# Supporting Information for 2014WR016503

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1. Figures S1 to S5
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**Introduction**

This supporting information contains several figures and tables, giving the data used in this study or supporting the its conclusions. Figure S1 gives the results of a grid convergence study indicating that grid induced effects did not affect the results obtained in this study. Figures S2 to S4 compare measured and modeled calcite distributions for experiments C4, D1 and BR, which are not shown in the manuscript itself. Further, Figure S5 compares measured and modeled effluent pH for experiment D2.

Table S1 gives relevant experimental design parameters and Table S2 the composition of the fluids injected during the experiments. Experimental measurements used as observations in inverse modeling are given in the Tables S3 to S7. Table S8 summarizes the sums of squared residuals of model predictions for selected parameter sets (see Table 2) to the experimental measurements of D2. This Table additionally gives the residuals measurements and the predictions of the previous model proposed by [*Ebigbo et al.*, 2012].

## References

Ebigbo, A., A. J. Phillips, R. Gerlach, R. Helmig, A. B. Cunningham, H. Class, and L. H. Spangler (2012), Darcy-scale modeling of microbially induced carbonate mineral precipitation in sand columns, *Water Resources Research*, *48*(7), W07,519, doi:10.1029/2011WR011714.

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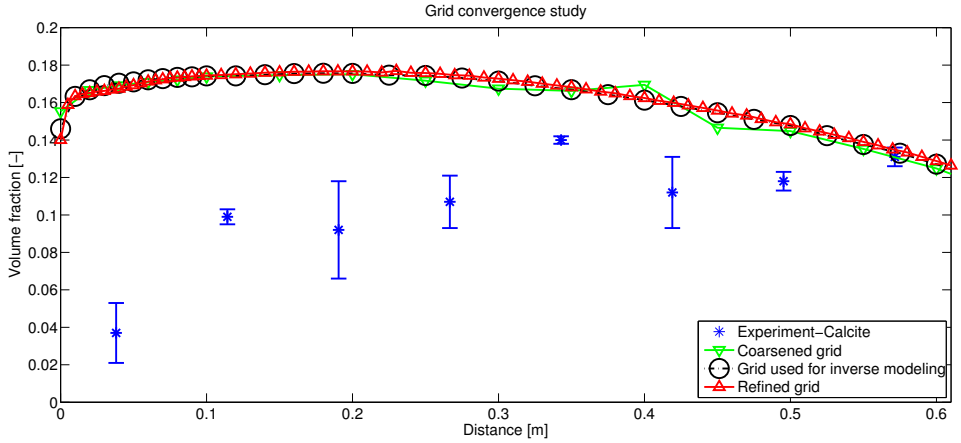


**Figure S1.** Results of a grid convergence study comparing different grid resolutions.

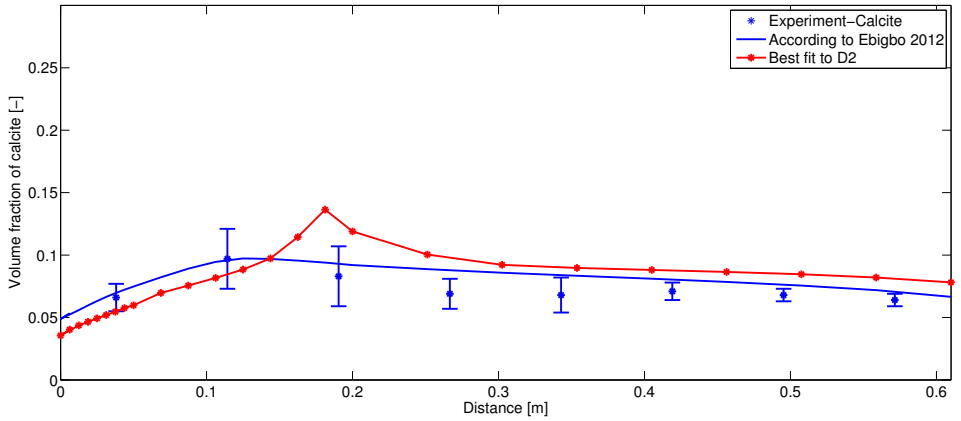


**Figure S2.** Comparison of the column C4 experiment results for calcite with predictions of the *Ebigbo et al.* [2012] model and the revised model. The fit to the data is approximately similar for both models.

**Table S1.** Experimental parameters of the experiments used in inverse modeling. Values of column C4 are taken from *Ebigbo et al.* [2012].

| Experiment | Inoculum $\left[\frac{\text{CFU}}{\text{ml}}\right]$ | Flow rate $\left[\frac{\text{ml}}{\text{min}}\right]$ | Residence time during flow [min] | No. of $Ca^{2+}$ rich pulses | Mineralization Period | No. of resuscitation events | Resuscitation frequency |
|---|---|---|---|---|---|---|---|
| Column C4 | $1.3 \cdot 10^7$ | 10 | 15 | 22 | Overnight no flow | 9 | Every 4-5 days |
| Column D1 | $2.7 \cdot 10^8$ | 10 | 15 | 30 | 4 h no flow | 29 | Daily |
| Column D2 | $5.6 \cdot 10^7$ | 10 | 15 | 30 | 4 h no flow | 29 | Daily |
| Bicycle Rim BR | $1.6 \cdot 10^8$ | 57 | 48 | 1 | 12 h constant flow | 0 | - |

**Table S2.** Injected fluid composition for the experiments used in inverse modeling. The given concentrations are in the units of $\frac{\text{g}}{\text{l}}$, except for *S. pasteurii*.

| Injection type | $CaCl_2$ | Urea | $NH_4Cl$ | $C_{tot}$ | Substrate[a] | $O_2$ | *S. pasteurii* | pH |
|---|---|---|---|---|---|---|---|---|
| Inoculation | 0 | 0 | 10 | 0.00058 | 3 | 0.008 | Exp. specific [b] | 6.2 |
| Resuscitation | 0 | 20 | 10 | 0.00058 | 3 | 0.008 | 0 | 6.2 |
| Calcium rich | 139.7 / 36.9[c] | 20 | 10 | 0.00058 | 3 | 0.008 | 0 | 5.4 |

[a] Substrate represents the carbon and energy source of *S. pasteurii* used in the experiments (Difco Nutrient Broth).

[b] The specific inoculation concentrations of each experiment are given in Table S1.

[c] The concentration of $CaCl_2$ is 139.7 $\frac{\text{g}}{\text{l}}$ for column 4 and 36.9 $\frac{\text{g}}{\text{l}}$ for all other experiments.

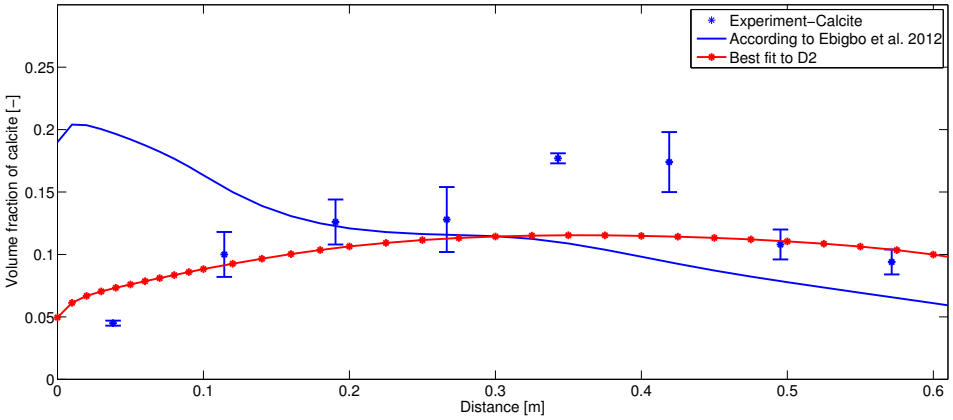


**Figure S3.** Comparison of the column D1 experiment results for calcite with predictions of the *Ebigbo et al.* [2012] model and the revised model. The model and parameters determined in this study for D2 provide a better fit to the D1 results than the model and parameters proposed by *Ebigbo et al.* [2012].

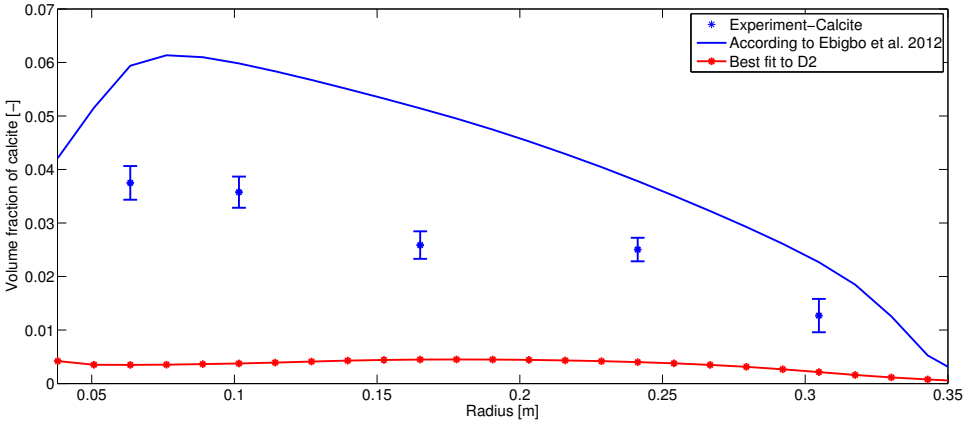


**Figure S4.** Comparison of the bicycle rim experiment results for calcite with predictions of the *Ebigbo et al.* [2012] model and the revised model. The *Ebigbo et al.* [2012] model overpredicts the amount of calcite precipitated, while the revised model with parameters determined for D2 underestimates it.

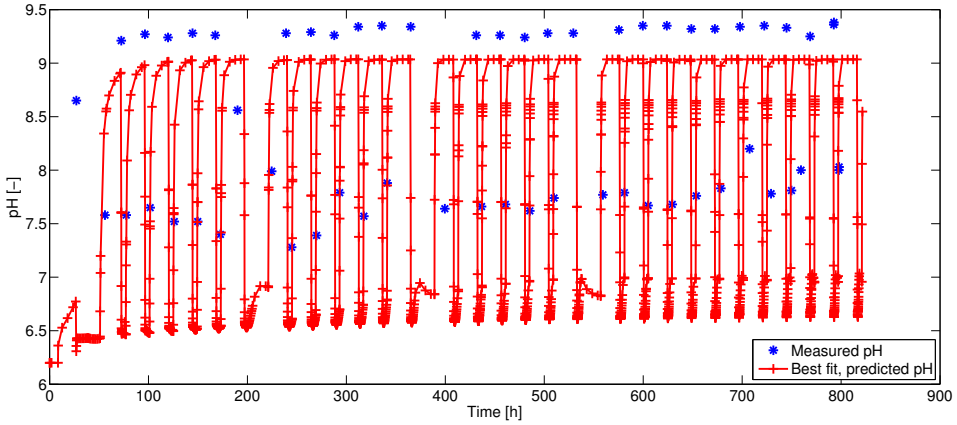


**Figure S5.** Comparison of experimentally measured pH of column experiment D2 to predictions of the revised model. Outgasing of $CO_2$ probably increased the measured pH, as the pH measurements were not conducted in-situ , but in samples extracted from the column and exposed to atmospheric conditions prior to pH measurement.

**Table S3.** Measured final volume fractions of calcite at given distance (Columns) or radius (Bicycle Rim) used as observations in inverse modeling. Values of C4 are taken from *Ebigbo et al.* [2012]. The values given here are the averages of triplicate measurements at each measurement location. For column D1 and D2, interpolated values are tabulated at locations that match the nearest grid point. These values were obtained through linear interpolation between the two surrounding measurements. The distance between measurement location and the nearest grid node was never greater than 1 cm. The experimental data presented here is also used in the Figures 9, S2, S3, and S4.

| Location measured | 3.81 cm | 11.43 cm | 19.05 cm | 26.67 cm | 34.29 cm | 41.91 cm | 49.53 cm | 57.15 cm |
|---|---|---|---|---|---|---|---|---|
| Column C4 | 0.066 | 0.097 | 0.083 | 0.069 | 0.068 | 0.071 | 0.068 | 0.064 |
| Column D1 | 0.045 | 0.100 | 0.126 | 0.128 | 0.177 | 0.174 | 0.108 | 0.094 |
| Column D2 | 0.037 | 0.099 | 0.092 | 0.107 | 0.140 | 0.112 | 0.118 | 0.131 |
| Location grid[a] | 4.0 cm | 12.0 cm | 20.0 cm | 27.5 cm | 35.0 cm | 42.5 cm | 50.0 cm | 57.5cm |
| Column D1[a] interpolated | 0.047 | 0.102 | 0.126 | 0.133 | 0.177 | 0.169 | 0.107 | 0.093 |
| Column D2[a] interpolated | 0.040 | 0.099 | 0.094 | 0.110 | 0.137 | 0.113 | 0.119 | 0.132 |
| Location measured | 6.35 cm | 10.16 cm | 16.51 cm | 24.13 cm | 30.48 cm | | | |
| Bicycle Rim BR[b] | 0.037 | 0.036 | 0.026 | 0.025 | 0.013 | | | |

[a] Grid location the measured calcite values were interpolated to in order to match the grid nodes and the interpolated values.

[b] The values given for the Bicycle Rim experiment are averages of measurements in 8 radial segments.

**Table S4.** Measured concentrations of ammonium $\left[\frac{\text{mol}}{\text{l}}\right]$ for column experiment D1 used as observations in inverse modeling.

| Pulse | Time [h] | 10 cm | 20 cm | 30 cm | 40 cm | 50 cm |
|---|---|---|---|---|---|---|
| 5 | 151.35 | 0.157 | 0.157 | 0.154 | 0.156 | 0.155 |
| | 151.85 | 0.173 | 0.170 | 0.177 | 0.184 | 0.190 |
| | 152.35 | 0.192 | 0.190 | 0.213 | 0.224 | 0.230 |
| | 153.35 | 0.206 | 0.212 | 0.274 | 0.287 | 0.302 |
| | 154.35 | 0.240 | 0.244 | 0.357 | 0.353 | 0.367 |
| | 155.35 | 0.260 | 0.287 | 0.430 | 0.407 | 0.416 |
| 7 | 218.85 | 0.150 | 0.155 | 0.149 | 0.155 | 0.159 |
| | 219.35 | 0.171 | 0.166 | 0.180 | 0.192 | 0.198 |
| | 219.85 | 0.192 | 0.183 | 0.191 | 0.224 | 0.247 |
| | 220.85 | 0.235 | 0.230 | 0.275 | 0.323 | 0.326 |
| | 221.85 | 0.283 | 0.289 | 0.370 | 0.421 | 0.436 |
| | 222.85 | 0.326 | 0.365 | 0.456 | 0.544 | 0.516 |
| 10 | 290.85 | 0.151 | 0.161 | 0.161 | 0.158 | 0.163 |
| | 291.35 | 0.215 | 0.211 | 0.238 | 0.214 | 0.187 |
| | 291.85 | 0.286 | 0.290 | 0.395 | 0.290 | 0.219 |
| | 292.85 | 0.375 | 0.419 | 0.547 | 0.431 | 0.257 |
| | 293.85 | 0.463 | 0.552 | 0.613 | 0.592 | 0.293 |
| | 294.85 | 0.518 | 0.642 | 0.685 | 0.657 | 0.408 |
| 22 | 626.85 | 0.160 | 0.163 | 0.167 | 0.172 | 0.174 |
| | 627.35 | 0.242 | 0.234 | 0.251 | 0.227 | 0.204 |
| | 627.85 | 0.294 | 0.269 | 0.288 | 0.244 | 0.202 |
| | 628.85 | 0.397 | 0.386 | 0.411 | 0.300 | 0.244 |
| | 630.85 | 0.511 | 0.551 | 0.521 | 0.360 | 0.273 |
| 24 | 698.85 | 0.184 | 0.191 | 0.191 | 0.207 | 0.213 |
| | 699.35 | 0.279 | 0.268 | 0.266 | 0.260 | 0.249 |
| | 699.85 | 0.384 | 0.362 | 0.372 | 0.344 | 0.310 |
| | 700.85 | 0.456 | 0.460 | 0.472 | 0.332 | 0.345 |
| | 701.85 | 0.522 | 0.612 | 0.552 | 0.429 | 0.349 |
| | 702.85 | 0.616 | 0.660 | 0.602 | 0.454 | 0.395 |
| 30 | 866.85 | 0.159 | 0.163 | 0.160 | 0.163 | 0.162 |
| | 867.35 | 0.259 | 0.255 | 0.276 | 0.299 | 0.294 |
| | 867.85 | 0.340 | 0.321 | 0.366 | 0.417 | 0.378 |
| | 868.85 | 0.495 | 0.511 | 0.558 | 0.586 | 0.357 |
| | 869.85 | 0.596 | 0.609 | 0.644 | 0.612 | 0.432 |
| | 870.85 | 0.628 | 0.679 | 0.690 | 0.679 | 0.397 |

**Table S5.** Measured concentrations of calcium $\left[\frac{\text{mol}}{\text{l}}\right]$ for column experiment D1 used as observations in inverse modeling.

| Pulse | Time [h] | 10 cm | 20 cm | 30 cm | 40 cm | 50 cm |
|---|---|---|---|---|---|---|
| 5 | 151.35 | 0.277 | 0.275 | 0.270 | 0.254 | 0.273 |
| | 151.85 | 0.196 | 0.277 | 0.263 | 0.264 | 0.266 |
| | 152.35 | 0.218 | 0.262 | 0.265 | 0.235 | 0.250 |
| | 153.35 | 0.241 | 0.262 | 0.224 | 0.207 | 0.206 |
| | 154.35 | 0.161 | 0.249 | 0.189 | 0.176 | 0.171 |
| | 155.35 | 0.175 | 0.227 | 0.154 | 0.164 | 0.152 |
| 7 | 218.85 | 0.258 | 0.256 | 0.249 | 0.252 | 0.250 |
| | 219.35 | 0.239 | 0.245 | 0.241 | 0.220 | 0.230 |
| | 219.85 | 0.204 | 0.234 | 0.202 | 0.193 | 0.211 |
| | 220.85 | 0.159 | 0.218 | 0.199 | 0.179 | 0.163 |
| | 221.85 | 0.158 | 0.210 | 0.172 | 0.144 | 0.133 |
| | 222.85 | 0.137 | 0.168 | 0.128 | 0.089 | 0.091 |
| 10 | 290.85 | 0.260 | 0.264 | 0.262 | 0.253 | 0.254 |
| | 291.35 | 0.231 | 0.248 | 0.232 | 0.239 | 0.255 |
| | 291.85 | 0.175 | 0.209 | 0.156 | 0.210 | 0.239 |
| | 292.85 | 0.120 | 0.156 | 0.086 | 0.133 | 0.218 |
| | 293.85 | 0.083 | 0.061 | 0.047 | 0.047 | 0.193 |
| | 294.85 | 0.042 | 0.022 | 0.013 | 0.024 | 0.138 |
| 22 | 626.85 | 0.263 | 0.262 | 0.256 | 0.255 | 0.255 |
| | 627.35 | 0.217 | 0.227 | 0.228 | 0.235 | 0.246 |
| | 627.85 | 0.193 | 0.203 | 0.191 | 0.210 | 0.216 |
| | 628.85 | 0.117 | 0.153 | 0.137 | 0.171 | 0.217 |
| | 630.85 | 0.070 | 0.076 | 0.092 | 0.181 | 0.202 |
| 24 | 698.85 | 0.303 | 0.299 | 0.286 | 0.288 | 0.290 |
| | 699.35 | 0.236 | 0.255 | 0.252 | 0.258 | 0.264 |
| | 699.85 | 0.187 | 0.222 | 0.205 | 0.224 | 0.241 |
| | 700.85 | 0.134 | 0.164 | 0.153 | 0.150 | 0.231 |
| | 701.85 | 0.113 | 0.083 | 0.115 | 0.177 | 0.222 |
| | 702.85 | 0.068 | 0.062 | 0.080 | 0.180 | 0.196 |
| 30 | 866.85 | 0.257 | 0.262 | 0.247 | 0.243 | 0.239 |
| | 867.35 | 0.193 | 0.209 | 0.188 | 0.179 | 0.188 |
| | 867.85 | 0.163 | 0.162 | 0.124 | 0.120 | 0.140 |
| | 868.85 | 0.085 | 0.084 | 0.058 | 0.050 | 0.063 |
| | 869.85 | 0.036 | 0.023 | 0.014 | 0.038 | 0.127 |
| | 870.85 | 0.017 | 0.001 | 0.001 | 0.004 | 0.136 |

**Table S6.** Measured concentrations of ammonium $\left[\frac{\text{mol}}{\text{l}}\right]$ for column experiment D2 used as observations in inverse modeling. The measurements at 20 cm distance from the inlet are used in Figure 8

| Pulse | Time [h] | 10 cm | 20 cm | 30 cm | 40 cm | 50 cm |
|---|---|---|---|---|---|---|
| 3 | 97 | 0.154 | 0.154 | 0.158 | 0.157 | 0.161 |
| | 97.5 | 0.160 | 0.163 | 0.167 | 0.171 | 0.174 |
| | 98 | 0.166 | 0.173 | 0.163 | 0.186 | 0.194 |
| | 99 | 0.178 | 0.184 | 0.192 | 0.216 | 0.227 |
| | 100 | 0.192 | 0.213 | 0.218 | 0.248 | 0.243 |
| | 101 | 0.215 | 0.218 | 0.269 | 0.257 | 0.289 |
| 6 | 169 | 0.162 | 0.166 | 0.169 | 0.171 | 0.172 |
| | 169.5 | 0.189 | 0.181 | 0.217 | 0.229 | 0.272 |
| | 170 | 0.222 | 0.214 | 0.238 | 0.284 | 0.323 |
| | 171 | 0.227 | 0.251 | 0.304 | 0.357 | 0.391 |
| | 172 | 0.245 | 0.325 | 0.394 | 0.423 | 0.462 |
| | 173 | 0.263 | 0.365 | 0.418 | 0.441 | 0.444 |
| 9 | 265 | 0.159 | 0.163 | 0.156 | 0.188 | 0.198 |
| | 265.5 | 0.229 | 0.274 | 0.315 | 0.346 | 0.392 |
| | 266 | 0.322 | 0.340 | 0.386 | 0.401 | 0.430 |
| | 267 | 0.371 | 0.453 | 0.521 | 0.498 | 0.500 |
| | 268 | 0.436 | 0.516 | 0.577 | 0.582 | 0.583 |
| | 269 | 0.444 | 0.562 | 0.637 | 0.625 | 0.646 |
| 15 | 433 | 0.157 | 0.168 | 0.179 | 0.184 | 0.199 |
| | 433.5 | 0.208 | 0.303 | 0.328 | 0.346 | 0.354 |
| | 434 | 0.264 | 0.457 | 0.471 | 0.517 | 0.532 |
| | 435 | 0.364 | 0.710 | 0.663 | 0.686 | 0.652 |
| | 436 | 0.545 | 0.723 | 0.709 | 0.658 | 0.690 |
| | 437 | 0.582 | 0.714 | 0.706 | 0.686 | 0.697 |
| 19 | 533.5 | 0.156 | 0.157 | 0.159 | 0.169 | 0.173 |
| | 534 | 0.170 | 0.258 | 0.282 | 0.291 | 0.332 |
| | 534.5 | 0.253 | 0.390 | 0.411 | 0.409 | 0.441 |
| | 535.5 | 0.293 | 0.503 | 0.591 | 0.669 | 0.625 |
| | 536.5 | 0.361 | 0.608 | 0.691 | 0.734 | 0.628 |
| | 537.5 | 0.398 | 0.641 | 0.723 | 0.677 | 0.644 |
| 21 | 601 | 0.190 | 0.206 | 0.236 | 0.171 | 0.180 |
| | 601.5 | 0.246 | 0.301 | 0.457 | 0.308 | 0.317 |
| | 602 | 0.290 | 0.298 | 0.465 | 0.440 | 0.421 |
| | 603 | 0.357 | 0.456 | 0.585 | 0.608 | 0.589 |
| | 604 | 0.398 | 0.639 | - | 0.683 | 0.658 |
| | 605 | 0.448 | 0.703 | 0.710 | 0.696 | 0.634 |
| 28 | 769 | 0.085 | 0.085 | 0.092 | 0.092 | 0.100 |
| | 769.5 | 0.114 | 0.162 | 0.181 | 0.165 | 0.165 |
| | 770 | 0.155 | 0.236 | 0.252 | 0.232 | 0.224 |
| | 771 | 0.524 | 0.722 | 0.732 | 0.642 | 0.649 |
| | 772 | 0.636 | 0.788 | 0.780 | 0.754 | 0.741 |
| | 773 | 0.650 | 0.766 | 0.740 | 0.743 | 0.715 |

**Table S7.** Measured concentrations of calcium $\left[\frac{\text{mol}}{\text{l}}\right]$ for column experiment D2 used as observations in inverse modeling. The measurements at 20 cm distance from the inlet are used in Figure 7

| Pulse | Time [h] | 10 cm | 20 cm | 30 cm | 40 cm | 50 cm |
|---|---|---|---|---|---|---|
| 3 | 97 | 0.286 | 0.287 | 0.290 | 0.292 | 0.287 |
| | 97.5 | 0.272 | 0.288 | 0.287 | 0.285 | 0.293 |
| | 98 | 0.289 | 0.286 | 0.270 | 0.277 | 0.274 |
| | 99 | 0.269 | 0.263 | 0.258 | 0.249 | 0.249 |
| | 100 | 0.260 | 0.274 | 0.250 | 0.231 | 0.215 |
| | 101 | 0.277 | 0.246 | 0.233 | 0.197 | 0.219 |
| 6 | 169 | 0.298 | 0.298 | 0.295 | 0.292 | 0.285 |
| | 169.5 | 0.280 | 0.289 | 0.285 | 0.260 | 0.236 |
| | 170 | 0.258 | 0.294 | 0.259 | 0.238 | 0.218 |
| | 171 | 0.258 | 0.254 | 0.222 | 0.182 | 0.185 |
| | 172 | 0.250 | 0.224 | 0.176 | 0.169 | 0.149 |
| | 173 | 0.241 | 0.187 | 0.167 | 0.157 | 0.116 |
| 9 | 265 | 0.287 | 0.284 | 0.251 | 0.273 | 0.270 |
| | 265.5 | 0.261 | 0.241 | 0.217 | 0.197 | 0.157 |
| | 266 | 0.218 | 0.186 | 0.172 | 0.176 | 0.134 |
| | 267 | 0.189 | 0.149 | 0.123 | 0.123 | 0.114 |
| | 268 | 0.161 | 0.111 | 0.082 | 0.083 | 0.078 |
| | 269 | 0.128 | 0.091 | 0.047 | 0.052 | 0.038 |
| 15 | 433 | 0.276 | 0.304 | 0.284 | 0.268 | 0.266 |
| | 433.5 | 0.250 | 0.206 | 0.201 | 0.191 | 0.179 |
| | 434 | 0.210 | 0.112 | 0.103 | 0.114 | 0.094 |
| | 435 | 0.169 | 0.017 | 0.029 | 0.037 | 0.040 |
| | 436 | 0.097 | 0.007 | 0.016 | 0.037 | 0.025 |
| | 437 | 0.058 | 0.009 | 0.016 | 0.022 | 0.027 |
| 19 | 533.5 | 0.277 | 0.266 | 0.266 | 0.271 | 0.250 |
| | 534 | 0.228 | 0.219 | 0.208 | 0.211 | 0.183 |
| | 534.5 | 0.223 | 0.179 | 0.136 | 0.162 | 0.129 |
| | 535.5 | 0.151 | 0.098 | 0.052 | 0.044 | 0.062 |
| | 536.5 | 0.132 | 0.043 | 0.009 | 0.002 | 0.028 |
| | 537.5 | 0.096 | 0.014 | 0.003 | - | 0 |
| 21 | 601 | 0.334 | 0.378 | 0.372 | 0.255 | 0.247 |
| | 601.5 | 0.314 | 0.247 | 0.280 | 0.190 | 0.187 |
| | 602 | 0.273 | 0.166 | 0.161 | 0.169 | 0.153 |
| | 603 | 0.215 | 0.116 | 0.057 | 0.045 | 0.052 |
| | 604 | 0.139 | 0.064 | 0.086 | 0.035 | 0.014 |
| | 605 | 0.124 | 0.025 | 0.007 | 0.024 | 0.021 |
| 28 | 769 | 0.279 | 0.283 | 0.273 | 0.254 | 0.261 |
| | 769.5 | 0.206 | 0.194 | 0.180 | 0.193 | 0.177 |
| | 770 | 0.153 | 0.144 | 0.120 | 0.159 | 0.138 |
| | 771 | 0.087 | 0.023 | 0.021 | 0.057 | 0.052 |
| | 772 | 0.042 | - | 0.003 | 0.011 | 0.018 |
| | 773 | 0.021 | 0.002 | 0.002 | 0.002 | 0.012 |

**Table S8.** Sum of squared residuals and normailzed squared residuals of model predictions for the data sets $NH_4^+$, $Ca^{2+}$, and $CaCO_3$. The squared residuals are summed over the 7 measurement pulses with each 6 measurements at the 5 locations for data sets $NH_4^+$ (total of 419 measurements; See Table 6) and $Ca^{2+}$ (total of 418 measurements; See Table S7) and the 8 measurements along the column length for $CaCO_3$ (See Table S3). The values presented here are for the selected parameter sets from Table 2 using the revised model and the parameters and equations as given in *Ebigbo et al.* [2012].

| | Data set | *Ebigbo et al.* [2012] | Low attachment | Low $\rho_f$ | Low $k_{ub}$ | Best fit |
|---|---|---|---|---|---|---|
| Sum of squared residuals | $NH_4^+$ | 4.11 | 12.25 | 11.37 | 13.90 | 3.42 |
| | $Ca^{2+}$ | 2.05 | 2.56 | 4.54 | 2.56 | 0.97 |
| | $CaCO_3$ | 0.024 | 0.034 | 0.008 | 0.037 | 0.003 |
| | Total | 6.18 | 14.84 | 15.92 | 16.50 | 4.40 |
| Sum of normalized squared residuals | $NH_4^+$ | 95 | 295 | 207 | 283 | 82 |
| | $Ca^{2+}$ | 3890 | 240 | 142 | 129 | 278 |
| | $CaCO_3$ | 9.3 | 14.3 | 2.3 | 13.3 | 0.9 |
| | Total | 3995 | 546 | 351 | 425 | 360 |