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PARAMETER DELIMITATION OF THE WEAK SOLVABILITY FOR A PSEUDO-PARABOLIC SYSTEM COUPLING CHEMICAL REACTIONS, DIFFUSION AND MOMENTUM EQUATIONS

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Abstract. The weak solvability of a nonlinearly coupled system of parabolic and pseudo-parabolic equations describing the interplay between mechanics, chemical reactions, diffusion and flow modelled within a mixture theory framework is studied via energy-like estimates and Gronwall inequalities. In analytically derived parameter regimes, these estimates ensure the convergence of discretized-in-time partial differential equations. These regimes are tested and extended numerically. Especially, the dependence of the temporal existence domain of physical behaviour on selected parameters is shown.

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1 Introduction

We investigate the existence of weak solutions to a system of partial differential equations coupling chemical reaction, momentum transfer and diffusion, cast in the framework of mixture theory [5]. For simplicity, we restrict ourselves to a model with a single non-reversible chemical reaction in a one-dimensional bounded spatial domain $[0, 1]$ enclosed by unlimited (or instantly replenished) reservoirs of the reacting chemicals. The chemical reaction is of the $N+1$-to-1-type with the reacting chemicals consisting out of N solids and a single fluid, while the produced chemical is a solid. New mathematical challenges arise due to the strong nonlinear coupling between all unknowns and their transport fluxes.
Evolution systems, in which chemical reactions, momentum transfer, diffusion and stresses interplay, thereby satisfying the balances of masses and forces occur in physical systems or biological processes; see e.g. [7, 11, 15, 25]. Here, the interest lies in capturing the interactions between flows, deformations, chemical reactions and structures. Such a system is, for instance, used in biology to better understand and eventually forecast plant growth and plant development [25], and in structural engineering to describe ambiental corrosion, for example sulfate attack in sewer pipes [15], in order to increase the durability of an exposed concrete sample. Our initial interest in this topic originates from mathematical descriptions of sulfate corrosion [4]. The mathematical techniques used for a system describing sulfate attack - when within a porous media (concrete) sulfuric acid reacts with slaked lime to produce gypsum - could be equally well applied to systems sharing similar features (e.g. types of flux couplings and nonlinearities).

At a general level, the system outlined in this paper is a combination of parabolic equations of diffusion-drift type with production terms by chemical reactions and pseudo-parabolic stress equations containing elastic and viscoelastic terms. On their own, both parabolic equations, cf. [13, 21, 22], and pseudo-parabolic equations, see [3, 14, 16, 27, 28, 31], are well understood from mathematical and numerical analysis perspectives. However, coupling these objects leads to systems of equations with a less understood structure. Many systems in the literature seem similar to ours at a first glance. A coupling resembling our case appears in [1], but with different nonlinear terms due to the combination of Navier-Stokes and Cahn-Hilliard systems. Other systems do not use chemical reactions or diffusion like in [7], where multi-dimensional Navier-Stokes-like stress equations are used; refer to a composite domain situation [11]; do not use stress equations [15]; or contain a hyperbolic stress equation [25].

We investigate in this paper the simplest case: a one-dimensional bounded domain. The one-dimensional setting allows one to control the nonlinearities by relying on the embedding $H^1 \hookrightarrow L^\infty$. In higher-dimensions, this embedding does not hold, and hence, nonlinearities become difficult to control.
The main target here is to probe the parameter region for which the system is weakly solvable. To this aim we search for explicit expressions of a priori parameter-dependent bounds. These bounds delimit the parameter region where the existence of our concept of weak solutions holds. Our numerical simulations show that the existence region is

actually larger.

In Section 2 we introduce our mathematical model together with a set of assumptions based on which the existence of weak solutions can be proven. In Section 3 we present two theorems: the main existence theorem for the continuous-time system with certain physical constraints and an auxilliary existence theorem for the time-discretized version of the system. In Section 4 we prove the auxilliary existence theorem and, then, in Section 5 we prove the main existence theorem by using the auxilliary existence theorem. In Section 6, we validate numerically the existence of solutions and, additionally, we show numerically that the assumptions seem to be more restrictive than necessary. Moreover, we show in what manner the existence of weak solutions depends on certain crucial parameters.

2 Formulation of the model equations

Consider a 1-d body, modeled as a d-component ($d \geq 2$) mixture of $(d-1)$ solid components and one fluid component. The body will deform under the action of chemical reactions. This process is described by a system of partial differential equations (PDEs) and initial and boundary conditions.
We define our system on a time-space domain $[0, T] \times [0, 1]$, where T is the not yet determined final time of the process. The unknowns of our system are two vector functions, $\phi : ([t_0, T] \times [0, 1])^d \to \mathbf{R}^d$ and $w : ([t_0, T] \times [0, 1])^{d-1} \to \mathbf{R}^{d-1}$, and two scalar functions $v : [0, T] \times [0, 1] \to \mathbf{R}$ and $W : [0, T] \to \mathbf{R}$ denoting respectively the volume fractions of the d chemical components active in a target chemical reaction, the displacements of the solid mixture components with respect to the initial domain as reference coordinate system, the velocity of the fluid, and the domain size. We identify the different components of the vectors with the different chemicals and use the following notation convention: The subscript 1 is related to the produced chemical, the subscript d is related to the fluid, all other subscripts are related to the remaining solid chemicals.
The time evolution of the unknowns is described by the following system of coupled partial differential equations: For $l \in \mathfrak{L} = \{1, \ldots, d-2, d\}$, the index of the reacting chemicals, and $m \in \mathfrak{M} = \{1, \ldots, d-1\}$, the index of the solid chemicals, we have

$$\partial_t \phi_l - \delta_l \partial_z^2 \phi_l + I_l(\phi) \partial_z \left(\Gamma(\phi) v\right) + \sum_{m \in \mathfrak{M}} \sum_{i,j=0}^{1} \partial_z^i \left(B_{lijm}(\phi) \partial_t^j w_m\right) = G_{\phi,l}(\phi), \tag{1a}$$

$$\partial_z \left(\Gamma(\phi) v\right) + \sum_{m \in \mathfrak{M}} \sum_{j=0}^{1} \partial_z \left(H_{jm}(\phi) \partial_t^j w_m\right) = G_v(\phi), \tag{1b}$$

$$\partial_t w_m - D_m \partial_z^2 w_m - \gamma_m \partial_z^2 \partial_t w_m + F_m(\phi) v \tag{1c}$$

$$+ \sum_{j \in \mathfrak{M}} \sum_{\substack{i+n=0 \\ i,n \geq 0}}^{1} \partial_z \left(E_{minj}(\phi) \partial_z^i \partial_t^n w_j\right) = G_{w,m}, (\phi)$$

with constants δ_l, D_m, $\gamma_m \in \mathbf{R}_+$ and functions I_l, Γ, B_{lijm}, H_{jm}, F_m, E_{minj}, $G_{\phi,l}$, G_v, $G_{w,m}$ that are actually products of functions $f_i(\cdot) \in C^1([0,1])$, satisfying

$$f(\phi) = \prod_{i=1}^{d} f_i(\phi_i). \tag{2}$$

Furthermore, we abuse notation with $\|f(\cdot)\|_{C^1([0,1])^d} \leq f \in \mathbf{R}_+$ for reducing the amount of constants.

Physically, Equation (1a) can be interpreted as a generalized reaction-diffusion-advection equation obtained from a mass balance law, Equation (1b) can be interpreted as a transport equation indicating the consequences of retaining incompressibility, and Equation (1c) is a pseudo-parabolic equation obtained from a generalized momentum balance law. Note that the system (1a) - (1c) must satisfy the constraint $\sum_{l=1}^{d} \phi_l = 1$, the fundamental equation of fractions, which allowed for the elimination of ϕ_{d-1}.
We assume the volume fractions are insulated at the boundary: $\partial_z \phi = 0$ at $z = 0$ and $z = 1$. The boundary at $z = 0$ is assumed to be fixed, while the boundary at $z = 1$ has a displacement $W(t) = h(t) - 1$, where $h(t)$ is the height of the reaction layer at the present time t and $h(0) = 1$. The Rankine-Hugoniot relations, see e.g. [23], state that the velocity of a chemical at a boundary is offset from $\mathcal{V}_0 = 0$ or $\mathcal{V}_1 = \partial_t W(t)$, the velocity of the boundary at $z = 0$ or $z = 1$, respectively, by influx or outflux of this chemical, i.e.

$$\text{at } z = 0 \text{ and } z = 1 \text{ hold } \begin{cases} \phi_m \left(\mathcal{V}_{0,1} - \partial_t w_m\right) \cdot \hat{n} = \hat{J}_m \mathcal{L}\left(\phi_{m,res} - \phi_m\right) \\ \phi_d \left(\mathcal{V}_{0,1} - v\right) \cdot \hat{n} = \hat{J}_d \mathcal{L}\left(\phi_{d,res} - \phi_d\right) \end{cases} \tag{3}$$

with $\hat{J}_d, \hat{J}_m \geq 0$ for $m \in \mathfrak{M}$, $\phi_{d,res}, \phi_{m,res} \in [0,1]$ for $m \in \mathfrak{M}$ and $\sum_{j=1}^{d} \phi_{l,res} = 1$. We assume $\mathcal{L}(\cdot)$, the concentration jump across the boundary, to have the semi-permeable form $\mathcal{L}(f) := f_+$, the positive part of f. Furthermore, we assume all chemicals have only one reservoir. The fluid chemical reservoir is assumed to be at $z = 1$: $\phi_{d,res} \geq 0$ at $z = 1$, $\phi_{d,res} = 0$ at $z = 0$. The solid chemical reservoirs are assumed to be at $z = 0$: $\phi_{m,res} = 0$ at $z = 1$, $\phi_{m,res} \geq 0$ at $z = 0$ for $m \in \mathfrak{M}$. We generalize the Rankine-Hugoniot relations by replacing ϕ_m with $H_{1m}(\phi)$ and ϕ_d with $\Gamma(\phi)$ in Equation (3).
The influx due to the Rankine-Hugoniot relations shows that the displacement $w_m|_{z=1}$ will not be equal to the boundary displacement $W(t)$. This will result in stresses, which we incorporate within a Robin boundary condition at these locations [24, Section 5.3]. Collectively for all $t \in [0,T]$, these boundary conditions are, for $m \in \mathfrak{M}$, $l \in \mathfrak{L}$, given by

$$\begin{cases} \partial_z \phi_l|_{z=0} &= 0, \\ \partial_z \phi_l|_{z=1} &= 0, \end{cases} \tag{4a}$$

$$\begin{cases} H_{1m}(\phi)\partial_t w_m|_{z=0} &= \hat{J}_m \mathcal{L}\left(\phi_{m,res} - \phi_m|_{z=0}\right), \\ \partial_z w_m|_{z=1} &= A_m \left(w_m|_{z=1} - W(t)\right), \\ v|_{z=0} &= 0, \\ \Gamma(\phi)\left(\partial_t W(t) - v\right)|_{z=1} &= \hat{J}_d \mathcal{L}\left(\phi_{d,res} - \phi_d|_{z=1}\right), \end{cases} \tag{4b}$$

where $A_m \in \mathbf{R}$. Additionally there are positive lower bounds for $\Gamma(\phi)$ and all H_{1m}: $\Gamma_\alpha := \inf\limits_{\phi \in \mathcal{I}_\alpha^d} \Gamma(\phi) > 0$ and $H_\alpha := \min\limits_{m \in \mathfrak{M}} \inf\limits_{\phi \in \mathcal{I}_\alpha^d} H_{1m}(\phi) > 0$, with $\mathcal{I}_\alpha = (\alpha, 1 - (d-1)\alpha)$ for

all $0 < \alpha < 1/d$. It is worth noting, that in the limit $|A_m| \to \infty$ one formally obtains Dirichlet boundary conditions.
The initial conditions describe a uniform and stationary equilibrium solution at $t = 0$:

$$\phi_l(0,z) = \phi_{l0} \qquad \text{and} \qquad w_m(0,z) = 0 \quad \text{for all } z \in [0,1] \qquad \text{and} \qquad W(0) = 0. \tag{5}$$

Note that $v(0,z) \in H^1(0,1)$ needs not to be specified as $v(0,z)$ follows from Equations (1b), (1c), and (4a) on $\{0\} \times (0,1)$.
The system of PDEs including initial and boundary conditions described above is called the *continuous-time system* for later reference in this paper.

3 Main existence result

Introduce $\phi_{\min} \in (0, 1 - C_{1,0}(d-1)/d]$. Moreover, $C_{1,0}$, the optimal Sobolev constant of the embedding $H^1(0,1) \subset C^0[0,1]$, is given by $C_{1,0} = \coth(1)$, see [33].
We assume that the following set of restrictions are satisfied.

Assumption 1.
We assume the parameters of the continuous-time system to satisfy:

(i) $\delta_l > 0$,

(ii) $|A_m| < 1$,

(iii) $E_{m01j}^2 < \frac{4}{9(d-1)^2} \min\{3/5, \gamma_m(1-|A_m|)\} \min\{3, \gamma_j(1-|A_j|)\}$,

(iv) $4\Gamma(\phi_0)^2 > (5d-4)^2 F_m(\phi_0)^2 H_{1j}(\phi_0)^2$,

(v) $\phi_{i0} \geq \phi_{\min}$ *and* $\sum_{i \neq \tilde{i}} \phi_{i0} < \frac{1-\phi_{\min}}{C_{1,0}}$ *for all* $1 \leq \tilde{i} \leq d$, *while* $\sum_{i=1}^{d} \phi_{i0} = 1$,

(vi) $(3d-2)(5d-4)\gamma_j A_j^2 < 1$,

(vii) $4\gamma_j > (3d-2)(5d-4)H_{1m}(\phi_0)^2/\Gamma(\phi_0)^2$

for all $j, m \in \mathfrak{M}$, *all* $l \in \mathfrak{L}$, *and all* $i \in \{1, \dots, d\}$.
Additionally, we assume that the parameters are such that there exist positive constants $\eta_{m1}, \eta_{m2}, \eta_{m01j1}, \eta_{m01j2} > 0$ *for* $j, m \in \mathfrak{M}$ *satisfying*

$$(viii) \quad \mathfrak{C}_{1m} = 1 - \sum_{j \in \mathfrak{M}} E_{j01m} \frac{\eta_{j01m1}}{2} > 0,$$

$$(ix) \quad \mathfrak{C}_{2m} = \gamma_m(1-|A_m|) - \frac{\eta_{m1}+\eta_{m2}}{2} - \frac{1}{2}\sum_{j \in \mathfrak{M}} \left(\frac{E_{m01j}}{\eta_{m01j1}} + \frac{E_{m01j}}{\eta_{m01j2}} + E_{j01m}\eta_{j01m2} \right) > 0,$$

$$(x) \quad \frac{7d-5}{\Gamma_{\phi_{\min}}^2} \max_{m \in \mathfrak{M}} \left\{ \frac{H_{1m}^2}{\mathfrak{C}_{2m}} \right\} \sum_{m \in \mathfrak{M}} \left(\frac{\gamma_m^2 |A_m|^2}{2\eta_{m1}} + \frac{F_m^2}{2\eta_{m2}} \right) < 1$$

for all $m \in \mathfrak{M}$.

Note, conditions (i), (ii), (viii) and (ix) are necessary conditions for coercivity in order to obtain a-priori estimates. Conditions (iii), (iv), (vi) and (vii) are necessary conditions for coercivity of a special system in Appendix A for the existence of a special physical v^0. Condition (v) guarantees the physical condition $\phi^k \in (\phi_{\min}, 1-(d-1)\phi_{\min})^d$, while condition (x) guarantees boundedness of $\|v\|_{L^2(0,T;H^1(0,1))}$.

Accepting Assumption 1, we can now formulate the main result of this paper.

Theorem 1.
Let $d \in \{2,3,4\}$ and let the parameters satisfy Assumption 1. Then there exist constants $T > 0$ and $V > 0$ and functions

$$
\begin{aligned}
\phi_l &\in L^2(0,T;H^2([0,1])) \cap L^\infty(0,T;H^1(0,1)) \cap C^0([0,T];C^0[0,1]) \\
&\quad \cap H^1(0,T;L^2(0,1)), \\
v &\in L^2(0,T;H^1(0,1)), \\
w_m &\in L^\infty(0,T;H^2(0,1)) \cap C^0([0,T];C^1[0,1]) \cap H^1(0,T;H^1(0,1)), \\
W &\in H^1(0,T),
\end{aligned}
$$

for all $l \in \mathfrak{L}$, $m \in \mathfrak{M}$ such that $(\phi_1,\ldots,\phi_{d-2},\phi_d,v,w_1,\ldots,w_{d-1},W)$ satisfies the weak version of the continuous system (1a)-(1c), (4a), (4b), and (5), such that

(I) $\|v\|_{L^2(0,T;L^2(0,1))} \le V$,

(II) $\|\partial_z v\|_{L^2(0,T;L^2(0,1))} \le V$,

(III) $\min\limits_{1\le l\le d}\min\limits_{t\in[0,T]}\min\limits_{z\in[0,1]} \phi_l(t,z) \ge \phi_{\min}$ *with* $\phi_{d-1} = 1 - \sum\limits_{l\in\mathfrak{L}} \phi_l$.

The proof of this theorem is given in Section 5, and consists out of the following three steps.

Step 1.
First, we assume conditions (I), (II), and (III) to hold. We discretise the continuous-time system in time with a regular grid of step size Δt, and apply a specific Euler scheme. This is the so-called Rothe method, see [18, 29]. Our chosen discretization is such that the equations become linear elliptic equations with respect to evaluation at time slice $\{t = t_k\}$ and only contain evaluations at time slices $\{t = t_k\}$ and $\{t = t_{k-1}\}$. The time derivative $\partial_t u$ is replaced with the standard first order finite difference $\mathcal{D}^k_{\Delta t}(u) := (u^k - u^{k-1})/\Delta t$,

where we use the notation $u^k(z) := u(t_k, z)$. The discretised system has the form

$$\mathcal{D}^k_{\Delta t}(\phi_l) - \delta_l \partial_z^2 \phi_l^k + I_l(\phi^{k-1})\partial_z\left(\Gamma(\phi^{k-1})v^{k-1}\right) \tag{8a}$$
$$+\sum_{m\in\mathfrak{M}}\sum_{i=0}^{1}\partial_z^i\left(B_{li0m}(\phi^{k-1})w_m^{k-1} + B_{li1m}(\phi^{k-1})\mathcal{D}^k_{\Delta t}(w_m)\right) = G_{\phi,l}(\phi^{k-1}),$$

$$\sum_{m\in\mathfrak{M}}\partial_z\left(H_{0m}(\phi^{k-1})w_m^{k-1} + H_{1m}(\phi^{k-1})\mathcal{D}^k_{\Delta t}(w_m)\right) \tag{8b}$$
$$+\partial_z\left(\Gamma(\phi^{k-1})v^k\right) = G_v(\phi^{k-1}),$$

$$\mathcal{D}^k_{\Delta t}(w_m) - D_m\partial_z^2 w_m^k - \gamma_m\partial_z^2\mathcal{D}^k_{\Delta t}(w_m) + F_m(\phi^{k-1})v^{k-1} \tag{8c}$$
$$+\sum_{j\in\mathfrak{M}}\sum_{i=0}^{1}\partial_z\left(E_{mi0j}(\phi^{k-1})\partial_z^i w_j^{k-1} + E_{m01j}(\phi^{k-1})\mathcal{D}^k_{\Delta t}(w_j)\right) = G_{w,m}(\phi^{k-1}),$$

with initial conditions Equation (5) and boundary conditions (3), (4a), and (4b) become:

$$\begin{cases} \partial_z\phi_l^k\Big|_{z=0} &= 0, \\ \partial_z\phi_l^k\Big|_{z=1} &= 0, \end{cases} \tag{9a}$$

$$\begin{cases} H_{1m}(\phi^{k-1}|_{z=0})\mathcal{D}^k_{\Delta t}(w_m)\Big|_{z=0} = \hat{J}_m\mathcal{L}\left(\phi_{m,res} - \phi_m^{k-1}\big|_{z=0}\right) \\ \partial_z w_m^k\Big|_{z=1} = A_m\left(w_m^k\big|_{z=1} - W^k\right) \\ v^k\Big|_{z=0} = 0 \\ \Gamma\left(\phi^{k-1}|_{z=1}\right)\left(\mathcal{D}^k_{\Delta t}(W) - v^{k-1}\right)\Big|_{z=1} = \hat{J}_d\mathcal{L}\left(\phi_{d,res} - \phi_d^{k-1}\big|_{z=1}\right), \end{cases} \tag{9b}$$

for $l \in \mathfrak{L}$ and $m \in \mathfrak{M}$, with the notation $W^k := W(t_k)$.
For convenience, we refer to the discretised system (8a)-(8c), (9a), and (9b) as the *discrete-time system.*
A powerful property of this discrete-time system is its sequential solvability at time t_k: the existence of a natural hierarchy in attacking this problem. First, we obtain results for Equation (8c), then we use these results to obtain results for both Equations (8a) and (8b). Moreover, the structure of the discrete-time system is that of an elliptic system. Hence, the general existence and uniqueness theory for elliptic systems can be extended directly to cover our situation. One can either apply standard results from ordinary differential equations (ODEs), cf. [26, p.130], or from elliptic theory, cf. Chapter 6 in [13], since the discrete-time system at each time slice $\{t = t_k\}$ can be put into the form $A(u^k, v^k) = F^{k-1}v^k$ with A a continuous coercive bilinear form and F^{k-1} a continuous operator depending on the previous time slice $\{t = t_{k-1}\}$ allowing Lax-Milgram to be applied. We take the elliptic theory option.

Step 2.
We prove Theorem 2, the discretized version of Theorem 1, in Section 4 by testing the time-discrete system with specific test functions such that we obtain quadratic inequalities by using conditions (I), (II) and (III). By application of Young's inequality and using Gronwall-like lemmas we obtain energy-like estimates, which are step size Δt-independent upper bounds of the Sobolev norms of the weak solutions. These bounds allow for weakly convergent sequences in Δt small parameter. Moreover, the upper bounds of the energy-like estimates are monotonically increasing functions of T and V, the parameters used in

(I), (II) and (III). With these upper bounds, we test whether or not the conditions (I), (II) and (III) can be satisfied: the consistency check of our assumption. This leads to the conditions of Assumption 1 to guarantee overlapping regions in (T, V)-space for which Theorem 2 holds for Δt small enough, including the conditions (I), (II) and (III). Since $T > 0$ and $V > 0$ only have to exist, it is sufficient to find a non-empty intersection of all the overlapping regions.

Theorem 2.
Let $d \in \{2, 3, 4\}$ and let the parameters satisfy Assumption 1, then there exist $T > 0$, $V > 0$, $\hat{\tau} > 0$ and $\mathcal{C} > 0$ independent of Δt such that for all $0 < \Delta t < \hat{\tau}$ there exists a sequence of functions $(\phi_1^k, \ldots, \phi_{d-2}^k, \phi_d^k, v^k, w_1^k, \ldots, w_{d-1}^k, W^k)$ for $0 \le t_k \le T$ satisfying the weak version of the discrete-time system given by Equations (8a)-(8c), (9a), (9b), and (5) as well as the following a priori bounds

$$\begin{aligned}
\sum_{j=0}^{k} \left\| \partial_z v^j \right\|_{L^2(0,1)}^2 \Delta t, \sum_{j=0}^{k} \left\| v^j \right\|_{L^2(0,1)}^2 \Delta t &\le V^2, \\
\min_{1 \le l \le d} \min_{z \in [0,1]} \phi_l^k(z) &\ge \phi_{\min}, \\
\left\| \phi_1^k \right\|_{H^1(0,1)}, \ldots, \left\| \phi_d^k \right\|_{H^1(0,1)} &\le \mathcal{C}, \\
\sum_{j=1}^{k} \left\| \phi_1^j \right\|_{H^2(0,1)}^2 \Delta t, \ldots, \sum_{j=1}^{k} \left\| \phi_d^j \right\|_{H^2(0,1)}^2 \Delta t &\le \mathcal{C}, \\
\sum_{j=1}^{k} \left\| \mathcal{D}_{\Delta t}^k(\phi_1^j) \right\|_{L^2(0,1)}^2 \Delta t, \ldots, \sum_{j=1}^{k} \left\| \mathcal{D}_{\Delta t}^k(\phi_d^j) \right\|_{L^2(0,1)}^2 \Delta t &\le \mathcal{C}, \\
\left\| w_1^k \right\|_{H^2}, \ldots, \left\| w_{d-1}^k \right\|_{H^2(0,1)} &\le \mathcal{C}, \\
\sum_{j=1}^{k} \left\| \mathcal{D}_{\Delta t}^k(w_1^j) \right\|_{H^1(0,1)}^2 \Delta t, \ldots, \sum_{j=1}^{k} \left\| \mathcal{D}_{\Delta t}^k(w_{d-1}^j) \right\|_{H^1(0,1)}^2 \Delta t &\le \mathcal{C}, \\
\left| W^k \right|, \sum_{j=1}^{k} \left| \mathcal{D}_{\Delta t}^k(W) \right|^2 \Delta t &\le \mathcal{C},
\end{aligned}$$

for all $0 \le t_k \le T$, where $\phi_{d-1}^k = 1 - \sum_{l \in \mathfrak{L}} \phi_l^k$.

Step 3.
We introduce temporal interpolation functions $\hat{u}(t) = u^{k-1} + (t - t_{k-1})\mathcal{D}_{\Delta t}^k(u)$ on $[t_0, T] \times [0, 1]$. Then we use Theorem 2 to show that the interpolation functions are measurable, bounded and converge weakly. With the Lions-Aubin-Simon lemma, see [8, 10], in combination with the Rellich-Kondrachov theorem, see [2, p.143] and [6], we show strong convergence as well. The proof concludes by showing that the weak solution of the time-discrete system converges to a weak solution of the continuous-time system.

4 Proof of Theorem 2

The proof of Theorem 2 is done in three steps. First, energy bounds are obtained by assuming there exist $\phi_{\min} > 0$, $V > 0$ and $T > 0$ for which the three inequalities of Theorem 2 hold.* Second, we apply two discrete variants of Gronwall's inequality to the quadratic inequalities to obtain a-priori estimates independent of Δt. Lastly, we show that $\phi_{\min} > 0$, $V > 0$ and $T > 0$ can be chosen if Assumption 1 is satisfied by the parameters of the continuous-time system.

Before we can do these three steps, we must show that the discrete-time system is well-posed. We do this iteratively in k, such that the solution of time slice t_{k-1} implies the well-posedness of the solution of time slice k. Since the initial conditions (5) are smooth and v^0 follows from a second order system, we obtain the well-posedness for all $t_k \in [0, T]$. In more detail see Appendix A.

We obtain the weak form of the discrete-in-time system by multiplying the model equations with a function in $H^1(0,1)$, integrating over $(0,1)$ and applying the boundary conditions where needed. We test Equation (8a) with ϕ_l^k and $\mathcal{D}_{\Delta t}^k(\phi_l)$, and Equation (8c) with w_m^k and $\mathcal{D}_{\Delta t}^k(w_m)$ to obtain the quadratic inequalities below:

$$
\begin{aligned}
&\mathcal{D}_{\Delta t}^k\left(\sum_{m\in\mathfrak{M}} \|w_m\|_{L^2}^2 + a_{1m}\|\partial_z w_m\|_{L^2}^2\right) \\
&\qquad\qquad + \sum_{m\in\mathfrak{M}} \left[a_{2m}(\Delta t)\left\|\mathcal{D}_{\Delta t}^k(w_m)\right\|_{L^2}^2 + a_{3m}(\Delta t)\left\|\mathcal{D}_{\Delta t}^k\left(\partial_z w_m\right)\right\|_{L^2}^2\right] \\
&\qquad \le a_4 + \sum_{m\in\mathfrak{M}} \Bigg[a_{5m}\|w_m^k\|_{L^2}^2 + a_{6m}\|\partial_z w_m^k\|_{L^2}^2 + a_{7m}\|w_m^{k-1}\|_{L^2}^2 + a_{8m}\|\partial_z w_m^{k-1}\|_{L^2}^2 \\
&\qquad + a_{9m}\left\|\mathcal{D}_{\Delta t}^k(w_m)\right\|_{L^2}^2 + a_{10m}\left\|\mathcal{D}_{\Delta t}^k(\partial_z w_m)\right\|_{L^2}^2\Bigg] + a_{11}\|v^{k-1}\|_{L^2}^2 + a_{12}\|\partial_z v^{k-1}\|_{L^2}^2, \quad (11)
\end{aligned}
$$

*We would like to point out that for a given time T, which is not defined as the size of the temporal domain for which (I), (II), and (III) in Theorem 1 hold, the common procedure for applying the Rothe method is the procedure as followed in [9], since one can choose sequences Δt decreasing to 0 such that $T/\Delta t$ is an integer. However, in our case we cannot a-priori claim that $T \geq \Delta t$ is satisfied or that $T/\Delta t$ is an integer. We shows that there is a delicate relation between T, V and Δt and that a $T > \Delta t$ and $V > 0$, both independent of Δt, for sufficiently small Δt can be chosen from a connected set of (T, V) points for which (I) and (II) hold for all sufficiently small Δt, especially for sequences Δt such that $T/\Delta t$ is an increasing integer. Moreover, one can even choose (T, V)-points independent of Δt such that (I), (II), and (III) in Theorem 1 hold for all Δt sufficiently small and $T/\Delta t$ an increasing sequence of integers.

for all $l \in \mathfrak{L}$

$$\mathcal{D}^k_{\Delta t}\left(\|\phi_l\|^2_{L^2}\right) + b_{1l}\|\partial_z\phi^k_l\|^2_{L^2} + b_{2l}\,(\Delta t)\left\|\mathcal{D}^k_{\Delta t}(\phi_l)\right\|^2_{L^2} \le b_{3l} + b_{4l}\|\partial_z v^{k-1}\|^2_{L^2} + b_{5l}\|\phi^k_l\|^2_{L^2} + \sum_{n\in\mathfrak{L}}\left[b_{6ln}\|\partial_z\phi^{k-1}_n\|^2_{L^2}\right] + \sum_{m\in\mathfrak{M}}\sum_{i=0}^{1}\left[b_{7lim}\left\|\partial^i_z w^{k-1}_m\right\|^2_{L^2} + b_{8lim}\left\|\mathcal{D}^k_{\Delta t}(\partial^i_z w_m)\right\|^2_{L^2}\right], \quad (12)$$

and

$$\mathcal{D}^k_{\Delta t}\left(\sum_{l\in\mathfrak{L}}\|\partial_z\phi_l\|^2_{L^2}\right) + \sum_{l\in\mathfrak{L}}\left[c_{1l}\left\|\mathcal{D}^k_{\Delta t}(\phi_l)\right\|^2_{L^2} + c_{2l}(\Delta t)\left\|\mathcal{D}^k_{\Delta t}\left(\partial_z\phi_l\right)\right\|^2_{L^2}\right] \le c_3 + c_4\|\partial_z v^{k-1}\|^2_{L^2} + \sum_{l\in\mathfrak{L}}\left[c_{5l}\left\|\mathcal{D}^k_{\Delta t}(\phi_l)\right\|^2_{L^2} + c^k_{6l}\|\partial_z\phi^{k-1}_l\|^2_{L^2}\right] + \sum_{m\in\mathfrak{M}}\sum_{i=0}^{1}\left[c_{7im}\left\|\partial^i_z w^{k-1}_m\right\|^2_{L^2} + c_{8im}\left\|\mathcal{D}^k_{\Delta t}(\partial^i_z w_m)\right\|^2_{L^2}\right]. \quad (13)$$

For details of the derivation of these quadratic inequalities and the exact definition of the 'a', 'b', and 'c'-coefficients, see Appendix B.
For coercivity, which is needed to obtain bounds on $\|\mathcal{D}^k_{\Delta t}(w_m)||_{H^1}$ and $\|\mathcal{D}^k_{\Delta t}(\phi_l)||_{L^2}$, we need the conditions $a_{2m}(0) - a_{9m} > 0$, $a_{3m}(0) - a_{10m} > 0$ and $c_{1l} - c_{5l} > 0$. It follows that these conditions can be satisfied by choosing the right values for the free parameters η_x if conditions (viii) and (ix) of Assumption 1 are satisfied, which is only possible if conditions (i), (ii) and (iii) of Assumption 1 are satisfied.

Before we make use of the quadratic inequalities (11), (12), and (13), we introduce two versions of the discrete Gronwall lemma, see [12] and Theorem 4 in [17], which we modified slightly by using the inequalities $1/(1-a) \le e^{a+a^2} \le e^{1.6838a}$ for $0 \le a \le 0.6838$, and $1 + a \le e^a \le 1 + ae^a$ for $a \ge 0$.

Lemma 1 (1st Discrete Gronwall lemma)**.**
Suppose $h \in (0, H)$. Let (x^k), (y^{k+1}) and (z^k) for $k = 0, 1, \ldots$ be sequences in $\mathbf{R}_+$ satisfying

$$y^k + \frac{x^k - x^{k-1}}{h} \le A + z^{k-1} + Bx^k + Cx^{k-1} \quad \textit{and} \quad \sum_{j=0}^{k-1} z^j h \le Z \quad (14)$$

for all $k = 1, \ldots$ with constants A,B,C and Z independent of h satisfying

$$A > 0, \quad Z > 0, \quad B + C > 0, \quad \textit{and} \quad BH \le 0.6838,$$

then

$$x^k \le \left(x^0 + Z + 1.6838Akh\right)e^{(C+1.6838B)kh} \quad \textit{and}$$

$$\sum_{j=1}^{k} y^j h \le \left(x^0 + Z + Ahk\right)e^{(C+1.6838B)kh}.$$

Proof. We multiply Equation (14) with h and rewrite it to

$$(1-Bh)x^k \le y^k h + (1-Bh)x^k \le Ah + z^{k-1}h + \frac{1+Ch}{1-Bh}(1-Bh)x^{k-1},$$

leading to the inequality below by making use of the partial geometric sum identity.

$$(1-Bh)x^k \le (1-Bh)\left(\frac{1+Ch}{1-Bh}\right)^k \left[\frac{A}{B+C} + \frac{Z}{1+Ch} + x^0\right] - (1-Bh)\frac{A}{B+C}$$

With $1+a \le e^a$ for $a \ge 0$ and $1/(1-a) \le e^{a+a^2} \le e^{1.6838a}$ for $0 \le a \le 0.6838$, we obtain $(1+Ch)/(1-Bh) \le \exp(Ch+Bh+B^2h^2) \le \exp(Ch+1.6838Bh)$, since $0 \le Bh < BH \le 0.6838$. Together with $e^a - 1 \le ae^a$ for $a \ge 0$, we see

$$x^k \le \left[A\frac{C+1.6838B}{C+B}kh + Z + x^0\right] e^{(C+1.6838B)kh}.$$

Multiplying Equation (14) with h and summing over k, we obtain

$$\sum_{j=1}^{k} y^j h \le \sum_{j=1}^{k} y^j h + (1-Bh)x^k \le Akh + Z + x^0 + (C+B)h\sum_{j=0}^{k-1} x^j,$$

which with our newly obtained identity for x^k and the partial geometric sum identity yields

$$\sum_{j=1}^{k} y^j h \le \left[Akh + Z + x^0\right] e^{(C+1.6838B)kh},$$

which concludes the proof. □

Lemma 2 (2nd Discrete Gronwall lemma)**.**
Let $c > 0$ and (y_k), (g_k) be sequences of positive numbers satisfying

$$y_k \le c + \sum_{0 \le j < k} g_j y_j \quad \text{for } k \ge 0,$$

then

$$y_k \le c \exp\left(\sum_{0 \le j < k} g_j\right) \quad \text{for } k \ge 0.$$

We are now able to apply Lemma 1 and Lemma 2 to the quadratic inequalities (11), (12), and (13). The result:

Lemma 3.
Let $\Delta t \in (0, H)$ with

$$H \le \min\left\{\frac{0.6838}{\max\limits_{m \in \mathfrak{M}}\left\{a_{5m}, \frac{a_{6m}}{a_{1m}}\right\}}, \frac{0.6838}{\min\limits_{l \in \mathfrak{L}}\{b_{5l}\}}\right\}.$$

There exist positive constants $\tilde{a}_{index}$, $\tilde{d}_{index}$, $\tilde{e}_{index}$ and parameter functions $a(T,V)$, $d_0(T,V)$, $d_1(T,V)$, $d_2(T,V)$, $e_1(T,V)$, and $e_2(T,V)$ such that for all $l \in \mathfrak{L}$, for all $m \in \mathfrak{M}$, and for all $t_k \in [0,T]$ the following estimates hold:

$$\|\phi_l^k\|_{L^2}^2 \leq \big(\phi_{l0}^2 + e_{2l}(T,V) + e_{1l}(T,V)T\big)e^{1.6838 b_{5l} T},$$

$$\frac{1}{d-1}\|\partial_z \phi_{d-1}^k\|_{L^2}^2 \leq \sum_{l\in\mathfrak{L}} \|\partial_z \phi_l^k\|_{L^2}^2 \leq d_1(T,V)e^{d_2(T,V)},$$

$$\frac{1}{d-1}\|\phi_{d-1}^k - \phi_{d-1,0}\|_{L^2}^2 \leq T\frac{d_1(T,V)\left(1 + d_2(T,V)e^{d_2(T,V)}\right)}{\min\limits_{l\in\mathfrak{L}}\{c_{1l} - c_{5l}\}},$$

$$\sum_{j=1}^{k}\sum_{l\in\mathfrak{L}}(c_{1l} - c_{5l})\left\|\mathcal{D}_{\Delta t}^j(\phi_l)\right\|_{L^2}^2 \Delta t \leq d_1(T,V)\left(1 + d_2(T,V)e^{d_2(T,V)}\right),$$

$$\sum_{m\in\mathfrak{M}} \|w_m^k\|_{L^2}^2 \leq d_0(T,V),$$

$$\sum_{m\in\mathfrak{M}} a_{1m}\|\partial_z w_m^k\|_{L^2}^2 \leq d_0(T,V),$$

$$\sum_{j=1}^{k}\sum_{m\in\mathfrak{M}}(a_{2m}(0) - a_{9m})\left\|\mathcal{D}_{\Delta t}^j(w_m)\right\|_{L^2}^2 \Delta t \leq d_0(T,V),$$

$$\sum_{j=1}^{k}\sum_{m\in\mathfrak{M}}(a_{3m}(0) - a_{10m})\left\|\mathcal{D}_{\Delta t}^j(\partial_z w_m)\right\|_{L^2}^2 \Delta t \leq d_0(T,V),$$

$$\sum_{j=1}^{k}\left|\mathcal{D}_{\Delta t}^j(W)\right|^2 \Delta t \leq 2V^2 + \frac{2\hat{J}_d^2\phi_{d,res}^2}{\Gamma_{\phi_{\min}}^2}T,$$

$$|W^k|^2 \leq \left(|W^0| + \frac{\hat{J}_d\phi_{d,res}}{\Gamma_{\phi_{\min}}}T + V\sqrt{T}\right)^2$$

with

$$\begin{aligned}
d_0(T,V) &= \left((a_{11} + a_{12})V^2 + 1.6838 a_4 T\right)e^{\tilde{d}_{01}T},\\
d_1(T,V) &= c_3 T + c_4 V^2 + (\tilde{d}_{11} + \tilde{d}_{12}T)d_0(T,V),\\
d_2(T,V) &= \sum_{l\in\mathfrak{L}} c_{6l1}V^2 + (\tilde{d}_{21} + \tilde{d}_{22}T)d_0(T,V),\\
e_{1l}(T,V) &= b_{3l} + \min_{n\in\mathfrak{L}}\{b_{6ln}\}d_1(T,V)e^{d_2(T,V)} + \tilde{e}_{11}d_0(T,V),\\
e_{2l}(T,V) &= b_{4l}V^2 + \tilde{e}_{21}d_0(T,V).
\end{aligned}$$

and with

$$\begin{aligned}
\tilde{d}_{01} &= \max_{m\in\mathfrak{M}}\left\{a_{7m}, \frac{a_{8m}}{a_{1m}}\right\} + 1.6838\max_{m\in\mathfrak{M}}\left\{a_{5m}, \frac{a_{6m}}{a_{1m}}\right\}\\
\tilde{d}_{11} &= \max_{m\in\mathfrak{M}}\left\{\frac{c_{80m}}{a_{2m}(0) - a_{9m}} + \frac{c_{81m}}{a_{3m}(0) - a_{10m}}\right\}
\end{aligned}$$

$$\begin{aligned}
\tilde{d}_{12} &= \max_{m\in\mathfrak{M}}\left\{c_{70m}+\frac{c_{71m}}{a_{1m}}\right\}\\
\tilde{d}_{21} &= \max_{m\in\mathfrak{M}}\left\{\frac{\sum_{l\in\mathfrak{L}}c_{6l3m}}{a_{2m}(0)-a_{9m}}+\frac{\sum_{l\in\mathfrak{L}}c_{6l3m}}{a_{3m}(0)-a_{10m}}\right\}\\
\tilde{d}_{22} &= \max_{m\in\mathfrak{M}}\left\{\sum_{l\in\mathfrak{L}}c_{6l2m}\left(1+\frac{1}{a_{1m}}\right)\right\}\\
\tilde{e}_{11} &= \max_{m\in\mathfrak{M}}\left\{b_{7l0m}+\frac{b_{7l1m}}{a_{1m}}\right\}\\
\tilde{e}_{21} &= \max_{m\in\mathfrak{M}}\left\{\frac{b_{8l0m}}{a_{2m}(0)-a_{9m}}+\frac{b_{8l1m}}{a_{3m}(0)-a_{10m}}\right\}
\end{aligned}$$

Proof.
The conditions $c_{5l} < c_{1l}$, $a_{9m} < a_{2m}(0)$ and $a_{10m} < a_{3m}(0)$ are satisfied due to conditions (i), (viii) and (ix) of Assumption 1, respectively. Apply Lemma 1 to Equation (11) in order to obtain all four w^k bounds.
For the bounds of ϕ^k_{d-1}, we use $\sum_{l=1}^{d}\phi^k_l = 1$ in two ways. First, we apply ∂_z to this identity and use $|x|_1^2 \leq n|x|_2^2$ for $x \in \mathbf{R}^n$ to obtain the upper bound $\sum_{l\in\mathfrak{L}}\|\partial_z\phi^k_l\|^2_{L^2}$. Second, we subtract the same identity at time-slice $t = 0$ to obtain an upper bound in $\sum_{l\in\mathfrak{L}}(\phi^k_l - \phi_{l,0})$ and, then, apply again $|x|_1^2 \leq n|x|_2^2$ for $x \in \mathbf{R}^n$ using the telescoping series for k to obtain the upper bound $k\Delta t\sum_{j=1}^{k}\sum_{l\in\mathfrak{L}}\|\mathcal{D}^k_{\Delta t}(\phi_{d-1})\|^2_{L^2}\Delta t$.
All the ϕ-bounds now follow from applying Lemma 1 to Equation (12) and Lemma 2 to Equation (13) and inserting the newly obtained w^k bounds.
The use of the Gronwall inequalities are only allowed for Δt small enough, as given by the conditions for H in Lemma 1. □

Remark: The a priori estimates in Lemma 3 depend on $T > 0$ and $V > 0$. We need to prove that $T > 0$ and $V > 0$ can be chosen for $\Delta t > 0$ small enough. On closer inspection, we see that we can work with upper bounds only.

Lemma 4.
Let $0 \leq t_k = k\Delta t \leq T$. *Let* $\mathbf{P}_d$ *be the set of cyclic permutations of* $(1, \ldots, d)$. *The constraints* $\phi^k_l(z) \in [\phi_{\min}, 1-(d-1)\phi_{\min}]$ *for* $1 \leq l \leq d$, $\sum_{j=0}^{k}\|v^j\|^2_{L^2}\Delta t \leq V^2$, *and* $\sum_{j=0}^{k}\|\partial_z v^j\|^2_{L^2}\Delta t \leq V^2$ *are implied by*

$$\sum_{j\in\mathfrak{M}}\left\|\phi^k_{\alpha_j}\right\|_{H^1} \leq \frac{1-\phi_{\min}}{C_{1,0}} \text{ for all } \alpha \in \mathbf{P}_d \quad \text{and} \quad \sum_{j=0}^{k}\left\|\partial_z v^j\right\|^2_{L^2}\Delta t \leq V^2,$$

with $C_{1,0}$ *given by (ii) from Section 3.*

Proof.
The boundary condition (9b) allows the application of the Poincaré inequality to v^k, which gives the bound $\|v^j\|_{L^2} \leq \|\partial_z v^j\|_{L^2}$.
For the constraints on ϕ^k_l we pick arbitrarily an $\alpha \in \mathbf{P}_d$ and start with the inequality

$\sum_{j\in\mathfrak{M}} \left\|\phi^k_{\alpha_j}\right\|_{H^1} \le (1-\phi_{\min})/C_{1,0}$. This inequality is transformed by the Sobolev embedding theorem on $[0,1]$ into $\sum_{j\in\mathfrak{M}} \left\|\phi^k_{\alpha_j}\right\|_{C^0} \le 1-\phi_{\min}$. Hence, we obtain $\inf_{z\in(0,1)} \phi^k_{\alpha_d} \ge \phi_{\min}$ from the volume fraction identity $1 = \sum_{1\le l\le d} \phi^k_l$. Since α was chosen arbitrarily, we conclude that this result holds for all $\alpha \in \mathbf{P}_d$. Hence, $\min\limits_{1\le l\le d} \inf\limits_{z\in(0,1)} \phi^k_l(z) \ge \phi_{\min}$. With the d infima established it yields that the d suprema follow automatically from the same volume fraction identity. □

We prove the simultaneous validity of the two inequalities of Lemma 4 with elementary arguments based on the Intermediate Value Theorem (IVT) for the continuous functions given as upper bounds in the inequalities of Lemma 3 having parameters T, V as variables.

Lemma 5.
Let $2 \le d \le C_{1,0}/(C_{1,0}-1) \approx 4.194528$, $0 < \phi_{\min} \le 1 - C_{1,0}(d-1)/d$ and let $\phi^0 = (\phi_{10},\dots,\phi_{d0}) \in \Phi_d(\phi_{\min},(1-\phi_{\min})/C_{1,0})$, where the set $\Phi_d(s,r)$ is defined as the non-empty set of points $(x_1,\dots,x_d) \in \mathbf{R}^d$ satisfying

$$\begin{cases} \sum\limits_{j\ne i} x_j < r & \text{for all } 1 \le i \le d, \\ x_i \ge s & \text{for all } 1 \le i \le d, \\ \sum\limits_{i=1}^{d} x_i = 1. \end{cases}$$

Then there exist an open simply connected region $S \subset \mathbf{R}^2$ containing $(0,0)$ such that

$$(T,V) \in S \Rightarrow P_\alpha(T,V) < \frac{1-\phi_{\min}}{C_{1,0}} \text{ for all } \alpha \in \mathbf{P}_d,$$
$$(T,V) \in \partial S \Rightarrow P_\alpha(T,V) \le \frac{1-\phi_{\min}}{C_{1,0}} \text{ for all } \alpha \in \mathbf{P}_d,$$
$$(T,V) \notin \overline{S} \Rightarrow P_\alpha(T,V) > \frac{1-\phi_{\min}}{C_{1,0}} \text{ for at least one } \alpha \in \mathbf{P}_d,$$

where $P_\alpha(T,V)$ denotes the upper bound of $\sum_{j\in\mathfrak{M}} \|\phi^k_{\alpha_j}\|_{H^1}$ obtained from the a-priori estimates of Lemma 3.

Proof.
First, we note that the set $\Phi_d(\phi_{\min},(1-\phi_{\min})/C_{1,0})$ is non-empty if the following inequalities are satisfied

$$0 < (d-1)\phi_{\min} \le \frac{d-1}{d} < \frac{1-\phi_{\min}}{C_{1,0}}.$$

This is because $(d-1)\phi_{\min}$ and $(d-1)/d$ are the minimal and the maximal value of the sum $\sum_{j\in\mathfrak{M}} x_{\alpha_j}$ over all $\alpha \in \mathbf{P}_d$ when minimizing for each $\alpha \in \mathbf{P}_d$ over all $(x_1,\dots,x_d)$ satisfying $\min_{1\le i\le d} x_i \ge \phi_{\min}$ and $\sum_{i=1}^d x_i = 1$. Hence, we obtain the inequalities

$$0 < \phi_{\min} < 1 - C_{1,0}\frac{d-1}{d} \le \frac{1}{d}$$

for $2 \le d < C_{1,0}/(C_{1,0}-1) \approx 4.194528$ integer.
Second, from Lemma 3, $P_\alpha(T,V)$ are monotonic increasing continuous functions with respect to the product ordering on $\mathbf{R}_+^2$ for all $\alpha \in \mathbf{P}_d$. Therefore, there exists a simply connected open set S_α such that $P_\alpha(T,V) < (1-\phi_{\min})/C_{1,0}$ for all $(T,V) \in S_\alpha$. Moreover, from Lemma 3 we deduce that $P_\alpha(0,0) = \sum_{j\in\mathfrak{M}} \phi_{\alpha_j 0} < (1-\phi_{\min})/C_{1,0}$ for all $\alpha \in \mathbf{P}_d$, which implies $(0,0) \in S_\alpha$ for all $\alpha \in \mathbf{P}_d$. Thus $S = \bigcap_{\alpha\in\mathbf{P}_d} S_\alpha$ is non-empty and satisfies all the desired inequalities. □

Lemma 6.
There exist a $\tau > 0$ such that for all $0 < \Delta t < \tau$ there exists an open simply connected region $\mathcal{R}_{\Delta t} \subset \mathbf{R}^2$ with the properties

$$\begin{aligned}(T,V) \in \mathcal{R}_{\Delta t} &\Rightarrow Q_{\Delta t}(T,V) < V^2,\\ (T,V) \in \partial\mathcal{R}_{\Delta t} &\Rightarrow Q_{\Delta t}(T,V) = V^2,\\ (T,V) \notin \overline{\mathcal{R}_{\Delta t}} &\Rightarrow Q_{\Delta t}(T,V) > V^2,\end{aligned}$$

where $Q_{\Delta t}(T,V)$ denotes the upper bound of $\sum_{t_k\in[0,T]} \|\partial_z v^k\|_{L^2}^2 \Delta t$ obtained from applying the a-priori estimates of Lemma 3 to Equation (8b) and is given by

$$\begin{aligned}Q_{\Delta t}(T,V) = \tilde{Q}_0\Delta t + \tilde{Q}_1 T + (\tilde{Q}_2 + \tilde{Q}_3 T)d_0(T,V)&\\ + [\tilde{Q}_4(T)T + (\tilde{Q}_5 + \tilde{Q}_6 T)d_0(T,V)]d_1(T,V)e^{d_2(T,V)}&\end{aligned}$$

with $\tilde{Q}_0, \tilde{Q}_1, \tilde{Q}_2, \tilde{Q}_3, \tilde{Q}_4, \tilde{Q}_5, \tilde{Q}_6 > 0$, if

$$1 > Q_1 := \tilde{Q}_2(a_{11}+a_{12}) = \frac{7d-5}{\Gamma_{\phi_{\min}}^2} \max_{m\in\mathfrak{M}} \left\{ \frac{H_{1m}^2}{a_{3m}(0) - a_{10m}} \right\} (a_{11}+a_{12}).$$

Moreover, the limit $\lim\limits_{\Delta t\downarrow 0} \mathcal{R}_{\Delta t}$ exists and is denoted by $\mathcal{R}_0$.

Proof.
We assume that $\|\partial_z v^0\|_{L^2}^2 \Delta t \le V^2$ holds for a not yet determined value of $V > 0$. By induction we will prove $\sum_{j=0}^k \|\partial_z v^j\|_{L^2}^2 \Delta t \le V^2$ for the same value $V > 0$. By our assumption this identity holds for $k = 0$.
Note, for all $\Delta t \le T$ we can choose any K such that $K\Delta t \in [0,T]$. Thus, there are sequences of Δt decreasing to 0 such that $T/\Delta t$ equals an integer for all Δt in these sequences. Hence, the induction is valid for all $k\Delta t = t_k \in [0,T]$ when $0 < \Delta t < \tau$, where τ has to be determined at a later stage. Remark, for $\Delta t > T$ we have $\sum_{t_k\in[0,T]} \|\partial_z v^k\|_{L^2}^2 \Delta t = \|\partial_z v^0\|_{L^2}^2 \Delta t \le V^2$ by assumption. In this case, the induction ends immediately at $k = 0$, which is a reflection of the fact that the Δt-sized temporal discretization is too coarse and smaller Δt should be chosen.
Thus for our induction step, we take $0 < k = K \le T/\Delta t$ for the case $\Delta t < T$ (a-priori assumed to be valid, since T is not yet determined, but only defined.).
We integrate (8b) from 0 to z. This yields:

$$\left[\Gamma(\phi^{k-1})v^k\right]_0^z = \int_0^z G_v(\phi^{k-1})\mathrm{d}z - \left[\sum_{m\in\mathfrak{M}} \left(H_{0m}(\phi^{k-1})w_m^{k-1} + H_{1m}(\phi^{k-1})\mathcal{D}_{\Delta t}^k(w_m)\right)\right]_0^z.$$

Inserting the boundary conditions (9b) and using $w_m^0 = 0$ gives:

$$\Gamma(\phi^{k-1})v^k = \int_0^z G_v(\phi^{k-1})\mathrm{d}z - \sum_{m\in\mathfrak{M}} \big(H_{0m}(\phi^{k-1})w_m^{k-1} + H_{1m}(\phi^{k-1})\mathcal{D}_{\Delta t}^k(w_m)\big)$$
$$+ \sum_{m\in\mathfrak{M}} \left(H_{0m}(\phi^{k-1}\big|_{z=0}) \sum_{K=1}^{k-1} \frac{\hat{J}_m \mathcal{L}(\phi_{m,res} - \phi_m^K\big|_{z=0})}{H_{1m}(\phi^K\big|_{z=0})}\Delta t \right.$$
$$\left. + \hat{J}_m \mathcal{L}(\phi_{m,res} - \phi_m^{k-1}\big|_{z=0}) \right).$$

Dividing both sides by $\Gamma(\phi^{k-1})$ and then applying the derivative ∂_z to both sides, leads to the identity

$$\partial_z v^k = -\frac{1}{\Gamma(\phi^{k-1})^2} \left(\sum_{i=1}^{d} \frac{\partial \Gamma_i(\phi_i^{k-1})}{\partial \phi_i^{k-1}} \frac{\partial \phi_i^{k-1}}{\partial z} \prod_{j\neq i} \Gamma_j(\phi_j^{k-1}) \right) \times$$
$$\times \left[\int_0^z G_v(\phi^{k-1})\mathrm{d}z - \sum_{m\in\mathfrak{M}} \big(H_{0m}(\phi^{k-1})w_m^{k-1} + H_{1m}(\phi^{k-1})\mathcal{D}_{\Delta t}^k(w_m)\big) \right.$$
$$+ \sum_{m\in\mathfrak{M}} \left(H_{0m}(\phi^{k-1}\big|_{z=0}) \sum_{K=1}^{k-1} \frac{\hat{J}_m \mathcal{L}(\phi_{m,res} - \phi_m^K\big|_{z=0})}{H_{1m}(\phi^K\big|_{z=0})}\Delta t \right.$$
$$\left.\left. + \hat{J}_m \mathcal{L}(\phi_{m,res} - \phi_m^{k-1}\big|_{z=0}) \right) \right]$$
$$+ \frac{1}{\Gamma(\phi^{k-1})} \left[G_v(\phi^{k-1}) - \sum_{m\in\mathfrak{M}} \big(H_{0m}(\phi^{k-1})\partial_z w_m^{k-1} + H_{1m}(\phi^{k-1})\mathcal{D}_{\Delta t}^k(\partial_z w_m)\big) \right.$$
$$- \sum_{m\in\mathfrak{M}} \left(\sum_{i=1}^{d} \frac{\partial H_{0m,i}(\phi_i^{k-1})}{\partial \phi_i^{k-1}} \frac{\partial \phi_i^{k-1}}{\partial z} \prod_{j\neq i} H_{0m,j}(\phi_j^{k-1}) \right) w_m^{k-1}$$
$$\left. - \sum_{m\in\mathfrak{M}} \left(\sum_{i=1}^{d} \frac{\partial H_{1m,i}(\phi_i^{k-1})}{\partial \phi_i^{k-1}} \frac{\partial \phi_i^{k-1}}{\partial z} \prod_{j\neq i} H_{1m,j}(\phi_j^{k-1}) \right) \mathcal{D}_{\Delta t}^k(w_m) \right].$$

Recalling (2) for $f(\phi^{k-1})$ and the notation $\|f(\cdot)\|_{C^1([0,1])^d} \leq f$, using Minkowski's inequality, Hölder's inequality, the embedding $H^1(0,1) \hookrightarrow L^\infty(0,1)$ with optimal constant $C_{1,0}$, the definition of $\Gamma_{\phi_{\min}}$ and $H_{\phi_{\min}}$,and the inequality $|(x_1,\ldots,x_n)|_1^2 \leq n|(x_1,\ldots,x_n)|_2^2$ for

$(x_1, \ldots, x_n) \in \mathbf{R}^n$, we obtain

$$\|\partial_z v^k\|_{L^2}^2 \leq \frac{d(7d-5)\Gamma^2}{\Gamma_{\phi_{\min}}^4} \sum_{i=1}^{d} \|\partial_z \phi_i^{k-1}\|_{L^2}^2 \times$$
$$\times \left[G_v^2 + C_{1,0}^2 \sum_{m \in \mathfrak{M}} \left(H_{0m}^2 \|w_m^{k-1}\|_{H^1}^2 + H_{1m}^2 \left\|\mathcal{D}_{\Delta t}^k(w_m)\right\|_{H^1}^2 \right) \right.$$
$$\left. + \sum_{m \in \mathfrak{M}} \left(H_{0m} \frac{\hat{J}_m \phi_{m,res}}{H_{\phi_{\min}}} T + \hat{J}_m \phi_{m,res} \right)^2 \right]$$
$$+ \frac{7d-5}{\Gamma_{\phi_{\min}}^2} \left[G_v^2 + \sum_{m \in \mathfrak{M}} \left(H_{0m}^2 \|\partial_z w_m^{k-1}\|_{L^2}^2 + H_{1m}^2 \left\|\mathcal{D}_{\Delta t}^k(\partial_z w_m)\right\|_{L^2}^2 \right) \right.$$
$$+ dC_{1,0}^2 \sum_{m \in \mathfrak{M}} H_{0m}^2 \sum_{i=1}^{d} \|\partial_z \phi_i^{k-1}\|_{L^2}^2 \|w_m^{k-1}\|_{H^1}^2$$
$$\left. + dC_{1,0}^2 \sum_{m \in \mathfrak{M}} H_{1m}^2 \sum_{i=1}^{d} \|\partial_z \phi_i^{k-1}\|_{L^2}^2 \left\|\mathcal{D}_{\Delta t}^k(w_m)\right\|_{H^1}^2 \right].$$

Summing over $k = 1$ to $k = K$ with $K\Delta t \leq T$, multiplying by Δt, and using the inequalities of Lemma 3, we obtain

$$\begin{aligned}
\sum_{k=0}^{K} \|\partial_z v^k\|_{L^2}^2 \Delta t \quad \leq \quad & \|\partial_z v^0\|_{L^2}^2 \Delta t + \frac{7d-5}{\Gamma_{\phi_{\min}}^2} G_v^2 T \\
& + \frac{7d-5}{\Gamma_{\phi_{\min}}^2} \left[\max_{m \in \mathfrak{M}} \left\{ \frac{H_{1m}^2}{a_{3m}(0) - a_{10m}} \right\} + \max_{m \in \mathfrak{M}} \left\{ \frac{H_{0m}^2}{a_{1m}} \right\} T \right] d_0(T,V) \\
& + \frac{d^2(7d-5)}{\Gamma_{\phi_{\min}}^2} \left[\frac{\Gamma^2}{\Gamma_{\phi_{\min}}^2} \left(G_v^2 + \sum_{m \in \mathfrak{M}} \left[H_{0m} \frac{\hat{J}_m \phi_{m,res}}{H_{\phi_{\min}}} T + \hat{J}_m \phi_{m,res} \right]^2 \right) T \right. \\
& \quad + C_{1,0}^2 \left(1 + \frac{\Gamma^2}{\Gamma_{\phi_{\min}}^2} \right) \left(\max_{m \in \mathfrak{M}} \left\{ \frac{H_{1m}^2}{a_{2m}(0) - a_{9m}} + \frac{H_{1m}^2}{a_{3m}(0) - a_{10m}} \right\} \right. \\
& \quad \left. \left. + \max_{m \in \mathfrak{M}} \left\{ H_{0m}^2 + \frac{H_{0m}^2}{a_{1m}} \right\} T \right) d_0(T,V) \right] d_1(T,V) e^{d_2(T,V)} \\
= \quad & Q_{\Delta t}(T,V).
\end{aligned}$$

Hence, we can rewrite $Q_{\Delta t}(T,V)$ as

$$Q_{\Delta t}(T,V) = \tilde{Q}_0 \Delta t + \tilde{Q}_1 T + (\tilde{Q}_2 + \tilde{Q}_3 T) d_0(T,V)$$
$$+ [\tilde{Q}_4(T) T + (\tilde{Q}_5 + \tilde{Q}_6 T) d_0(T,V)] d_1(T,V) e^{d_2(T,V)}.$$

This yields

$$\begin{aligned} Q_{\Delta t}(0,V) &= \tilde{Q}_0\Delta t + \tilde{Q}_2 d_0(0,V) + \tilde{Q}_5 d_0(0,V) d_1(0,V) e^{d_2(0,V)} \\ &= \|\partial_z v^0\|^2_{L^2}\Delta t + \frac{7d-5}{\Gamma^2_{\phi_{\min}}} \max_{m\in\mathfrak{M}} \left\{ \frac{H^2_{1m}}{a_{3m}(0)-a_{10m}} \right\} (a_{11}+a_{12})V^2 \\ &\quad + \frac{d^2(7d-5)C^2_{1,0}}{\Gamma^2_{\phi_{\min}}} \left(1+\frac{\Gamma^2}{\Gamma^2_{\phi_{\min}}}\right) \max_{m\in\mathfrak{M}} \left\{ \frac{H^2_{1m}}{a_{2m}(0)-a_{9m}} + \frac{H^2_{1m}}{a_{3m}(0)-a_{10m}} \right\} \times \\ &\quad \times (a_{11}+a_{12}) \left(c_4 + \tilde{d}_{11}(a_{11}+a_{12})\right) V^4 e^{(\sum_{l\in\mathfrak{L}} c_{6l1} + \tilde{d}_{21}(a_{11}+a_{12}))V^2}. \end{aligned}$$

Hence, we have

$$Q_{\Delta t}(0,V) = Q_0\Delta t + Q_1 V^2 + Q_2 V^4 e^{Q_3 V^2}$$

with

$$Q_1 = \frac{7d-5}{\Gamma^2_{\phi_{\min}}} \max_{m\in\mathfrak{M}} \left\{ \frac{H^2_{1m}}{a_{3m}(0)-a_{10m}} \right\} (a_{11}+a_{12}).$$

If $Q_1 < 1$, then by the Intermediate Value Theorem there is a $V^* \in \left(0, \sqrt[4]{\frac{1-Q_1}{Q_2 Q_3}}\right)$ for all $\Delta t > 0$ such that

$$\left.\frac{\partial Q_{\Delta t}(0,V)}{\partial (V^2)}\right|_{V=V^*} = 1 > Q_1 = \left.\frac{\partial Q_{\Delta t}(0,V)}{\partial (V^2)}\right|_{V=0},$$

because $\partial Q_{\Delta t}(0,V)/\partial(V^2) = Q_1 + Q_2 V^2(2+Q_3V^2)e^{Q_3V^2} \geq Q_1 + Q_2Q_3V^4$.
Immediately we see that $Q_{\Delta t}(0,V^*) < (V^*)^2$ for $0 < \Delta t < \tau$ if we choose

$$\tau = \min\left\{ \frac{1-Q_1}{Q_0}\left(1-\frac{1}{2+Q_3(V^*)^2}\right)(V^*)^2, H \right\},$$

where H denotes the upper bound of $\Delta t > 0$ as found in Lemma 3. Moreover, for $0 < \Delta t < \tau$ we have the inequalities $Q_{\Delta t}(0,0) > 0$, $Q_{\Delta t}(0,V^*) < (V^*)^2$, and $Q_{\Delta t}(0,\tilde{V}) > \tilde{V}^2 = (1-Q_1)/Q_2 > (V^*)^2$ due to $Q_{\Delta t}(0,V) > Q_1V^2 + Q_2V^4$ for $V > 0$. Hence, by the Intermediate Value Theorem, there exist $V_{1,\Delta t} \in (0,V^*)$ and $V_{2,\Delta t} \in (V^*,\tilde{V})$ such that $Q_{\Delta t}(0,V_{1,\Delta t}) = V^2_{1,\Delta t}$ and $Q_{\Delta t}(0,V_{2,\Delta t}) = V^2_{2,\Delta t}$.
We see that $Q_{\Delta t}(T,V)$ is a monotonic increasing continuous function with respect to the product ordering on $\mathbf{R}^2_+$ for $0 < \Delta t < \tau$. Therefore, there exists a simply connected open set $\mathcal{R}_{\Delta t}$ such that $Q_{\Delta t}(T,V) < V^2$ for all $(T,V) \in \mathcal{R}_{\Delta t}$. Thus $\sum_{k=0}^{K} \|\partial_z v^k\|^2_{L^2}\Delta t \leq V^2$ for $(T,V) \in \mathcal{R}_{\Delta t}$
Hence, induction states that $\sum_{t_k\in[0,T]} \|\partial_z v^k\|^2_{L^2}\Delta t \leq V^2$ for $(T,V) \in \mathcal{R}_{\Delta t}$.
Our assumption of $\|\partial_z v^0\|^2_{L^2}\Delta t \leq V^2$ for some $V > 0$ can now be lifted for $\Delta t \leq T$. We have

$$\|\partial_z v^0\|^2_{L^2}\Delta t = Q_0\Delta t \leq Q_{\Delta t}(0,V_{1,\Delta t}) = V^2_{1,\Delta t} \leq V^2 \text{ for all } (0,V) \in \overline{\mathcal{R}_{\Delta t}}$$

and, by monotonicity in T, this inequality holds for all $(T,V) \in \overline{\mathcal{R}_{\Delta t}}$. Do note that τ depends on $Q_0 = \|\partial_z v^0\|^2_{L^2}$. Thus for all $v^0 \in L^2(0,1)$ with $v^0(0) = 0$ there exist a $\tau > 0$

such that our assumption and, therefore, our induction holds if $(T,V) \in \overline{\mathcal{R}_{\Delta t}}$.
Note, the region $\mathcal{R}_{\Delta t}$ contains the cylinder $[0,T) \times (\|\partial_z v^0\|_{L^2}\sqrt{\Delta t}, \infty)$ such that the case $\Delta t > T$ satisfies the assumption $\|\partial_z v^0\|^2_{L^2}\Delta t \le V^2$ and the three domain properties.

$\mathcal{R}_0$, the limit set of $\mathcal{R}_{\Delta t}$, exists because the construction of $\mathcal{R}_{\Delta t}$ is only dependent on Δt when using the Intermediate Value Theorem to guarantee the existence of $V_{1,\Delta t}$ and $V_{2,\Delta t}$, which directly follows from the fact that $Q_{\Delta t}(T,V)$ is a right-continuous monotonic increasing function in $\Delta t \in \mathbf{R}_+$. Moreover, the cylinder $[0,T) \times (\|\partial_z v^0\|_{L^2}\sqrt{\Delta t}, \infty)$ becomes the empty set in the limit $\Delta t = 0$, since this cylinder represents the case $\Delta t > T$ and is, therefore, Δt-thick. Therefore, $\mathcal{R}_0$ can be seen as the limit of the part of the set $\mathcal{R}_{\Delta t}$, where the case $\Delta t > T$ is satisfied. □

Lemma 7.
Let $1 < d \le C_{1,0}/(C_{1,0}-1)$, $0 < \Delta t < \tau$, $0 < \phi_{\min} \le 1 - C_{1,0}(d-1)/d$ and $\phi^0 \in \Phi_d(\phi_{\min}, (1-\phi_{\min})/C_{1,0})$, where the set $\Phi_d(s,r)$ is as defined in Lemma 5 and τ has the value as determined in the proof of Lemma 6. Then there exists a $\tau^* > 0$ such that

$$\{(\Delta t, \infty) \times \mathbf{R}_+\} \cap S \cap \mathcal{R}_{\Delta t} \neq \emptyset \quad \textit{for all } 0 \le \Delta t < \tau^*,$$

where S is the set as defined in Lemma 5 and $\mathcal{R}_{\Delta t}$ is the set as defined in Lemma 6.

Proof.
Due to the monotonicity of both S and $\mathcal{R}_{\Delta t}$ with respect to T, we only have to check for all $\alpha \in \mathbf{P}_d$ that there exists a $V_\alpha > 0$ such that $P_\alpha(0, V_\alpha) < (1-\phi_{\min})/C_{1,0}$. For $T = 0$ and using the equivalence of $\mathbf{R}^n$-norms, we obtain

$$\begin{aligned} P_\alpha(0,V) \;\le\; & \sum_{j\in\mathfrak{M}} \phi_{\alpha_j 0} + \sum_{j\in\mathfrak{M},\alpha_j\neq d-1} \sqrt{b_{4\alpha_j} + \tilde{e}_{21}(a_{11}+a_{12})}V \\ & + e^{\left(\sum_{l\in\mathfrak{L}} c_{6l1} + \tilde{d}_{21}(a_{11}+a_{12})\right)\frac{V^2}{2}} \sqrt{(d-1)(c_4 + \tilde{d}_{11}(a_{11}+a_{12}))}V. \end{aligned}$$

From Lemma 5 and condition (v) in Assumption 1, there exists $\phi^0 \in \Phi_d(\phi_{\min}, (1-\phi_{\min})/C_{1,0})$ such that $\sum_{j\in\mathfrak{M}} \phi_{\alpha_j 0} < (1-\phi_{\min})/C_{1,0}$ for all $\alpha \in \mathbf{P}_d$. Since $P_\alpha(0,V)$ is strictly increasing in V, there exists a $\hat{V}_\alpha > 0$ such that $P_\alpha(0,\hat{V}_\alpha) = (1-\phi_{\min})/C_{1,0}$. Construct $\hat{V} = \min_{\alpha\in\mathbf{P}_d} \hat{V}_\alpha$.
Now we have two cases: either $\hat{V} \ge V_{1,\tau}$ or $0 < \hat{V} < V_{1,\tau}$, where $V_{1,\tau} = \lim_{\Delta t \uparrow \tau} V_{1,\Delta t}$ with $V_{1,\Delta t}$ and τ from the proof of Lemma 6. In the first case, we can introduce $\tau^{**} = \tau$, because $(\{0\} \times (0,\hat{V}]) \cap \overline{\mathcal{R}_\tau} \neq \emptyset$. In the second case, we have $(\{0\} \times (0,\hat{V}]) \cap \overline{\mathcal{R}}_\tau = \emptyset$. Fortunately, $V_{1,\Delta t}$ is a monotonically increasing function of Δt, because $Q_{\Delta t}(T,V)$ is monotonically increasing in Δt for all $(T,V) \in \mathbf{R}^2_+$ and $Q_0(0,0) = 0$. Thus the Intermediate Value Theorem states there exists a $\tau^{**} < \tau$ such that $\hat{V} = V_{1,\tau^{**}}$ and thus $(\{0\} \times (0,\hat{V}]) \cap \overline{\mathcal{R}_{\tau^{**}}} \neq \emptyset$. Hence $S \cap \mathcal{R}_{\Delta t} \neq \emptyset$ for all $0 \le \Delta t < \tau^{**}$. However, $T < \Delta t$ is not allowed, as $k > 0$ integer such that $k\Delta t \le T$ was implicitly used up to now in the proofs of Lemmas 3, 4, 5, and 6. Since $(0,V^*) \in \overline{\mathcal{R}_{\Delta t}}$, there are $(T,V) \in \mathcal{R}_{\Delta t}$ with $T < \Delta t$. Thus, even though $S \cap \mathcal{R}_{\Delta t} \neq \emptyset$ for all $0 \le \Delta t < \tau^{**}$, we still need to prove $\{(\Delta t, \infty) \times \mathbf{R}_+\} \cap S \cap \mathcal{R}_{\Delta t} \neq \emptyset$.

For all $0 \le \Delta t < \tau$, we have $Q_{\Delta t}(0,V^*) < (V^*)^2$ with V^* the unique value, independent of Δt, for which $\frac{dQ_{\Delta t}(T,V)}{d(V^2)}\Big|_{V=V^*} = 1$. Since $Q_{\Delta t}(T,V)$ is monotonic increasing in both Δt and T, we can define the new function $\mathbb{Q}(\Delta t) = Q_{\Delta t}(\Delta t, V^*) - (V^*)^2$. Due to $\overline{\mathcal{R}_\tau} = \{0\} \times \{V^*\}$ by construction, we find $\mathbb{Q}(\tau) > 0$, while $\mathbb{Q}(0) < 0$. Hence, by the Intermediate Value Theorem there exists a $0 < \tau^{***} < \tau$ such that $\mathbb{Q}(\tau^{***}) = 0$ and, therefore, $\{(\Delta t, \infty) \times \mathbf{R}_+\} \cap \mathcal{R}_{\Delta t} \neq \emptyset$ for all $0 \le \Delta t < \tau^{***}$. Introduce $\tilde{V}_{\Delta t}$ as the minimal value of V such that $\underline{Q_{\Delta t}(\Delta t, V) \le V^2}$ if such a V exists. For $0 \le \Delta t < \tau^{***}$, there exists a $(\Delta t, \tilde{V}_{\Delta t}) \in \overline{\{(\Delta t,\infty) \times \mathbf{R}_+\} \cap \mathcal{R}_{\Delta t}}$. Introduce $\mathbb{P}(\Delta t) = \max_{\alpha \in \mathbf{P}_d} P_\alpha(\Delta t, \tilde{V}_{\Delta t})$. For $\tau^{***} \le \tau^{**}$, if $\lim_{\Delta t \to \tau^{***}} \mathbb{P}(\Delta t) \le \frac{1-\phi_{\min}}{C_{1,0}}$, then $(\Delta t, \tilde{V}_{\Delta t}) \in \mathcal{S}$ for all $0 \le \Delta t < \tau^* = \tau^{***} = \min\{\tau^{**}, \tau^{***})$. If $\lim_{\Delta t \to \tau^{***}} \mathbb{P}(\Delta t) > \frac{1-\phi_{\min}}{C_{1,0}}$, which also occurs for $\tau^{**} \le \tau^{***}$, then we recall $Q_0(0,0) = 0$ and $P_\alpha(0,0) < \frac{1-\phi_{\min}}{C_{1,0}}$ for all $\alpha \in \mathbf{P}_d$. Hence, $\mathbb{P}(0) < \frac{1-\phi_{\min}}{C_{1,0}}$. By continuity of $Q_{\Delta t}(T,V)$ and $P_\alpha(T,V)$ in the parameters Δt, T and V, follows the continuity of $\mathbb{P}(\Delta t)$. Thus by the Intermediate Value Theorem, there is a $\tau^* \in (0, \tau^{**}) = (0, \min\{\tau^{**}, \tau^{***}\})$ such that $\mathbb{P}(\tau^*) = \frac{1-\phi_{\min}}{C_{1,0}}$. Thus there exists a $\tau^* \in (0, \min\{\tau^{**}, \tau^{***}\}]$ such that $(\Delta t, \tilde{V}_{\Delta t}) \in \overline{\{(\Delta t, \infty) \times \mathbf{R}_+\} \cap \mathcal{R}_{\Delta t}} \cap \mathcal{S}$ for all $0 \le \Delta t < \tau^*$.
Hence, for all $0 \le \Delta t < \tau^* \in (0, \min\{\tau^{**}, \tau^{***}\}]$, we have $\{(\Delta t, \infty) \times \mathbf{R}_+\} \cap \mathcal{R}_{\Delta t} \cap \mathcal{S} \neq \emptyset$ due to the monotonicity of $Q_{\Delta t}(T,V)$ and $P_\alpha(T,V)$ on the parameters Δt, T and V. □

We have shown that the conditions $c_{5l} < c_{1l}$, $a_{9m} < 1$ and $a_{10m} < a_{3m}(0)$ are satisfied by the conditions (i), (viii) and (ix) in Assumption 1. Moreover, the conditions $\phi_{\min} \le 1 - C_{1,0}(d-1)/d$ and $\phi^0 \in \Phi_d(\phi_{\min}, (1-\phi_{\min})/C_{1,0})$ of Lemma 5 follows from (v), while the conditions (ii), (iii), (iv), (vi) and (vii) are needed for coercivity.
The condition $Q_1 < 1$ of Lemma 6 is equivalent to

$$1 > \frac{7d-5}{\Gamma^2_{\phi_{\min}}} \max_{m \in \mathfrak{M}} \left\{ \frac{H^2_{1m}}{a_{3m}(0) - a_{10m}} \right\} (a_{11} + a_{12}),$$

which can be satisfied if (x) in Assumption 1 is satisfied.

We finish the proof of Theorem 2 with remarking that we can choose any pair $(T,V) \in S \cap \operatorname{int}(\mathcal{R}_0)$ to satisfy the theorem, since $\lim_{\Delta t \downarrow 0} \{(\Delta t, \infty) \times \mathbf{R}_+\} \cap S \cap \mathcal{R}_{\Delta t} = S \cap \operatorname{int}(\mathcal{R}_0)$.

5 Proof of Theorem 1

The proof of Theorem 1 is straightforward. We use an interpolation function $\hat{u}_{\Delta t}(t) := u^{k-1} + (t - t_{k-1})\mathcal{D}^k_{\Delta t}(u)$ on each interval $[t_{k-1}, t_k] \subset [0,T]$ for all functions $u \in \{\phi_l, v, w_m, W\}$ with $l \in \mathfrak{L}$ and $m \in \mathfrak{M}$ to extend the discrete-time solutions of Theorem 2 to $[0,T] \times [0,1]$ and $[0,T]$. We see that $\hat{u}_{\Delta t}$ is measurable on $[0,T] \times [0,1]$ for $u \in \{\phi_l, v, w_m\}$ and $[0,T]$ for $u = W$, has a time-derivative on $[0,T] \times [0,1]$ a.e. for $u \in \{\phi_l, v, w_m\}$ and $[0.T]$ a.e. for $u = W$, and has a Δt-independent bound in an appropriate Bochner space (cf. Theorem

2). Hence, we obtain the following weak convergence results

(1) $\hat{\phi}_{l,\Delta t} \rightharpoonup \hat{\phi}_l \in H^1(0,T;L^2(0,1)) \cap L^\infty(0,T;H^1(0,1)) \cap L^2(0,T;H^2(0,1)),$

(2) $\hat{v}_{\Delta t} \rightharpoonup \hat{v} \in L^2(0,T;H^1(0,1)),$

(3) $\hat{w}_{m,\Delta t} \rightharpoonup \hat{w}_m \in H^1(0,T;H^1(0,1)) \cap L^\infty(0,T;H^2(0,1)),$ and

(4) $\hat{W}_{\Delta t} \rightharpoonup \hat{W} \in H^1(0,T)$

for $l \in \mathfrak{L}$ and $m \in \mathfrak{M}$.
As the time-continuous system has non linear terms, we need strong convergence of the $\hat{\phi}_{l,\Delta t}$ and $\hat{w}_{m,\Delta t}$ terms in order to pass to the limit $\Delta t \to 0$. The strong convergence is obtained here by combining two versions of the Lions-Aubin-Simon lemma, see [10, Theorem 1] for the version for piecewise constant functions and [32, Theorem 3] for the standard Lions-Aubin-Simon, which is used for the piecewise linear functions.

Theorem 3 (Lions-Aubin-Simon lemma for piecewise constant functions)**.**
Let X, B, and Y be Banach spaces such that the embedding $X \hookrightarrow B$ is compact and the embedding $B \hookrightarrow Y$ is continuous. Furthermore, let either $1 \le p < \infty$, $r = 1$ or $p = \infty$, $r > 1$, and let $(u_{\Delta t})$ be a sequence of functions, which are constant on each subinterval (t_{k-1}, t_k), satisfying

$$\|\mathcal{D}_{\Delta t}(u_{\Delta t})\|_{L^r(\Delta t,T;Y)} + \|u_{\Delta t}\|_{L^p(0,T;X)} \le C_0 \quad \textit{for all} \quad \Delta t \in (0,\tau), \tag{21}$$

where $C_0 > 0$ is a constant which is independent of Δt. If $p < \infty$, then $(u_{\Delta t})$ is relatively compact in $L^p(0,T;B)$. If $p = \infty$, there exists a subsequence of $(u_{\Delta t})$ which converges in each space $L^q(0,T;B)$, $1 \le q < \infty$, to a limit which belongs to $C^0([0,T];B)$.

Theorem 4 (Standard Lions-Aubin-Simon lemma)**.**
Let X and B be Banach spaces, such that $X \hookrightarrow B$ is compact. Let $f \in \mathbb{F} \subset L^p(0,T;B)$ where $1 \le p \le \infty$, and assume

(A) $\mathbb{F}$ is bounded in $L^1_{loc}(0,T;X)$,

(B) $\|f(t+\Delta t) - f(t)\|_{L^p(0,T-\Delta t;B)} \to 0$ as $\Delta t \to 0$, uniformly for $f \in \mathbb{F}$.

Then $\mathbb{F}$ is relatively compact in $L^p(0,T;B)$ (and in $C(0,T;B)$ if $p = \infty$).

We apply Theorem 3 and Theorem 4 with the triples

$$(X,B,Y) = (H^2(0,1), C^1([0,1]), L^2(0,1))$$

or

$$(X,B,Y) = (H^1(0,1), C^0([0,1]), L^2(0,1)),$$

depending on the situation, together with the Rellich-Kondrachov theorem on $[0,1]$, see [2, p.143] and [6], ensuing $X \hookrightarrow B$ compactly. We obtain the existence of a subsequence $\Delta t \downarrow 0$ for which we also have strong convergence next to the weak convergence:

$$\hat{\phi}_{l,\Delta t} \to \hat{\phi}_l \in C^0([0,T];C^0[0,1]) \quad \text{for } l \in \mathfrak{L},$$
$$\hat{w}_{m,\Delta t} \to \hat{w}_m \in C^0([0,T];C^1[0,1]) \quad \text{for } m \in \mathfrak{M}.$$

The limit functions $\hat{\phi}_l$, $\hat{v}$ and $\hat{w}_m$ satisfy the weak formulation of the continuous-time equations (1a)-(1c).
Using the interpolation-trace inequality, $\|u\|_{C(\overline{\Omega})} \leq C\|u\|_{H^1(\Omega)}^{1-\theta}\|u\|_{L^2(\Omega)}^{\theta}$ (for $\theta = 1/2$, see [34, Example 21.62 on p.285]), the weak convergence for Theorem 2 applies up to the boundary, which together with the smoothness of the functions satisfying Equation (2) ensure the passage of the limit so that the boundary conditions are recovered. The initial conditions are satisfied by construction.
Hence, there exist $\phi_{\min} > 0$, $T > 0$, $V > 0$ such that $\phi_l := \hat{\phi}_l$, $v := \hat{v}$, $w_m := \hat{w}_m$ and $W := \hat{W}$ satisfy Theorem 1.

6 Numerical exploration of allowed parameter sets

In this section we simulate numerically the model (5), (8a)-(8c), (9a), and (9b). This model is already in a format that allows a straightforward numerical implementation next to allowing some analytical evaluation of observed (numerical) behaviors. The chosen model has $d = 3$ and is determined by the following functions and constants, for all $l \in \mathfrak{L}$ and $m \in \mathfrak{M}$

$$\begin{array}{rclrcl}
\delta_l &=& \delta & \Gamma(\phi) &=& 4\phi_d \\
I_1(\phi) &=& 0 & I_3(\phi) &=& \epsilon \\
B_{l10l}(\phi) &=& \epsilon\phi_l & B_{lijm}(\phi) &=& 0 \text{ for } (i,j,m) \neq (1,0,l) \\
H_{1m}(\phi) &=& \phi_m & H_{0m}(\phi) &=& 0 \\
E_{m10j}(\phi) &=& \frac{1}{2}D_j\phi_m & E_{minj}(\phi) &=& 0 \text{ for } (i,j) \neq (1,0) \\
F_m(\phi) &=& 1 & \gamma_m &=& \gamma \\
G_{\phi,l}(\phi) &=& \epsilon\kappa_l G_v(\phi) & G_v(\phi) &=& \mathcal{L}(\phi_{1,sat} - \phi_1)\mathcal{L}(\phi_3 - \phi_{3,thr}) \\
G_{w,m}(\phi) &=& 0 & A_m &=& A
\end{array}$$

The conditions of Assumption 1 have to be satisfied. To this end, we choose $\eta_m = \zeta\gamma|A|$ for $m \in \mathfrak{M}$ with $\zeta > 0$ in conditions (ix) and (x) of Assumption 1. This yields for $\phi_{\min} \in (0, 1 - 2\coth(1)/3) \approx (0, 0.124643143)$ the conditions

(i) $\delta > 0$

(ii) $|A| < 1$

(iii) $\frac{1}{4}D_j^2\phi_m^2 < \frac{1}{9}\min\{3, \gamma(1-A)\}\min\{3/5, \gamma(1-A)\}$

(iv) $64\phi_{d0}^2 > 36\phi_{l0}^2$ for all $l \in \mathfrak{L}$.

(v) $\phi_{j0} \geq \phi_{\min}$, $\sum_{i\neq j} \phi_{i0} < \frac{1-\phi_{\min}}{\coth(1)}$ and $\sum_{i=1}^{d} \phi_{i0} = 1$ for all $1 \leq j \leq d$,

(vi) $77\gamma A^2 < 1$,

(vii) $\gamma > \frac{77\phi_m^2}{64\phi_d^2}$,

(viii) $0 < \mathfrak{C}_{1m} = 1 - \sum_{j \in \mathfrak{M}} D_m \frac{\eta_{j01m1}}{4}$,

(ix) $0 < \mathfrak{C}_{2m} = \gamma\left(1 - \left(1 + \frac{\zeta}{2}\right)|A|\right) - \frac{\eta_{m2}}{2} - \frac{1}{4}\sum_{j \in \mathfrak{M}}\left(\frac{D_j}{\eta_{m01j1}} + \frac{D_j}{\eta_{m01j2}} + D_m \eta_{j01m2}\right)$,

(x) $1 > \frac{1}{2}\left(\frac{1-2\phi_{\min}}{\phi_{\min}}\right)^2 \max_{m \in \mathfrak{M}}\left\{\frac{1}{\mathfrak{C}_{2m}}\right\} \sum_{m \in \mathfrak{M}}\left(\frac{\gamma|A|}{\zeta} + \frac{1}{\eta_{m2}}\right)$.

An upper bound for $|A|$ can be determined with (ix) and (x) by taking $D_m = 0$ and by removing both the η_{m2} terms and $\mathfrak{C}_{1m}$. This yields the conditions

$$|A| < \frac{2}{2+\zeta} \text{ and } 1 > \left(\frac{1-2\phi_{\min}}{\phi_{\min}}\right)^2 \frac{|A|}{\zeta(2-(2+\zeta)|A|)}.$$

Using $\phi_{\min} < 1/8$, we obtain for $\zeta = 6$ the maximal value

$$|A| < \frac{2}{2+\zeta+\frac{36}{\zeta}} \leq \frac{1}{7},$$

which is not even attainable due to the approximations made in the derivation. In any case, (x) is a stronger condition than (ii).
For γ, we need to first determine the values of η_{m01j1} and η_{m01j2}. For these we choose the values that are the square root of the product of their lower and upper limits obtained by letting all undetermined terms in (viii) and (ix) have an equal part such that $\mathfrak{C}_{1m} = 0$ and $\mathfrak{C}_{2m} = 0$ for $\zeta = 1$. This yields, for $|A| \leq \frac{1}{7}$, the positive numbers

$$\eta_{m01j1} = \sqrt{\frac{7d-5}{d-1}\frac{1}{\gamma(1-\frac{3}{2}|A|)}} \text{ and } \eta_{m01j2} = 1$$

and the inequality

$$1 > \left(\frac{1-2\phi_{\min}}{\phi_{\min}}\right)^2 \left(\gamma|A| + \frac{1}{\eta}\right) \max_{m \in \mathfrak{M}}\left\{\frac{1}{1 - \frac{D_m}{2}\sqrt{\frac{8}{\gamma(1-\frac{3}{2}|A|)}}} + \frac{1}{\gamma(1-\frac{3}{2}|A|) - \frac{\eta}{2} - \frac{D_m}{2} - \frac{1}{4}\sum_{j \in \mathfrak{M}}\left(D_j\sqrt{\frac{\gamma(1-\frac{3}{2}|A|)}{8}} + D_j\right)}\right\}, \quad (23)$$

where we have chosen $\eta_{m2} = \eta$.
In the limit $|A| \downarrow 0$, choosing $D_m < 1$, we obtain the condition

$$1 > 2\left(\frac{1-2\phi_{\min}}{\phi_{\min}}\right)^2 \frac{1}{\eta}\left(\frac{1}{2-\sqrt{\frac{8}{\gamma}}} + \frac{1}{2\gamma - \eta - 2 - \sqrt{\frac{\gamma}{8}}}\right).$$

The second term yields a minimal value for $\eta = \gamma - 1 - \sqrt{\gamma/32}$, which leads to

$$1 > 2\left(\frac{1-2\phi_{\min}}{\phi_{\min}}\right)^2 \frac{1}{\gamma - 1 - \sqrt{\frac{\gamma}{32}}}\left(\frac{1}{2-\sqrt{\frac{8}{\gamma}}} + \frac{1}{\gamma - 1 - \sqrt{\frac{\gamma}{32}}}\right).$$

We obtain

$$\gamma > \gamma^* \approx 49.2186 \text{ with } \phi_{\min} < 0.124643143. \tag{24}$$

For a stricter upper bound of $|A|$, we take $D_j = \frac{2}{3}\sqrt{\min\{3, \gamma(1-|A|)\}\min\{3/5, \gamma(1-|A|)\}}$. With the γ^* of Equation (24) and the rough upper bound $|A| < 0.201$, we see that $D_j = 2/\sqrt{5}$. With this value of D_j, assuming $\gamma > \gamma^*$, $\eta = 1/(\gamma|A|)$, $\gamma \gg \sqrt{\gamma}$ and $1/\gamma \ll \gamma|A|$, we can remove some terms of Equation (23) and obtain

$$1 > 2\left(\frac{1-2\phi_{\min}}{\phi_{\min}}\right)^2 |A|\,(1+\gamma)\,.$$

Hence, we obtain

$$\frac{1}{\gamma^2} \ll |A| < A^*_\gamma = \frac{1}{2}\left(\frac{\phi_{\min}}{1-2\phi_{\min}}\right)^2 \frac{1}{1+\gamma} \approx \frac{1}{72.55(1+\gamma)} \text{ with } \phi_{\min} < 0.124643143, \tag{25}$$

and additionally

$$\gamma \gg \gamma^{**} \approx 73.55, \quad \frac{1}{\gamma^2} \ll |A| < A^*_{\gamma^{**}} \approx \frac{1}{5409}. \tag{26}$$

Using the values of (26), we see that $D_j^2 < 4/5$ must hold and that (vi) and (vii) are also automatically satisfied. Hence, there exists a non-empty parameter region where all conditions of Assumption 1 are satisfied and, therefore, a continuous solution exists.

The analytically obtained parameter region is very restrictive due to the sometimes crude estimates used in the proofs of the theorems. The actual parameter region is expected to be much larger. Numerically, this region can be probed. Moreover, it allows us to probe the size T of the time-interval satisfying the physical constraints (I), (II) and (III).

A fixed set of reference parameter values have been chosen after a deliberate numerical search for parameter values around which T changes significantly. The reference parameter values are

$$\begin{array}{rclrclrclrcl} A &=& 0.388 & \gamma &=& 10^4 & \delta &=& 1 & \epsilon &=& 0.0014 \\ D_1 &=& 0.38 & D_2 &=& 1 & \kappa_1 &=& 23.0 & \kappa_3 &=& -13.5 \\ \hat{J}_1 &=& 0 & \hat{J}_2 &=& 0.4 & \hat{J}_3 &=& 2.0 & \phi_{\min} &=& 0.1 \\ \phi_{1,sat} &=& 1 & \phi_{3,thr} &=& 0 & \phi_{2,res} &=& 1 & \phi_{3,res} &=& 1 \\ \phi_{10} &=& 0.3 & \phi_{30} &=& 0.4 & & & & & & \end{array}$$

We solve the time-discrete system for the small time step $\Delta t = 0.001$. This value has been chosen arbitrarily, although it is large enough for keeping the computational costs and duration of the simulation acceptable and small enough for showing continuous temporal

behaviour.
Following the concept of Rothe method, we only need to solve numerically a 1D spatial problem at each time slice $\{t = t_k\}$. At $\{t = 0\}$ we still need to solve a different 1D spatial problem in order to obtain v^0. We implemented the time-discrete system in MATLAB using the `BVP5c` solver, although one can also use the `bvp4c` solver. These solvers take a grid, a guess for the solution, and the BVP system as input. Then they automatically readjust the grid and interpolate the guess solution to obtain a starting point for the numerical scheme, controlling a certain error metric to determine the solution based on user-defined-convergence criteria. For an in depth description and performance analysis of the solvers, see [19, 30] for `bvp4c` and [20] for `bvp5c`.
Initially, we take a uniform grid of 300 intervals. As initial guess for the solution, we take the solution at time slice $\{t = t_{k-1}\}$ or the zero function.

Tests that check the conditions of Theorem 1 at each time slice, including $\{t = 0\}$, are incorporated in the numerical method. For these conditions, we use the value $V = 10^6$ and $\phi_{\min} = 0.1$. At the start of our numerical method additional tests are implemented to test the pseudo-parabolicity of the system. Failure to pass any of these tests ends the simulation.
To guarantee the end of any simulation, we incorporate an end time $T_{end} = 0.5$, which coincides with the time slice $\{t = t_{500}\}$.

The criteria for stopping a simulation in this numerical program allow one to probe the boundary of $S \cap \text{int}(\mathcal{R}_{\Delta t})$ at fixed V-value lines and determine T in Δt increments for different parameter values. Smaller Δt will yield better approximations to T.

The simulation of the time-discrete system for the reference parameter values gives interesting results. All volume fractions ϕ_l are practically spatially constant functions at all time slices. Numerically, we expect a much larger area in (γ, A)-space for which Theorem 1 holds. As $(\gamma, A) = (10^4, 0.388)$ is well outside the analytically obtained existence region, we conclude that the conditions Assumption 1 are more restrictive than practically necessary. The simulation ends at time slice $\{t = t_{194}\}$ due to a violation of one of the condition of Theorem 1 with $\phi_3 < 0.1 = \phi_{\min}$ as shown in Figure 1. This indicates that $193\Delta t \leq T < 194\Delta t$ for these parameter values.

Next to the volume fraction conditions, we have the conditions on the velocity v as stated in Theorem 1. A clear supra-exponential growth of the $L^2(0, t; H_0^1(0, 1))$ norm of v is seen in Figure 2 in the region where in Figure 1 the volume fractions exhibited sudden drastic changes in value. Surprisingly the supra-exponential growth was not large enough to breach the $V = 10^6$ threshold of Theorem 1. Hence, the simulation was stopped only because the volume fraction condition was breached. The graph of $W(t)$ in Figure 2 looks similar to the graph of the norm, which is due to (4b) and the logarithmic scale of the axis.

We conclude that the reference parameter values allow a discrete solution that satisfies Theorem 2, even though the reference parameter values do not satisfy Assumption 1.

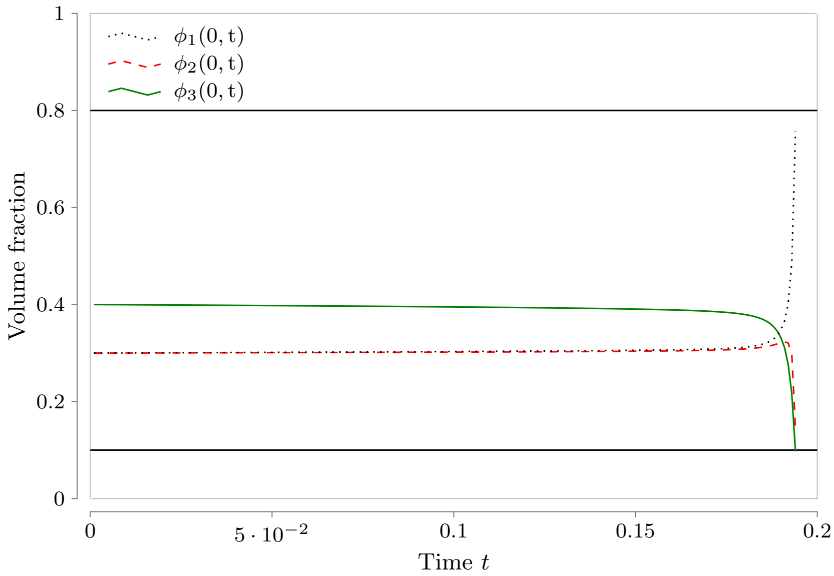

Figure 1: The time evolution of the volume fractions of the simulation at the reference values. The simulation automatically ended at time slice $\{t = t_{194}\}$ due to $\phi_3(0, t_{194}) < 0.1 = \phi_{\min}$. The other volume fractions stayed between the two black-lines, which indicates a guaranteed breach of $\phi_l < \phi_{\min}$ by one of the volume fractions.

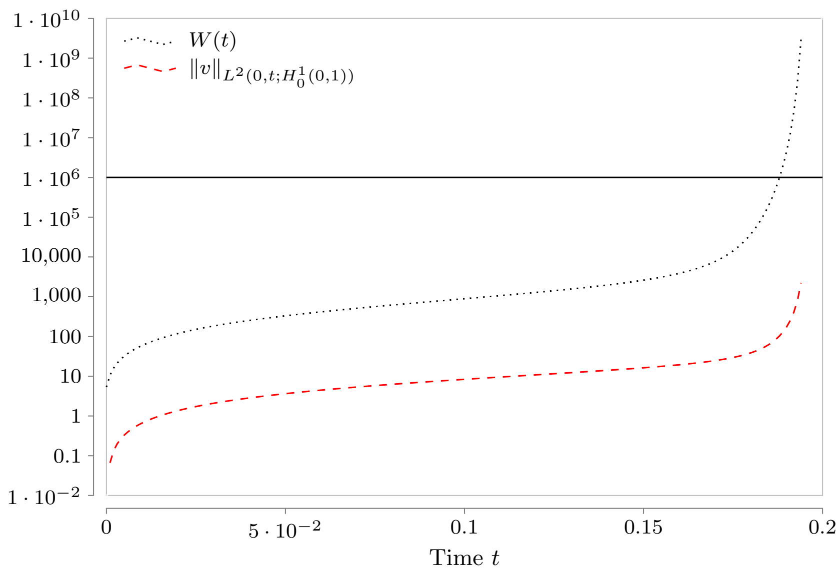

Figure 2: The time evolution of $W(t)$ and $\|v\|_{L^2(0,t;H_0^1(0,1))}$ of the simulation at the reference values. The simulation automatically ended at time slice $\{t = t_{194}\}$ due to $\phi_3(0, t_{194}) < 0.1 = \phi_{\min}$. The upper bound $V = 10^6$ was not yet reached. Both graphs show supra-exponential growth in the region where the volume fraction values changed dramatically.

This result showed us a method of probing the parameter space dependence as the simulation was ended prematurely at $t = t_{194}$. From now on, we denote $t = t_{194}$ with $N_R = 194$,

while a completed simulation is denoted by $N_R = 500$. By tracking the value of N_R at different parameter values, we indicate the dependence of T on the parameters, i.e. $(N_R - 1)\Delta t \leq T < N_R \Delta t$. We probed a grid in (γ, A)-space, a grid in ϵ-space and a grid in $(\phi_{10}, \phi_{20}, \phi_{30})$-space. We restricted our attention to these parameters because ϵ should highly affect the volume fractions ϕ_l, and we have specific existence restrictions given by Assumption 1 for the other parameters.
It turns out that γ has a negligible effect on N_R in our (γ, A)-space grid. We choose the values $\gamma \in \{10^{3.5}, 10^4, 10^{4.5}, 10^5, 10^{5.5}, 10^6, 10^{6.5}, 10^7, 10^{7.5}, 10^8\}$ and
$A \in \{0.376, 0.379, 0.382, 0.385, 0.388, 0.391, 0.394, 0.397, 0.400\}$.

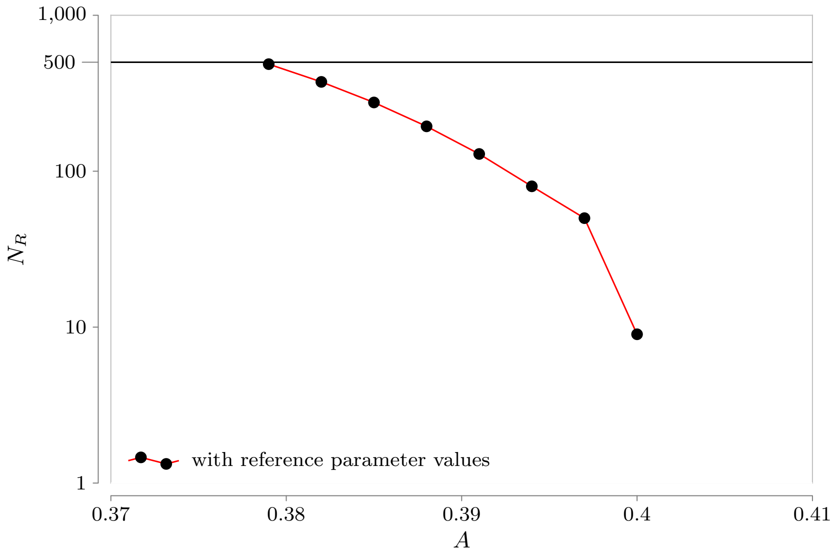

Figure 3: The dependence of N_R with respect to A with the other parameters taking their reference values. An approximately exponential dependence of N_R on A can be discerned. Note that A can be much larger than $\frac{1}{72.55(1+\gamma)}$ and still lead to a positive time T.

The dependence of A on N_R with $\gamma = 10^4$ is shown in Figure 3. An approximately exponential dependence of N_R on A can be seen. Moreover, the values of N_R decrease rapidly to almost 0 for A approaching 0.4. This indicates that the actual threshold of A is much larger than $\frac{1}{72.55(1+\gamma)}$.

Since condition (viii) of Assumption 1 has been shown to be an underestimation of the actual existence region with respect to the parameter A, we expect a similar effect to happen for the initial conditions $(\phi_{10}, \phi_{20}, \phi_{30})$. The restriction $\phi_{10} + \phi_{20} + \phi_{30} = 1$ hints at the use of barycentric coordinates to represent the dependence of N_R on the initial conditions in the best way. In Figure 4 a grid, where the cells have edge size 0.1, has been placed on the region of nonnegative initial volume fractions. Additionally, the central gridpoint, where all volume fractions have the identical value 1/3, has been added to the grid. At each gridpoint the actual value of N_R is shown for the simulation with that particular set of parameters. The inner shaded small triangle represents the region where Assumption 1 holds, while the shaded area between the two outer triangles represents the region where the initial conditions violate the condition of Theorem 1.

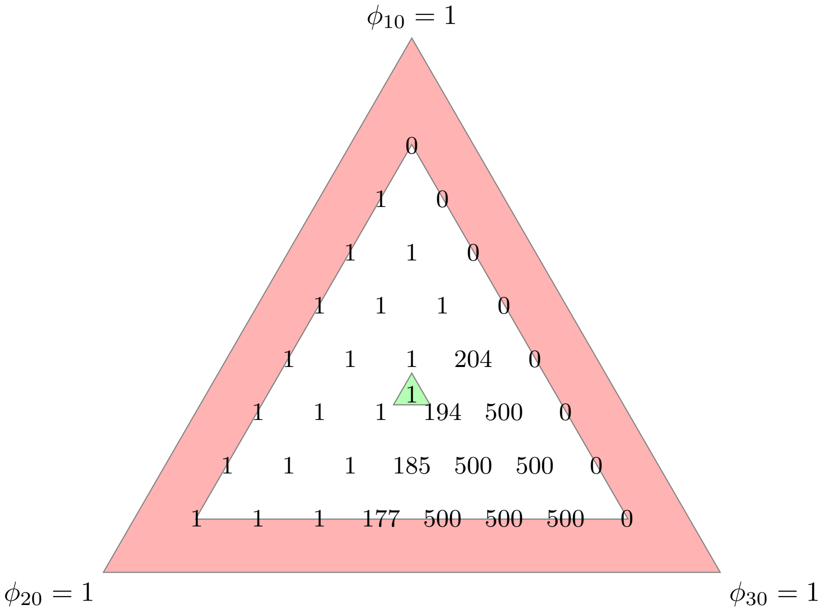

Figure 4: The dependence of N_R with respect to the initial conditions $(\phi_{10}, \phi_{20}, \phi_{30})$ with the other parameters taking their reference values. The inner triangle represents the region where Assumption 1 holds, while the shaded area between the two outer triangles represents the region where the initial conditions violate the condition of Theorem 1.

In Figure 4, the values of N_R increase with larger values of ϕ_{30}, which is expected since ϕ_3 is transformed in the reaction and can therefore decrease. Moreover, v is sensitive to the values of ϕ_3 and changes in v directly effect ϕ_3. Larger values of ϕ_{30} deminishes the influence of other terms on v and, therefore, the change in ϕ_3 itself. As it was shown in Figure 1 that ϕ_3 crossed the lower threshold set by Theorem 1, we expect N_R to increase with larger ϕ_{30} due to both the stabilizing effect and the higher starting value of the simulation.
Again, we see that the simulation gives $N_R > 1$ outside of the region defined by Assumption 1 indicating that the analytical condition in Assumption 1 is more restrictive than practically necessary. It is worth noting that the outer triangle of N_R values are on the boundary of the region where the condition of Theorem 1 holds. Due to machine-precision inaccuracies some simulations have $N_R = 0$, what indicates an unlawful starting value, or $N_R > 0$, what indicates that the starting values satisfied all conditions of Theorem 1.

The parameter ϵ indicates how strong certain terms influence the time-derivative of the volume fractions. In Figure 4, we see that there is a strong dependence between ϕ_3 and N_R. Therefore, we expect ϵ to have a significant effect on N_R as well. To this end we took a set of ϵ values and solved the time-discrete system for each of these values supplemented with the reference values of the other parameters. The used ϵ values here are: $\{1.4 \cdot 10^{-5}, 1.4 \cdot 10^{-4.5}, 1.4 \cdot 10^{-4}, \ldots, 1.4 \cdot 10^{-0.5}, 1.4\}$. In Figure 5 a polynomial relation between N_R and ϵ can be discerned. This confirms our expectation that ϵ has a significant effect on N_R.

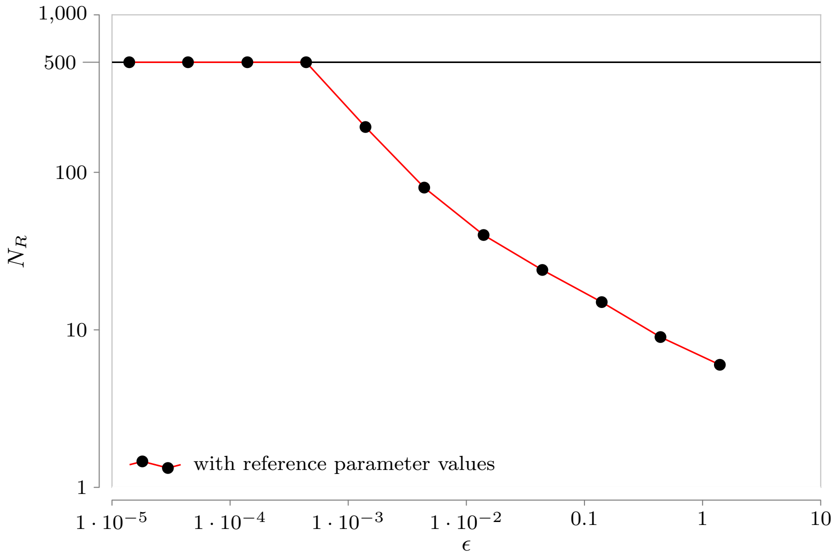

Figure 5: The dependence of N_R with respect to ϵ with the other parameters taking their reference values. A polynomial relation between N_R and ϵ can be discerned.

7 Conclusion

We have employed Rothe's method to prove Theorem 1, which essentially states that there exists a weak solution on $[0,T] \times (0,1)$ of the continuous-time system given by Equations (1a)-(1c), (4a), (4b), and (5) for $(T,V) \in S \cap \text{int}(\mathcal{R}_0)$ provided a suitable parameter regime is chosen (cf. Assumption 1).

Numerically, we have validated that the conditions of Theorem 1 can be violated for t large enough. Moreover, we have shown using numerical simulations that the parameter region for the existence of weak solutions as given by Assumption 1 is restrictive. Both in (γ, A)-space as in $(\phi_{10}, \phi_{20}, \phi_{30})$-space the numerical simulations showed existence for points well outside the regions given by Assumption 1. Additionally, we have shown that A, ϕ_{30} and ϵ have a significant influence on T, as was expected. Moreover, we could indicate that γ has no significant effect on T in the numerical simulations. This was against the prediction of the shape of the existence region of Assumption 1.
This means that sharper inequality results probably hold, which would finally lead to a relaxation of conditions (v) and (viii) in Assumption 1.

Acknowledgments

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A Existence of solutions to discrete-time system

The subsystem (8a) with (9a) is a standard elliptic system in ϕ_l^k, which has a unique solution in $\phi_l^k \in H^1(0,1)$ if $\phi_l^{k-1}, v^{k-1}, w_m^{k-1} \in H^1(0,1)$ and $w_m^k \in H^1(0,1)$. Similarly, by direct integration, the subsystem (8b) with (9b) has a unique solution $v^k \in L^2(0,1)$ if there are unique $\phi_l^{k-1}, v^{k-1}, w_m^{k-1} \in L^2(0,1)$, $\phi_{\min} \leq \phi_l^{k-1} \leq 1$ almost everywhere, and $w_m^k \in L^2(0,1)$. Moreover, this subsystem has a unique solution $v^k \in H^1(0,1)$ if there are unique $\phi_l^{k-1}, v^{k-1}, w_m^{k-1} \in H^1(0,1)$ and $w_m^k \in H^1(0,1)$.
The existence of a unique $v^0 \in H^1(0,1)$ is slightly more complicated. Even though any $v^0 \in H^1(0,1)$ will give a unique solution, we do realize that the numerical method might be highly sensitive to the choice of $v^0 \in H^1(0,1)$. Physically, we expect $v^0 \in H^1(0,1)$ to be close to the solution of continuous-time system with the initial conditions filled in. Unfortunately, we do not have sufficient temporal regularity to extend the system to the $t = 0$ boundary. However, since any $v^0 \in H^1(0,1)$ would suffice, we just choose the function $v^0 \in H^1(0,1)$ that would be the solution if there was sufficient regularity.
To this end, we integrate (1b) and insert the initial conditions (5) in the continuous-time system. This yields, at $t = 0$, a system for v and $\partial_t w_m$.

$$\Gamma(\phi_0)v + \sum_{m\in\mathfrak{M}} H_{1m}(\phi_0)\partial_t w_m = G_v(\phi_0)z + \sum_{m\in\mathfrak{M}} \hat{J}_m \mathcal{L}(\phi_{m,res} - \phi_{m0}), \tag{27a}$$

$$\partial_t w_m - \gamma_m \partial_z^2 \partial_t w_m + F_m(\phi_0)v + \sum_{j\in\mathfrak{M}} E_{m01j}(\phi_0)\partial_z \partial_t w_j = G_{w,m}(\phi_0), \tag{27b}$$

with boundary conditions

$$v|_{z=0} = 0, \tag{28a}$$

$$\partial_t w_m|_{z=0} = \frac{\hat{J}_m}{H_{1m}(\phi_0)} \mathcal{L}(\phi_{m,res} - \phi_{m0}), \tag{28b}$$

$$\partial_z \partial_t w_m|_{z=1} = A_m \left(\partial_t w_m|_{z=1} + \sum_{j\in\mathfrak{M}} \frac{H_{1j}(\phi_0)}{\Gamma(\phi_0)} \partial_t w_j|_{z=1} \right) \tag{28c}$$

$$- \frac{A_m}{\Gamma(\phi_0)} \left[G_v(\phi_0) + \sum_{j\in\mathfrak{M}} \hat{J}_j \mathcal{L}(\phi_{j,res} - \phi_{j0}) + \hat{J}_d \mathcal{L}(\phi_{d,res} - \phi_{d0}) \right]^{z=1}.$$

Inserting Equation (27a) in Equation (27b), we obtain

$$B(\partial_t w_m, \psi) = \sum_{m\in\mathfrak{M}} \mathfrak{G}_m(\psi),$$

where

$$B_m(u,\psi) = \int_0^1 \gamma_m \partial_z u_m \partial_z \psi_m + \sum_{j\in\mathfrak{M}} E_{m01j}(\phi_0)(\partial_z u_j)\psi_m - \sum_{j\in\mathfrak{M}} \frac{F_m(\phi_0)H_{1j}(\phi_0)}{\Gamma(\phi_0)} u_j\psi_m \\ + u_m\psi_m - \gamma_m A_m \left[\partial_z(u_m\psi_m) + \sum_{j\in\mathfrak{M}} \frac{H_{1j}(\phi_0)}{\Gamma(\phi_0)}\partial_z(u_j\psi_m)\right] \mathrm{d}z$$

and

$$\mathfrak{G}_m(\psi) = G_{w,m}(\phi_0)\psi_m - \frac{F_m(\phi_0)}{\Gamma(\phi_0)}\left[G_v(\phi_0)z + \sum_{j\in\mathfrak{M}} \hat{J}_j\mathcal{L}(\phi_{j,res}-\phi_{j0})\right]\psi_m \\ - \left[\frac{\gamma_m A_m}{\Gamma(\phi_0)}\left(G_v(\phi_0) + \sum_{j\in\mathfrak{M}} \hat{J}_j\mathcal{L}(\phi_{j,res}-\phi_{j0}) + \hat{J}_d\mathcal{L}(\phi_{d,res}-\phi_{d0})\right)\psi_m\right]^{z=1}.$$

Clearly, $B(\cdot,\cdot) = \sum_{m\in\mathfrak{M}} B_m(\cdot,\cdot)$ is a bilinear form on $H^1_{0,free}(0,1)^{d-1}$, which is defined as $H^1_{0,free}(0,1)^{d-1} = \{f \in H^1(0,1)^d \mid f(0) = 0\}$. This bilinear form and $\sum_{m\in\mathfrak{M}} \mathfrak{G}_m(\cdot)$ are obviously continuous. However, $B(\cdot,\cdot)$ is only coercive if the following conditions are satisfied for all $j, m \in \mathfrak{M}$:

$$E_{m01j}(\phi_0)^2 < \frac{4\gamma_j}{(3d-2)(5d-4)}, \tag{29a}$$

$$4\Gamma(\phi_0)^2 > (5d-4)^2 F_m(\phi_0)^2 H_{1j}(\phi_0)^2. \tag{29b}$$

$$\gamma_j A_j^2 < \frac{1}{(3d-2)(5d-4)}, \tag{29c}$$

$$\frac{H_{1m}(\phi_0)^2}{\Gamma(\phi_0)^2} < \frac{4\gamma_j}{(3d-2)(5d-4)}. \tag{29d}$$

Condition (29a) follows from condition (iii) in Assumption 1, while conditions (29b), (29c), (29d) are exactly conditions (iv), (vi) and (vii) in Assumption 1, respectively.
Unfortunately, due to the boundary conditions $\partial_t w_m$ is not an element of $H^1_{0,free}(0,1)^{d-1}$. However, using the decomposition $\partial_t w_m = \tilde{w}_m + \tilde{a}_m(1-z)^2 + \tilde{b}z^{A_m}\sin\left(\frac{\pi}{2}z\right) = \tilde{w}_m + \tilde{c}_m(z)$ with

$$\tilde{w} \in \left\{ f \in H^2(0,1)^{d-1} \,\middle|\, f_m(0) = 0,\ (\partial_z f)_m(1) = A_m\left(f_m(1) + \sum_{j\in\mathfrak{M}} \frac{H_{1j}(\phi_0)}{\Gamma(\phi_0)} f_j(1)\right)\right\} = \tilde{\mathfrak{W}}$$

and the bounded values

$$\tilde{a}_m = \frac{\hat{J}_m}{H_{1m}(\phi_0)}\mathcal{L}(\phi_{m,res}-\phi_{m0}),$$

$$\tilde{b} = \frac{G_v(\phi_0) + \sum_{j\in\mathfrak{M}} \hat{J}_j \mathcal{L}(\phi_{j,res} - \phi_{j0}) + \hat{J}_d \mathcal{L}(\phi_{d,res} - \phi_{d0})}{\sum_{j\in\mathfrak{M}} H_{1j}(\phi_0)},$$

which follow from the identities

$$\begin{aligned}
\partial_t w_m(0) &= \tilde{w}_m(0) + \tilde{a}_m - \lim_{z\to 0} \tilde{b} \frac{\pi}{2A_m} \frac{\cos(\frac{\pi}{2}z)}{z^{-A_m-1}} = \begin{cases} \tilde{w}_m(0) + \tilde{a}_m & \text{for } A_m > -1, \\ \tilde{w}_m(0) + \tilde{a}_m + \frac{\pi}{2}\tilde{b} & \text{for } A_m = -1, \\ \infty & \text{for } A_m < -1, \end{cases} \\
\partial_t w_m(1) &= \tilde{w}_m(1) + \tilde{b}, \\
\partial_z \partial_t w_m(1) &= \partial_z \tilde{w}_m(1) + A_m \tilde{b},
\end{aligned}$$

we see that $\tilde{\mathfrak{W}} \subset H^1_{0,free}(0,1)^{d-1}$.
Via Lax-Milgram we obtain a unique solution $\tilde{w}$ in $H^1_{0,free}(0,1)^{d-1}$ that satisfies

$$B(\tilde{w}, \psi) = -B(\tilde{c}(z), \psi) + \sum_{m\in\mathfrak{M}} \mathfrak{G}_m(\psi). \tag{30}$$

Since, $B(\cdot,\cdot)$ is a coercive bilinear form, there exists a constant $C > 0$ such that the inequality $\left|\sum_{m\in\mathfrak{M}} \int_0^1 \partial_z \tilde{w}_m \partial_z \psi_m \mathrm{d}z\right| \leq C\|\psi\|_{C^1_c(0,1)^{d-1}}$ holds for $\psi_m \in C^1_c(0,1)$, the space of C^1 functions with compact support on $(0,1)$. Hence, by Proposition 8.3 of [6], we have $\tilde{w} \in H^2(0,1)^{d-1}$.
Applying a partial integration to (30), we see that $\tilde{w} + \tilde{c}(z)$ can only satisfy (27a)-(28c) if $\tilde{w} \in \tilde{\mathfrak{W}}$. Hence, there exists a unique solution $\partial_t w_m \in H^2(0,1)$ and, therefore, a unique solution $v^0 \in H^1_{0,free}(0,1)$ satisfying (27a)-(28c).

For the existence of a unique weak solution $w^k \in H^2(0,1)^{d-1}$, we follow a similar procedure and use induction on k. Of course, $k = 0$ is satisfied by $w = 0$. For the induction step we use $0 < k = K \leq T/\Delta t$ and assume that $w^{k-1} \in H^2(0,1)^{d-1}$. We test Equation (8c) with $\psi \in H^1(0,1)^{d-1}$. Using the decomposition $w^k_m = \hat{w}^k_m + \hat{a}^k_m(1-z)^2 + \hat{b}^k z^{A_m/2} \sin\left(\frac{\pi}{2}z\right) = \hat{w}^k + \hat{c}^k(z)$ with

$$\hat{w}^k \in \left\{ f \in H^2(0,1)^{d-1} \,\middle|\, f_m(0) = 0,\ (\partial_z f)_m(1) = A_m(f_m(1)) \right\} = \hat{\mathfrak{W}} \subset H^1_{0,free}(0,1)^{d-1}$$

and

$$\hat{a}^k_m = w^{k-1}_m(0) + \frac{\hat{J}_m \Delta t}{H_{1m}(\phi^{k-1})} \mathcal{L}(\phi_{m,res} - \phi^{k-1}_m),$$

$$\hat{b}^k = 2W^k,$$

which are straightforwardly bounded from (9b), we obtain a bilinear form $A_{\Delta t}(\hat{w}, \psi)$ on $H^1_{0,free}(0,1)^{d-1}$:

$$A^k_{\Delta t}(\hat{w}^k, \psi) = \sum_{m\in\mathfrak{M}} \int_0^1 (\gamma_m + D_m \Delta t) \partial_z \hat{w}^k_m \partial_z \psi_m + \hat{w}^k_m \psi_m - \sum_{j\in\mathfrak{M}} E_{m01j}(\phi^{k-1}) \hat{w}^k_j \partial_z \psi_m \mathrm{d}z.$$

Unfortunately, this bilinear form is used in the equation

$$
\begin{aligned}
A^k_{\Delta t}(\hat{w}^k,\psi) &= A^k_{\Delta t}(w^{k-1},\psi) - A^k_{\Delta t}\left(\hat{c}^k(z),\psi\right)\\
&\quad + \sum_{m\in\mathfrak{M}}\left[(\gamma_m + D_m\Delta t)(\partial_z \hat{w}^k_m)\psi_m - \sum_{j\in\mathfrak{M}} E_{m01j}(\phi^{k-1})\hat{w}^k_j\psi_m\right]_0^1\\
&\quad + \sum_{m\in\mathfrak{M}}\left[(\gamma_m + D_m\Delta t)(\partial_z \hat{c}^k_m)\psi_m - \sum_{j\in\mathfrak{M}} E_{m01j}(\phi^{k-1})\hat{c}^k_j\psi_m\right]_0^1\\
&\quad - \sum_{m\in\mathfrak{M}}\left[\gamma_m(\partial_z w^{k-1}_m)\psi_m - \sum_{j\in\mathfrak{M}} E_{m01j}(\phi^{k-1})w^{k-1}_m\psi_m\right]_0^1\\
&\quad + \Delta t\sum_{m\in\mathfrak{M}}\int_0^1 G_{w,m}(\phi^{k-1})\psi_m - F_m(\phi^{k-1})v^{k-1}\psi_m + \sum_{j\in\mathfrak{M}}\sum_{i=0}^{1} E_{mi0j}\partial_z^i w_j^{k-1}\partial_z\psi_m \mathrm{d}z\\
&\quad - \Delta t\sum_{m\in\mathfrak{M}}\left[\sum_{j\in\mathfrak{M}}\sum_{i=0}^{1} E_{mi0j}\partial_z^i w_j^{k-1}\psi_m\right]_0^1\\
&= \sum_{m\in\mathfrak{M}}\left[(\gamma_m + D_m\Delta t)(\partial_z \hat{w}^k_m)\psi_m - \sum_{j\in\mathfrak{M}} E_{m01j}(\phi^{k-1})\hat{w}^k_j\psi_m\right]_0^1 + \mathfrak{F}^k(\psi),
\end{aligned}
$$

which has a right-hand-side that violates the conditions of Lax-Milgram. However, we can create a new bilinear form $a^k_{\Delta t}(\hat{w}^k_m,\psi)$ on $H^1_{0,free}(0,1)^{d-1}$ such that we can apply Lax-Milgram. Due to the behaviour of elements of $\hat{\mathfrak{W}}$ on the boundary of $(0,1)$, we obtain

$$
\begin{aligned}
a^k_{\Delta t}(\hat{w}^k,\psi) = A^k_{\Delta t}(\hat{w}^k,\psi) &- \sum_{m\in\mathfrak{M}}(\gamma_m + D_m\Delta t)A_m\int_0^1 \partial_z(\hat{w}^k_m\psi_m)\mathrm{d}z\\
&+ \sum_{m\in\mathfrak{M}}\sum_{j\in\mathfrak{M}} E_{m01j}(\phi^{k-1}(1))\int_0^1 \partial_z(\hat{w}^k_j\psi_m)\mathrm{d}z = \mathfrak{F}^k(\psi). \quad (31)
\end{aligned}
$$

Remark that the trace $\phi^{k-1}(1)$ exists due to $\phi^{k-1}\in H^1(0,1)$.
The continuity of $a^k_{\Delta t}(\hat{w},\psi)$ and $\mathfrak{F}^k(\psi)$ is straightforward. The coercivity of $a^k_{\Delta t}(\hat{w},\psi)$ is equivalent to the conditions

$$
\begin{aligned}
&0 < 1 - \sum_{j\in\mathfrak{M}} E_{j01m}\frac{\eta_{j01m1}}{2},\\
&0 < \gamma_m(1-|A_m|) - \frac{1}{2}\sum_{j\in\mathfrak{M}}\left(\frac{E_{m01j}}{\eta_{m01j1}} + \frac{E_{m01j}}{\eta_{m01j2}} + E_{j01m}\eta_{j01m2}\right),
\end{aligned}
$$

for $\eta_{m01j1},\eta_{m01j2} > 0$, which follow from conditions (ii), (viii) and (ix) in Assumption 1 if E_{m01j}, γ_m and A_m satisfy condition (iii) in Assumption 1.
Thus Lax-Milgram gives a unique solution $\hat{w}^k \in H^1_{0,free}(0,1)^{d-1}$. By the coercivity, we obtain again via proposition 8.3 of [6] that $\hat{w}^k\in H^2(0,1)^{d-1}$. Applying a partial integration

to (31), we see that equation (8c) with boundary conditions (4b) can only be satisfied if $\hat{w}^k \in \hat{\mathfrak{W}}$. Hence, there is a unique weak solution $w^k \in H^2(0,1)^{d-1}$. Thus induction gives us that there is a unique weak solution $w^k \in H^2(0,1)^{d-1}$ for all $t_k \in [0,T]$.

B Derivation of discrete-time quadratic inequalities

In the derivation of the quadratic inequalities (12), (13), (11), we use the following identities

$$2(a-b)a = a^2 - b^2 + (a-b)^2, \tag{33a}$$
$$2(a-b)b = a^2 - b^2 - (a-b)^2, \tag{33b}$$

which are valid for all $a, b \in \mathbf{R}$.

The quadratic inequality (12) is obtained by testing Equation (8a) with ϕ_l, partially integrating the Laplacian terms, and using Young's inequality, leading to the following identities for the "b"-coefficients, where $\eta_1, \eta_2, \eta_{3n}, \eta_{lijm}, \eta_{l1jmn} > 0$.

$$\begin{aligned}
b_{1l} &= 2\delta_l, & b_{6ln} &= \eta_{3n} + \sum_{m\in\mathfrak{M}}\sum_{j=0}^{1}\eta_{l1jmn},\\
b_{2l}(\Delta t) &= \Delta t, & b_{7l0m} &= \frac{B_{l00m}^2}{\eta_{l00m}} + \sum_{n\in\mathfrak{L}}\frac{4B_{l10m}^2}{\eta_{l10mn}},\\
b_{3l} &= \frac{G_{\phi,l}^2}{\eta_1}, & b_{7l1m} &= \frac{B_{l10m}^2}{\eta_{l10m}},\\
b_{4l} &= \frac{4I_l^2\Gamma^2}{\eta_2} + I_l^2\Gamma^2\sum_{n\in\mathfrak{L}}\frac{1}{\eta_{3n}}, & b_{8l0m} &= \frac{B_{l01m}^2}{\eta_{l01m}} + \sum_{n\in\mathfrak{L}}\frac{4B_{l11m}^2}{\eta_{l11mn}},\\
b_{5l} &= \eta_1 + \eta_2 + \sum_{m\in\mathfrak{M}}\sum_{i,j=0}^{1}\eta_{lijm}, & b_{8l1m} &= \frac{B_{l11m}^2}{\eta_{l11m}}.
\end{aligned} \tag{34}$$

Similarly, the quadratic inequality (13) is obtained by testing Equation (8a) with $\mathcal{D}_{\Delta t}^k(\phi_l)$, partially integrating the Laplacian terms, and using Young's inequality, leading to the following identities for the "c"-coefficients, where $\eta_1, \eta_2, \eta_{3n}, \eta_{lijm}, \eta_{l1jmn} > 0$.

$$\begin{aligned}
c_{1l} &= \frac{2}{\delta_l}, \quad c_{5l} = \frac{2}{\delta_l}\Bigg(\eta_1 + \eta_2 + \sum_{n\in\mathcal{L}}\eta_{3n}\\
&\qquad + \sum_{n\in\mathcal{L}}\sum_{m\in\mathfrak{M}}\sum_{j=0}^{1}\eta_{l1jmn} + \sum_{m\in\mathfrak{M}}\sum_{j=0}^{1}\sum_{i=0}^{1}\eta_{lijm}\Bigg),\\
c_{2l}(\Delta t) &= \Delta t, \quad c_{6l}^k = \sum_{n\in\mathcal{L}}\Bigg[\frac{2I_l^2\Gamma^2}{\delta_l\eta_{3n}}\|\partial_z v^{k-1}\|_{L^2}^2 + \sum_{m\in\mathfrak{M}}\Bigg[\frac{2B_{l10m}^2C_{1,0}^2}{\delta_l\eta_{l10mn}}\|w_m^{k-1}\|_{H^1}^2\\
&\qquad + \frac{2B_{l11m}^2C_{1,0}^2}{\delta_l\eta_{l11mn}}\left\|\mathcal{D}_{\Delta t}^k(w_m)\right\|_{H^1}^2\Bigg]\Bigg],\\
c_3 &= \frac{G_{\phi,l}^2}{2\delta_l\eta_1}, \quad c_{7im} = \frac{B_{li0m}^2}{2\delta_l\eta_{li0m}},\\
c_4 &= \frac{I_l^2\Gamma^2}{2\delta_l\eta_2}, \quad c_{8im} = \frac{B_{li1m}^2}{2\delta_l\eta_{li1m}}.
\end{aligned} \tag{35}$$

Note that

$$\sum_{t_k\in[0,T]} c_{6l}^k \Delta t \le \sum_{n\in\mathfrak{L}} \left[\frac{2I_l^2\Gamma^2}{\delta_l \eta_{3n}} V^2 + \sum_{m\in\mathfrak{M}} \left[\frac{2B_{l10m}^2 C_{1,0}^2}{\delta_l \eta_{l10mn}} \left(\sum_{t_k\in[0,T]} \|w_m^{k-1}\|_{H^1}^2 \Delta t \right) + \frac{2B_{l11m}^2 C_{1,0}^2}{\delta_l \eta_{l11mn}} \left(\sum_{t_k\in[0,T]} \left\| \mathcal{D}_{\Delta t}^k(w_m) \right\|_{H^1}^2 \Delta t \right) \right] \right]$$

$$= c_{6l1} V^2 + \sum_{m\in\mathfrak{M}} \left[c_{6l2m} \left(\sum_{t_k\in[0,T]} \|w_m^{k-1}\|_{H^1}^2 \Delta t \right) + c_{6l3m} \left(\sum_{t_k\in[0,T]} \left\| \mathcal{D}_{\Delta t}^k(w_m) \right\|_{H^1}^2 \Delta t \right) \right]. \quad (36)$$

The quadratic inequality (11) is not so easy to obtain. First, we rewrite Equation (8c) into a more structured form:

$$\mathcal{D}_{\Delta t}^k(w_m) - \partial_z \mathbb{S}_m^k = G_{w,m}(\phi^{k-1}) - F_m(\phi^{k-1}) v^{k-1}, \quad (37)$$

where $\mathbb{S}_m^k = \mathbb{S}_{m0}^k + \mathbb{S}_{m1}^k$ is given by

$$\begin{cases} \mathbb{S}_{m0}^k = -\sum_{j\in\mathfrak{M}} \left[E_{m00j}(\phi^{k-1}) w_j^{k-1} + E_{m01j}(\phi^{k-1}) \mathcal{D}_{\Delta t}^k(w_j) \right], \\ \mathbb{S}_{m1}^k = D_m \partial_z w_m^k + \gamma_m \mathcal{D}_{\Delta t}^k(\partial_z w_m) - \sum_{j\in\mathfrak{M}} E_{mi0j}(\phi^{k-1}) \partial_z w_j^{k-1}, \end{cases}$$

a term with boundary evaluations at only $z = 0$, $\mathbb{S}_{m0}^k$, and a term with boundary evaluations at only $z = 1$, $\mathbb{S}_{m1}^k$. Second, we test Equation (37) with both w_m^k and $\mathcal{D}_{\Delta t}^k(w_m)$, apply a partial integration to the $\partial_z \mathbb{S}_m^k$ term, obtain two quadratic inequalities and sum them. The partial integration of the $\partial_z \mathbb{S}_m^k$ term yields a boundary evaluation, which we can bound:

$$\left| \left[\mathbb{S}_m^k \psi \right]_0^1 \right| \le \left| \mathbb{S}_m^k(1) - \mathbb{S}_m^k(0) \right| |\psi(0)| + \left[\left| \mathbb{S}_{m0}^k(0) \right| + \left| \mathbb{S}_{m1}^k(1) \right| + \left| \mathbb{S}_{m0}^k(1) - \mathbb{S}_{m0}^k(0) \right| \right] \|\partial_z \psi\|_{L^2},$$

where we use the following bounds

$$\begin{aligned} \left| \mathbb{S}_m^k(1) - \mathbb{S}_m^k(0) \right| &\le \|\mathcal{D}_{\Delta t}^k(w_m)\|_{L^2} + G_{w,m} + F_m \|v^{k-1}\|_{L^2}, \\ \left| \mathbb{S}_{m0}^k(0) \right| &\le \sum_{j\in\mathfrak{M}} \frac{\hat{J}_j \phi_{j,res}}{H_{\phi_{\min}}} \left[E_{m00j} T + E_{m01j} \right], \\ \left| \mathbb{S}_{m1}^k(1) \right| &\le |A_m| (\gamma_m + D_m T) \left[\frac{\hat{J}_m \phi_{m,res}}{H_{\phi_{\min}}} + \frac{\hat{J}_d \phi_{d,res}}{\Gamma_{\phi_{\min}}} \right] \\ &\quad + D_m |A_m| \left[|\mathcal{W}^0| + V\sqrt{T} \right] + \gamma_m |A_m| \left[\|\mathcal{D}_{\Delta t}^k(\partial_z w_m)\|_{L^2} + \|\partial_z v^{k-1}\|_{L^2} \right], \\ \left| \mathbb{S}_{m0}^k(1) - \mathbb{S}_{m0}^k(0) \right| &\le \sum_{j\in\mathfrak{M}} \left[E_{m00j} \|\partial_z w_j^{k-1}\|_{L^2} + E_{m01j} \|\mathcal{D}_{\Delta t}^k(\partial_z w_j)\|_{L^2} \right. \\ &\quad \left. + \frac{\hat{J}_j \phi_{j,res}}{H_{\phi_{\min}}} \left(E_{m00j} T + E_{m01j} \right) \right]. \end{aligned}$$

With the above bounds, we can test Equation (37) with both w_m^k and $\mathcal{D}_{\Delta t}^k(w_m)$, apply Young's inequality and sum the two inequalities. This leads to the following identities for the 'a'-coefficients with all η's positive:

$$
\begin{aligned}
a_{1m} &= \gamma_m + D_m, \qquad (38)\\
a_{2m}(\Delta t) &= 2 + \Delta t,\\
a_{3m}(\Delta t) &= 2\gamma_m + (\gamma_m + D_m)\Delta t,\\
a_4 &= D_m^2|A_m|^2|\mathcal{W}^0|^2\left(\frac{1}{\eta_{m8}} + \frac{1}{\eta_{am8}}\right) + D_m^2|A_m|^2V^2T\left(\frac{1}{\eta_{m9}} + \frac{1}{\eta_{am9}}\right)\\
&\quad + G_{w,m}^2\left(\frac{1}{\eta_{m1}} + \frac{1}{\eta_{am1}}\right) + \left(\frac{\hat{J}_m\phi_{m,res}}{H_{\phi_{\min}}}T\right)^2\left(\frac{1}{\eta_{m3}} + \eta_0 + \frac{1}{\eta_{am3}} + \eta_{a0}\right)\\
&\quad + \left(\sum_{j\in\mathfrak{M}}\frac{\hat{J}_j\phi_{j,res}}{H_{\phi_{\min}}}(E_{m00j}T + E_{m01j})\right)^2\left(\frac{4}{\eta_{m4}} + \frac{4}{\eta_{am4}}\right)\\
&\quad + \left(\frac{\hat{J}_m\phi_{m,res}}{H_{\phi_{\min}}} + \frac{\hat{J}_d\phi_{d,res}}{\Gamma_{\phi_{\min}}}\right)^2(D_mT + \gamma_m)^2|A_m|^2\left(\frac{1}{\eta_{m5}} + \frac{1}{\eta_{am5}}\right)\\
&\quad + 2G_{w,m}\frac{\hat{J}_m\phi_{m,res}}{H_{\phi_{\min}}}(T+1),\\
a_{5m} &= \eta_{m1} + \eta_{m2},\\
a_{6m} &= \max\left\{0, \sum_{i=4}^{9}\eta_{mi} - 2D_m(1 - |A_m|) + \frac{D_m^2|A_m|^2}{\eta_{am6}}\right.\\
&\qquad \left. + \sum_{j\in\mathcal{M}}(\eta_{m00j} + \eta_{m10j} + \eta_{m01j} + \eta_{m00j1} + \eta_{m01j1})\right\},\\
a_{7m} &= \sum_{j\in\mathfrak{M}} E_{j00m}^2\left(\frac{1}{\eta_{j00m}} + \frac{1}{\eta_{aj00m}}\right),\\
a_{8m} &= \sum_{j\in\mathfrak{M}}\left[E_{j10m}^2\left(\frac{1}{\eta_{j10m}} + \frac{1}{\eta_{aj10m}}\right) + E_{j00m}^2\left(\frac{1}{\eta_{j00m1}} + \frac{1}{\eta_{aj00m1}}\right)\right],\\
a_{9m} &= \eta_{m3} + \eta_{am3} + \sum_{j\in\mathfrak{M}}\left(\frac{E_{j01m}^2}{\eta_{j01m}} + E_{j01m}\eta_{aj01m}\right),\\
a_{10m} &= \frac{\gamma_m^2|A_m|^2}{\eta_{m6}} + 2\gamma_m|A_m| + \eta_{am1} + \eta_{am2} + \sum_{i=4}^{9}\eta_{ami}\\
&\quad + \sum_{j\in\mathfrak{M}}\left(\frac{E_{j01m}^2}{\eta_{j01m1}} + \eta_{am00j1} + \eta_{am00j} + \eta_{am10j}\right)\\
&\quad + \sum_{j\in\mathfrak{M}}\left(\frac{E_{m01j}}{\eta_{am01j}} + \frac{E_{j01m}}{\eta_{aj01m1}} + E_{m01j}\eta_{am01j1}\right),\\
a_{11} &= F_m^2\left(\frac{1}{\eta_0} + \frac{1}{\eta_{m2}} + \frac{1}{\eta_{a0}} + \frac{1}{\eta_{am2}}\right),\\
a_{12} &= \gamma_m^2|A_m|^2\left(\frac{1}{\eta_{m7}} + \frac{1}{\eta_{am7}}\right).
\end{aligned}
$$

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