

Supporting information

Additional file 1: PEST++: Influence of input parameter value

Figure 1 - 5 show the resulting boxplots when the input parameter is varied for the simulation of the experiment of inducing air into tap water.

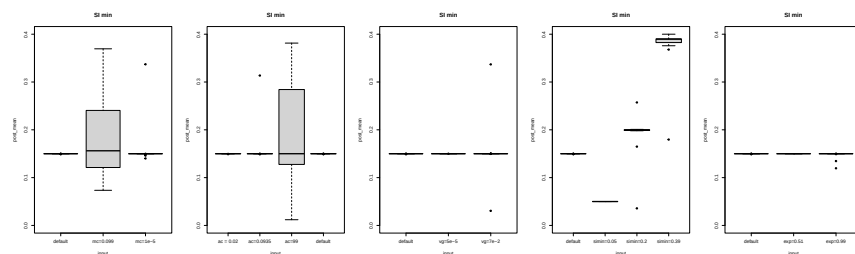


Figure 1: Parameter analysis: Box plots of the SI min value for the simulations of the experiments of inducing air into tap water, when the input values are changed.

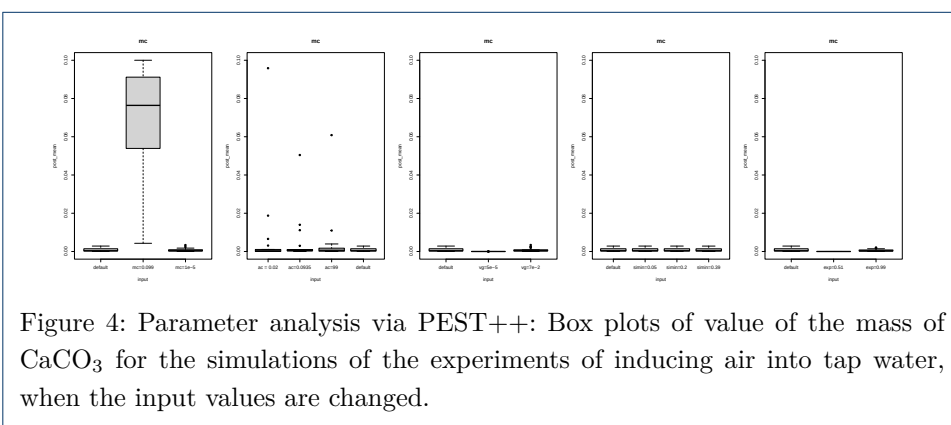
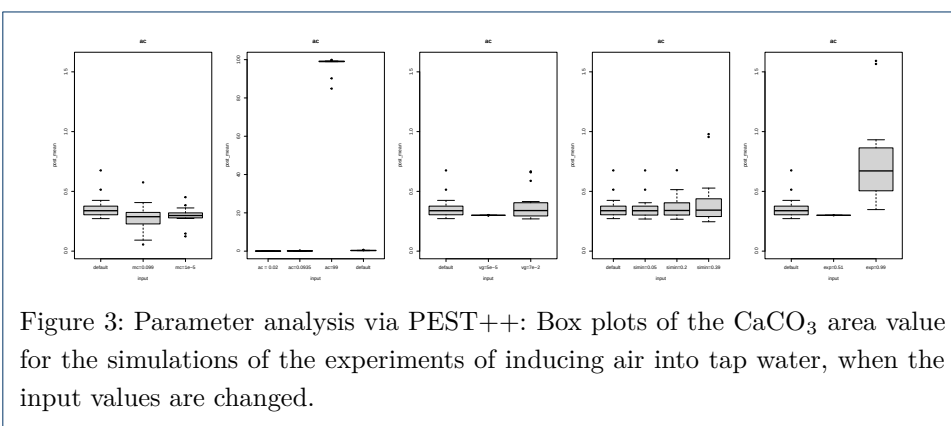


Figure 4: Parameter analysis via PEST++: Box plots of value of the mass of CaCO_3 for the simulations of the experiments of inducing air into tap water, when the input values are changed.

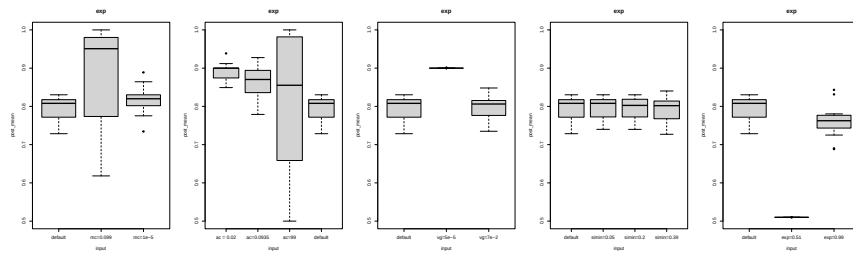


Figure 5: Parameter analysis via PEST++: Box plots of exp CaCO_3 for the simulations of the experiments of inducing air into tap water, when the input values are changed.

Additional file 2: Ion concentrations of the experiment with $I = 1.40 \times 10^{-2} \text{ mol/L}$.
Summary of ionic concentrations determined by IC of the experiments of injecting air into water with an ionic strength of $I = 1.40 \times 10^{-2} \text{ mol/L}$ are shown in Table [1](#).

Table 1: Concentration of the ions of the solutions in mg/L ($\pm$ standard deviation) before and after injecting air into water with an ionic strength of 1.40×10^{-2} mol/L as well as the mass balance and acidification of the column (in mg).

	before mg/L	after mg/L	$\sum$ after mg	$\sum$ before mg	Δ mg	acidification mg
Na^+	105	93.1	5870	6620	752	64.3 $\pm$ 34.7
NH_4^+	± 21.0	± 12.2	n.d.	n.d.	n.d.	n.d.
K^+	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
Ca^{2+}	1.19 $\pm$ 0.454	1.05 $\pm$ 0.299	66.4	74.9	8.54	n.d.
Mg^{2+}	95.2 $\pm$ 4.90	22.2 $\pm$ 1.59	1400	6000	4600	3750 $\pm$ 58.1
Cl^-	21.8 $\pm$ 2.04	20.4 $\pm$ 0.795	1280	1370	90.0	60.7 $\pm$ 0.372
NO_2^-	78.7 $\pm$ 16.8	92.9 $\pm$ 0.762	4360	4960	599	120 $\pm$ 0.142
NO_3^-	n.d.	n.d.	n.d.	n.d.	n.d.	9.97 $\pm$ 0.0839
PO_4^{3-}	4.72 $\pm$ 0.352	5.29 $\pm$ 0.266	301	298	3.72	29 500 $\pm$ 24.4
SO_4^{2-}	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	5.27 $\pm$ 0.853	4.80 $\pm$ 0.0289	339	332	7.35	36.9 $\pm$ 0.0575

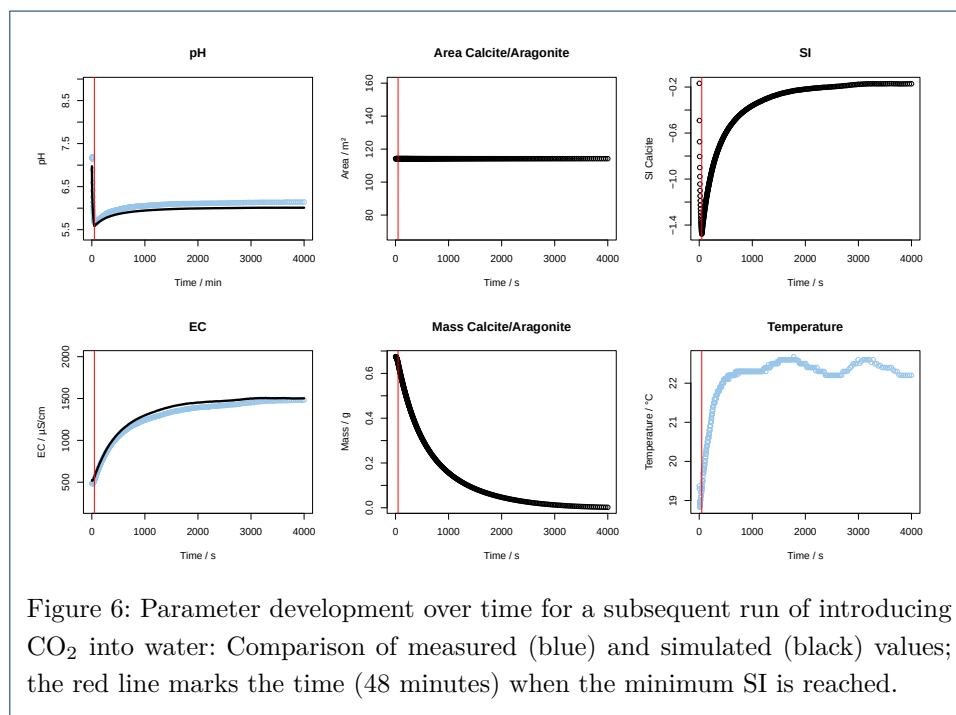
Additional file 3: Example for subsequent run of inducing CO_2 into water

Figure 6: Parameter development over time for a subsequent run of introducing CO_2 into water: Comparison of measured (blue) and simulated (black) values; the red line marks the time (48 minutes) when the minimum SI is reached.

Additional file 4: Parameter development of the injection of air into a solution with $I = 2.97 \text{ mol/L}$, area set to zero.

