Simulation Results for the Calcite Precipitation with reactants $NaHCO_3 + CaCl_2$ with Nucleation and Growth only during Addition period

Analysed cases:

- Supersaturation:

$$S = \sqrt{\frac{\gamma_{Ca^{2+}} x_{Ca^{2+}} \gamma_{CO^{2-}} x_{CO^{2-}}}{K_{sp}}}$$

and

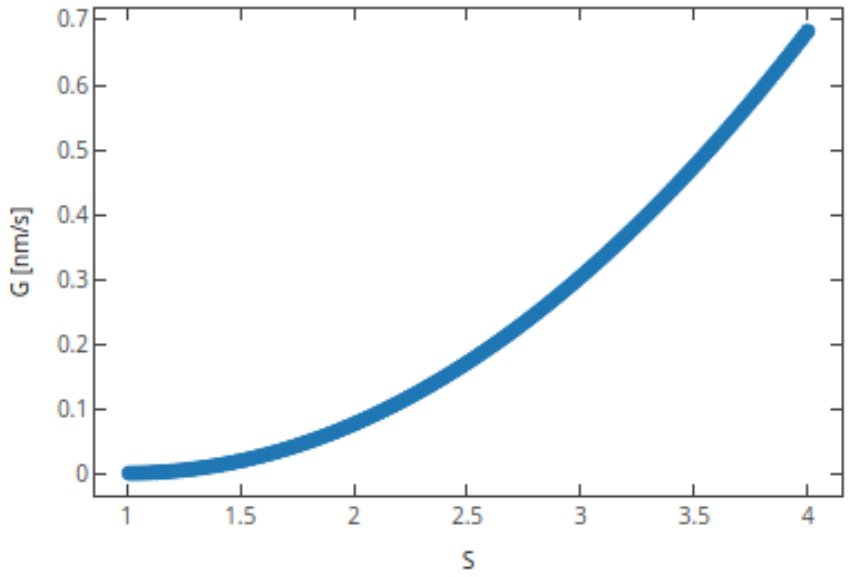
$$S = \frac{\gamma_{Ca^{2+}} x_{Ca^{2+}} \gamma_{CO^{2-}} x_{CO^{2-}}}{K_{sp}}$$

- Growth rates:

1. Reis et al. (2018):

$$G(t) = k_g (S-1)^2$$

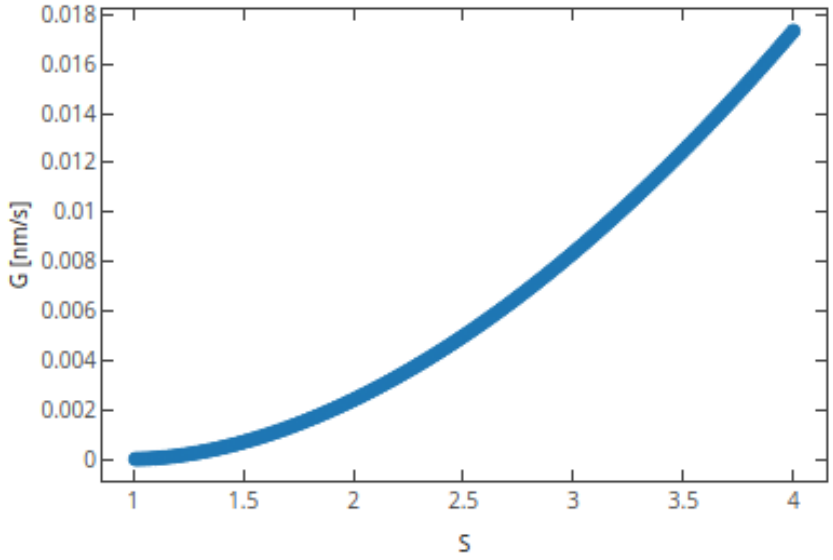
$$\log k_g = -0.275 + 0.228 \left[\frac{I^{1/2}}{1 + I^{1/2}} - 0.3I \right]$$



2. Verdoes, Kashchiev, and Rosmalen (1992)

$$G(t) = k_g(S-1)^1.8$$

Verdoes, Kashchiev, and Rosmalen (1992) provides the growth kinetics in a similar form, but with $g = 1.8$ and $k_g = 2.4e-12m/s$



- Nucleation

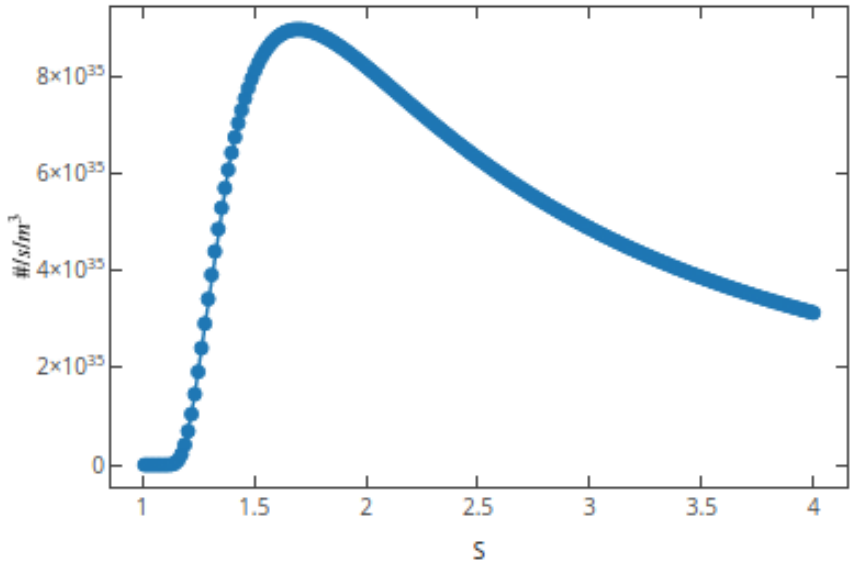
1. Reis et al. (2018):

$$B_0(t) = A \exp\left[-\frac{\beta\sigma^3\nu^2}{2.30k_b^3T^3(\log S)^2}\right]$$

where $\beta = 16.75$ for spherically symmetric particles, $\sigma = 0.068N/m$; $\nu = 6.132 \cdot 10^{-29}$. An approximation for A is given:

$$A = \frac{D}{\epsilon^5 S^{5/3}}$$

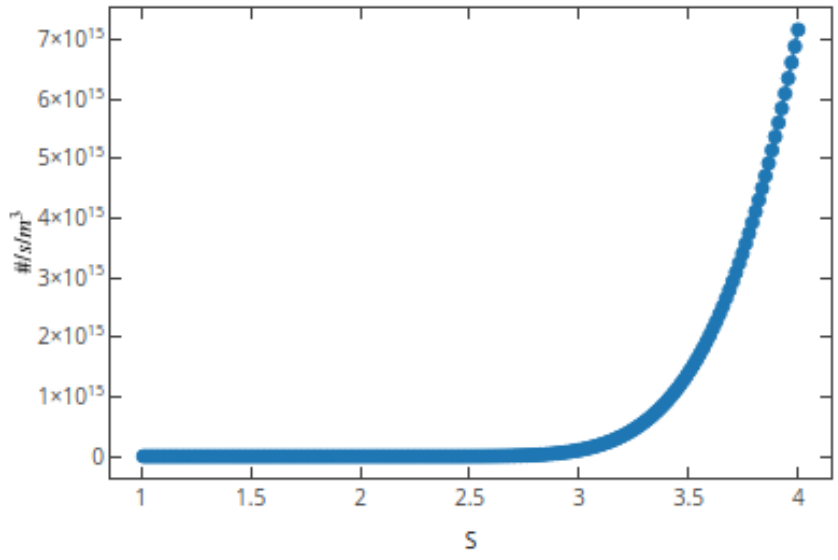
$$D = 8.67 \cdot 10^{-10}m^2/s \text{ and } \epsilon = 7.62 \cdot 10^{-10}$$



2. Verdoes, Kashchiev, and Rosmalen (1992)

$$B_0 = K_s S \exp\left(-\frac{E_b}{\ln^2 S}\right)$$

where $K_s = 1.4e181/m^3/s$ and $E_b = 12.8$



Results

Case	Eq. S.	Growth	Nucleation	Note
1	sqrt	Reis	Reis	Failed - Nucleation low for working S
2	sqrt	Reis	Verdoes	Ok.
3	sqrt	Verdoes	Reis	Not tested See (1)
4	sqrt	Verdoes	Verdoes	Failed - Growth low (check the modification)
5	sqrt	Verdoes-Mod	Verdoes	Issues with sundials but running
6	non sqrt	Reis	Reis	Not tested See (1)
7	non sqrt	Reis	Verdoes	Not tested
8	non sqrt	Verdoes	Reis	Not tested
9	non sqrt	Verdoes	Verdoes	Not tested

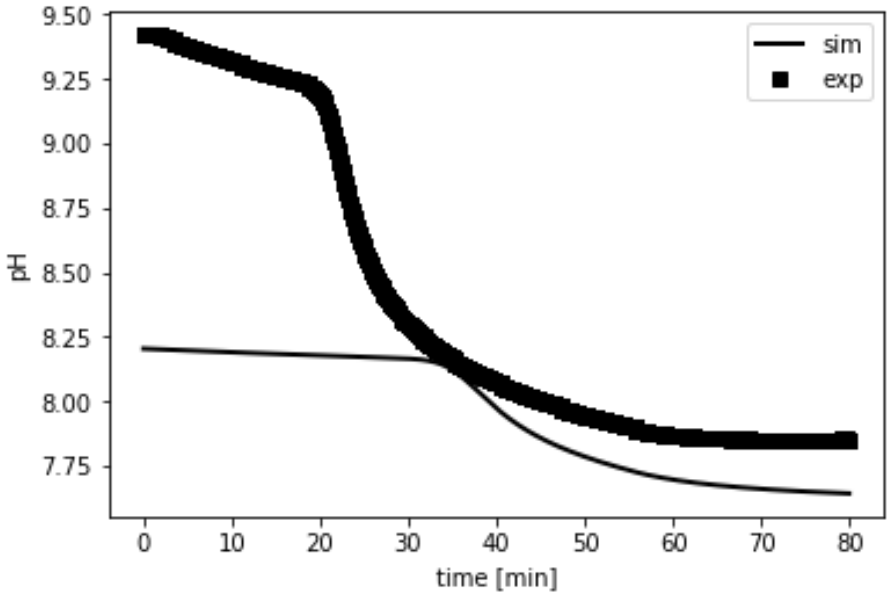
Case (1)

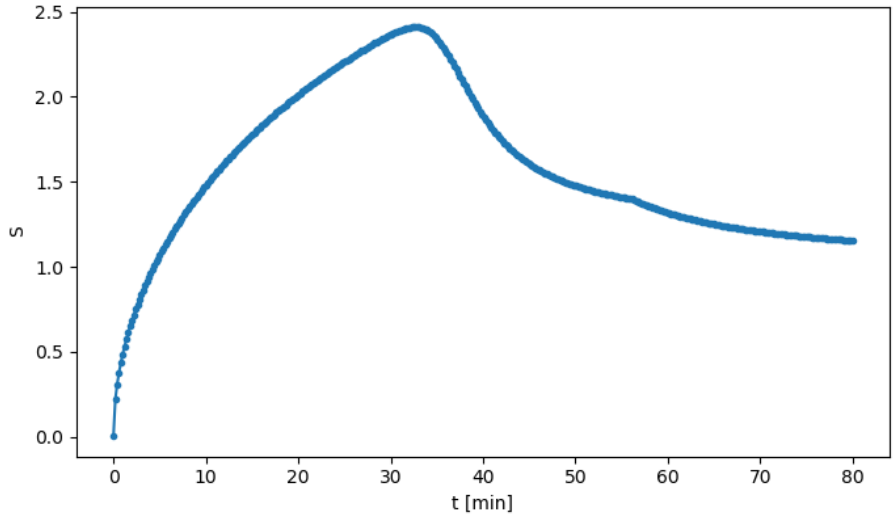
(1 | sqrt | Reis | Reis)

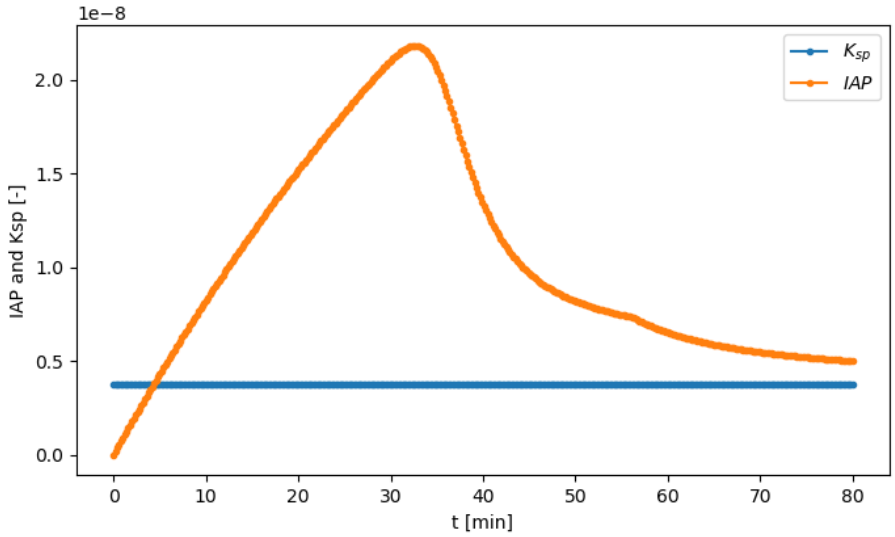
Numerical error when using Reis Nucleation Rate.

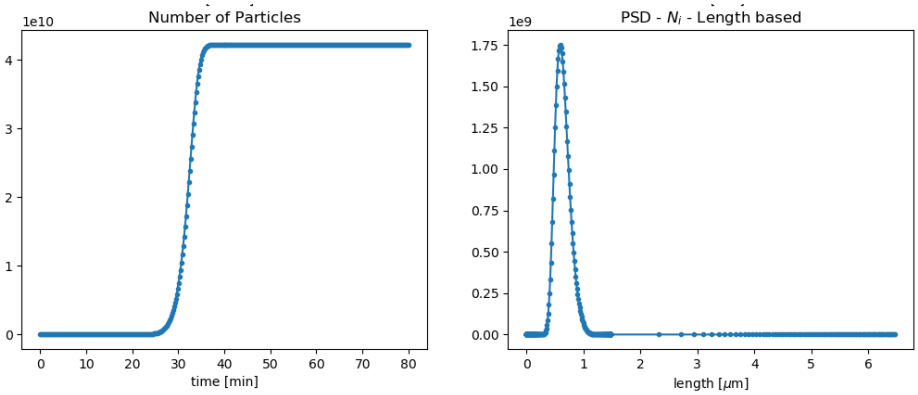
Case (2)

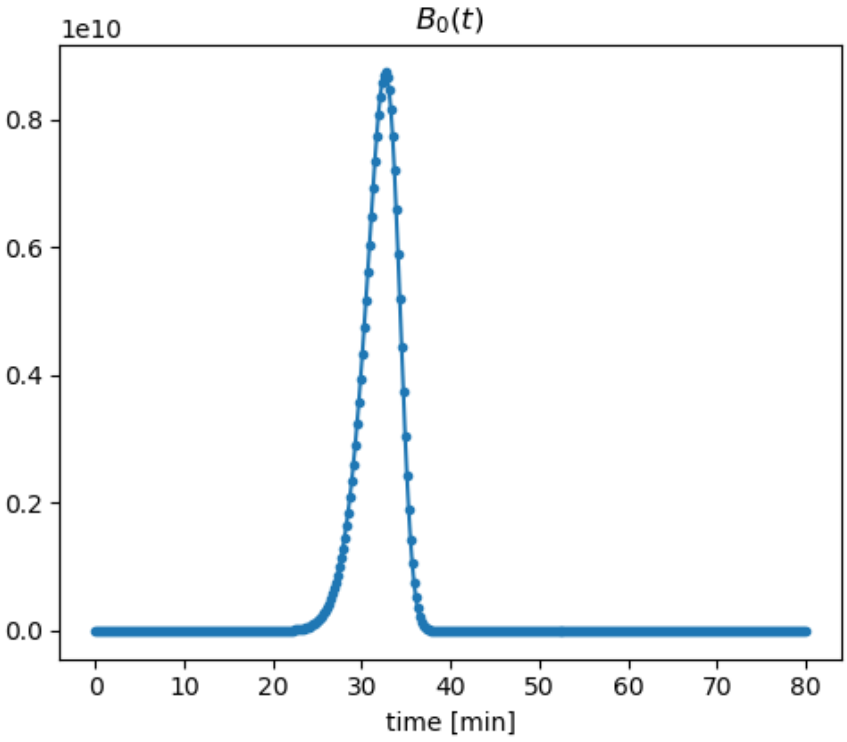
(2 | sqrt | Reis | Verdoes)




S
t [min]


1e−8
IAP and Ksp [-]
t [min]
K_{sp}
IAP



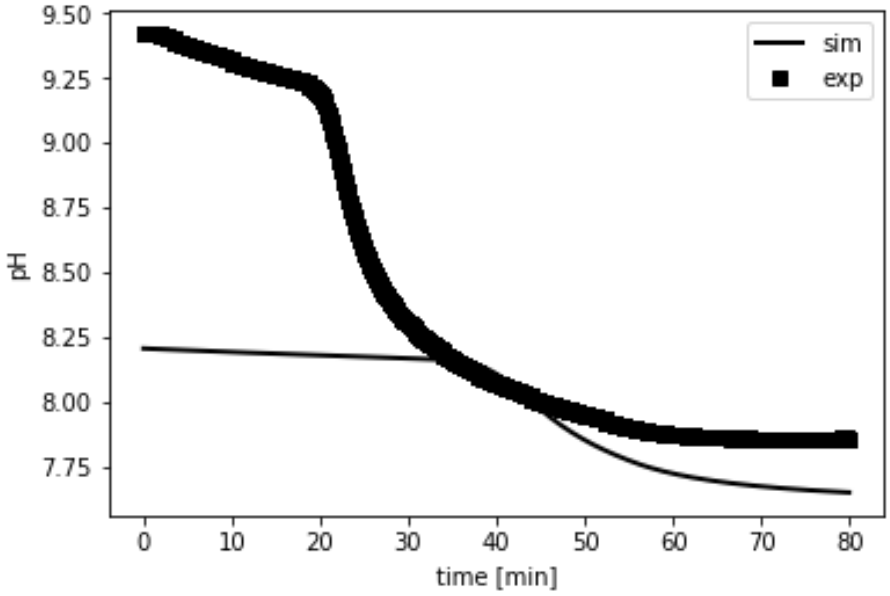


Case (4)

(4 | sqrt | Verdoes | Verdoes)

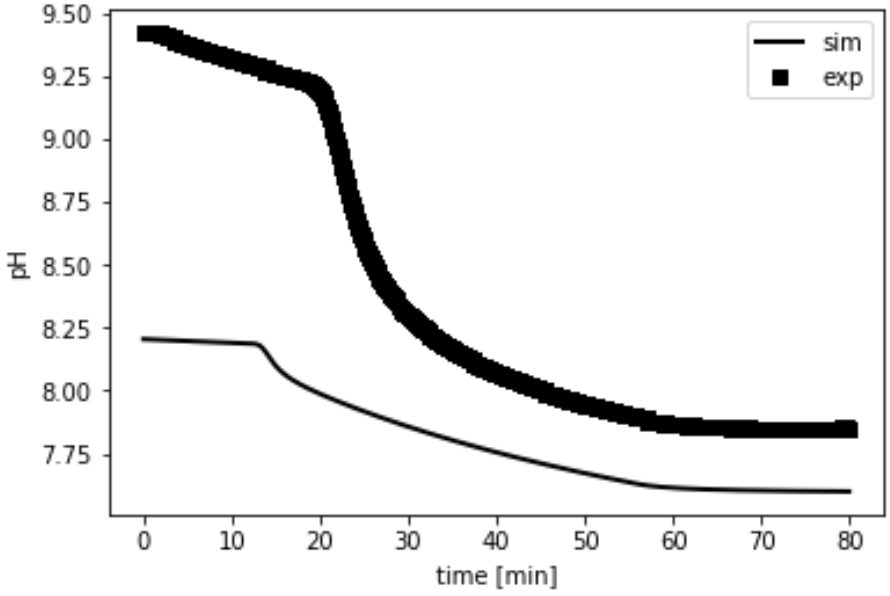
Numerical error when using Verdoes Growth Rate. The author suggest other references using $K_g \cdot 10^2$

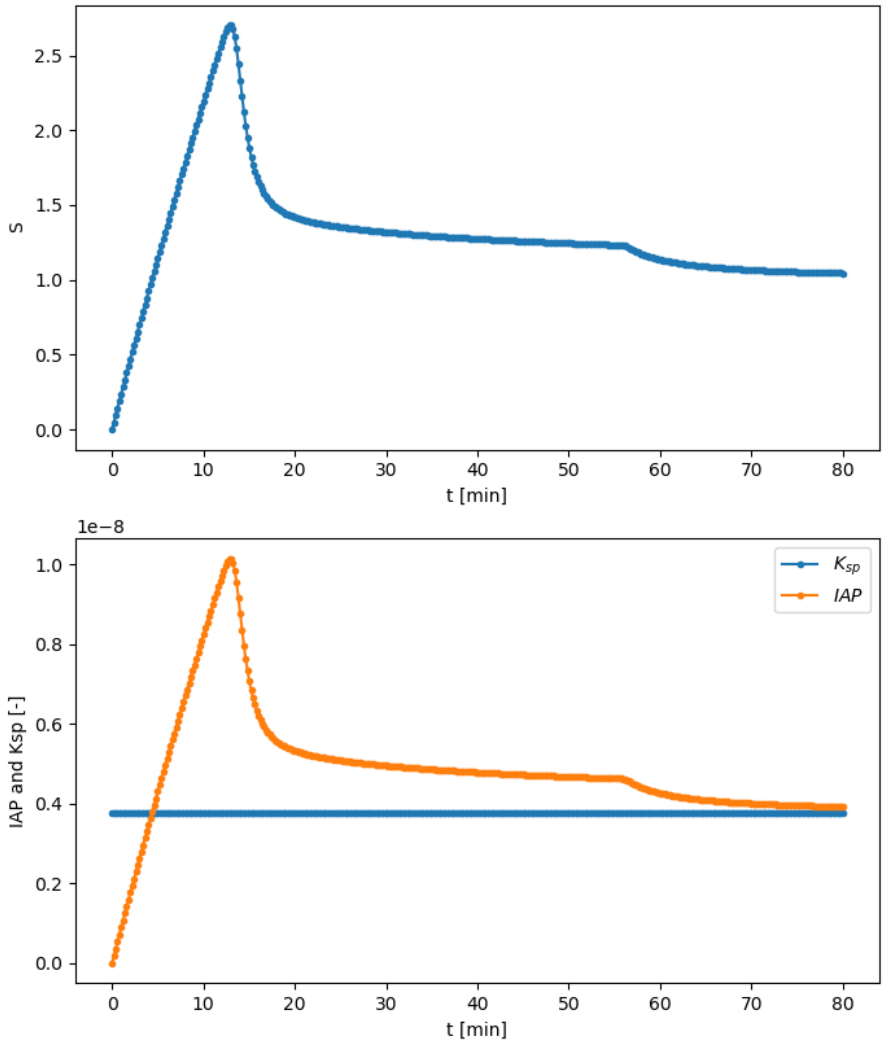
Case (5)



Case (6)

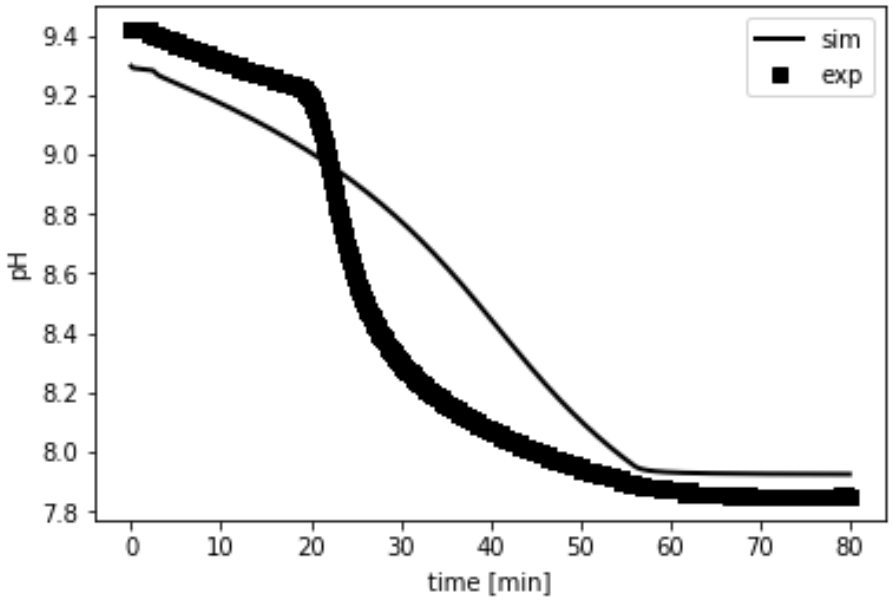
(6 | non sqrt | Reis | Reis)



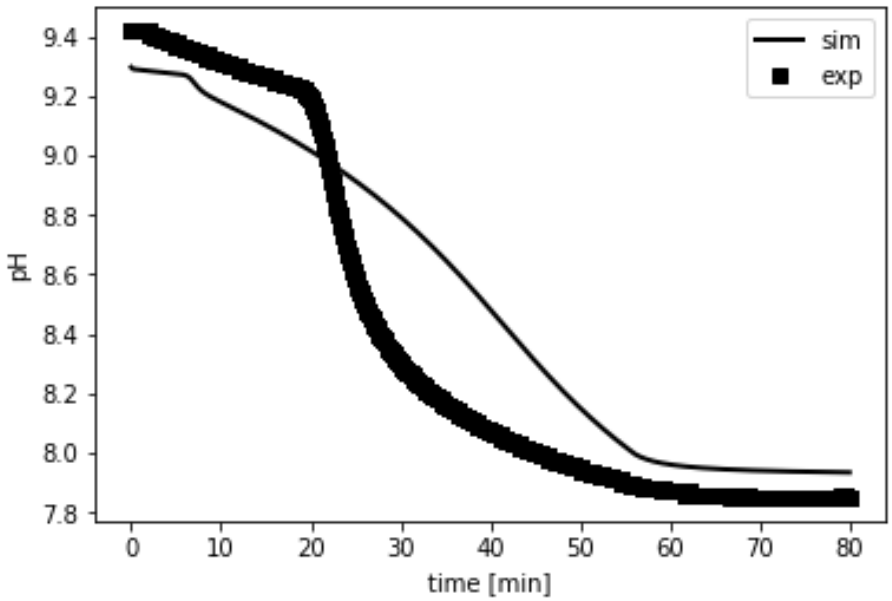


Case - Partial Result: Using new pH calculation method

(Not listed yet | non sqrt | Reis | Verdoes)



(Not listed yet | sqrt | Reis | Verdoes)



Reis, MC, MFB Sousa, F Alobaid, CA Bertran, and Y Wang. 2018. "A Two-Fluid Model for Calcium Carbonate Precipitation in Highly Supersaturated Solutions." *Advanced Powder Technology* 29 (7): 1571–81.

Verdoes, D, D. Kashchiev, and G. M. van Rosmalen. 1992. "Determination of nucleation and growth rates from induction times in seeded and unseeded precipitation of calcium carbonate." *Journal of Crystal Growth* 118 (3-4): 401–13. https://doi.org/10.1016/0022-0248(92)90089-2.