Supplementary Materials: Aqueous Free-Radical Polymerization of Non-Ionized and Fully Ionized Methacrylic Acid

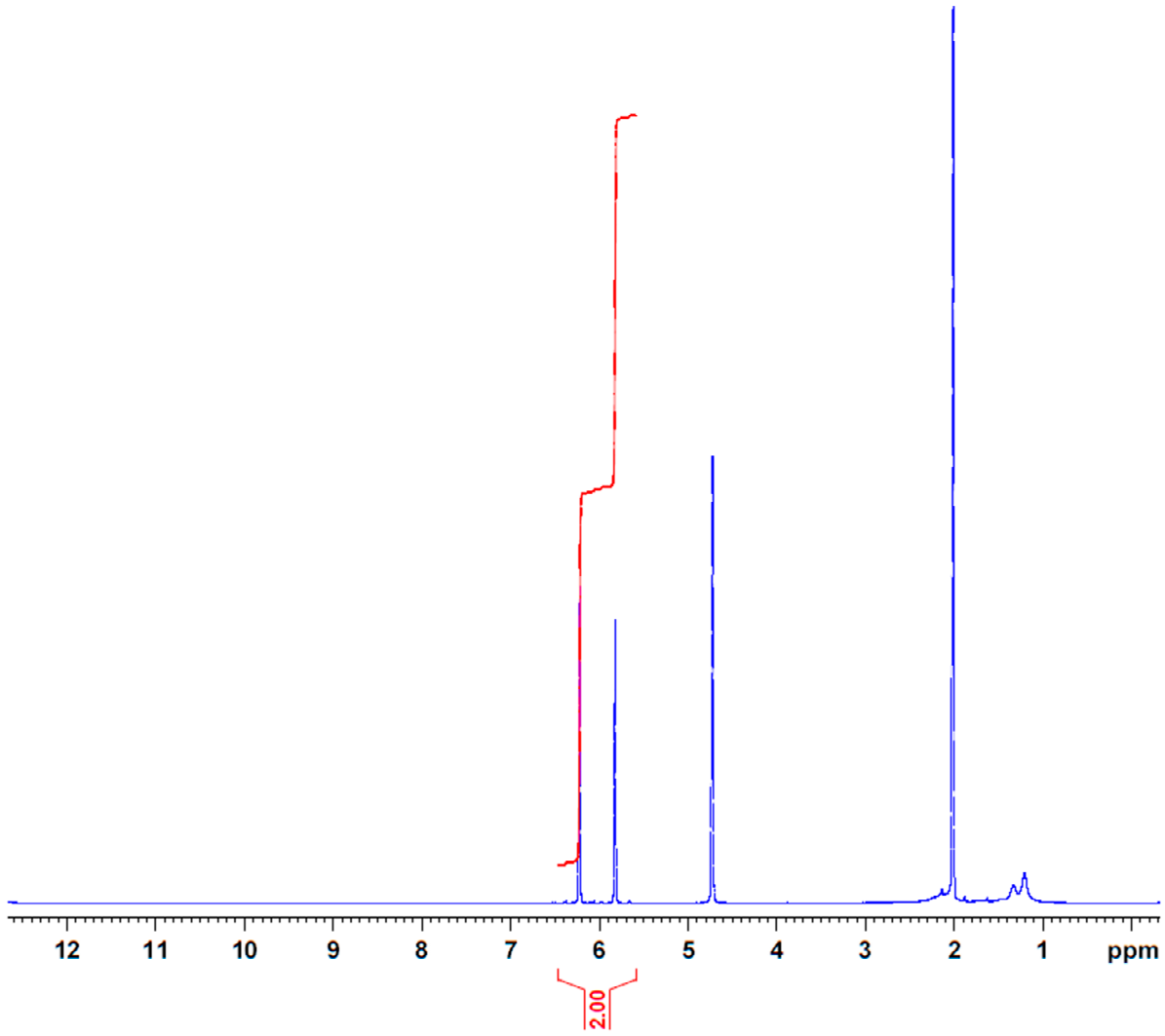

Figure S1. Details about the monomer peak area selected for the calculation of the monomer conversion from the ^{1}H NMR analysis for the polymerization of non-ionized MAA.

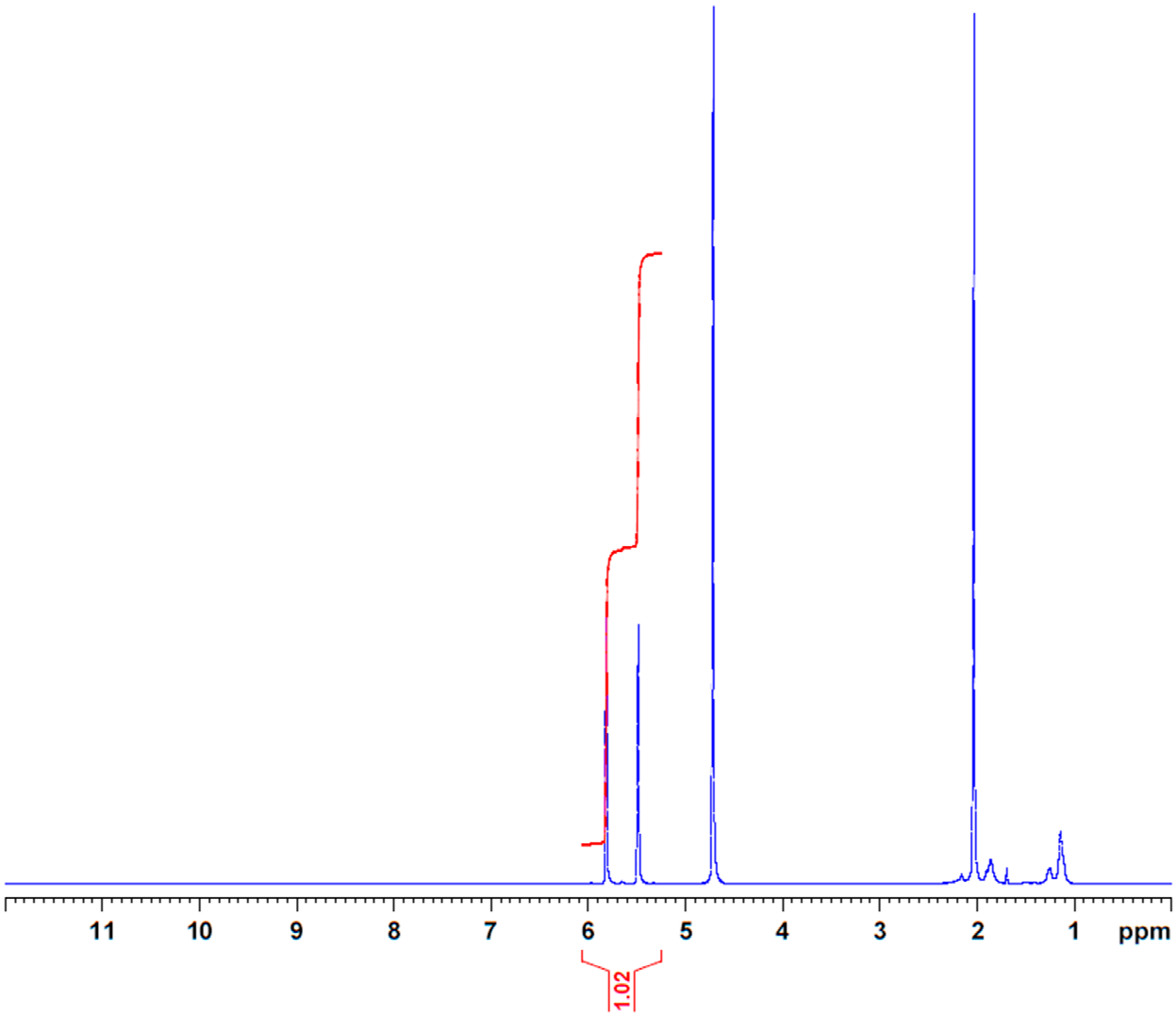

Figure S2. Details about the monomer peak area selected for the calculation of the monomer conversion from the ^{1}H NMR analysis for the polymerization of fully ionized MAA.

Table S1. Full list of reactions with non-ionized (0.02 wt % initiator V-50) and fully ionized MAA (0.1 wt % initiator V-50) including repeated experiments.

Reaction No.	alpha	Initial monomer concentration w%	Ionic strength corresponding to	Ionic strength [kg mol^{-1}]	pH
0-1	0	1	-	-	3.4
0-1-a	0	1	-	-	3.6
0-2	0	5	-	-	3.1
0-3	0	10	-	-	3.1
0-3-a	0	10	-	-	2.9
1-1	1	1	1	0.12	7.6
1-1-a	1	1	1	0.12	6.9
1-2	1	2.5	2.5	0.29	7.2
1-3	1	5	5	0.58	7.0
1-4	1	10	10	1.16	7.0
1-4-a	1	10	10	1.16	6.9
1-4-b	1	10	10	1.16	6.7
1-5	1	1	5	0.58	7.5
1-6	1	1	10	1.16	7.1
1-7	1	5	10	1.16	6.3
1-8	1	5	15	1.74	6.4
1-9	1	5	20	2.32	7.6
1-10	1	5	30	3.48	6.6

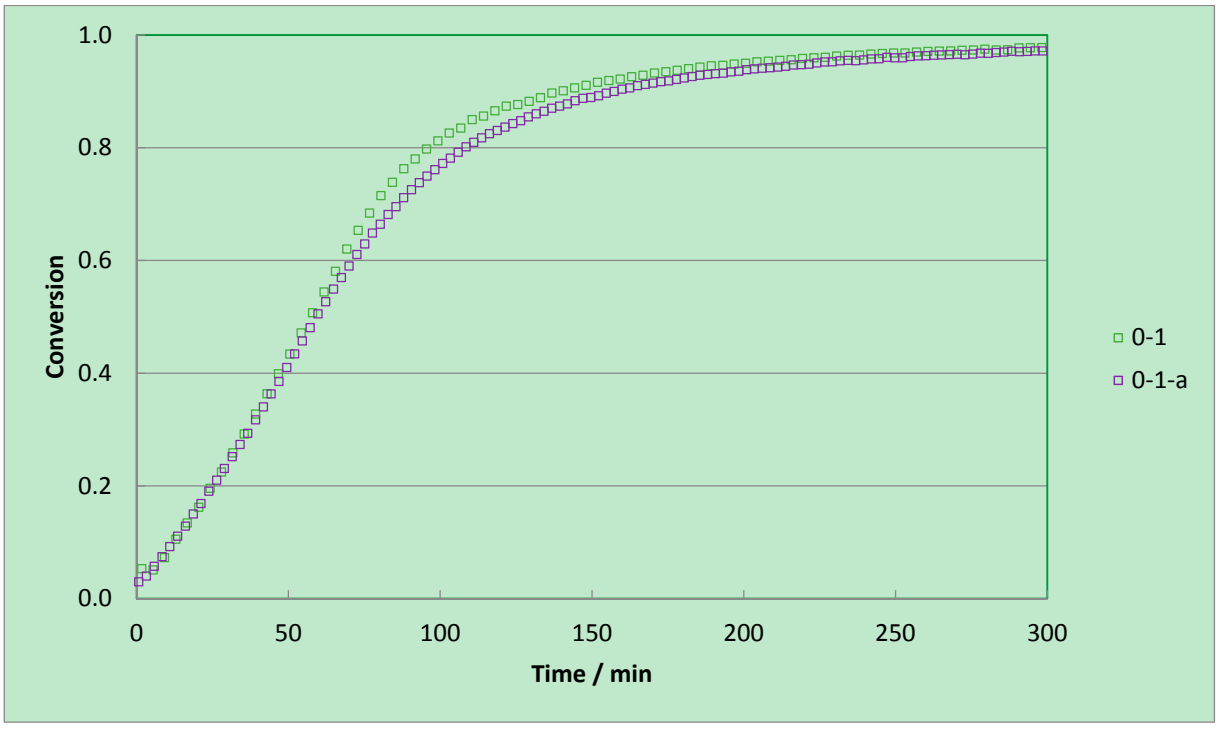

Figure S3. Reproducibility of the monomer conversion versus time profiles of the radical batch polymerization of non-ionized MAA in aqueous solution at 50 °C, 0.02 wt % of V-50 initiator and 1 wt % MAA.

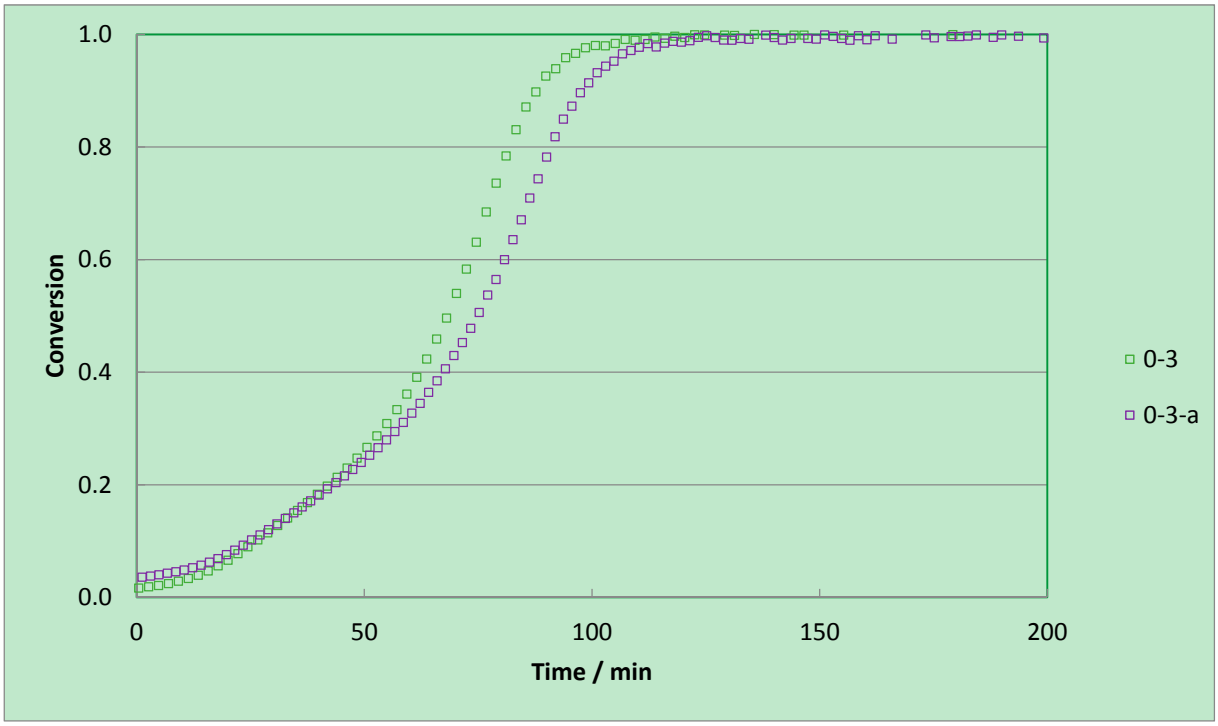

Figure S4. Reproducibility of the monomer conversion versus time profiles of the radical batch polymerization of non-ionized MAA in aqueous solution at 50 °C, 0.02 wt % of V-50 initiator and 10 wt % MAA.

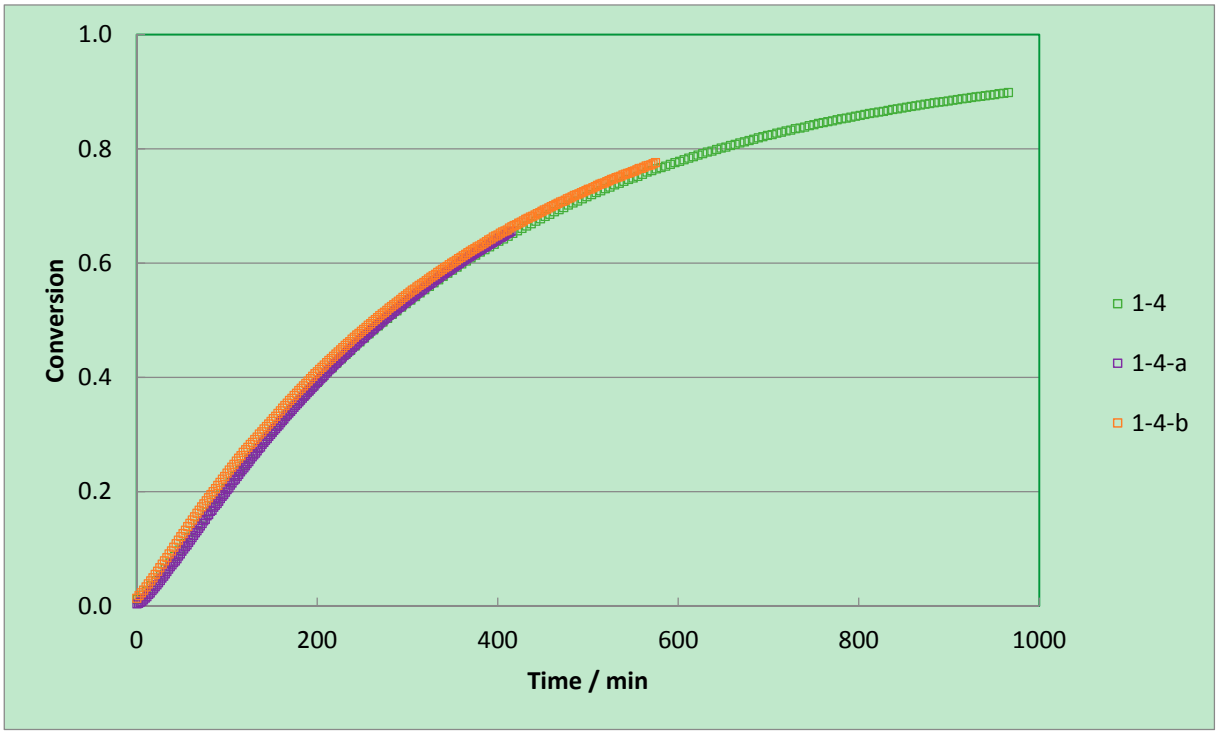

Figure S5. Reproducibility of the monomer conversion versus time profiles of the radical batch polymerization of fully ionized MAA in aqueous solution at 50 °C, 0.1 wt % of V-50 initiator and 10 wt % MAA.

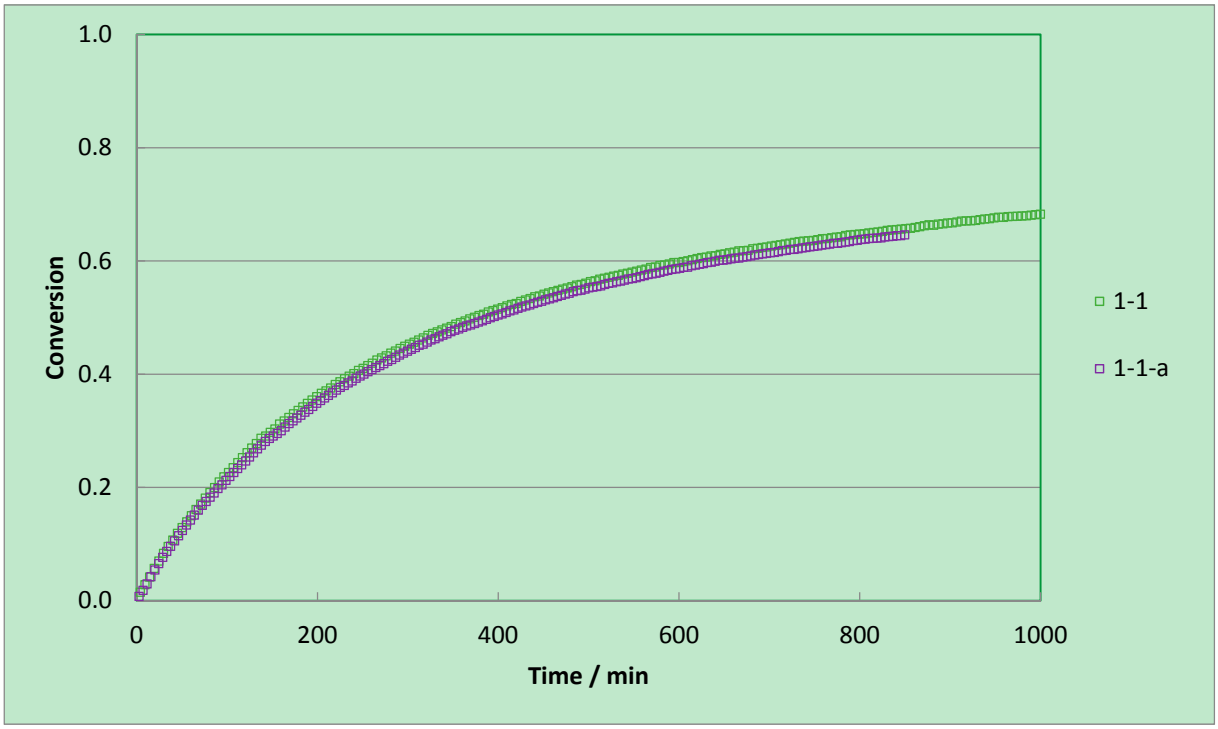

Figure S6. Reproducibility of the monomer conversion versus time profiles of the radical batch polymerization of fully ionized MAA in aqueous solution at 50 °C, 0.1 wt % of V-50 initiator and 1 wt % MAA.

Table S2. Comparison of intrinsic vs. electrostatic contributions to the propagation rate.

Reaction No.	$w_{M,0}$ / wt %	Ionic strength eq. to wt %	$k_{p,i}^{0}\exp(-w_{M,0}B)$ / $(L\ mol^{-1}s^{-1})$	$k_{D,0}C_E^{\beta}$ / $(L\ mol^{-1}s^{-1})$	k_p / $(L\ mol^{-1}s^{-1})$
3	5	5	689	279	198
4	10	10	626	1263	418
5	1	5	744	279	203
6	1	10	744	1263	468
7	5	10	689	1263	446

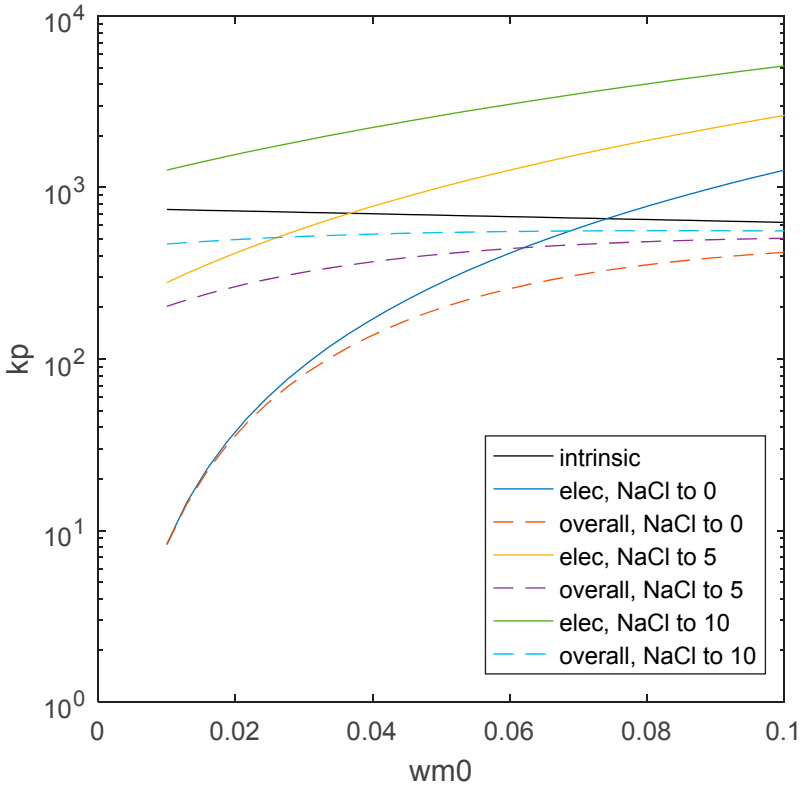

Figure S7. Representation of the intrinsic and electrostatic contributions to the overall propagation reaction rate, based on the parameter set provided in Table 6.

Table S3. Sensitivity analysis on the parameter values. The total error (mean-square error) between the experiments at α = 1 and simulations is calculated upon a 10% increase of each model parameter with respect to its optimized value reported in Table 6. The error corresponding to the set of unchanged parameters is reported as a reference (bottom line in the table).

$k_{p,i}^0$	$k_{D,0}$	β	B	Total error
1.1	1	1	1	2.33%
1	1.1	1	1	2.52%
1	1	1.1	1	2.33%
1	1	1	1.1	1.93%
1	1	1	1	0.01%