A $P^1 - P^0$ FINITE ELEMENT METHOD FOR A MODEL OF POLYMER CRYSTALLIZATION*

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Abstract. We consider a practical finite element approximation of a 3D model for the crystallization of polymers. The model is a system consisting of a parabolic PDE for the thermal balance coupled with several nonlinear ODEs for the crystallization kinetics. The isokinetic assumption implies a non-Lipschitz continuous dependence of the kinetic equations on the crystalline volume fraction. Piecewise linear elements are used for temperature and piecewise constants for the kinetic variables. The numerical algorithm is simple, easy to implement on a computer, and a linear system with the same symmetric positive definite matrix has to be solved per time step. We prove optimal linear $L^\infty L^1$ a priori error estimates in terms of both discretization parameters, using monotonicity and L^1 techniques. A relevant simulation in 3D with axial symmetry shows qualitative agreement of the mathematical model with experimental results.

Key words. polymer crystallization, parabolic equations, finite elements, error estimates

AMS subject classification. 80A22, 65M60, 65M15, 35K55, 35Q80.

1. Introduction.

This paper examines a practical finite element method for a 3D model of crystallization of polymers, which was introduced in [4] and further studied in [5,17]. For 3-dimensional growth, the model couples the thermal balance equation (heat equation) with a system of non-Lipschitz ODEs for the crystallization kinetics, which models the growth of the crystalline phase in terms of (averaged) number and sizes of crystals.

Assuming that the polymer fills a (smooth) bounded domain $\Omega \subset \mathbb{R}^3$, and setting $\Omega_{t^*} = \Omega \times (0, t^*)$ for $t^* > 0$, the heat equation in Ω_{t^*} takes the form

$$c\rho\partial_t T - k\Delta T = \lambda\rho\partial_t\chi, \tag{1.1}$$

where T is the temperature, c the specific heat, ρ the density, and k the thermal conductivity. Moreover, λ is the latent heat of crystallization per unit of mass, and χ is the crystalline volume fraction, $\chi \in [0,1]$. The term $\lambda\rho\partial_t\chi$ represents the heat released by the crystallization process. The system of ODEs for the crystallization kinetics in Ω_{t^*} reads

$$\partial_t\chi = 4G(T)(1-\chi)^\beta M_2, \tag{1.2}$$

$$\partial_t M_2 = \pi G(T)(1-\chi)^\beta M_1, \tag{1.3}$$

$$\partial_t M_1 = 2G(T)(1-\chi)^\beta M_0, \tag{1.4}$$

$$\partial_t M_0 = F(T)(1-\chi)^\beta, \tag{1.5}$$

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where $0 < \beta < 1$ depends on the polymeric species. The variables M_i have the following geometrical meaning: M_0 is the number of crystals (assumed to be spherical) per unit of volume, while $4M_2/M_0$ and M_1/M_0 are the averaged surface area and the averaged diameter of the crystals, respectively. The factors G and F are non-negative growth rate coefficients, typically vanishing outside a finite temperature range, so that crystallization can take place only if T belongs to such a range. The corrective term $(1-\chi)^\beta$ slows down the crystal growth as χ approaches $\chi = 1$, which accounts for the effect of impingement, namely collisions between expanding crystals. This obviously becomes more significant as the crystalline fraction increases, and so the non-Lipschitz structure of $(1-\chi)^\beta$ may allow χ to reach the value $\chi = 1$ in a finite time. However we do not expect, in general, the crystallization to be complete (i.e., $\chi = 1$), after T has dropped below the crystallization temperature range. Instead, the asymptotic value of χ will be determined by the history of the process.

The PDE (1.1) must be supplied with suitable initial and boundary conditions, namely

$$T(\cdot, 0) = T_0(\cdot) \quad \text{in } \Omega, \tag{1.6}$$

$$-k\partial_\nu T = H(T - T_a) \quad \text{on } \Sigma_{t^*} = \partial\Omega \times (0, t^*), \tag{1.7}$$

whereas vanishing initial conditions are given for the ODEs (1.2)-(1.5)

$$\chi(\cdot, 0) = M_2(\cdot, 0) = M_1(\cdot, 0) = M_0(\cdot, 0) = 0 \quad \text{in } \Omega. \tag{1.8}$$

Both existence and continuous dependence on the data of a weak solution to the problem introduced above have been proved in [5], using the monotonicity intrinsic to (1.1)-(1.8), to by-pass the lack of smoothness, combined with classical L^1 techniques.

We refer to [3,4,12,14,16,17], and to the references quoted therein, for further discussion of the physical phenomenon and of the model, as well as of related models. Let us focus here on the parameter β. The identification of the value of β has been undertaken either by means of comparison with experimental data or by theoretical approach [1,16,17]. It turns out that, invoking the isokinetic assumption along with the Hoffman theory of regimes of crystallization [12], values $\beta < 1$ are predicted [17]. Also, in [2] the classical model of Avrami [6,7,8] is shown to be approximated by the model investigated here for values $\beta \simeq 0.7$. Therefore, it seems interesting to consider (1.1)-(1.8) for $\beta \in (0, 1)$.

We study a $P^1 - P^0$ finite element approximation of problem (1.1)-(1.8). The ODEs (1.2)-(1.5), being space independent, are discretized with piecewise constant elements in space and advanced explicitly in time. This entails an elementwise algebraic calculation per time step, and is equivalent to assuming an isothermal crystallization over small time intervals. The heat equation (1.1) is instead discretized implicitly, which guarantees the scheme to be inconditionally stable. The corresponding space discretization of (1.1) is based on piecewise linear finite elements and leads to a symmetric positive definite linear system, which is solved with a preconditioned conjugate gradient method. The resulting numerical algorithm is simple and effective [17]. Our primary goal here is to prove *optimal* first-order a priori error estimates in $L^\infty(0,t^*;L^1(\Omega))$ for all discrete variables. The main difficulty is the lack of regularity associated with the non-Lipschitz structure of the ODEs. We compensate with discrete monotonicity. A special parabolic duality argument is also used to deal with $L^1(\Omega)$, a non-standard space in the finite element literature.

In §2 we introduce the discrete problem along with notation. Essential discrete properties, such as monotonicity, are discussed in §3. In §4 we derive basic stability estimates for the fully discrete problem. They are subsequently applied in §5 to prove error estimates. A relevant simulation in 3D with axial symmetry, which shows qualitative agreement of the mathematical model with experimental results, is presented in §6. Conclusions are finally drawn in §7.

2. Fully Discrete Model. The following regularity properties will be assumed

$$c,\rho,k,\lambda\in(0,+\infty),\quad 0<\beta<1, \tag{2.1}$$

$$G,F\geq 0,\quad G,F\in W^1_\infty(\mathbb{R}),\quad \tfrac{F(s)}{G(s)}\leq\mu\ \ \forall\, s\geq 0, \tag{2.2}$$

$$T_0\in H^3(\Omega),\quad T_0\geq 0, \tag{2.3}$$

$$\begin{aligned}&T_a\in W^2_1(0,t^*;L^2(\partial\Omega))\cap H^1(0,t^*;H^{1/2}(\partial\Omega))\cap L^\infty(0,t^*;H^{3/2}(\partial\Omega))\\ &\quad\cap W^1_1(0,t^*;W^1_\infty(\partial\Omega)),\quad T_a\geq 0,\end{aligned} \tag{2.4}$$

$$-k\partial_\nu T_0=H(T_0-T_a)\quad \text{at } \partial\Omega\times\{0\}, \tag{2.5}$$

$$H\in W^1_\infty(\partial\Omega),\quad H\geq 0. \tag{2.6}$$

In view of (2.4) and (2.6) we may consider T_a and H extended in Ω to functions $T_a\in W^1_1(0,t^*;W^1_\infty(\Omega))$ and $H\in W^1_\infty(\Omega)$. We denote by L_f the Lipschitz constant of any function f, and by C_f the L^∞ norm of f (whenever such quantities are finite). We also indicate by γ a positive constant depending on the data, that may change at the various occurrences; in particular, γ will be independent of the discretization parameters τ and h. We denote by $\langle\cdot,\cdot\rangle$ the inner product in $L^2(\Omega)$ and by $\langle\!\langle\cdot,\cdot\rangle\!\rangle$ the inner product in $L^2(\partial\Omega)$.

We consider the following weak formulation of problem (1.1)-(1.8): *Find*

$$T\in H^1(0,t^*;L^2(\Omega))\cap L^2(0,t^*;H^2(\Omega))\cap L^\infty(\Omega_{t^*}), \tag{2.7}$$

$$\chi,M_0,M_1,M_2\in W^1_\infty(0,t^*;L^\infty(\Omega)), \tag{2.8}$$

such that (1.6) *and* (1.8) *hold a.e. in* Ω, (1.2)-(1.5) *are fulfilled a.e. in* Ω_{t^*}, *and for a.e.* $t\in(0,t^*)$ *and for all* $\varphi\in H^1(\Omega)$ *it holds*

$$c\rho\langle\partial_t T,\varphi\rangle+k\langle\nabla T,\nabla\varphi\rangle+\langle\!\langle H(T-T_a),\varphi\rangle\!\rangle=\lambda\rho\langle\partial_t\chi,\varphi\rangle. \tag{2.9}$$

Note that the initial conditions (1.6) and (1.8) are meaningful because $H^1(0,t^*;L^2(\Omega))\cap L^2(0,t^*;H^2(\Omega))\subset C^0([0,t^*];H^1(\Omega))$ [15]. Existence and uniqueness of the weak solution have been proved in [5], along with the extra regularity

$$\partial_{tt}T,\ \ \partial_{tx_jx_l}T,\ \ \partial_{tt}\chi,\ \ \partial_{tt}M_i\in L^p(0,t^*;L^p(\Omega)),\quad i=0,1,2,\ \ j,l=1,2,3, \tag{2.10}$$

for all $1<p<\frac{1-\beta}{1-2\beta}$ if $0<\beta\leq\frac{1}{3}$ and $p=2$ if $\frac{1}{3}<\beta<1$. In particular

$$T\in L^\infty(0,t^*;W^2_p(\Omega))\cap W^1_\infty(0,t^*;L^p(\Omega)). \tag{2.11}$$

All variables exhibit Lipschitz dependence in $L^\infty(0,t^*;L^1(\Omega))$ with respect to data [5]. This strongly suggests that the error analysis is to be carried out in $L^\infty(0,t^*;L^1(\Omega))$, a non-standard Banach space in the finite element literature.

Let $\{\mathcal{S}_h\}_h$ be a family of regular partitions of Ω into simplexes [10, p.132]; as usual $h>0$ stands for the meshsize. We assume, for simplicity, that $\overline{\Omega}=\Omega_h=\cup_{S\in\mathcal{S}_h}S$. Since quasi-uniformity [10, p.140] is not required, local refinements are allowed. In addition we assume $\mathcal{S}_h$ is acute, which guarantees the validity of the discrete maximum principle and helps compensate for the lack of regularity in several occasions [11].

The finite element spaces we deal with are $V_h^1\subset W^1_\infty(\Omega)$ and $V_h^0\subset L^\infty(\Omega)$ given by

$$V_h^1|_S=P^1(S),\quad V_h^0|_S=P^0(S),\quad \forall\ S\in\mathcal{S}_h.$$

Let $\{x_S\}_{S\in\mathcal{S}_h}$ be the barycentres of $\mathcal{S}_h$. Let $\{\phi_j\}_{j=1}^J$ denote the canonical basis of V_h^1 and $\{\psi_k\}_{k=1}^K$ the canonical basis of V_h^0. Let Π_h be the local Lagrange interpolation operator $\Pi_h|_S:C^0(S)\to P^1(S)$ for all $S\in\mathcal{S}_h$. We associate with $\langle\cdot,\cdot\rangle$ and $\langle\!\langle\cdot,\cdot\rangle\!\rangle$ discrete bilinear forms which, for piecewise uniformly continuous functions ζ and ϕ, are defined by

$$\langle\zeta,\phi\rangle_h=\sum_{S\in\mathcal{S}_h}\int_S\Pi_h|_S(\zeta\phi)dx,\quad \langle\!\langle\zeta,\phi\rangle\!\rangle_h=\sum_{S\in\mathcal{S}_h}\int_{S\cap\partial\Omega}\Pi_h|_S(\zeta\phi)d\sigma.$$

Note that $\langle\zeta,\phi\rangle_h$ and $\langle\!\langle\zeta,\phi\rangle\!\rangle_h$ can be evaluated elementwisely by the vertex quadrature rule, which is exact for piecewise linear functions [10]. We can define the following stiffness and mass matrices:

$$\mathbf{K}=\left\{k\langle\nabla\phi_j,\nabla\phi_l\rangle\right\}_{j,l=1}^J,\quad \mathbf{M}=\left\{c\rho\langle\phi_j,\phi_l\rangle_h\right\}_{j,l=1}^J,$$
$$\mathbf{B}=\left\{\langle\!\langle H\phi_j,\phi_l\rangle\!\rangle_h\right\}_{j,l=1}^J,\quad \mathbf{N}=\left\{\lambda\rho\langle\phi_j,\psi_k\rangle\right\}_{j=1,k=1}^{J\quad K}.$$

Note that $\mathbf{K}$ is symmetric and positive definite, whereas $\mathbf{M}$ and $\mathbf{B}$ are diagonal.

We finally denote by $\tau=\frac{t^*}{N}$ the (uniform) time step; hereafter $N\geq 1$ indicates the number of time steps.

The fully discrete approximations to problem (1.1)-(1.8) read as follows: *Set*

$$T_h^0 = \Pi_h T_0, \quad \chi_h^0 = M_{2h}^0 = M_{1h}^0 = M_{0h}^0 = 0 \quad \text{in } \Omega$$

and, for any $1 \le n \le N$, *find* $T_h^n \in V_h^1$ *and* $\chi_h^n, M_{2h}^n, M_{1h}^n, M_{0h}^n \in V_h^0$ *such that*

$$c\rho\langle T_h^n - T_h^{n-1}, \phi\rangle_h + k\tau\langle \nabla T_h^n, \nabla\phi\rangle + \tau\langle\!\langle H(T_h^n - T_a^n), \phi\rangle\!\rangle_h = \lambda\rho\langle \chi_h^n - \chi_h^{n-1}, \phi\rangle \tag{2.12}$$

for all $\phi \in V_h^1$ *and, on each element* $S \in \mathcal{S}_h$,

$$\chi_h^n = \min\left(1, \chi_h^{n-1} + 4\tau G(T_h^{n-1}(x_S))(1-\chi_h^{n-1})^\beta M_{2h}^{n-1}\right), \tag{2.13}$$

$$M_{2h}^n = M_{2h}^{n-1} + \pi\tau G(T_h^{n-1}(x_S))(1-\chi_h^{n-1})^\beta M_{1h}^{n-1}, \tag{2.14}$$

$$M_{1h}^n = M_{1h}^{n-1} + 2\tau G(T_h^{n-1}(x_S))(1-\chi_h^{n-1})^\beta M_{0h}^{n-1}, \tag{2.15}$$

$$M_{0h}^n = M_{0h}^{n-1} + \tau F(T_h^{n-1}(x_S))(1-\chi_h^{n-1})^\beta. \tag{2.16}$$

Existence and uniqueness of the discrete solution $\{(T_h^n, \chi_h^n, M_{2h}^n, M_{1h}^n, M_{0h}^n)\}_{0\le n\le N}$ are obvious. In fact, (2.13)-(2.16) can be solved elementwise explicitly for χ_h^n and M_{ih}^n, $i = 2, 1, 0$, in terms of the solution at previous time step $(T_h^{n-1}, \chi_h^{n-1}, M_{2h}^{n-1}, M_{1h}^{n-1}, M_{0h}^{n-1})$, whereas (2.12) reduces to the symmetric positive definite linear system:

$$(\mathbf{M} + \tau\mathbf{K} + \tau\mathbf{B})T_h^n = \mathbf{M}T_h^{n-1} + \mathbf{N}(\chi_h^n - \chi_h^{n-1}) + \tau\mathbf{B}T_a^n,$$

whose matrix is invariant in time. This algebraic problem is solved via a conjugate gradient method preconditioned with an incomplete Choleski factorization. Note the truncation $\min(1, \cdot)$ used in (2.13), so that

$$0 \le \chi_h^n \le 1 \quad \forall\, S \in \mathcal{S}_h, \;\; \forall\, 1 \le n \le N.$$

3. Preliminary Properties. The following simple lemma is the crucial tool used in [5] for proving Lipschitz dependence and will be instrumental also in our numerical analysis.

LEMMA 3.1. *Assume* (2.1)-(2.6). *Then for any weak solution* (T, χ, M_2, M_1, M_0) *to* (1.1)-(1.8) *and all* $\overline{\chi} \in [0,1]$ *we have*

$$|(1-\chi)^\beta - (1-\overline{\chi})^\beta| \le 4|\chi - \overline{\chi}| + 8C_G t^* M_2 |(1-\chi)^\beta - (1-\overline{\chi})^\beta| \quad \text{a.e. } (x,t) \in \Omega_{t^*}. \tag{3.1}$$

Proof. we repeat the argument of [5] for completeness. First we claim that $\chi(x,t) \ge \frac{1}{2}$ implies $M_2(x,t) \ge \frac{1}{8C_G t}$. Indeed, integrating (1.2) we have

$$4C_G \int_0^t M_2(x,s)ds \ge 4\int_0^t G(T(x,s))M_2(x,s)(1-\chi(x,s))^\beta ds = \chi(x,t) \ge \tfrac{1}{2},$$

which, employing also $\partial_t M_2 \geq 0$, i.e., $M_2(x,t) \geq M_2(x,s)$ for $s \leq t$, proves the claim. Then, if $\chi(x,t) \geq \frac{1}{2}$ it follows that

$$|(1-\chi)^\beta - (1-\overline{\chi})^\beta| \leq 8C_G t^* M_2 |(1-\chi)^\beta - (1-\overline{\chi})^\beta|. \tag{3.2}$$

It remains to consider the case $\chi(x,t) < \frac{1}{2}$. We distinguish between the cases: (i) $\overline{\chi} \geq \frac{3}{4}$, (ii) $\overline{\chi} < \frac{3}{4}$. In case (i),

$$|\chi - \overline{\chi}| \geq \tfrac{1}{4} \geq \tfrac{1}{4}|(1-\chi)^\beta - (1-\overline{\chi})^\beta|. \tag{3.3}$$

If (ii) holds, we note that, from Lagrange's mean value theorem,

$$|(1-\chi)^\beta - (1-\overline{\chi})^\beta| \leq \beta\big(\min(1-\chi, 1-\overline{\chi})\big)^{\beta-1}|\chi - \overline{\chi}| \leq 4|\chi - \overline{\chi}|. \tag{3.4}$$

Collecting (3.2)-(3.4), we obtain (3.1). $\square$

For any $0 \leq n \leq N$, set $t^n = n\tau$ and

$$f^n(\cdot) = f(\cdot, t^n), \quad \partial_t f^n(\cdot) = \partial_t f(\cdot, t^n),$$

for a given function f defined in Ω_{t^*}. If f satisfies $\partial_{tt} f \in L^1(\Omega_{t^*})$, then it easily follows

$$\sum_{n=1}^{N} \int_\Omega \big|\partial_t f^n - \tfrac{1}{\tau}(f^n - f^{n-1})\big| dx \leq \|\partial_{tt} f\|_{L^1(\Omega_{t^*})}. \tag{3.5}$$

Using the elementary identity $2a(a-b) = a^2 - b^2 + (a-b)^2$, for $a, b \in \mathbb{R}$, we get the following discrete integration by parts formulae which will be used later: for $a_n, b_n \in \mathbb{R}$,

$$2\sum_{n=1}^{m} a_n(a_n - a_{n-1}) = a_m^2 - a_0^2 + \sum_{n=1}^{m}(a_n - a_{n-1})^2 \geq a_m^2 - a_0^2, \tag{3.6}$$

$$\sum_{n=1}^{m} a_n(b_n - b_{n-1}) = a_m b_m - a_0 b_0 - \sum_{n=1}^{m}(a_n - a_{n-1})b_{n-1}. \tag{3.7}$$

We now collect some useful properties of finite elements. We first observe that $\langle\cdot,\cdot\rangle_h$ and $\langle\!\langle\cdot,\cdot\rangle\!\rangle_h$ are equivalent to $\langle\cdot,\cdot\rangle$ and $\langle\!\langle\cdot,\cdot\rangle\!\rangle$ when restricted to V_h^1, namely

$$\|\phi\|^2_{L^2(\Omega)} \leq \langle\phi,\phi\rangle_h \leq C^*\|\phi\|^2_{L^2(\Omega)}, \quad \langle\!\langle\zeta,\phi\rangle\!\rangle_h \leq C^*\|\zeta\|_{H^1(\Omega)}\|\phi\|_{H^1(\Omega)}, \quad \forall\, \zeta,\phi \in V_h^1. \tag{3.8}$$

Moreover, using a well known local estimate for the Lagrange interpolation operator Π_h, their discrepance can be bounded as follows, for all $\zeta, \phi \in V_h^1$ [19, p.260]:

$$\|\zeta\phi - \Pi_h(\zeta\phi)\|_{L^1(\Omega)} \leq C^* h \|\nabla\zeta\|_{L^1(\Omega)}\|\phi\|_{L^\infty(\Omega)}, \tag{3.9}$$

$$\|\zeta\phi - \Pi_h(\zeta\phi)\|_{L^1(\partial\Omega)} \leq \begin{cases} C^* h \|\nabla\zeta\|_{L^2(\Omega)}\|\nabla\phi\|_{L^2(\Omega)}, \\ C^* h^{3/2}\|\nabla\zeta\|_{L^\infty(\Omega)}\|\nabla\phi\|_{L^2(\Omega)}. \end{cases} \tag{3.10}$$

In deriving (3.10) we have also used the following local inverse inequality, where h_S denotes the diameter of $S \in \mathcal{S}_h$: $\|f\|_{L^1(\partial S)} \le C^* h_S^{-1} \|f\|_{L^1(S)}$ for all $f \in P^2(S)$, $S \in \mathcal{S}_h$. In addition to Π_h we will also need some projection operators associated with the above discrete spaces. The L^2-projection operator P_h^0 onto V_h^0 is defined, for all $\varphi \in L^2(\Omega)$, by

$$\langle P_h^0 \varphi, \psi \rangle = \langle \varphi, \psi \rangle \quad \forall\, \psi \in V_h^0,$$

and satisfies the following approximation property [10]:

$$\|P_h^0 \varphi - \varphi\|_{L^2(\Omega)} \le C^* h \|\varphi\|_{H^1(\Omega)} \quad \forall\, \varphi \in H^1(\Omega). \tag{3.11}$$

Note that $P_h^0 \phi|_S = \phi(x_S)$ for all $S \in \mathcal{S}_h$ and $\phi \in V_h^1$. Hence, in (2.13)-(2.16) we are using $P_h^0 T_h^{n-1}$. The Riesz projection operator R_h onto V_h^1 is defined, for all $\varphi \in H^1(\Omega)$, by

$$k\langle \nabla R_h \varphi, \nabla \phi \rangle + \langle\!\langle H R_h \varphi, \phi \rangle\!\rangle + \langle R_h \varphi, \phi \rangle = k\langle \nabla \varphi, \nabla \phi \rangle + \langle\!\langle H \varphi, \phi \rangle\!\rangle + \langle \varphi, \phi \rangle \quad \forall\, \phi \in V_h^1, \tag{3.12}$$

and satisfies the following error estimate for $\varphi \in W_p^2(\Omega)$ [9, Chapter 7]:

$$\|R_h \varphi - \varphi\|_{L^p(\Omega)} + h \|\nabla (R_h \varphi - \varphi)\|_{L^p(\Omega)} \le C^* h^2 \|\varphi\|_{W_p^2(\Omega)} \quad \forall\, 1 < p < \infty. \tag{3.13}$$

We observe that (3.13) results from the stability bound $\|R_h \varphi\|_{W_p^1(\Omega)} \le C^* \|\varphi\|_{W_p^1(\Omega)}$, which could be derived for the Robin boundary condition (1.7) invoking weighted Sobolev norms as in [9]. Since $\mathcal{S}_h$ is weakly acute, the *discrete maximum principle* holds, that is

$$\langle \nabla \phi, \nabla \phi_j \rangle \ge 0 \quad \text{if } \phi \in V_h^1 \text{ attains its maximum at the node } x_j. \tag{3.14}$$

In dealing with estimates in $L^1(\Omega)$ in §5 we will resort to a *parabolic duality* technique [13,18]. For any $1 \le m \le N$, let $\{z^n\}_{n=1}^{m+1} \subset V_h^1$ be the solution to the following dual problem: let $z^{m+1} = \zeta \in V_h^1$ be given and, for $m \ge n \ge 1$, let z^n solve

$$c\rho \langle z^{n+1} - z^n, \phi \rangle_h - k\tau \langle \nabla z^n, \nabla \phi \rangle - \tau \langle\!\langle H z^n, \phi \rangle\!\rangle_h = 0 \quad \forall\, \phi \in V_h^1. \tag{3.15}$$

It is then easy to prove the following stability result.

LEMMA 3.2. *Let $\{z^n\}_{n=1}^{m+1}$ be the solution to the dual problem* (3.15). *Then*

$$\max_{1 \le n \le m} \|z^n\|_{L^\infty(\Omega)} \le \|\zeta\|_{L^\infty(\Omega)}, \qquad \sum_{n=1}^{m} \tau \|\nabla z^n\|_{L^2(\Omega)}^2 \le C^* \tfrac{c\rho}{2k} \|\zeta\|_{L^2(\Omega)}^2. \tag{3.16}$$

Proof. Let x_M be a node such that $z^n(x_M) = \max_x z^n(x)$. Applying (3.14) for $\phi = \phi_M$, we get $\langle \nabla z^n, \nabla \phi_M \rangle \ge 0$. Since $H \ge 0$, we obtain from (3.15)

$$\max_x z^n(x) \le \left(1 + \tfrac{\tau}{c\rho} H(x_M) \frac{\oint_{\partial\Omega} \phi_M \, d\sigma}{\int_\Omega \phi_M \, dx}\right) z^n(x_M) \le \max_x z^{n+1}(x);$$

a similar argument applies to the minimum. To prove the second stability estimate, we simply take $\phi = z^n$, add over n from 1 to m, and eventually use (3.6) and (3.8). $\square$

4. Stability. We establish here some a priori estimates for the discrete solutions that will be used in §5 to derive the error estimates. Before proving L^∞ bounds, we recall that $\gamma > 0$ stands for a constant depending on data but independent of τ and h.

LEMMA 4.1. *Assume* (2.1)-(2.6) *and let* $\{(T_h^n, \chi_h^n, M_{2h}^n, M_{1h}^n, M_{0h}^n)\}_{0\le n\le N}$ *be the discrete solution to* (2.12)-(2.16). *Then we have, for all* $x \in \Omega$ *and* $1 \le n \le N$,

$$0 \le T_h^n \le \gamma, \tag{4.1}$$

$$0 \le M_{ih}^n \le \gamma, \quad i = 0, 1, 2, \tag{4.2}$$

$$0 \le \chi_h^n - \chi_h^{n-1} \le \gamma\tau, \quad 0 \le M_{ih}^n - M_{ih}^{n-1} \le \gamma\tau, \quad i = 0, 1, 2. \tag{4.3}$$

Proof. Since $0 \le \chi_h^n \le 1$, we add (2.14)-(2.16) over n from 1 to any $m \le N$, to get

$$0 \le M_{0h}^m \le C_F t^m, \quad 0 \le M_{1h}^m \le C_G C_F (t^m)^2, \quad 0 \le M_{2h}^m \le \tfrac{\pi}{3} C_G^2 C_F (t^m)^3,$$

that is (4.2). Noting that (2.13) yields

$$0 \le \chi_h^n - \chi_h^{n-1} \le 4\tau G(P_h^0 T_h^{n-1})(1 - \chi_h^{n-1})^\beta M_{2h}^{n-1} \le \tfrac{4\pi}{3} C_G^3 C_F (t^{n-1})^3 \tau, \tag{4.4}$$

inserting (4.2) into (2.14)-(2.16) we obtain (4.3). In order to prove (4.1), we assume by induction that

$$0 \le T_h^{n-1} \le \|T_0\|_{L^\infty(\Omega)} + \|T_a\|_{L^\infty(\Sigma_{t^*})} + \tfrac{\lambda}{c}\tfrac{\pi}{3} C_G^3 C_F (t^{n-1})^4 = C^{n-1}.$$

Let x_M be a node where T_h^n attains its maximum, which we may suppose to satisfy $T_h^n(x_M) > C^{n-1}$ for otherwise there is nothing to prove. Taking $\phi = \phi_M$ in (2.12), and using (3.14), it follows that

$$k\langle \nabla T_h^n, \nabla \phi_M \rangle + \langle\!\langle H(T_h^n - T_a^n), \phi_M \rangle\!\rangle_h \ge 0,$$

because $T_h^n(x_M) > C^{n-1} \ge \|T_a\|_{L^\infty(\Sigma_{t^*})}$ and $H \ge 0$. Hence, using (4.4) we get

$$T_h^n(x_M) \le T_h^{n-1}(x_M) + \tfrac{\lambda}{c}\|\chi_h^n - \chi_h^{n-1}\|_{L^\infty(\Omega)} \le C^{n-1} + \tfrac{\lambda}{c}\tfrac{4\pi}{3} C_G^3 C_F (t^{n-1})^3 \tau,$$

which yields $T_h^n(x_M) \le C^n$. Similarly we obtain $T_h^n \ge 0$. ∎

Next lemma reproduces the energy a priori estimates for the discrete temperature.

LEMMA 4.2. *Assume* (2.1)-(2.6) *and let* $\{(T_h^n, \chi_h^n, M_{2h}^n, M_{1h}^n, M_{0h}^n)\}_{0\le n\le N}$ *be the discrete solution to* (2.12)-(2.16). *Then we have*

$$\sum_{n=1}^{N} \tfrac{1}{\tau}\|T_h^n - T_h^{n-1}\|_{L^2(\Omega)}^2 + \max_{1\le n\le N} \|T_h^n\|_{H^1(\Omega)} \le \gamma. \tag{4.5}$$

Proof. We take $\phi = \frac{1}{\tau}(T_h^n - T_h^{n-1})$ in (2.12) and add the resulting expression over n from 1 to any $m \leq N$. Using (3.8) we get

$$
\begin{aligned}
c\rho \sum_{n=1}^{m} \tfrac{1}{\tau} \|T_h^n - T_h^{n-1}\|_{L^2(\Omega)}^2 + k \sum_{n=1}^{m} \langle \nabla T_h^n, \nabla(T_h^n - T_h^{n-1})\rangle + \sum_{n=1}^{m} \langle\!\langle H T_h^n, T_h^n - T_h^{n-1}\rangle\!\rangle_h \\
\leq \sum_{n=1}^{m} \langle\!\langle H T_a^n, T_h^n - T_h^{n-1}\rangle\!\rangle_h + \lambda\rho \sum_{n=1}^{n} \tfrac{1}{\tau} \langle \chi_h^n - \chi_h^{n-1}, T_h^n - T_h^{n-1}\rangle,
\end{aligned}
\tag{4.6}
$$

which can be written as I+II+III=IV+V. Now we estimate each term separately. Owing to (3.6), (3.8) and (2.3), (2.6), and noting that $H^3(\Omega) \subset C^{1,1/2}(\overline{\Omega})$ by Sobolev embedding, we have $\|T_0\|_{W_\infty^1(\Omega)} \leq \gamma$ and

$$
\begin{aligned}
\tfrac{2}{k} \mathrm{II} &\geq \|\nabla T_h^m\|_{L^2(\Omega)}^2 - \|\nabla T_h^0\|_{L^2(\Omega)}^2 \geq \|\nabla T_h^m\|_{L^2(\Omega)}^2 - \gamma, \\
2\mathrm{III} &\geq \langle\!\langle H T_h^m, T_h^m\rangle\!\rangle_h - \langle\!\langle H T_h^0, T_h^0\rangle\!\rangle_h \geq -C^* C_H \|T_h^0\|_{H^1(\Omega)}^2 \geq -\gamma.
\end{aligned}
$$

We have also used the stability property of Π_h in $W_\infty^1(\Omega)$. On using the elementary inequality $2ab \leq \varepsilon a^2 + \frac{1}{\varepsilon} b^2$, for $a, b \in \mathbb{R}$, $\varepsilon > 0$, (3.7), (3.8), and (2.3), (2.4), (2.6), we get

$$
\begin{aligned}
\mathrm{IV} &= \langle\!\langle H T_a^m, T_h^m\rangle\!\rangle_h - \langle\!\langle H T_a^0, T_h^0\rangle\!\rangle_h - \sum_{n=1}^{m} \langle\!\langle H(T_a^n - T_a^{n-1}), T_h^{n-1}\rangle\!\rangle_h \\
&\leq \|T_0\|_{W_\infty^1(\Omega)}^2 + \tfrac{1}{\varepsilon} \gamma \|T_a\|_{W_1^1(0,t^*;W_\infty^1(\Omega))}^2 + \varepsilon \max_{1 \leq n \leq m} \|T_h^n\|_{H^1(\Omega)}^2,
\end{aligned}
$$

where $\varepsilon > 0$ is to be selected. Finally, owing to the estimate for $\chi_h^n - \chi_h^{n-1}$ in (4.3),

$$
2\mathrm{V} \leq c\rho \sum_{n=1}^{m} \tfrac{1}{\tau} \|T_h^n - T_h^{n-1}\|_{L^2(\Omega)}^2 + \gamma.
$$

Now we insert the preceding estimates into (4.6). Since

$$
\max_{1 \leq n \leq m} \|T_h^n\|_{L^2(\Omega)}^2 \leq 2\|T_h^0\|_{L^2(\Omega)}^2 + 2 \sum_{n=1}^{m} \tfrac{1}{\tau} \|T_h^n - T_h^{n-1}\|_{L^2(\Omega)}^2,
$$

on selecting $\varepsilon > 0$ sufficiently small we get (4.5). $\square$

We conclude this section by proving $L^1(0, t^*; L^\infty(\Omega))$ a priori estimates for time derivatives of the discrete momenta.

LEMMA 4.3. *Assume* (2.1)-(2.6) *and let* $\{(T_h^n, \chi_h^n, M_{2h}^n, M_{1h}^n, M_{0h}^n)\}_{0\le n\le N}$ *be the discrete solution to* (2.12)-(2.16). *Then we have, for all* $x \in \Omega$ *and* $i = 0, 1, 2$,

$$\sum_{n=1}^{N} \left|(1-\chi_h^n)^\beta - (1-\chi_h^{n-1})^\beta\right| \le 1, \tag{4.7}$$

$$\sum_{n=1}^{N} \int_\Omega \left|G(P_h^0 T_h^n)(1-\chi_h^n)^\beta M_{ih}^n - G(P_h^0 T_h^{n-1})(1-\chi_h^{n-1})^\beta M_{ih}^{n-1}\right| dx \le \gamma, \tag{4.8}$$

$$\sum_{n=1}^{N} \int_\Omega \left|F(P_h^0 T_h^n)(1-\chi_h^n)^\beta - F(P_h^0 T_h^{n-1})(1-\chi_h^{n-1})^\beta\right| dx \le \gamma. \tag{4.9}$$

Proof. Since $\chi_h^{n-1} \le \chi_h^n$, we readily have (4.7) because

$$\sum_{n=1}^{N} \left|(1-\chi_h^n)^\beta - (1-\chi_h^{n-1})^\beta\right| = \sum_{n=1}^{N} \left((1-\chi_h^{n-1})^\beta - (1-\chi_h^n)^\beta\right) = 1-(1-\chi_h^N)^\beta \le 1.$$

In order to prove (4.8), for $i = 0$, we decompose the integrand as follows:

$$\begin{aligned} G(P_h^0 T_h^n)(1-\chi_h^n)^\beta M_{0h}^n &- G(P_h^0 T_h^{n-1})(1-\chi_h^{n-1})^\beta M_{0h}^{n-1} \\ &= G(P_h^0 T_h^n)\big((1-\chi_h^n)^\beta - (1-\chi_h^{n-1})^\beta\big) M_{0h}^n \\ &+ \big(G(P_h^0 T_h^n) - G(P_h^0 T_h^{n-1})\big)(1-\chi_h^{n-1})^\beta M_{0h}^n \\ &+ G(P_h^0 T_h^{n-1})(1-\chi_h^{n-1})^\beta (M_{0h}^n - M_{0h}^{n-1}), \end{aligned}$$

and then use (2.2), (4.2), (4.3), (4.5), and (4.7). The remaining estimates in (4.8) and (4.9) can be proved similarly. □

5. Error Analysis. In this section we prove a first-order error estimate between continuous and fully discrete solutions in the $L^\infty(0, t^*; L^1(\Omega))$ norm. The result is *optimal* because time discretization is based on a first-order finite difference scheme and the momenta are approximated by piecewise constant functions. The proof combines the main idea used in [5] for proving Lipschitz dependence of solutions and a parabolic duality argument used in [13,18]. The error e_W corresponding to a quantity W is defined by

$$e_W(\cdot, t) = W(\cdot, t) - W_h^n(\cdot) \quad \forall\, t \in (t^{n-1}, t^n],\ 1 \le n \le N.$$

THEOREM 5.1. *Assume* (2.1)-(2.6). *Let* (T, χ, M_2, M_1, M_0) *be the weak solution to the continuous problem* (1.1)-(1.8) *and let* $\{(T_h^n, \chi_h^n, M_{2h}^n, M_{1h}^n, M_{0h}^n)\}_{0\le n\le N}$ *be the solution to the discrete problem* (2.12)-(2.16). *Then there exists* $\gamma > 0$ *solely depending on data such that*

$$\|e_T\|_{L^\infty(0,t^*;L^1(\Omega))} + \|e_\chi\|_{L^\infty(0,t^*;L^1(\Omega))} + \sum_{i=0}^{2} \|e_{M_i}\|_{L^\infty(0,t^*;L^1(\Omega))} \le \gamma(\tau + h). \tag{5.1}$$

Proof. In view of (2.10), we first write (1.2) at time t^n as follows:

$$\chi^n - \chi^{n-1} = (\chi^n - \chi^{n-1} - \tau\partial_t\chi^n) + 4\tau G(T^n)(1-\chi^n)^\beta M_2^n \quad \text{a.e. } x \in \Omega. \tag{5.2}$$

Then we subtract $\chi_h^n - \chi_h^{n-1}$ from (5.2) and multiply the resulting equation by $\operatorname{sign}(e_\chi^n)$, where the sign function is taken to be 0 for a vanishing argument. Integrating over Ω, adding over n from 1 to any $m \le N$, and reordering, we get

$$\begin{aligned}
\sum_{n=1}^m \langle e_\chi^n - e_\chi^{n-1}, \operatorname{sign}(e_\chi^n)\rangle &= \sum_{n=1}^m \langle \chi^n - \chi^{n-1} - \tau\partial_t\chi^n, \operatorname{sign}(e_\chi^n)\rangle \\
&+ \sum_{n=1}^m \langle 4\tau G(P_h^0 T_h^{n-1})(1-\chi_h^{n-1})^\beta M_{2h}^{n-1} - (\chi_h^n - \chi_h^{n-1}), \operatorname{sign}(e_\chi^n)\rangle \\
&+ \sum_{n=1}^m \tau\langle 4G(P_h^0 T_h^n)(1-\chi_h^n)^\beta M_{2h}^n - 4G(P_h^0 T_h^{n-1})(1-\chi_h^{n-1})^\beta M_{2h}^{n-1}, \operatorname{sign}(e_\chi^n)\rangle \\
&+ \sum_{n=1}^m \tau\langle 4(G(T_h^n) - G(P_h^0 T_h^n))(1-\chi_h^n)^\beta M_{2h}^n, \operatorname{sign}(e_\chi^n)\rangle \\
&+ \sum_{n=1}^m \tau\langle 4G(T^n)(1-\chi^n)^\beta M_2^n - 4G(T_h^n)(1-\chi_h^n)^\beta M_{2h}^n, \operatorname{sign}(e_\chi^n)\rangle,
\end{aligned} \tag{5.3}$$

which we write as I=II+III+IV+V+VI. Since $e_\chi^0(\cdot) = \chi(\cdot,0) - \chi_h^0(\cdot) = 0$, we have at once

$$\mathrm{I} \ge \sum_{n=1}^m \int_\Omega \left(|e_\chi^n| - |e_\chi^{n-1}|\right) dx = \int_\Omega |e_\chi^m| dx.$$

Owing to (2.10), (3.5), and to (4.8) for $i = 2$, we readily see that

$$\mathrm{II} \le \tau\|\partial_{tt}\chi\|_{L^1(\Omega_{t^*})} \le \gamma\tau, \quad \mathrm{IV} \le \gamma\tau.$$

For a.e. $x \in \Omega$, let $n^*(x)$ be the first time step for which $\chi_h^n(x)$ reaches 1, i.e., $n^*(x) = \min\{1 \le n \le N : \ \chi_h^{n-1}(x) < \chi_h^n(x) = 1\}$, and note that $\chi_h^n(x) = 1$ for all $n \ge n^*(x)$. Then (2.13) yields

$$4\tau G\big(P_h^0 T_h^{n-1}(x)\big)\big(1-\chi_h^{n-1}(x)\big)^\beta M_{2h}^{n-1}(x) - \big(\chi_h^n(x) - \chi_h^{n-1}(x)\big) = 0$$

for all $n < n^*(x)$ and $n > n^*(x)$. This, together with (4.4), implies

$$0 \le \mathrm{III} \le \int_\Omega 4\tau G(P_h^0 T_h^{n^*-1})(1-\chi_h^{n^*-1})^\beta M_{2h}^{n^*-1} dx \le \gamma\tau.$$

Using (3.11), (4.2), and (4.5) we infer that

$$\mathrm{V} \leq \sum_{n=1}^{m} \tau 4 L_G \|M_{2h}^n\|_{L^\infty(\Omega)} \|T_h^n - P_h^0 T_h^n\|_{L^1(\Omega)} \leq \gamma h.$$

Finally, we set

$$e_\beta(t) = \big(1-\chi(t)\big)^\beta - (1-\chi_h^n)^\beta \quad \text{for } t \in (t^{n-1}, t^n],\ \ 1 \leq n \leq N,$$

and note that monotonicity yields $e_\beta^n \operatorname{sign}(e_\chi^n) = -|e_\beta^n|$. Then, owing to (2.2), (2.8), and positivity of M_2, we can write

$$\begin{aligned}
\mathrm{VI} &= \sum_{n=1}^{m} \tau \langle 4G(T^n) M_2^n e_\beta^n, \operatorname{sign}(e_\chi^n)\rangle \\
&\quad + \sum_{n=1}^{m} \tau \langle 4\big(G(T^n) - G(T_h^n)\big) M_2^n (1-\chi_h^n)^\beta, \operatorname{sign}(e_\chi^n)\rangle \\
&\quad + \sum_{n=1}^{m} \tau \langle 4G(T_h^n) e_{M_2}^n (1-\chi_h^n)^\beta, \operatorname{sign}(e_\chi^n)\rangle \\
&\leq \sum_{n=1}^{m} \tau \big(-4\|G(T^n) M_2^n e_\beta^n\|_{L^1(\Omega)} + 4 L_G C_{M_2} \|e_T^n\|_{L^1(\Omega)} + 4 C_G \|e_{M_2}^n\|_{L^1(\Omega)}\big).
\end{aligned}$$

Inserting the preceding estimates into (5.3) we obtain

$$\begin{aligned}
&\|e_\chi^m\|_{L^1(\Omega)} + 4\sum_{n=1}^{m} \tau \|G(T^n) M_2^n e_\beta^n\|_{L^1(\Omega)} \\
&\qquad \leq \gamma \sum_{n=1}^{m} \tau \big(\|e_T^n\|_{L^1(\Omega)} + \|e_{M_2}^n\|_{L^1(\Omega)}\big) + \gamma(\tau + h).
\end{aligned} \tag{5.4}$$

By similar arguments, and using also that $\frac{F(s)}{G(s)} \leq \mu$ for $s > 0$, we find

$$\|e_{M_2}^m\|_{L^1(\Omega)} \leq \gamma \sum_{n=1}^{m} \tau \big(\|G(T^n) e_\beta^n\|_{L^1(\Omega)} + \|e_T^n\|_{L^1(\Omega)} + \|e_{M_1}^n\|_{L^1(\Omega)}\big) + \gamma(\tau + h), \tag{5.5}$$

$$\|e_{M_1}^m\|_{L^1(\Omega)} \leq \gamma \sum_{n=1}^{m} \tau \big(\|G(T^n) e_\beta^n\|_{L^1(\Omega)} + \|e_T^n\|_{L^1(\Omega)} + \|e_{M_0}^n\|_{L^1(\Omega)}\big) + \gamma(\tau + h), \tag{5.6}$$

$$\|e_{M_0}^m\|_{L^1(\Omega)} \leq \gamma \sum_{n=1}^{m} \tau \big(\mu \|G(T^n) e_\beta^n\|_{L^1(\Omega)} + \|e_T^n\|_{L^1(\Omega)}\big) + \gamma(\tau + h). \tag{5.7}$$

In view of (1.2), (2.10), and (3.12) we can write (2.9) at time t^n as follows:

$$
\begin{aligned}
&c\rho\langle R_hT^n - R_hT^{n-1},\phi\rangle_h + \tau k\langle\nabla R_hT^n,\nabla\phi\rangle + \tau\langle\!\langle H(R_hT^n - T_a^n),\phi\rangle\!\rangle_h\\
&\quad= \tau\langle T^n - R_hT^n,\phi\rangle + c\rho\langle T^n - T^{n-1} - \tau\partial_tT^n,\phi\rangle + 4\tau\lambda\rho\langle G(T^n)(1-\chi^n)^\beta M_2^n,\phi\rangle\\
&\quad+ c\rho\big(\langle R_hT^n - R_hT^{n-1},\phi\rangle_h - \langle T^n - T^{n-1},\phi\rangle\big)\\
&\quad+ \tau\big(\langle\!\langle H(R_hT^n - T_a^n),\phi\rangle\!\rangle_h - \langle\!\langle H(R_hT^n - T_a^n),\phi\rangle\!\rangle\big) \quad \forall\, \phi\in V_h^1.
\end{aligned}
\tag{5.8}
$$

We then subtract (2.12) from (5.8), take $\phi = z^n \in V_h^1$, and add the resulting expression over n from 1 to any $m \le N$; here $\{z^n\}_{n=1}^{m+1}$ is the solution of the dual problem (3.15). We employ (3.7) to integrate by parts the first term, that is

$$
\sum_{n=1}^m \langle R_he_T^n - R_he_T^{n-1}, z^n\rangle_h = \langle R_he_T^m,\zeta\rangle_h - \langle R_he_T^0, z^1\rangle_h - \sum_{n=1}^m \langle R_he_T^n, z^{n+1} - z^n\rangle_h.
$$

Let $\zeta = \Pi_h[\mathrm{sign}(R_he_T^m)] \in V_h^1$ and note that ζ is well defined because $\mathrm{sign}(0) = 0$. Inserting $\phi = R_he_T^n \in V_h^1$ into (3.15), we obtain

$$
\begin{aligned}
c\rho\langle R_he_T^m, \Pi_h[\mathrm{sign}(R_he_T^m)]\rangle_h &= c\rho\langle R_he_T^0, z^1\rangle_h + \sum_{n=1}^m \tau\langle T^n - R_hT^n, z^n\rangle\\
&+ \sum_{n=1}^m c\rho\langle T^n - T^{n-1} - \tau\partial_tT^n, z^n\rangle\\
&+ \sum_{n=1}^m \lambda\rho\langle 4\tau G(T^n)(1-\chi^n)^\beta M_2^n - (\chi_h^n - \chi_h^{n-1}), z^n\rangle\\
&+ \sum_{n=1}^m c\rho\big(\langle R_h(T^n - T^{n-1}), z^n\rangle_h - \langle T^n - T^{n-1}, z^n\rangle\big)\\
&+ \sum_{n=1}^m \tau\big(\langle\!\langle H(R_hT^n - T_a^n), z^n\rangle\!\rangle_h - \langle\!\langle H(R_hT^n - T_a^n), z^n\rangle\!\rangle\big).
\end{aligned}
\tag{5.9}
$$

We write the above equation as $\mathrm{VII} = \mathrm{VIII} + \mathrm{IX} + \mathrm{X} + \mathrm{XI} + \mathrm{XII} + \mathrm{XIII}$ and estimate each term separately. Using (3.13) and (2.11) it follows that

$$
\begin{aligned}
\tfrac{1}{c\rho}\mathrm{VII} = \langle R_he_T^m, \mathrm{sign}(R_he_T^m)\rangle_h &= \int_\Omega \Pi_h[|R_he_T^m|]dx \ge \|R_he_T^m\|_{L^1(\Omega)}\\
&\ge \|e_T^m\|_{L^1(\Omega)} - \|T^m - R_hT^m\|_{L^1(\Omega)}\\
&\ge \|e_T^m\|_{L^1(\Omega)} - C^*h^2\|T\|_{L^\infty(0,t^*;W_p^2(\Omega))} \ge \|e_T^m\|_{L^1(\Omega)} - \gamma h^2.
\end{aligned}
$$

Since $e_T^0 = T_0 - \Pi_hT_0$, (2.3), (3.13), (3.16) and interpolation properties of Π_h lead to

$$
\begin{aligned}
\tfrac{1}{c\rho}\mathrm{VIII} &\le \|R_hT_0 - \Pi_hT_0\|_{L^2(\Omega)}\|z^1\|_{L^2(\Omega)}\\
&\le |\Omega|^{1/2}\big(\|R_hT_0 - T_0\|_{L^2(\Omega)} + \|T_0 - \Pi_hT_0\|_{L^2(\Omega)}\big)\\
&\le |\Omega|^{1/2}C^*h^2\|T^0\|_{H^2(\Omega)} \le \gamma h^2.
\end{aligned}
$$

By (2.11), (3.13), and (3.16), we have

$$\mathrm{IX} \le C^* h^2 \sum_{n=1}^{m} \tau \|T^n\|_{W_p^2(\Omega)} \|z^n\|_{L^\infty(\Omega)} \le C^* t^* h^2 \|T\|_{L^\infty(0,t^*;W_p^2(\Omega))} \le \gamma h^2.$$

Arguing as for the right hand side of (5.3), and using (3.16) and (2.10), we find

$$\mathrm{X} \le c\rho\tau \|\partial_{tt} T\|_{L^1(\Omega_{t^*})} \le \gamma\tau,$$

$$\mathrm{XI} \le \gamma \sum_{n=1}^{m} \tau\big(\|G(T^n)e_\beta^n\|_{L^1(\Omega)} + \|e_T^n\|_{L^1(\Omega} + \|e_{M_2}^n\|_{L^1(\Omega)}\big) + \gamma(\tau + h).$$

We split term XII as follows:

$$\begin{aligned}\tfrac{1}{c\rho}\mathrm{XII} &= \sum_{n=1}^{m} \big(\langle R_h(T^n - T^{n-1}), z^n\rangle_h - \langle R_h(T^n - T^{n-1}), z^n\rangle\big) \\ &\quad + \sum_{n=1}^{m} \big(\langle R_h(T^n - T^{n-1}), z^n\rangle - \langle T^n - T^{n-1}, z^n\rangle\big) = \mathrm{XII}_1 + \mathrm{XII}_2.\end{aligned}$$

Since $\|\nabla R_h \varphi\|_{L^p(\Omega)} \le C^* \|\varphi\|_{W_p^1(\Omega)}$, (2.10), (3.9), and (3.16) yield

$$\begin{aligned}\mathrm{XII}_1 &\le C^* h \sum_{n=1}^{m} \|\nabla R_h(T^n - T^{n-1})\|_{L^p(\Omega)} \|z^n\|_{L^\infty(\Omega)} \\ &\le C^* h \sum_{n=1}^{m} \|T^n - T^{n-1}\|_{W_p^1(\Omega)} \le C^* h \|\partial_t T\|_{L^1(0,t^*;W_p^1(\Omega))} \le \gamma h.\end{aligned}$$

Using (2.10), (3.13), and (3.16) we get

$$\mathrm{XII}_2 \le C^* h^2 \sum_{n=1}^{m} \|T^n - T^{n-1}\|_{W_p^2(\Omega)} \|z^n\|_{L^\infty(\Omega)} \le C^* h^2 \|\partial_t T\|_{L^1(0,t^*;W_p^2(\Omega))} \le \gamma h^2.$$

We split term XIII as follows:

$$\begin{aligned}\mathrm{XIII} &= \sum_{n=1}^{m} \tau\big(\langle\!\langle H(R_h T^n - T_a^n), z^n\rangle\!\rangle_h - \langle\!\langle \Pi_h[\Pi_h H(R_h T^n - \Pi_h T_a^n)], z^n\rangle\!\rangle\big) \\ &\quad + \sum_{n=1}^{m} \tau\big(\langle\!\langle \Pi_h[\Pi_h H(R_h T^n - \Pi_h T_a^n)], z^n\rangle\!\rangle - \langle\!\langle \Pi_h H(R_h T^n - \Pi_h T_a^n)], z^n\rangle\!\rangle\big) \\ &\quad + \sum_{n=1}^{m} \tau\langle\!\langle \Pi_h H(T_a^n - \Pi_h T_a^n), z^n\rangle\!\rangle + \sum_{n=1}^{m} \tau\langle\!\langle (\Pi_h H - H)(R_h T^n - T_a^n), z^n\rangle\!\rangle \\ &= \mathrm{XIII}_1 + \mathrm{XIII}_2 + \mathrm{XIII}_3 + \mathrm{XIII}_4.\end{aligned}$$

For XIII_1, we resort to (3.10) and (3.16), in conjunction to (2.4), (2.6), and (2.7), to derive

$$
\begin{aligned}
\mathrm{XIII}_1 &\le C^* h \sum_{n=1}^{m} \tau \|\nabla[\Pi_h H(R_h T^n - \Pi_h T_a^n)]\|_{L^2(\Omega)} \|\nabla z^n\|_{L^2(\Omega)} \\
&\le C^* h \|H\|_{W^1_\infty(\Omega)} \Big(\sum_{n=1}^{m} \tau \|R_h T^n - \Pi_h T_a^n\|^2_{H^1(\Omega)} \Big)^{1/2} \Big(\sum_{n=1}^{m} \tau \|\nabla z^n\|^2_{L^2(\Omega)} \Big)^{1/2} \\
&\le \gamma h \|H\|_{W^1_\infty(\Omega)} \big(\|T\|_{L^\infty(0,t^*;H^1(\Omega))} + \|T_a\|_{L^\infty(0,t^*;W^1_\infty(\Omega))} \big) \le \gamma h.
\end{aligned}
$$

We have used the fact that $\|\nabla \Pi_h f\|_{L^2(\Omega)} \le C^* \|\nabla f\|_{L^2(\Omega)}$ if f is piecewise polynomial. Since $\|z^n\|_{L^\infty(\partial\Omega)} \le 1$, we get similarly

$$
\begin{aligned}
\mathrm{XIII}_2 &\le \sum_{n=1}^{m} \tau \|\Pi_h[\Pi_h H(R_h T^n - \Pi_h T_a^n)] - \Pi_h H(R_h T^n - \Pi_h T_a^n)\|_{L^1(\partial\Omega)} \|z^n\|_{L^\infty(\partial\Omega)} \\
&\le \gamma h^{3/2} \|\nabla H\|_{L^\infty(\Omega)} \big(\|T\|_{L^\infty(0,t^*;H^1(\Omega))} + \|T_a\|_{L^\infty(0,t^*;W^1_\infty(\Omega))} \big) \le \gamma h^{3/2}.
\end{aligned}
$$

On using standard interpolation estimates and (2.6), (3.16), we have for XIII_3

$$
\begin{aligned}
\mathrm{XIII}_3 \le& C^* h \|H\|_{L^\infty(\Omega)} |\Omega|^{1/2} \sum_{n=1}^{m} \tau \|T_a^n\|_{W^1_\infty(\Omega)} \|z^n\|_{L^2(\partial\Omega)} \\
\le& \gamma h \|H\|_{L^\infty(\Omega)} \|T_a\|_{L^\infty(0,t^*;W^1_\infty(\Omega))} \le \gamma h,
\end{aligned}
$$

and likewise for XIII_4

$$
\begin{aligned}
\mathrm{XIII}_4 \le& C^* h \|H\|_{W^1_\infty(\Omega)} \sum_{n=1}^{m} \tau \big(\|R_h T^n\|_{L^2(\partial\Omega)} + \|T_a^n\|_{L^2(\partial\Omega)} \big) \|z^n\|_{L^2(\partial\Omega)} \\
\le& \gamma h \|H\|_{W^1_\infty(\Omega)} \big(\|T\|_{L^\infty(0,t^*;H^1(\Omega))} + \|T_a\|_{L^\infty(0,t^*;H^1(\Omega))} \big) \le \gamma h.
\end{aligned}
$$

Hence, inserting the preceding estimates into (5.9), we get

$$
\|e_T^m\|_{L^1(\Omega)} \le \gamma \sum_{n=1}^{m} \tau \big(\|G(T^n) e_\beta^n\|_{L^1(\Omega)} + \|e_T^n\|_{L^1(\Omega)} + \|e_{M_2}^n\|_{L^1(\Omega)} \big) + \gamma(\tau + h). \tag{5.10}
$$

Let us multiply (5.4) by a constant $\Lambda > 1$ to be chosen. Adding the resulting inequality together with (5.5)-(5.7) and (5.10) it follows that

$$
\begin{aligned}
\|e_T^m\|_{L^1(\Omega)} + \Lambda \|e_\chi^m\|_{L^1(\Omega)} + \sum_{i=0}^{2} \|e_{M_i}^m\|_{L^1(\Omega)} &\le \gamma\Lambda(\tau + h) + \gamma\Lambda \sum_{n=1}^{m} \tau \|e_T^n\|_{L^1(\Omega)} \\
&+ \gamma\Lambda \sum_{i=0}^{2} \sum_{n=1}^{m} \tau \|e_{M_i}^n\|_{L^1(\Omega)} + \sum_{n=1}^{m} \tau \int_\Omega G(T^n) \big(\gamma |e_\beta^n| - 4\Lambda M_2^n |e_\beta^n| \big) dx.
\end{aligned} \tag{5.11}
$$

By means of Lemma 3.1, we estimate the last term in (5.11), say XIV, as follows:

$$
\begin{aligned}
\mathrm{XIV} &\le \sum_{n=1}^{m} \tau \int_\Omega G(T^n)\big(4\gamma|e_\chi^n| + 8C_G t^* \gamma M_2^n |e_\beta^n| - 4\Lambda M_2^n |e_\beta^n|\big)\,dx \\
&\le 4\gamma C_G \sum_{n=1}^{m} \tau \|e_\chi^n\|_{L^1(\Omega)},
\end{aligned} \tag{5.12}
$$

provided we choose, e.g., $\Lambda = 2\gamma C_G t^*$. Using (5.12) in (5.11), we find a discrete integral inequality to which we may apply the discrete Gronwall's lemma, thereby obtaining

$$
\max_{1\le n\le N} \|e_T^n\|_{L^1(\Omega)} + \max_{1\le n\le N} \|e_\chi^n\|_{L^1(\Omega)} + \sum_{i=0}^{2} \max_{1\le n\le N} \|e_{M_i}^n\|_{L^1(\Omega)} \le \gamma(\tau + h).
$$

The assertion (5.1) finally follows from (2.8) and (2.11) because

$$
\max_{1\le n\le N} \|f^n - f\|_{L^\infty(t^{n-1},t^n;L^1(\Omega))} \le \tau \|\partial_t f\|_{L^\infty(0,t^*;L^1(\Omega))} \quad \forall\ f \in W^1_\infty(0,t^*;L^1(\Omega)). \quad \square
$$

6. Simulation. We present a numerical simulation for the crystallization of a screw typically used in orthopaedics. The advantage of prostheses in polylactic acid, a biodegradable semicrystalline polymer, is mainly due to the fact that they do not need to be removed but, instead, they are simply consumed and absorbed as lactic acid by the body. On the other hand, the mechanical properties as well as the consumption kinetics of prostheses depend strongly on the crystalline structure developed during their solidification. It turns out that they have to be balanced in order to allow for bone healing right before consumption. The cost and complexity of lab experimentation explain the increasing interest in modeling and simulation of polymer crystallization processes.

Figure 6.1 shows the longitudinal section of the screw which is roughly assumed to be axially symmetric. The finite element mesh $\mathcal{S}_h$ is quasi-uniform with $h = 0.25$ mm whereas $\tau = 0.25$ sec is the time step. Termodynamic and kinetic constants are taken from [17]. In particular, the growth rate factors G and F are given by $F(T) = F_0\Phi(T)$ and $G(T) = G_0\Phi(T)$, where

$$
\Phi(T) = \exp\big(-\tfrac{\mathcal{U}^*}{\mathcal{R}(T-T_g)}\big)\exp\big(-\tfrac{K_g(T_m^0+T)}{2T^2(T_m^0-T)}\big).
$$

and $F_0 = 1.494 \times 10^{17}$ m^{2}sec^{-1}, $G_0 = 3.241 \times 10^4$ m sec^{-1}. Here $T_g = 261.2$ K is the glass transition temperature, $T_m^0 = 464.2$ K is the equilibrium melting temperature, $K_g = 4.87 \times 10^5$ K^2 is the thermodynamic nucleation constant, $\mathcal{U}^*/\mathcal{R} = 6280/8.314$ K is a universal constant related to polymer chain mobility energy activation over the gas constant. The crystalline volume fraction is normalized to the equilibrium value $\chi^* = 0.440$

FIGURE 6.1. Longitudinal section of the screw.

FIGURE 6.2. Crystalline volume fraction ($0 \leq \chi_h^N \chi^* \leq 0.265$).

FIGURE 6.3. Number of spherulites per mm^3 ($0 \leq M_{0h}^N \leq 480$).

FIGURE 6.4. Mean radius of spherulites ($0 \leq M_{1h}^N / 2M_{0h}^N \leq 0.0526$ mm).

and exponent β is $\beta = 0.765$. Finally we have $\rho = 903$ kg m^{-3}, $c = 2140$ J kg^{-1}K^{-1}, $k = 0.23$ W m^{-1}K^{-1}, and $\lambda = 209300$ J kg^{-1}. The initial temperature of the melt polymer is $T_0 = 494.2$ K and the boundary heat exchange efficiency is given by $H = 41860$ W m^{-2}K^{-1} for $T_a = 310.2$ K. We assume an adiabatic condition $H = 0$ only on the screw's head, where the melt is injected from into the mould, and next packed to compensate for volume reduction during solidification. Lab experiments show a core of relatively high crystallized material, whereas size and number of spherulites decrease toward the thread. This structure is confirmed by our numerical experiments. After $t^* = 200$ sec the polymer rests at $T = T_a$ and crystallization becomes complete. Figures 6.2-6.4 show the isoclines for crystalline volume fraction $\chi_h^N \chi^*$, number of nuclei M_{0h}^N per unit of volume (mm^3) and mean radius of spherulites $M_{1h}^N / 2M_{0h}^N$, respectively. Note the low crystalline volume fraction in the screw core of about 10% of the maximum value $\chi^* = 0.440$.

Orthopaedic screws must hold fractured bones together until complete healing, and only after be dissolved and absorbed by the body. However the fastest heat diffuses during solidification the smaller and fewer spherulites will grow, thereby leading to a soft material with short biological decomposition time. To achieve a proper balance between mechanical properties for stress resistance and time scale, the rate of heat diffusion must be carefully controlled. This entails acting on the efficiency of heat exchange on the thread, and numerics may be a rather cheap complement to more expensive lab experiments.

7. Conclusions. We have introduced and discussed a rather simple, easy to implement, $P^1 - P^0$ finite element method for a realistic model of polymer crystallization. We have examined its mathematical properties, and derived optimal linear error estimates in the natural $L^\infty L^1$ space, which provides solid basis to our approach. The analysis accounts for the lack of regularity associated with non-Lipschitz kinetic equations. Since our numerical simulation agrees qualitatively with experimental results [16,17], the above relatively simple model seems to be able to capture the essence of the crystallization process. Numerical simulation might then be able to complement a much more expensive lab experimentation. In improving local resolution, and making the method adaptive, a $P^1 - P^1$ scheme would be more desirable. This issue is under investigation.

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