

Determination of the Kinetics of the Ethoxylation of Octanol in Homogeneous Phase

Pascal D. Hermann,[†] Toine Cents,[‡] Elias Klemm,[†] and Dirk Ziegenbalg^{*,†}

[†]*Institute of Chemical Technology, University of Stuttgart, 70569 Stuttgart Germany*

[‡]*Sasol, Group Technology, 1947 Sasolburg, South Africa*

E-mail: dirk.ziegenbalg@itc.uni-stuttgart.de

Reaction Conditions of Various Published Work

Table S1: Process conditions and reactor types used in various publications on the kinetics of ethoxylation of fatty alcohols.

Source	Alcohol	Reactor	T / °C	p / kPa	System
Hall 1990 ¹	dodecanol	spray-loop	124 - 173	68 - 204	
Santacesaria 1992 ²	dodecanol	semibatch	68.5 - 197.5	101 - 304	2-phase
DiSerio 1995 ³	dodecanol	semibatch	150 - 180	203 - 507	2-phase
DiSerio 1996 ⁴	octanol	semibatch	100 - 130	203	2-phase
Fan 2000 ⁵	dodecanol	pipe-reactor	131 - 164.3	3 600	2-phase
Amaral 2011 ⁶	dodecanol	semibatch	130 - 180	343	2-phase
Rupp 2015 ⁷	octanol	microreactor	130 - 240	9 000 - 10 000	1-phase
This Work	octanol	microreactor	180 - 240	9 000 - 10 000	1-phase

Precision of the CFD-14-Species Model

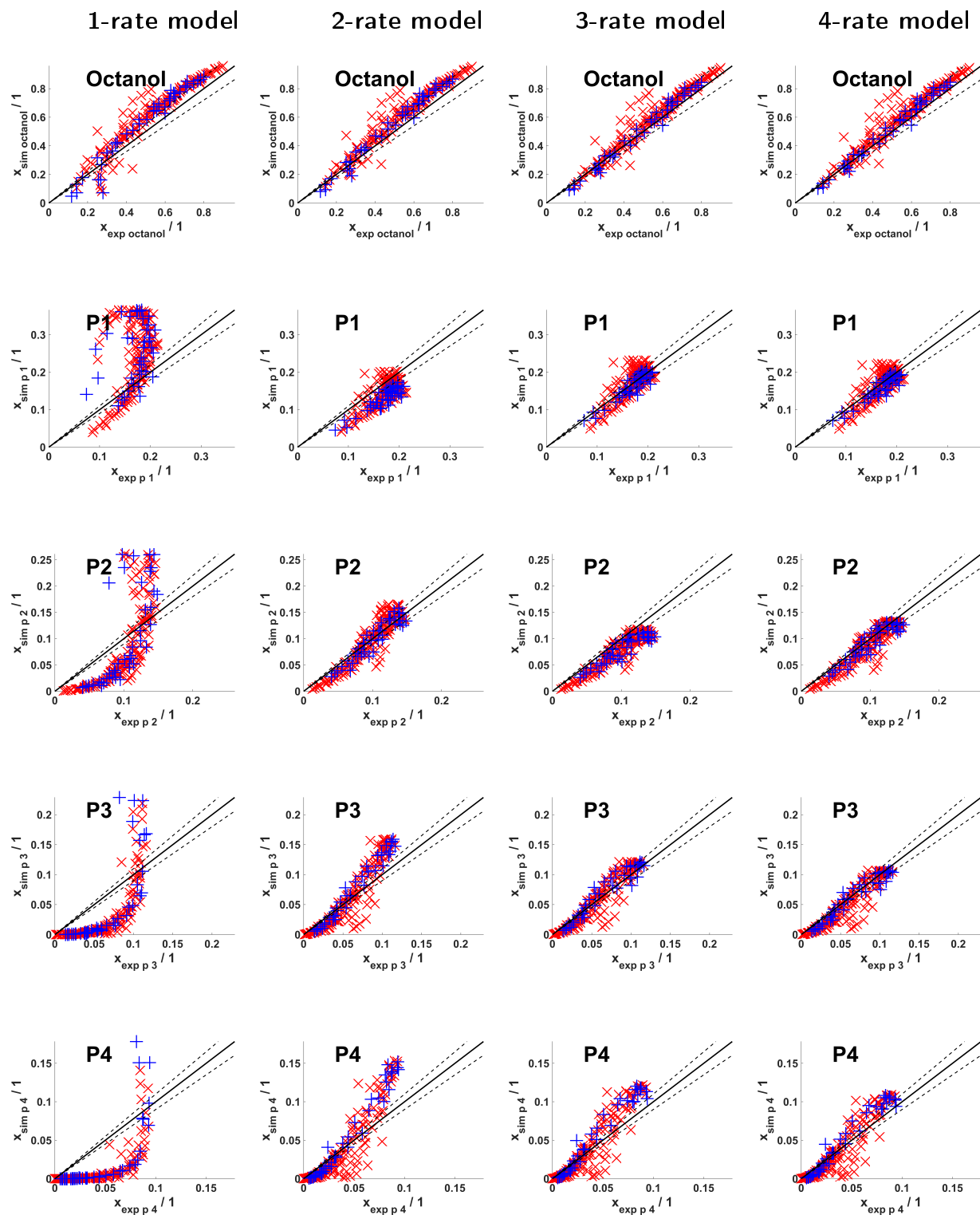


Figure S1: Parity plots for octanol to product 4. The black dotted lines gives the $\pm 10\%$ error.

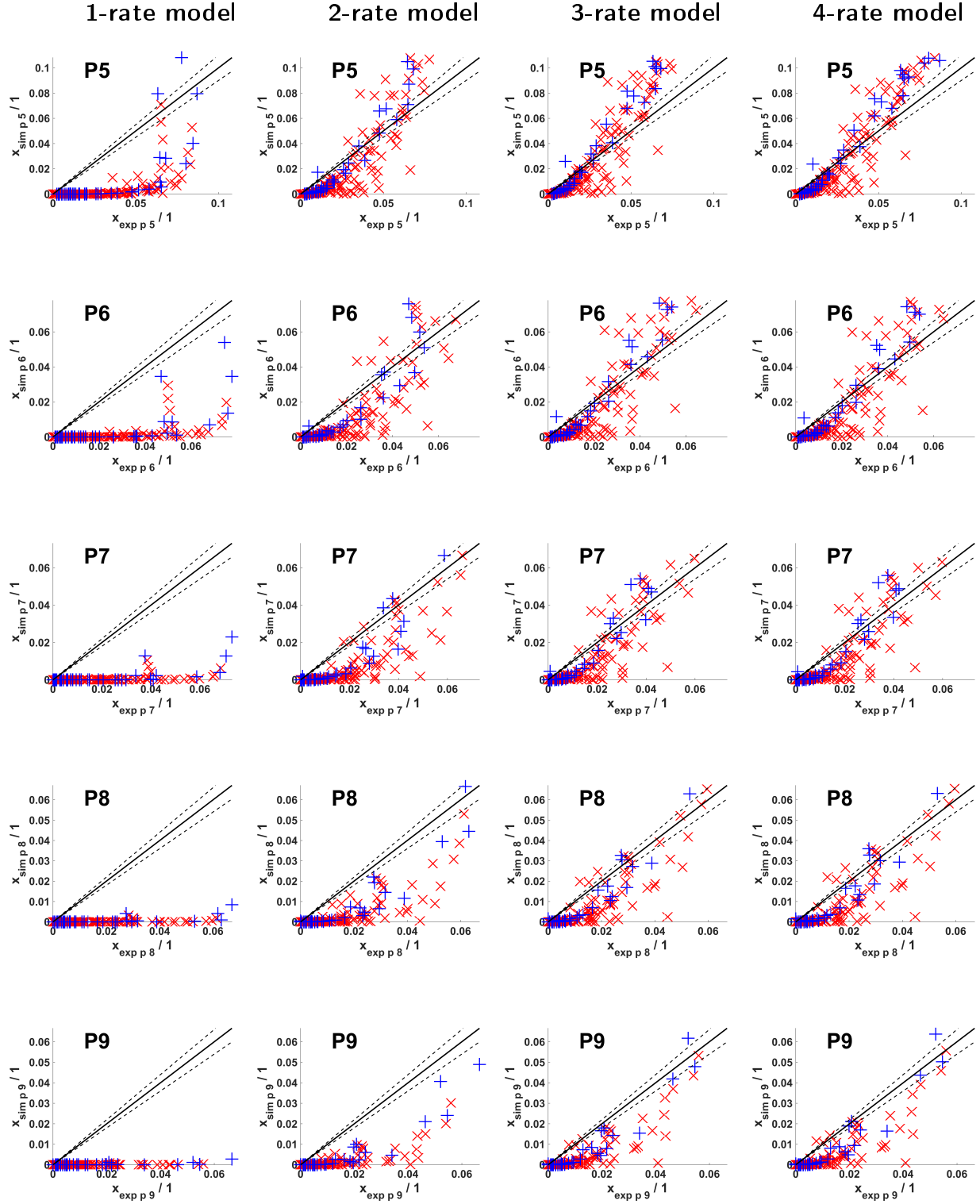


Figure S2: Parity plots for product 5 to product 9. The black dotted lines gives the $\pm 10\%$ error.

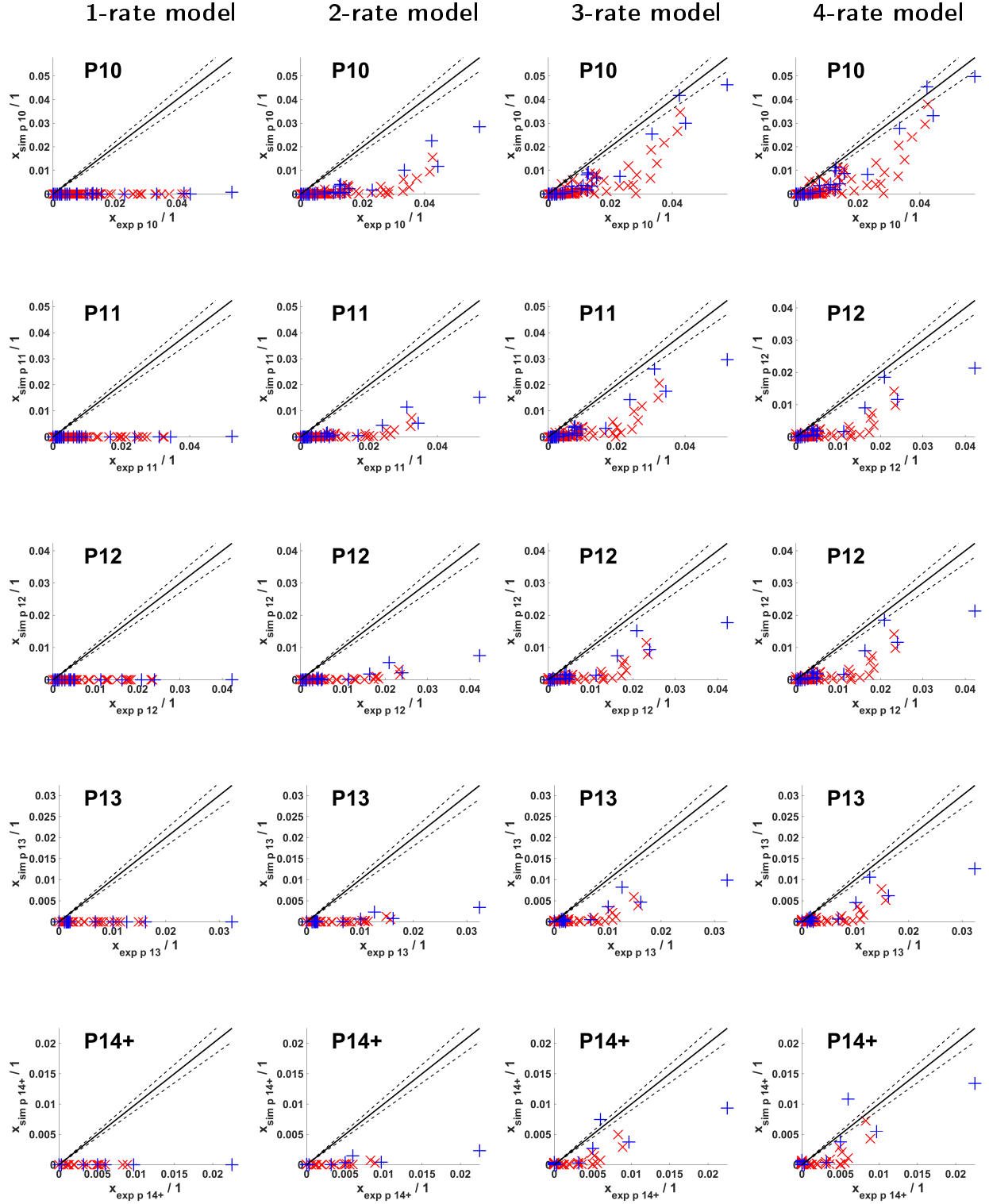


Figure S3: Parity plots for product 10 to product 14. The black dotted lines gives the $\pm 10\%$ error.

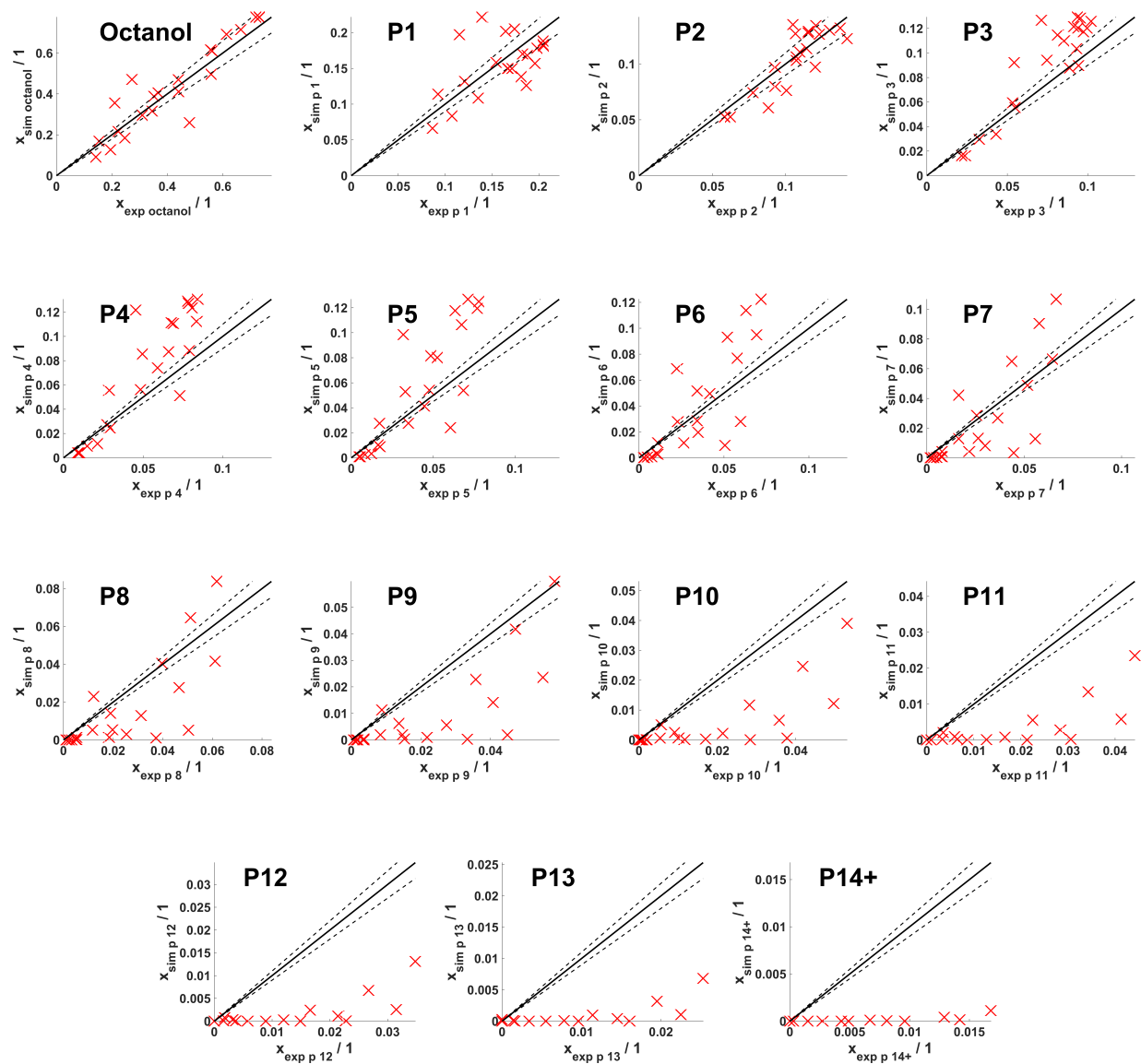


Figure S4: Parity plots for octanol to product 14 for a concentration of 0.83 mol% anionic species. The black dotted lines gives the $\pm 10\%$ error.

PFR-Model Kinetic and Precision

Table S2: Kinetic Parameters PFR Study

	1-rate	2-rate	3-rate	4-rate	5-rate	6-rate	7-rate	8-rate
E_{Ap}	73.7	75.7	76.6	75.1	74.8	74.4	74.2	74.0
/ kJ mol^{-1}	± 1.8	± 4.6	± 1.4	± 0.4	± 0.5	± 0.7	± 0.8	± 0.6
$k_{0p} \cdot 10^{-3}$	80	550	770	580	570	550	560	5603
/ $\text{m}^3 \text{mol}^{-1} \text{s}^{-1}$	± 2	± 380	± 220	± 25	± 14	± 24	± 18	± 21
E_{A1}		68.3	65.7	67.4	67.3	67.3	67.5	67.4
/ kJ mol^{-1}		± 1.5	± 2.5	± 0.6	± 0.7	± 0.7	± 1.1	± 0.7
$k_{01} \cdot 10^{-3}$		17	11	18	18	19	20	19
/ $\text{m}^3 \text{mol}^{-1} \text{s}^{-1}$		± 5	± 7	± 2	± 1	± 1	± 1	± 1
E_{A2}			78.3	77.2	77.0	77.4	76.7	76.8
/ kJ mol^{-1}			± 1.7	± 1	± 1	± 0.9	± 1.2	± 0.8
$k_{02} \cdot 10^{-3}$			603	506	495	544	467	498
/ $\text{m}^3 \text{mol}^{-1} \text{s}^{-1}$			± 73	± 32	± 58	± 25	± 32	± 28
E_{A3}				76.3	76.4	76.5	76.5	76.6
/ kJ mol^{-1}				± 1.0	± 1.1	± 1.0	± 1.0	± 0.7
$k_{03} \cdot 10^{-3}$				505	550	557	552	548
/ $\text{m}^3 \text{mol}^{-1} \text{s}^{-1}$				± 56	± 38	± 33	± 28	± 32
E_{A4}					75.8	75.7	75.6	75.3
/ kJ mol^{-1}					± 0.8	± 0.7	± 1.1	± 0.7
$k_{04} \cdot 10^{-3}$					536	545	543	544
/ $\text{m}^3 \text{mol}^{-1} \text{s}^{-1}$					± 20	± 45	± 36	± 28
E_{A5}						75.0	75.1	75.0
/ kJ mol^{-1}						± 0.7	± 0.7	± 1.7
$k_{05} \cdot 10^{-3}$						520	540	543
/ $\text{m}^3 \text{mol}^{-1} \text{s}^{-1}$						± 45	± 41	± 35
E_{A6}							75.1	75.1
/ kJ mol^{-1}							± 1.1	± 0.7
$k_{06} \cdot 10^{-3}$							564	549
/ $\text{m}^3 \text{mol}^{-1} \text{s}^{-1}$							± 38	± 29
E_{A67}								74.9
/ kJ mol^{-1}								± 0.7
$k_{07} \cdot 10^{-3}$								560
/ $\text{m}^3 \text{mol}^{-1} \text{s}^{-1}$								± 54

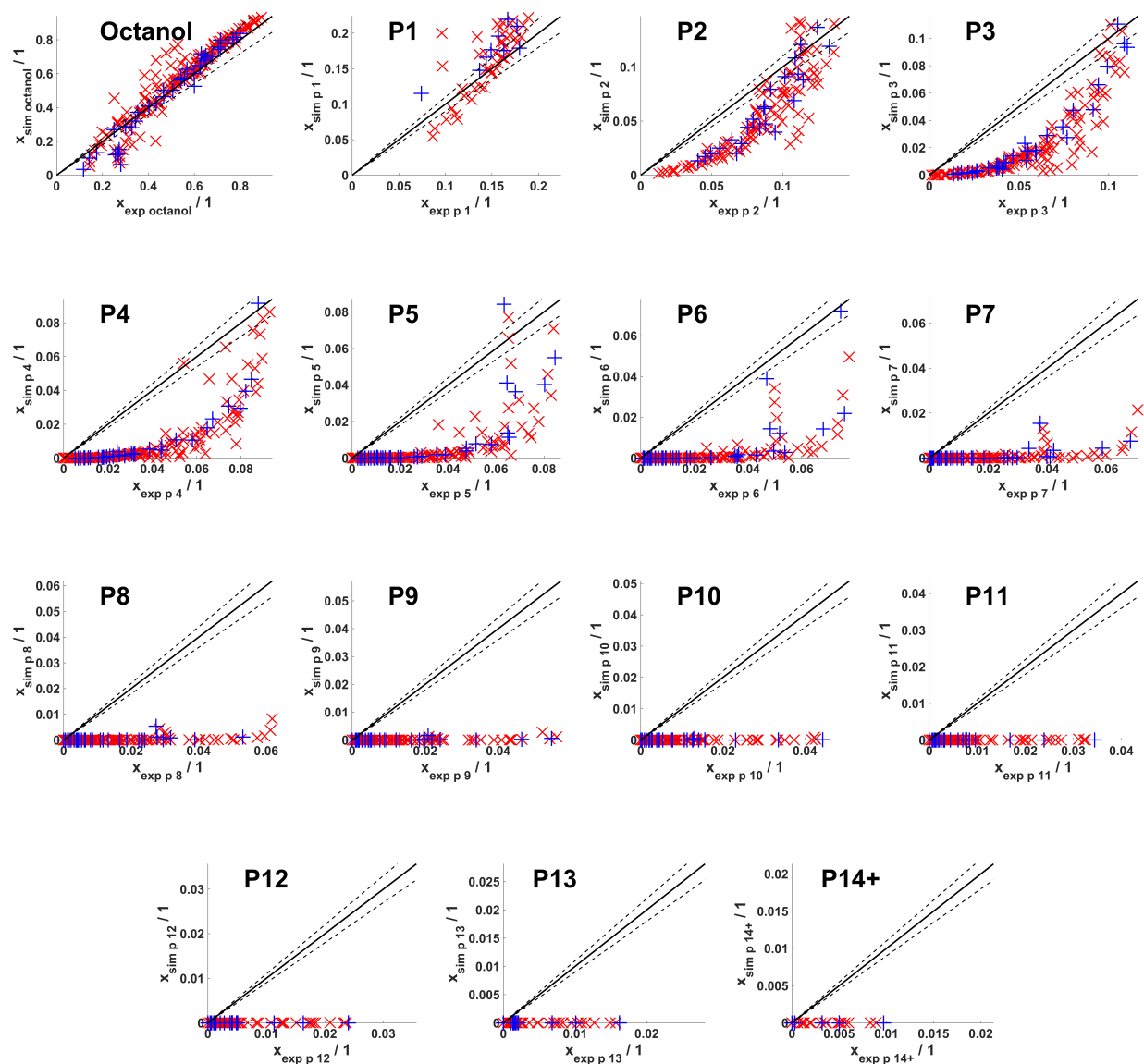


Figure S5: PFR-1-rate model parity plots for octanol to product 14 for a concentration of 0.66 mol% anionic species. The black dotted lines gives the $\pm 10\%$ error, the blue data points are used for determining the kinetic parameters, the red data points are predicted values.

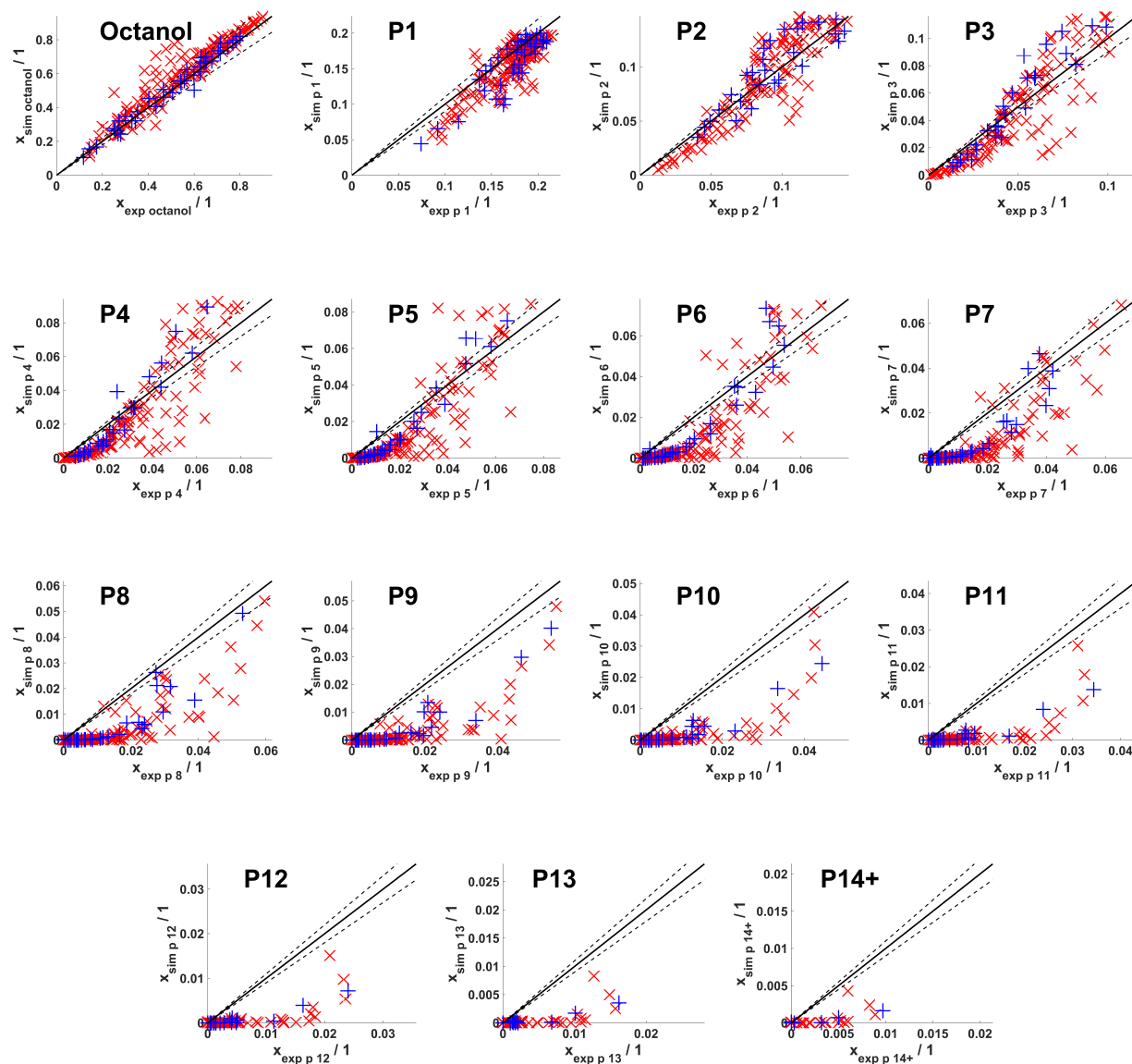


Figure S6: PFR-2-rate model parity plots for octanol to product 14 for a concentration of 0.66 mol% anionic species. The black dotted lines gives the $\pm 10\%$ error, the blue data points are used for determining the kinetic parameters, the red data points are predicted values.

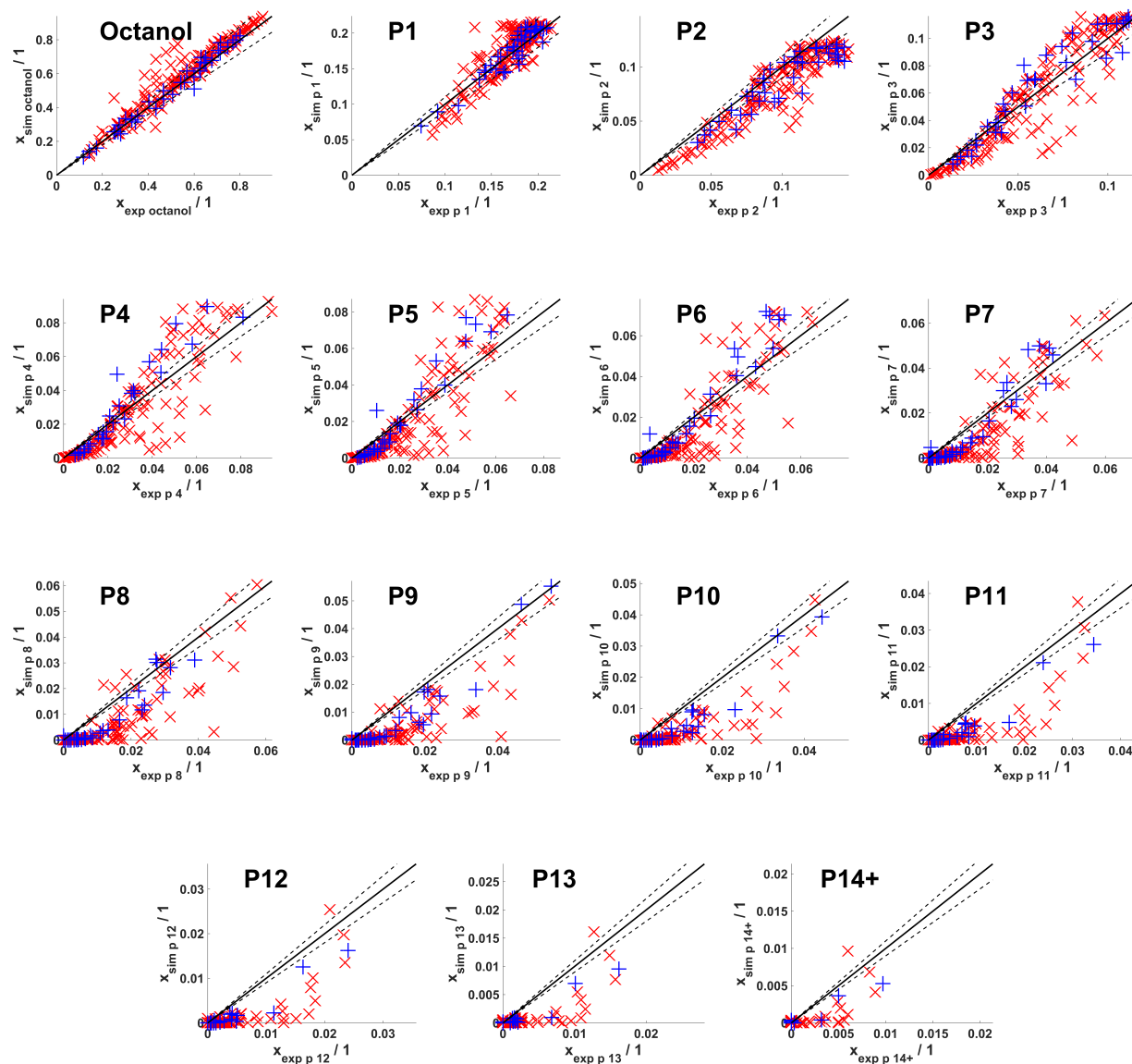


Figure S7: PFR-3-rate model parity plots for octanol to product 14 for a concentration of 0.66 mol% anionic species. The black dotted lines gives the $\pm 10\%$ error, the blue data points are used for determining the kinetic parameters, the red data points are predicted values.

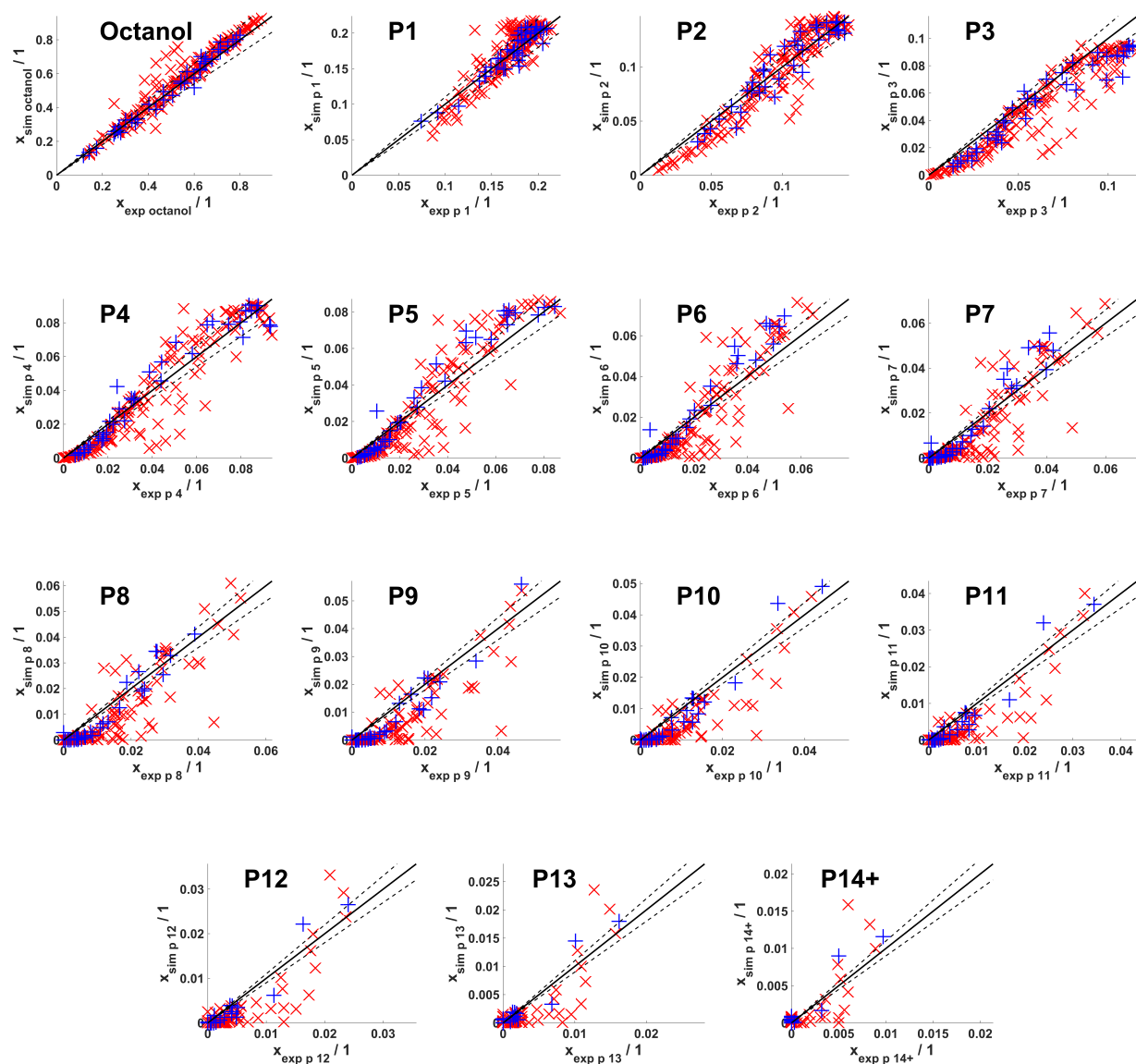


Figure S8: PFR-4-rate model parity plots for octanol to product 14 for a concentration of 0.66 mol% anionic species. The black dotted lines gives the $\pm 10\%$ error, the blue data points are used for determining the kinetic parameters, the red data points are predicted values.

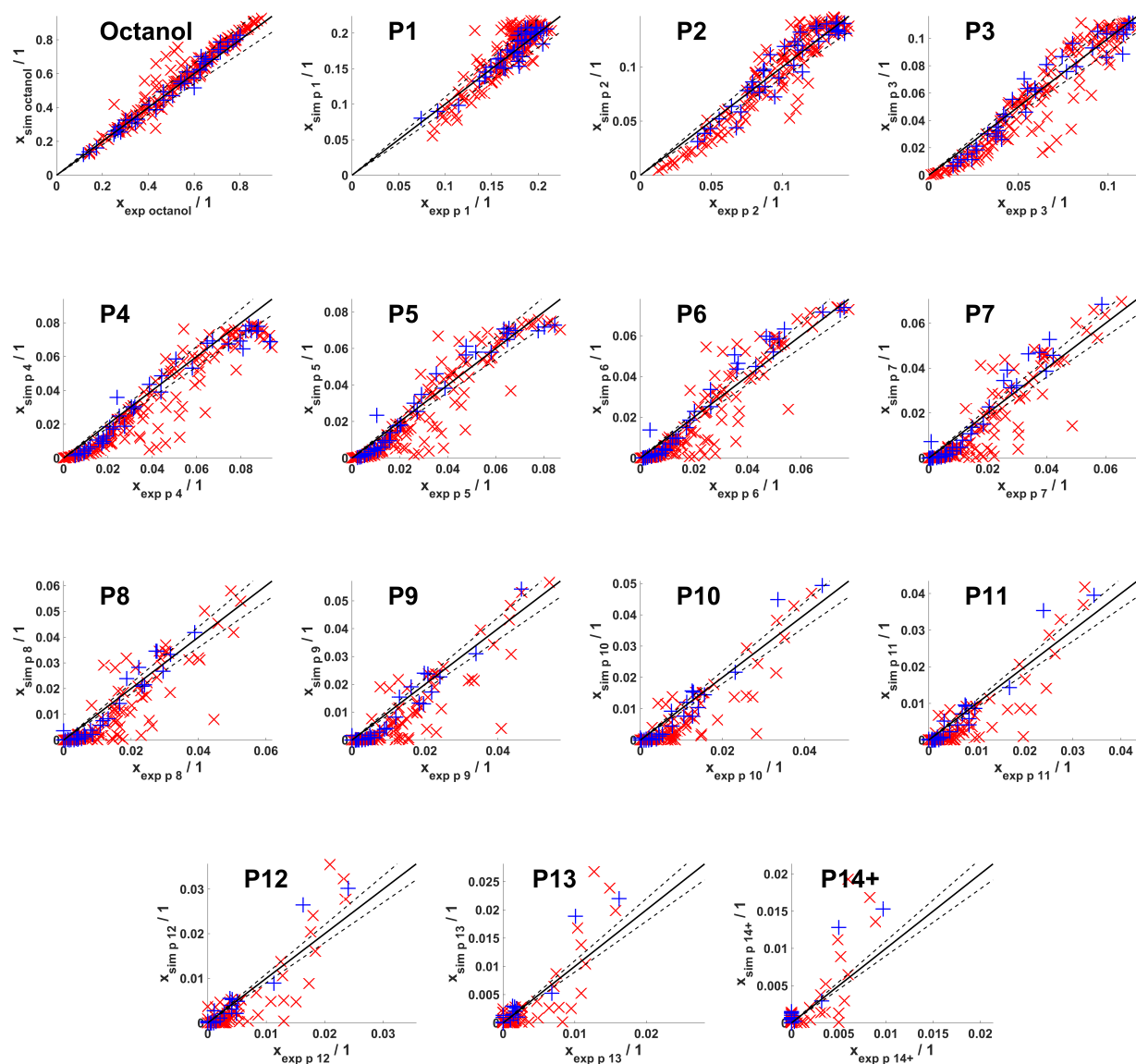


Figure S9: PFR-5-rate model parity plots for octanol to product 14 for a concentration of 0.66 mol% anionic species. The black dotted lines gives the $\pm 10\%$ error, the blue data points are used for determining the kinetic parameters, the red data points are predicted values.

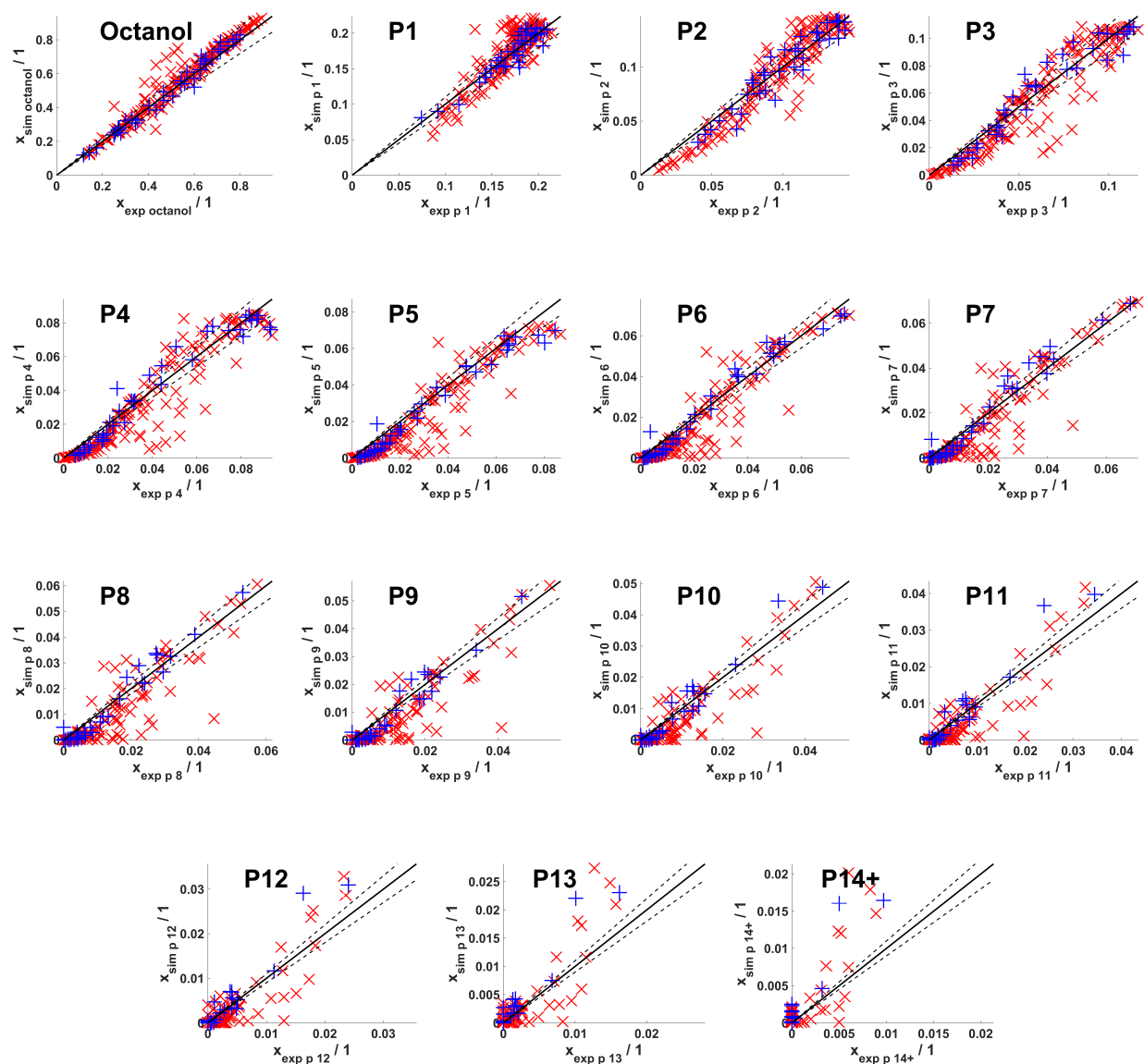


Figure S10: PFR-6-rate model parity plots for octanol to product 14 for a concentration of 0.66 mol% anionic species. The black dotted lines gives the $\pm 10\%$ error, the blue data points are used for determining the kinetic parameters, the red data points are predicted values.

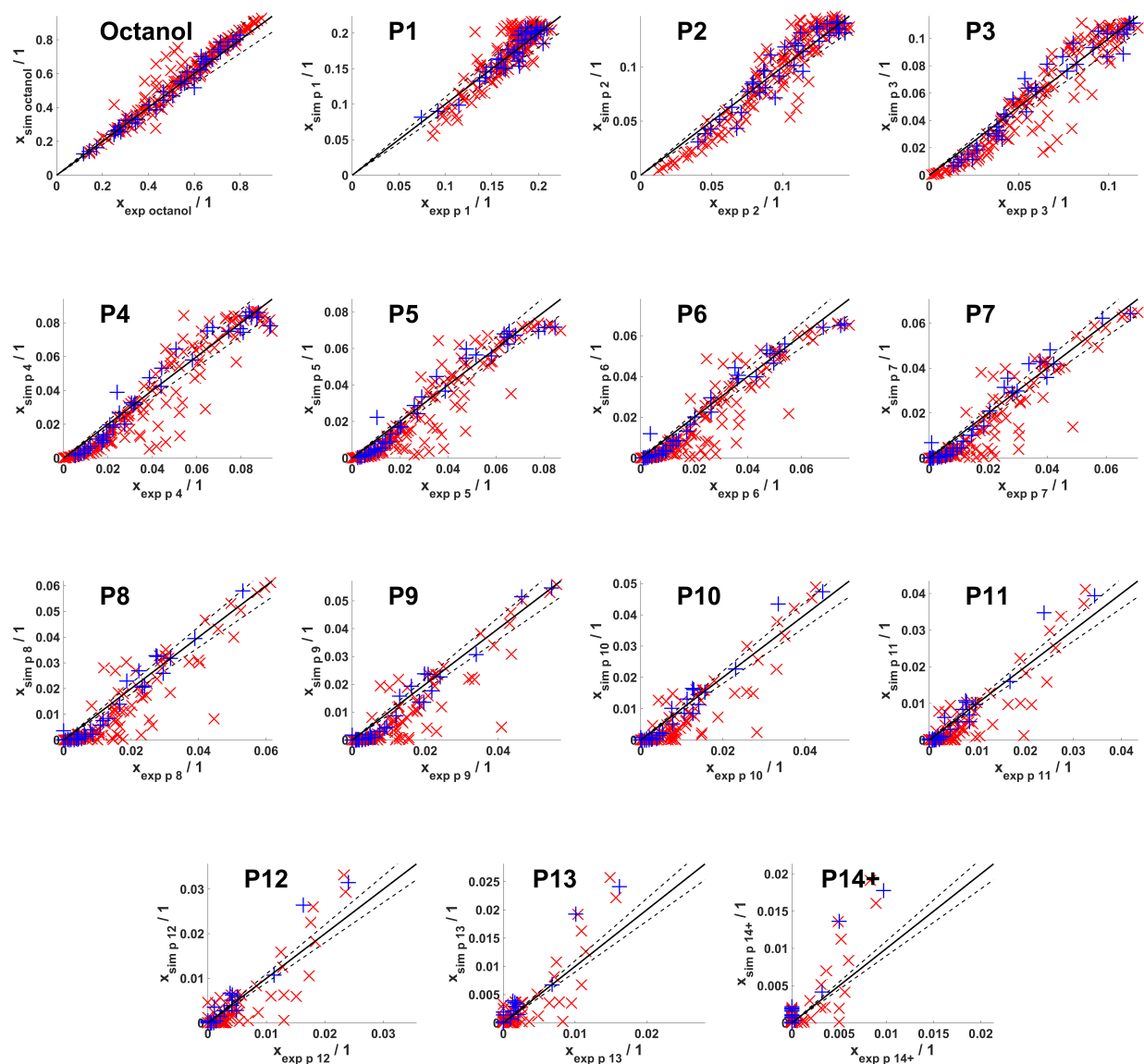


Figure S11: PFR-7-rate model parity plots for octanol to product 14 for a concentration of 0.66 mol% anionic species. The black dotted lines gives the $\pm 10\%$ error, the blue data points are used for determining the kinetic parameters, the red data points are predicted values.

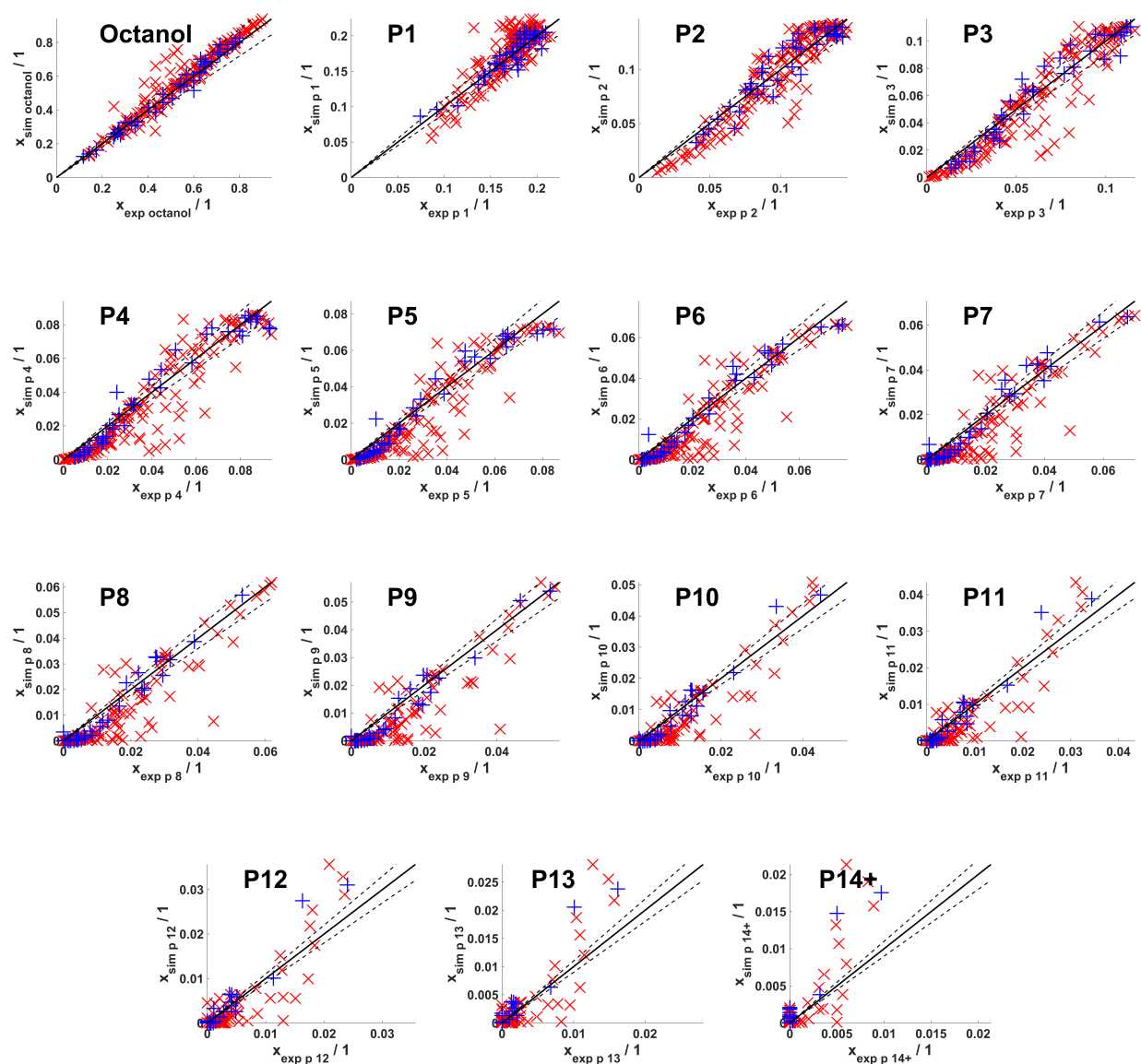


Figure S12: PFR-8-rate model parity plots for octanol to product 14 for a concentration of 0.66 mol% anionic species. The black dotted lines gives the $\pm 10\%$ error, the blue data points are used for determining the kinetic parameters, the red data points are predicted values.

References

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