

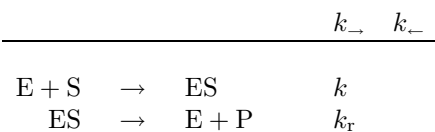
1 Fit of progress curves

1.1 Data

1. ./examples/reductase/data/i0.txt

1.2 Theoretical model

1.2.1 Reaction mechanism



1.2.2 Differential equations

$$\dot{c}_{\text{E}} = -k c_{\text{E}} c_{\text{S}} + k_{\text{r}} c_{\text{ES}} \quad (1)$$

$$\dot{c}_{\text{S}} = -k c_{\text{E}} c_{\text{S}} \quad (2)$$

$$\dot{c}_{\text{ES}} = +k c_{\text{E}} c_{\text{S}} - k_{\text{r}} c_{\text{ES}} \quad (3)$$

$$\dot{c}_{\text{P}} = +k_{\text{r}} c_{\text{ES}} \quad (4)$$

Set	Par.	No.	Initial	Fit	Error	%Error
	k	1	0.01	0.0299	0.0026	8.7
	k_{r}	2	1	0.611	0.048	7.9
	r_{P}	3	3.226	3.21	0.04	1.3
1	offset	4	6.41	-0.98	0.6	61

Table 1: Parameters and formal standard errors

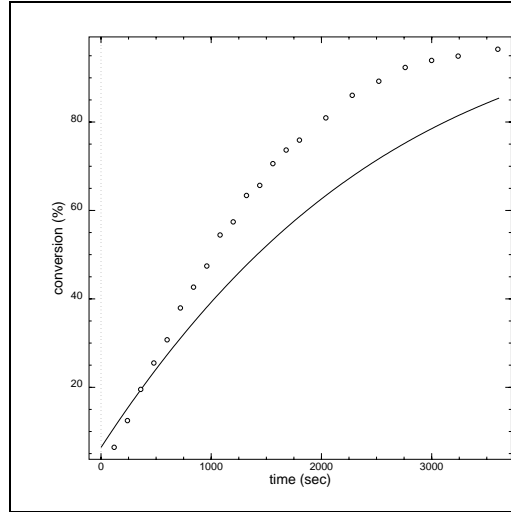


Figure 1: Data and model: initial estimate

Set	Par.	No.	Covariances		
	k	1	1		
	k_r	2	-96	2	
	r_P	3	-92	89	3
1	offset	4	61	-74	-78

Table 2: Covariance matrix

			Eigenvectors			
Eigenvalues			0.00	0.08	0.20	3.72
$\log_{10} C$			2.91	1.67	1.28	0.00
Set	Par.	No.	1	2	3	4
	k	1	-70	46	-15	51
	k_r	2	56	8	-65	49
	r_P	3	37	28	73	48
1	offset	4	-20	-83	9	50

Table 3: Eigenvalues and eigenvectors

		Index		3	2	1	0
Set	Par.	No.	<i>1</i>	<i>2</i>	<i>3</i>	<i>4</i>	
	k	<i>1</i>	49	21	2	26	
	k_r	<i>2</i>	31	0	42	24	
	r_p	<i>3</i>	14	8	53	23	
1	offset	<i>4</i>	4	69	0	25	

Table 4: Redundancy grades

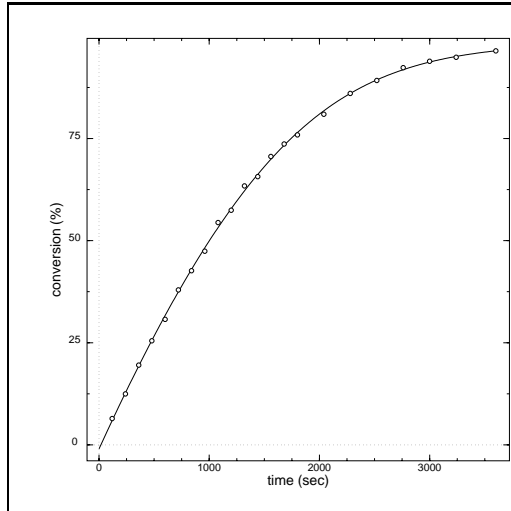


Figure 2: Data and model: least-squares fit

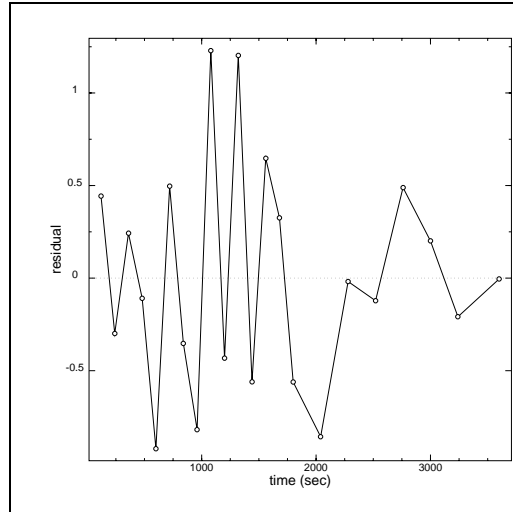


Figure 3: Residuals vs. independent variable

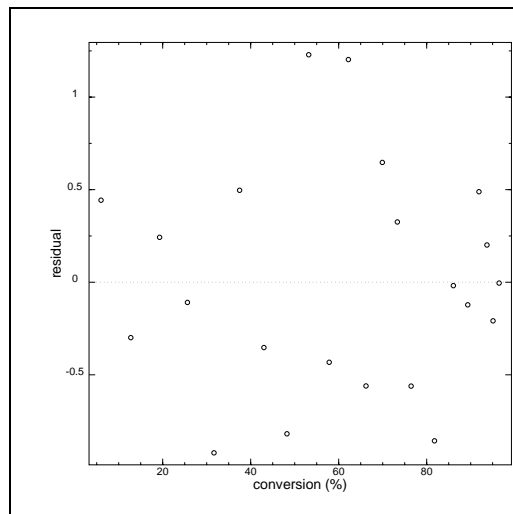


Figure 4: Residuals vs. dependent variable

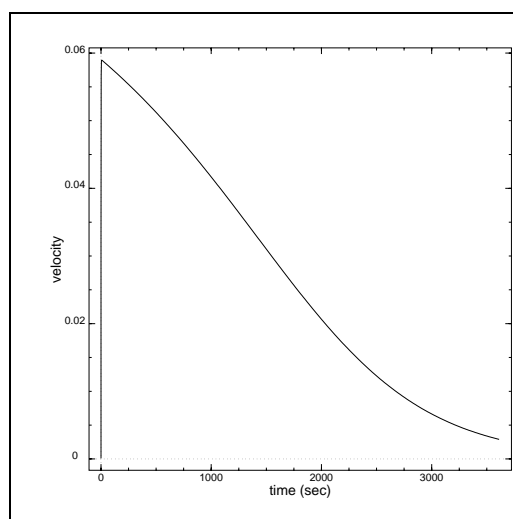


Figure 5: Reaction velocity curve