Finding a balance between accuracy and effort for modeling biomineralization

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Abstract

Microbially induced calcite precipitation (MICP) is a technology aiming at the mitigation of potential leakage from underground gas storage sites. A numerical model for MICP was previously developed and validated. The model complexity leads to high computation times, prohibiting at the moment the use of the model for designing field-scale MICP applications. This study investigates savings of the computational time by well-chosen model simplifications. Additionally, this approach is motivated by the high uncertainty of relevant input-parameters. Excessively detailed equations are unnecessary burdens to the MICP model, whose reliability is influenced by the input-parameter uncertainty.

Keywords: Microbially induced calcite precipitation; numerical modeling; model simplification; computational efficiency

1. Introduction

Previously, a numerical model for microbially induced calcite precipitation (MICP) was developed and validated using laboratory experiments [1]. This model was improved further and is now able to predict the resulting calcite precipitate distribution for a wide range of laboratory experiments [2]. But due to the various processes considered in the model, it is very complex. Examples for this complexity are the precipitation rate being dependend on the activities of calcium and carbonate, which in turn depend on the concentrations of all other ions in the aqueous phase, the change in the porous medium's porosity and permeability due to calcite precipitation and biomass accumulation, or the composition-dependent phase properties such as density and viscosity. All these interactions between the different component mass balances increase the non-linearity of the system of equations and by that the number of non-linear solver iterations necessary for convergence. As a results of this, the computational effort is relatively high, even for the

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relatively small laboratory-scale setups used in Ebigbo et al. [1] and Hommel et al. [2]. For field-scale applications, the simulation domain is typically larger and less information is available. As a consequence, the computational time increases both due to the size of the domain and due to the necessity to model different scenarios accounting for the uncertainty in the geometry and the porous medium's properties. All of this limits the use of the current model for designing field-scale applications of MICP, until its computational effort is reduced while maintaining its ability to make accurate predictions. Different strategies for reducing the computational effort are possible, e.g. optimized numerical approaches, optimized choice of numerical parameters, or simplified physics and chemistry.

Nomenclature

Δt	time-step size
ϕ_c	calcite volume fraction
ϕ_f	biofilm volume fraction
CT	computational time
E	error between the reference with a maximum time-step size of 100 s and the modified model results
E_{comp}	error introduced by assuming homogeneous permeability, estimated based on [3]
$E_{FC,8}$	error between the reference with unrestricted time-step size and the modified model results
LIT	number of linear solver iterations
N	convergence criterion of the non-linear (Newton) solver
NLIT	number of non-linear (Newton) solver iterations
R	maximum relative change of the non-linear (Newton) solver
r_{prec}	calcite precipitation rate
r_{urea}	ureolysis rate

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2. Options to reduce computational time

There are several options for reducing the computational time. What they have in common is that they mainly focus on reducing the number of unknowns or the non-linear coupling between the equations, which are the main sources of numerical difficulties [4,5].

2.1. Simplification of physics and chemistry

Models with simplified physics or chemistry are an engineering approach, since they neglect certain processes; these need to be identified beforehand dependent on the setup.

The main disadvantage of this approach is that the potential for simplification has to be identified prior to simulation, requiring additional investigations or expert knowledge, and that these potential simplifications are specific to a given setup, limiting the general applicability of such simplified models. For this approach, the reduction in computational effort is achieved by reducing the complexity of the governing equations or the source terms related to (bio)chemical reactions, which makes it easier to solve the system of equations. For example, reaction rates and phase properties like density or viscosity are in general dependent on concentrations of multiple components or even the total composition of the phase. A reduction of the coupling of the mass balance equations also reduces the computational time [5–7]. In some cases, even a reduction of the number of balance equations might be possible, which would additionally decrease the computational time.

In addition to a possible reduction of computational time, another motivation for the simplification approach is the uncertainty of important model input parameters (e.g. porosity and permeability) in the field. In light of this input-parameter uncertainty, excessively detailed equations might be an unnecessary burden on modeling as the overall reliability of the model predictions is already limited by the reliability of the input parameter estimation. Such simplified models might be able to increase the computational efficiency while, in contrast to sequential approaches, conserving the robustness of the globally implicit approach.

Two model simplifications are investigated and compared to the full complexity model (FC):

- an *initial biofilm* model (IB), neglecting the suspended biomass and starting with a pre-established biofilm;
- a *simple chemistry* model (SC), setting the precipitation rate equal to the ureolysis rate. This model assumes that the precipitation is instantaneous and stoichometrically follows the overall reaction equation (Eq. (1)).

$$CO(NH_2)_2 + 2H_2O + Ca^{2+} \xrightarrow{urease} 2NH_4^+ + CaCO_3 \downarrow . \tag{1}$$
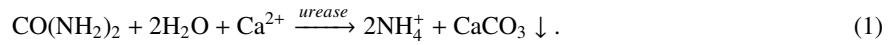
In addition to neglecting the component suspended biomass, the IB model avoids simulating the inoculation and the attachment periods, saving extra computational effort by a reduced process length to be simulated. This model simplification is motivated by the findings of Hommel et al. [8], who showed that accounting for suspended biomass is only relevant when biomass is added to the system. The initial biofilm distribution $\phi_{f,0}$ is assumed to follow the distribution dependent on the radius r of the radial simulation domain (see Section 3) as described by Equation (2) which is fitted to the FC model biofilm distribution predictions:

$$\phi_{f,0} = -0.00911r^3 - 0.000111r^2 - 0.000035r + 0.0000808. \tag{2}$$

Setting the precipitation rate equal to the ureolysis rate (Eq. (3)) in the SC model avoids the calculation of the precipitation rate and the associated calculation of the saturation state (Eq. (6)) and of the carbonate and calcium activities, which are expensive due to exponential functions and logarithms. Additionally, this reduces the coupling of the mass balance equations for the different components as the activities in the full model are dependent on the overall aqueous phase chemistry [2]. Further, the dissociation of carbonic acid (and ammonia) can be neglected, as the the molalities of bicarbonate and especially carbonate are no longer needed. This assumption of instantaneous, stoichiometric precipitation is commonly used in model studies on MICP, e.g. Cuthbert et al. [9] or van Wijngaarden et al. [10,11]. The rate of urea hydrolysis is:

$$r_{urea} = k_{urease}\, k_{ub}\, \rho_f\, \phi_f\, \frac{m^u}{m^u + K_u}. \tag{3}$$

Here, r_{urea} represents the rate of ureolysis according to Lauchnor et al. [12], k_{urease} the maximum activity of urease adapted from Lauchnor et al. [12], ρ_f and ϕ_f the density and volume fraction of biofilm respectively, k_{ub} the mass ratio of urease to biofilm as given in Bachmeier et al. [13], m^u the molality of urea calculated from the water phase composition, and K_u is the half saturation constant for urea adapted from Lauchnor et al. [12]. The precipitation rate of calcite for the FC and IB models is calculated as:

$$r_{prec} = k_{prec}A_{sw}\,(\Omega - 1)^{n_{prec}}\,;\ \text{for } \Omega \geq 1, \tag{4}$$

$$A_{sw} = A_{sw,0}\left(1 - \frac{\phi_c}{\phi_0}\right)^{\frac{2}{3}}, \tag{5}$$

$$\Omega = \frac{m^{Ca^{2+}}\gamma^{Ca^{2+}}m^{CO_3^{2-}}\gamma^{CO_3^{2-}}}{K_{sp}}, \tag{6}$$

where k_{prec} and n_{prec} are empirical precipitation parameters from Zhong and Mucci [14], A_{sw} and $A_{sw,0}$ are the current and initial interfacial areas respectively between the water phase and the solid phases, K_{sp} the calcite solubility product and $m^{Ca^{2+}}$ and $m^{CO_3^{2-}}$ the molalities of calcium and carbonate respectively. The activity coefficients γ^κ are calculated using Pitzer equations [15–17]. For the SC model, those complex calculations necessary to calculate the calcite precipitation rate reduce to:

$$r_{prec} = r_{urea}. \tag{7}$$

2.2. Optimized numerical solution approaches

The most commonly used solution approaches are the globally implicit approach (GIA) and sequential approaches such as the sequential iterative approach (SIA) and the sequential non-iterative approach (SNIA) [18]. All of the numerical solution approaches are able to accurately predict the distributions of components as well as the resulting reaction rates even for complex multicomponent reactive transport setups as shown in the benchmark of Carrayrou et al. [4].

Sequential approaches are often used in modeling reactive transport in porous media, since they allow the use of specific methods to solve the transport and chemical equations [19]. Sequential approaches are usually computationally more efficient than GIAs [20], but this is not always the case. For example, Saaltink et al. [21] demonstrated that for cases with high influence of the solid phases on the transport behavior, GIAs perform better. In general, SNIAs are more efficient than SIAs, as SNIAs do not iterate [19]. The MICP model of Hommel et al. [2] uses a GIA. However, due to the high effort related with implementing a SIA or a SNIA solution scheme, optimized numerical solution approaches are not investigated in this study.

2.3. Other possible ways of reducing computational effort

Optimizing the time-step size through adaptive time stepping is a good way of improving the computational efficiency [4]. The model of Hommel et al. [2] for MICP already uses adaptive time stepping based on the number of non-linear iterations needed for convergence. Thus, relaxing the convergence criterion of the non-linear Newton solver makes it easy to test the effect of increased time steps on the computational efficiency.

Multi-chemistry approaches are also a possible way. Such approaches can be implemented similarly to the multi-physics approaches investigated in Faigle et al. [22,23]. Multi-chemistry approaches can save computational time by calculating activity coefficients or complex reaction equations only in those parts of the domain where suitable indicators show the need for such expensive calculations. Indicators might be the Damköhler number, the presence of certain reactive components, or a threshold concentration of a certain reactive component. In the other parts of the domain, a simplified model can be used, see Section 2.1.

Refinement of the computational grid around heterogeneities also increases the computational efficiency compared with uniform grids, as this allows the grid to coarsen at other locations, thereby reducing the global number of unknowns [4]. For known heterogeneities in the simulation domain, this grid refinement can be done beforehand, but grid refinement might also be useful for refining concentration gradients or heterogeneities that develop during the simulation, e.g. due to the accumulation of biofilm of minerals. For such cases, which cannot be addressed by initially refining the grid, the use of adaptive grids might be a promising solution. Adaptive grid refinement schemes might refine the computational grid based on indicators dependent on concentration gradients or reaction rates. For example, refinement based on concentration gradients prevents numerical diffusion which usually increases the reaction rates by artificial mixing.

3. Investigation of the selected methods for increasing computational efficiency

This section presents the results of an investigation of selected options for reducing the computational effort, see Section 2, applied to the model of Hommel et al. [2] for MICP. For each option, the accuracy and the efficiency are evaluated. The efficiency is expressed using the computational time. Other numerical performance parameters such as the number of linear and non-linear (Newton) iterations are given as well. To determine the accuracy, the result for the precipitated calcite is compared with the resulting calcite precipitate for a simulation using the globally implicit model with high spatial resolution, a strict convergence criterion for the Newton solver of $N = 10^{-8}$, and a maximum time-step size of $\Delta t_{max} = 100$ s. This comparison is based on the error E introduced by the simplification, which is calculated as:

$$E = \sqrt{\sum_{i=1}^{\text{nodes}} \left(\phi_{c,i} - \phi_{c,\text{ref},i} \right)^2},$$
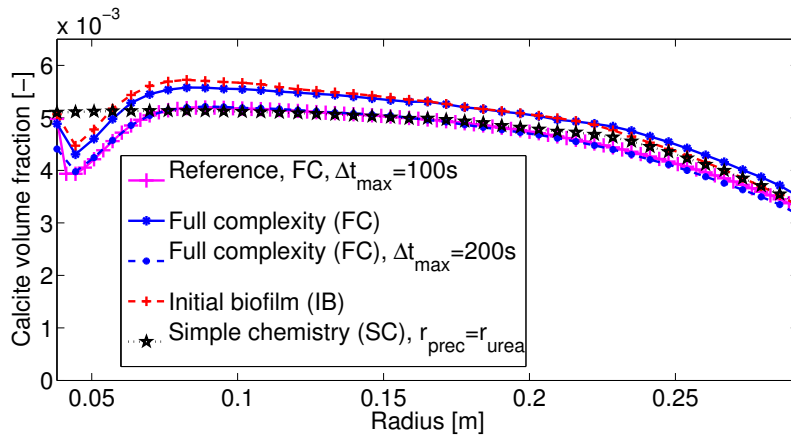
(8)

Fig. 1. Resulting calcite distribution for the BR experiment [2] obtained by the models: initial biofilm (IB), simple chemistry (SC), and full complexity (FC). For FC, three resulting calcite distributions are shown: the reference solution on a refined grid and a time-step size limited to 100 s in maximum, the solution on a non-refined grid with an unlimited time-step size as for the solutions shown for IB and SC, and the solution on a non-refined grid with a time-step size limited to 200 s in maximum.

where $\phi_{c,i}$ is the calcite volume fraction and $\phi_{c,ref,i}$ the reference calcite volume fraction at the node i.

The setup for the investigation is the BR Experiment presented in Hommel et al. [2]. In this experiment, cells and biomineralization media were injected in the center of a sand-filled radial reactor built using a bicycle rim and acrylic-glass plates at the top and the bottom. Outflow was at the outer radius through 16 ports. The simulation domain is the entire $360°$ to be able to compare the errors introduced by the model simplifications (Section 3.1) or the manipulation of the time-stepping scheme (Section 3.2) with the error introduced by the common assumption of a homogeneous porous medium permeability.

In a recent investigation by Kurz [3], the model error due to the assumption of a homogeneous permeability was estimated to be $6.6 \cdot 10^{-4}$ for the BR-experiment setup using Equation (8). This error was estimated using literature data for the heterogeneity of the permeability from Carsel and Parish [24] to create a realistic heterogeneous permeability distribution. To correct for the different number of grid nodes for this investigation and the grid used in Kurz [3], it is assumed that the average error per grid node is constant. The resulting error for comparison is $E_{comp} = {}^{720}/_{144} \cdot 6.6 \cdot 10^{-4} = 3.3 \cdot 10^{-3}$. For the following, it is important to note that E_{comp} is only an estimate based on literature values.

3.1. Simplification of physics and chemistry

Both simplified models (IB and SC) are compared with the full-complexity model (FC) discussed and published in Hommel et al. [2]. Further, all three models are compared with a reference solution obtained using the full complexity model on a refined grid and with a limited time-step size.

The predictions of the models are presented in Figure 1. The IB model and the full complexity model predict a very similar final distribution of calcite for the BR experiment [2]. Both models agree with the reference results in general but overestimate the amount of calcite precipitated compared with the reference solution. The difference between the FC model and the reference results is mainly due to the different time-step sizes. While the time-step size is unrestricted and only dependent on the convergence of the Newton solver, the time-step size is limited to 100 s for the reference. The FC model with a restricted time-step size of 200 s yields almost the same result on the coarse grid as the reference simulation with a maximum time-step size of 100 s on the refined grid. The SC model matches the reference solution quite well for a radius of more than 8 cm, but does not show the dynamics of the other models for smaller radii. However, all models show a satisfactory agreement in the amount and distribution of calcite.

For all models, the error E is less than or equal to $3E_{comp}$. When compared with the FC model with unlimited time-step size and non-refined grid, the error is lower for the FC and the IB model and comparable with the error of neglecting the heterogeneous permeability distribution, see Table 1. For the SC model, both E and $E_{FC,8}$ are identical.

Table 1. Numerical parameters and the error compared with the reference solution of the models (FC, IB, and SC). CT is the computational time, NLIT is the number of non-linear (Newton) iterations needed, LIT is the number of linear iterations needed, and E is the error defined in Equation (8). $E_{FC,8}$ is the error defined in Equation (8) using the FC model with a strict Newton convergence criterion ($N = 1 \cdot 10^{-8}$) but unlimited time-step size and non-refined grid as a reference solution. For comparison, the estimated error for neglecting the effect of a heterogeneous permeability distribution in the porous medium is $E_{comp} = 0.0033$.

Model	CT [s]	NLIT	LIT/NLIT	NLIT/Δt	E	$E_{FC,8}$
FC	32110	4971	15.2	8.6	0.009	0.003
IB	28089	5053	14.9	8.8	0.010	0.004
SC	5758	1094	14.9	5.5	0.007	0.007

Unlike the results, the numerical parameters show a difference between the models. While the IB model does not reduce the computational time (CT) much, but the SC model needs only 18% of the CT of the full model, see Table 1. The reduction of the CT in the IB model is only 13%, which corresponds to a reduction in the time simulated of 13% as well, because the initial inoculation and the first 8 h of growth are neglected. The number of linear iterations per non-linear Newton iteration is almost constant for the three models, suggesting that the reduction on CT of the SC model is mainly due to the reduced number of non-linear (Newton) iterations (NLIT). While the FC model needs 4971 NLIT, the SC model only needs 1094 NLIT, 22% of the NLIT of the FC model. Some part of this reduction in the number of NLIT for the SC model results from the SC model needing on average only 5.5 NLIT/Δt, while the FC and the IB model need 8.6 and 8.8 NLIT/Δt respectively. The remaining reduction in CT of the SC model results from the adaptive time-stepping scheme increasing Δt for low NLIT/Δt, which leads to larger time steps for the SC model [25].

3.2. Other possibilities for reducing computational effort

Of the potential other methods to optimize the computational effort discussed in Section 2.3, only the optimization of the time-stepping scheme was investigated. A significant reduction of the computational effort can be achieved by increasing the time-step size by relaxing the Newton convergence criterion controlling the time-step adaption scheme for the model of Hommel et al. [2] as well as for each of the simplified models IB and SC. For convergence, the maximum relative change R of any primary variable pV at any point of the simulation domain within an iteration of the Newton solver has to be less than the convergence criterion N. At each point and for each pV, the relative change R is calculated as:

$$R = \frac{|pV_{\text{before}} - pV_{\text{after}}|}{\max\left(1, \frac{pV_{\text{before}} + pV_{\text{after}}}{2}\right)}, \tag{9}$$

where pV_{before} and pV_{after} are the values of the primary variable before and after the update. Increasing the convergence criterion leads to fewer iterations necessary for convergence, increasing NLIT/Δt, and, through the adaptive time-stepping scheme [25], to increasing time steps. This is the case for all GIA models, the FC model and both the simplified models, IB and SC, see Table 2.

For all models, relaxing the Newton solver's convergence criterion N leads to decreasing NLIT/Δt, increasing the time-step size Δt [25], which leads to fewer but larger time steps. The number of linear iterations per non-linear iteration LIT/NLIT also decreases with decreasing N, further decreasing the computational time, except for the FC and the SC model and $N = 1 \cdot 10^{-8}$ (Table 2). The very high CT for the SC model with $N = 1 \cdot 10^{-8}$ is probably due to convergence problems of the Newton solver, which is indicated by the high ratio of NLIT/Δt = 12.2.

NLIT is the best predictor of the CT of a model. For the FC model, the CT needed for each NLIT is approximately 6.4 s for all N investigated. The NLIT for the IB model requires a constant time of 5.5 s. The CT/NLIT for the SC model is more variable, from 4.9 s for $N = 1 \cdot 10^{-8}$ to 5.3 s for $N = 1 \cdot 10^{-6}$.

The error introduced by relaxing the convergence criterion increases with an increasing convergence criterion. However, even for $1 \cdot 10^{-4}$, the error E is still less than an order of magnitude higher than the estimated error of the assumption of homogeneous permeability E_{comp} = 0.0033 (Table 2). The error is more dependent on the model simplification than on the convergence criterion and relaxing the convergence criterion does not dramatically increase

Table 2. Numerical parameters and the error compared with the reference solution of the models (FC, IB, and SC) for different convergence criteria N of the Newton solver (Eq. (9)). The values for $N = 1 \cdot 10^{-6}$ are already given in Table 1. $E_{\text{FC,8}}$ is the error defined in Equation (8) using the FC model with a strict Newton convergence criterion ($N = 1 \cdot 10^{-8}$) but unlimited time-step size and non-refined grid as a reference solution. For comparison, the estimated error for neglecting the effect of a heterogeneous permeability distribution in the porous medium is $E_{\text{comp}} = 0.0033$.

Model, N	CT [s]	NLIT	LIT	LIT/NLIT	NLIT/Δt	E	$E_{\text{FC,8}}$
FC, $1 \cdot 10^{-8}$	57533	9051	108437	12.0	9.3	0.007	0.0
FC, $1 \cdot 10^{-6}$	32110	4971	75335	15.2	8.6	0.009	0.003
FC, $1 \cdot 10^{-4}$	4861	776	5103	6.6	3.4	0.010	0.007
IB, $1 \cdot 10^{-8}$	48100	8687	143591	16.5	9.3	0.008	0.003
IB, $1 \cdot 10^{-6}$	28089	5053	75335	14.9	8.8	0.010	0.004
IB, $1 \cdot 10^{-4}$	3816	689	6160	8.9	3.8	0.008	0.005
SC, $1 \cdot 10^{-8}$	111662	22745	126870	5.6	12.2	0.007	0.008
SC, $1 \cdot 10^{-6}$	5758	1094	16303	14.9	5.5	0.007	0.007
SC, $1 \cdot 10^{-4}$	2002	396	5203	13.1	2.6	0.008	0.010

the error compared with the assumption of homogeneous permeability, which is difficult to avoid for realistic scenarios where the permeability distribution is unknown.

Using the FC model with $N = 1 \cdot 10^{-8}$ results in $E = 0.007$ compared with $E = 0.010$ using $N = 1 \cdot 10^{-4}$. Thus, the increase in E for increasing the tolerance of the Newton solver by 10^4, is still in the range of E_{comp}, but the reduction in the computational effort is more than one order of magnitude (91.6%). For the IB model, the computational effort is reduced similarly to 7.9%, while E does not change. For the SC model, the reduction is even more than 98%, resulting from the very high computational time using $N = 1 \cdot 10^{-8}$.

4. Conclusions

As presented in Section 3.1, model simplification can reduce the computational time significantly. Other simplifications than those investigated might include: a single-phase model for MICP as most applications of MICP do not include two-phase systems, a model with fewer components, e.g. substrate might be neglected in addition to suspended biomass as substrate is usually injected in excess compared with oxygen and thus does not influence biomass growth, total nitrogen might be neglected in the SC model, or a model using simplified physical equations of state to calculate e.g. density and viscosity. Further simplifying the SC model, e.g. a single-phase SC model, might result in a model with a computational time reduced by an order of magnitude or more compared with the FC model. The SC model has a relatively low error of $E = 0.008$, which is still comparable to $E_{\text{comp}} = 0.0033$.

Optimizing the time-step size also has a high potential to reduce the computational time, see Section 3.2. For the cases investigated, relaxing the convergence criterion of the Newton solver does not significantly increase the error compared with the reference solution, see Table 2. Thus, it is a first important step for reducing the computational time to choose optimized convergence criteria to improve the adaptive time-step size.

The errors introduced by the model simplifications or a relaxed convergence criterion still seem tolerable when compared with the assumption of homogeneous permeability, which is difficult to avoid for application scenarios where the permeability distribution is unknown. It is important to balance the modeling error introduced by the choice of the model simplification and other modeling assumptions with the possible associated gain in computational efficiency.

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