta_\tau^X) \tag{20}$$

Get k_{AB} from

$$\theta_{\tau+1}^B - \theta_\tau^B = k_{AB}\Delta\tau\theta_\tau^A(M - \theta_\tau^X) \tag{21}$$

Get k_{AO} from

$$\theta_{\tau+1}^A - (1 - k_{AB}\Delta\tau(M - \theta_\tau^X))\theta_\tau^A = -k_{AO}\Delta\tau\theta_\tau^A \tag{22}$$

Get k_{BA} from

$$\theta_{\tau+1}^B - \theta_\tau^B - k_{AB}\Delta\tau\theta_\tau^A(M - \theta_\tau^X) = -k_{BA}\Delta\tau P\theta_\tau^B \tag{23}$$

Get k_{OA} from

$$\theta_{\tau+1}^X - \theta_\tau^X + k_{AO}\Delta\tau\theta_\tau^A = -k_{OA}\Delta\tau P(M - \theta_\tau^X) \tag{24}$$

Results

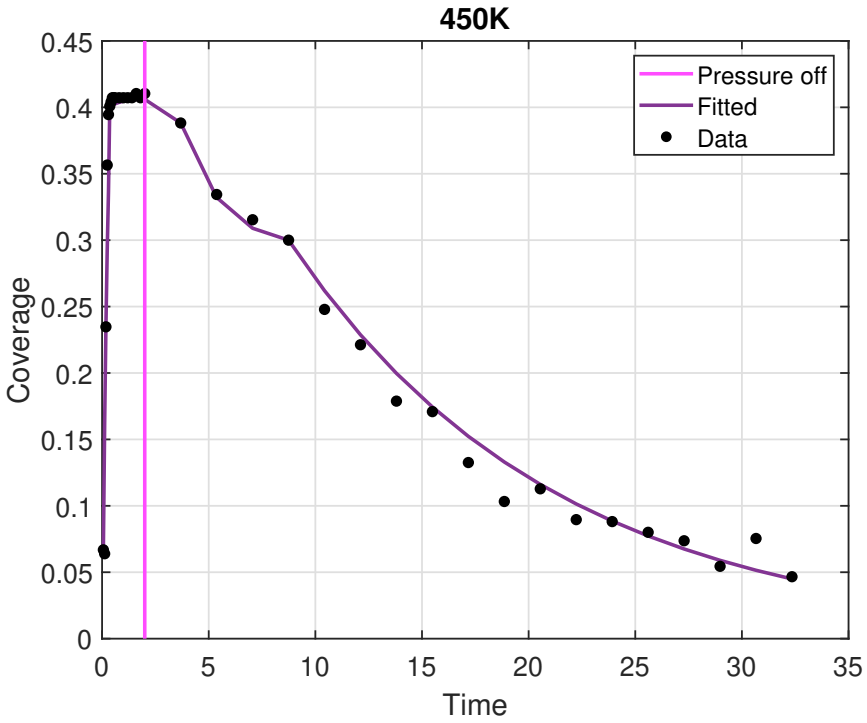

Figure 1: Overall 450K

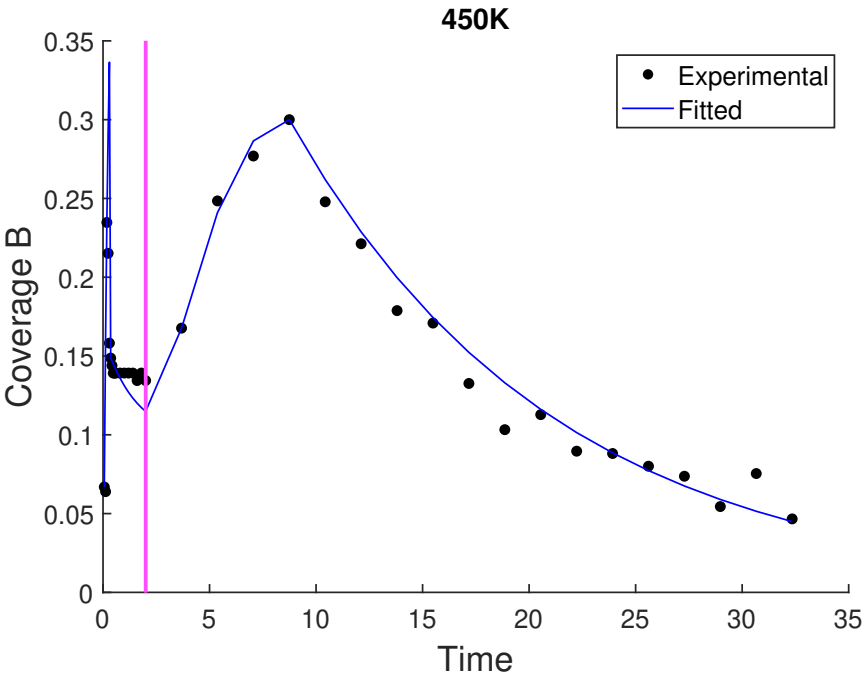

Figure 2: State B 450K

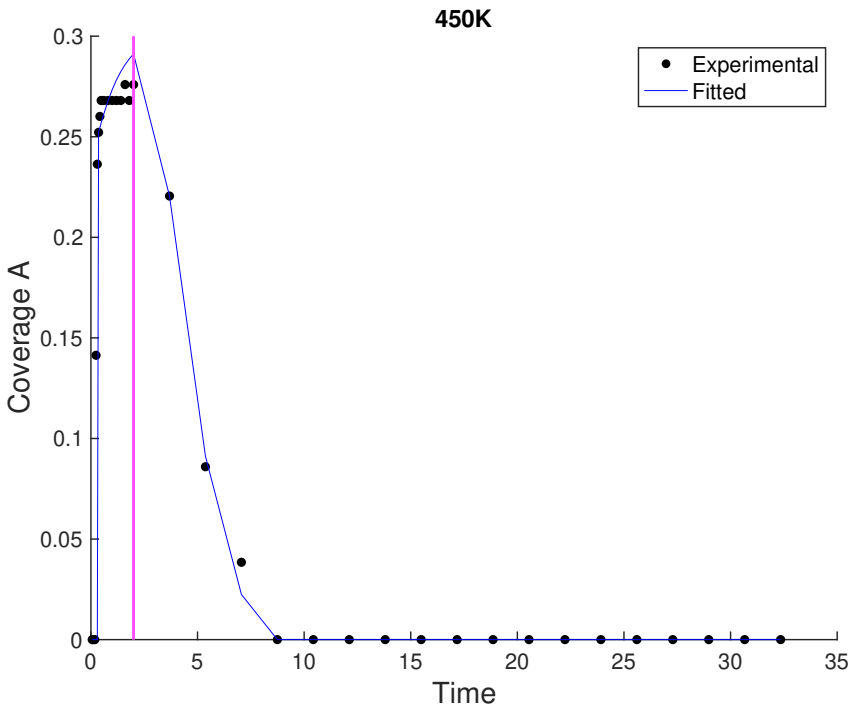

Figure 3: State A 450K

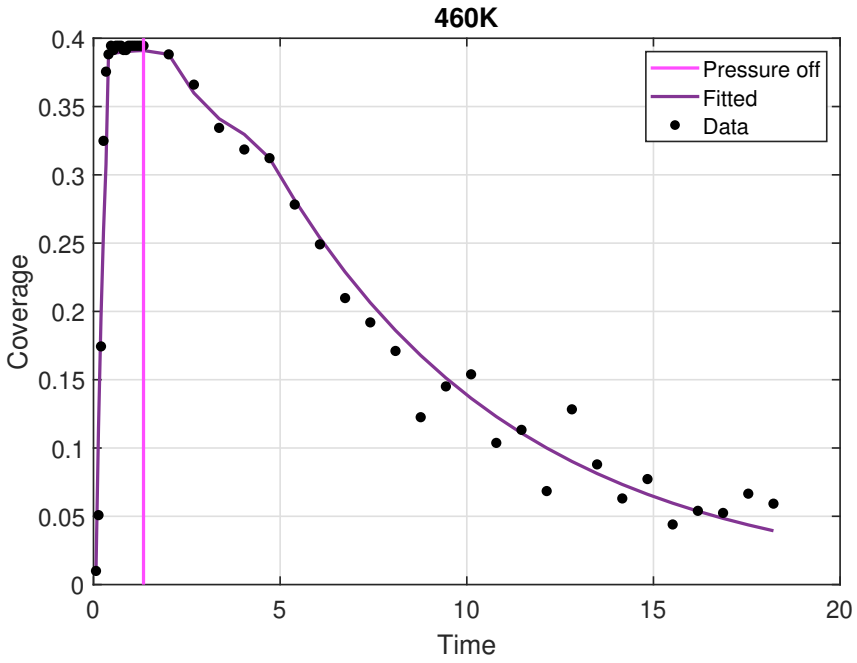

Figure 4: Overall 460K

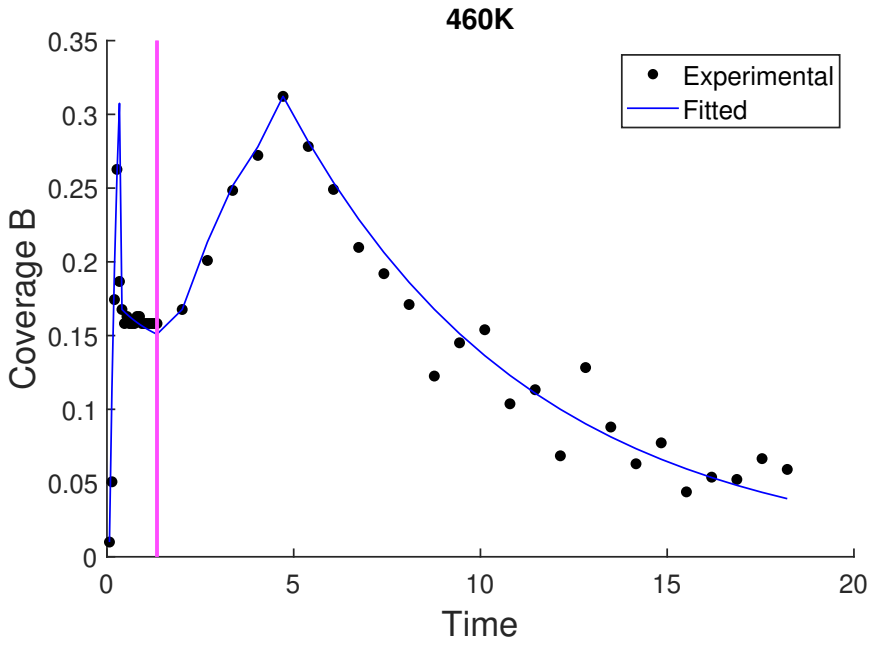

Figure 5: State B 460K

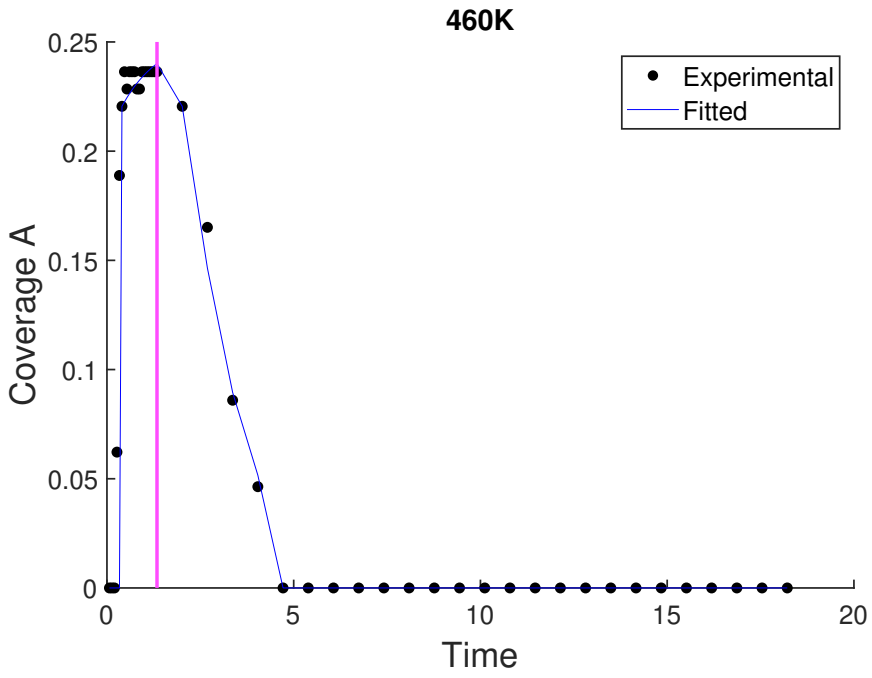

Figure 6: State A 460K

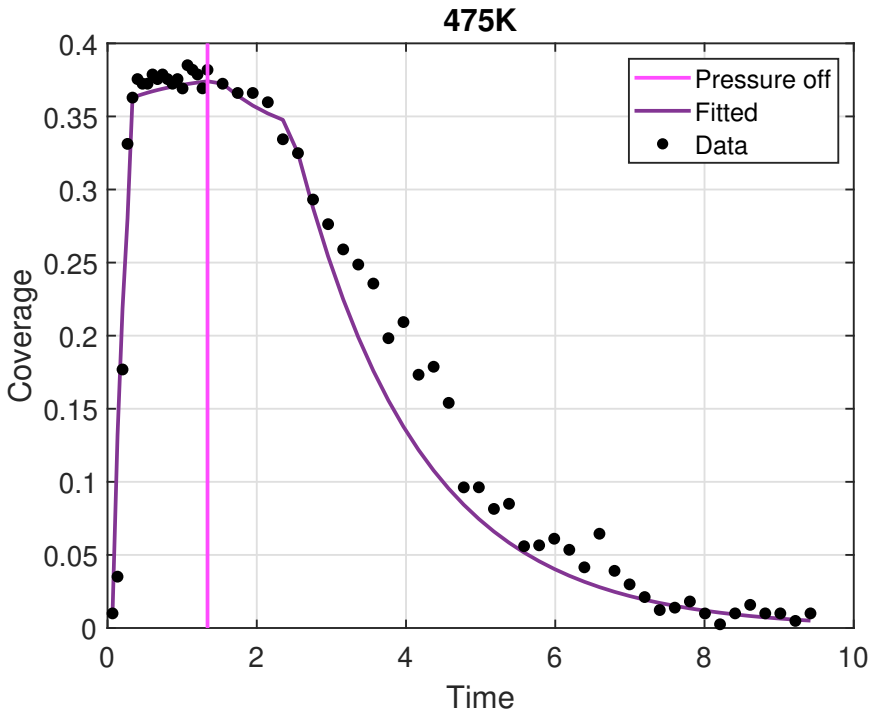

Figure 7: Overall 475K

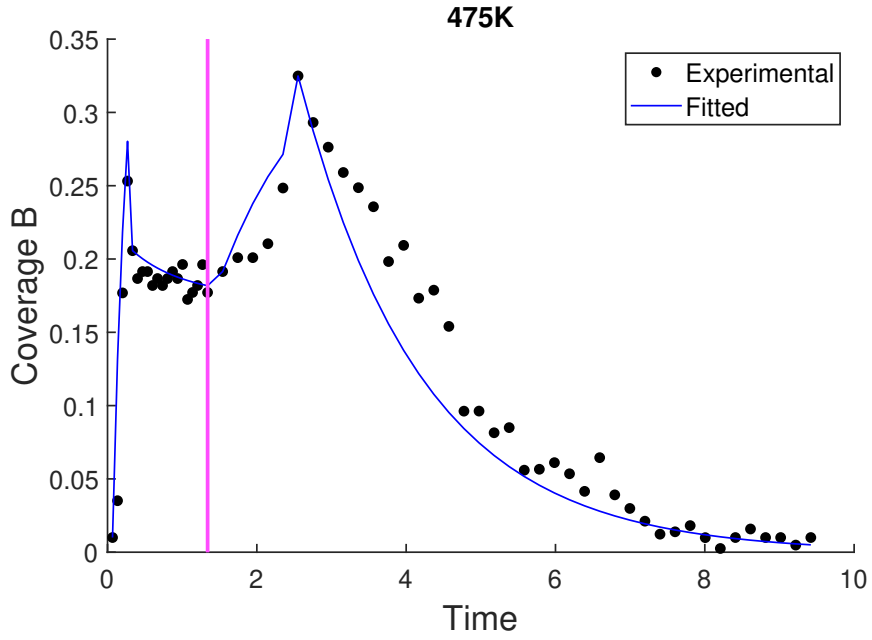

Figure 8: State B 475K

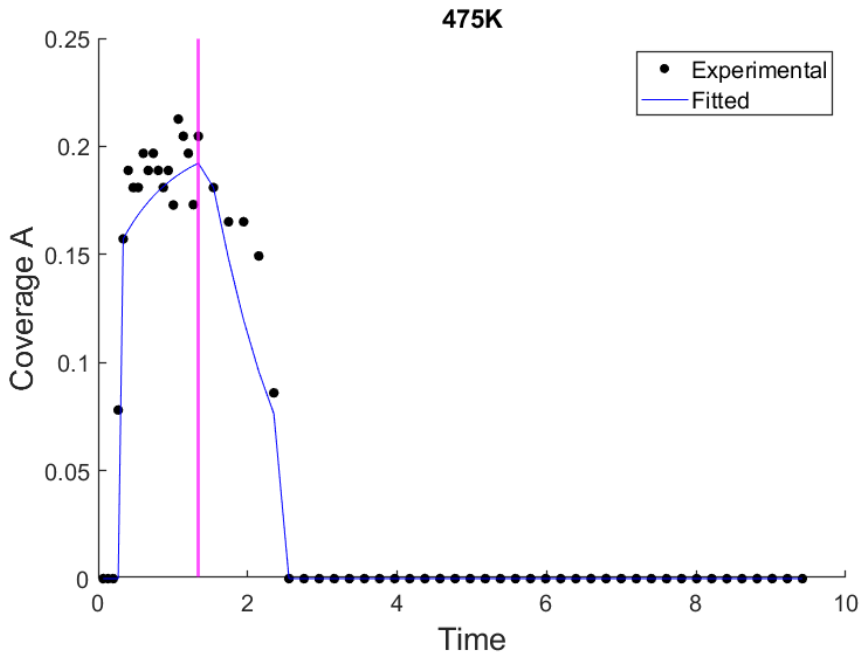

Figure 9: State A 475K

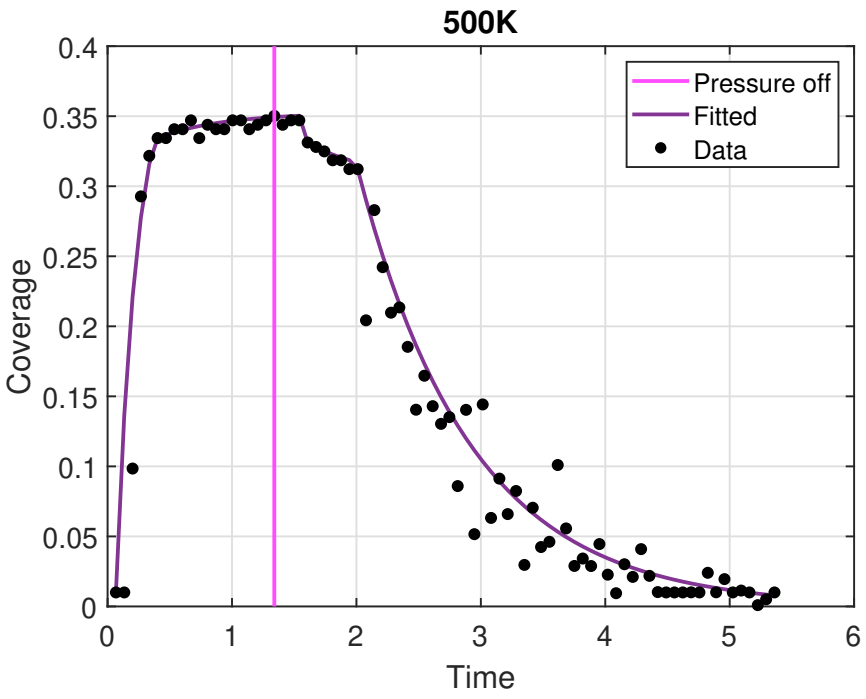

Figure 10: Overall 500K

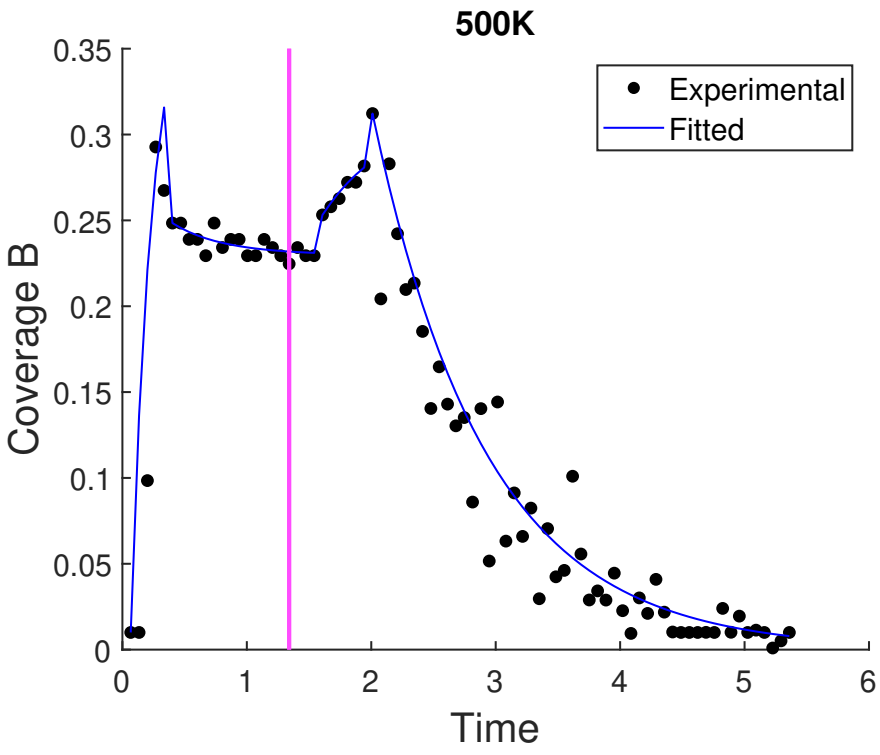

Figure 11: State B 500K

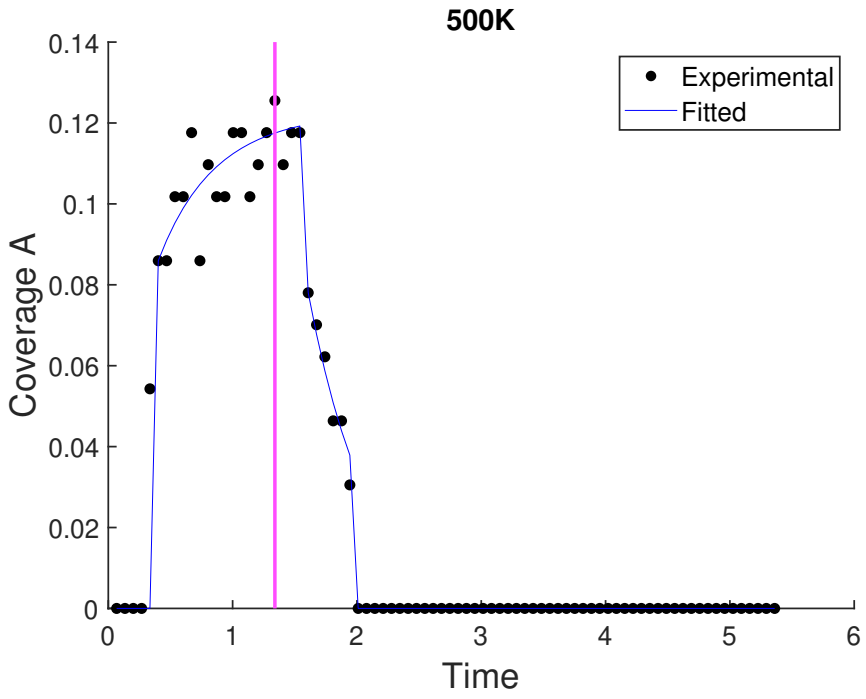

Figure 12: State A 500K