A PRIORI ERROR ESTIMATES FOR FINITE ELEMENT GALERKIN APPROXIMATIONS TO A FREE BOUNDARY PROBLEM IN POLYMER TECHNOLOGY

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1. INTRODUCTION.

In this paper, we examine a finite element Galerkin method for a free boundary problem arising in the polymer industry which models the penetration of a solvent into a glassy polymer. Initially, we briefly discuss the model proposed by Astarita and Sarti[**1**], and the related existence and uniqueness results.

Consider a semi-infinite slab of glassy polymer occupying the half space $x \geq 0$, which is in contact with a solvent. When the solvent concentration at the face of the polymer at $x = 0$ exceeds some threshold, the solvent moves into the polymer creating a swollen zone through which the solvent diffuses according to Fick's law. The interface that is the free boundary between the swollen zone and the glassy polymer obeys an empirical penetration law, which guarantees that the speed of the penetration increases with the excess of concentration above the threshold. In addition, in order to fully specify the free boundary, an additional condition must be imposed in the form of a mass conservation condition. In the present model, we assume that the penetration process has commenced so that a free boundary has already formed and that the swelling takes place instantaneously at the interface. With appropriate non-dimensional normalised variables, the above model leads to the following parabolic free boundary problem.

Problem $\tilde{\mathbf{P}}$. Find a pair $\{U(y,t), s(t)\}$ such that

(1.1) $$U_t - U_{yy} = 0, 0 < y < s(t), \quad 0 < t \leq T$$

(1.2) $$U(y,0) = g(y), \quad 0 < y \leq 1,$$

$$U(0,t) = U^*, \quad 0 < t \leq T, \tag{1.3}$$

$$U_y(s(t),t) = -\frac{ds}{dt}[U(s(t),t) + q(t)], \tag{1.4}$$

and

$$\frac{ds}{dt} = f(U(s(t),t)), \quad 0 < t \leq T \tag{1.5}$$

with

$$s(0) = 1.$$

Here, $U(y,t)$ represents the concentration of the solvent, and equation (1.5) states the empirical penetration law where $f(r)$ may be of the form αr^m, with both α and m positive constants. The additional condition (1.4), on the free boundary $s(t)$, is the mass conservation with $q \geq 0$ defining the threshhold concentration for penetration. The term U^* in equation (1.3) denotes the normalised concentration so that the normalised solvent concentration is given by $U + q$. By redefining U, we henceforth assume that $U^* = 0$. This parabolic free boundary problem is non-standard because of the unusual boundary conditions (1.4) and (1.5).

We make the following assumptions about the Problem $\tilde{\mathrm{P}}$:

A_1. Problem $\tilde{\mathrm{P}}$ has a unique smooth solution pair $\{U, s\}$, with $s(t) \geq c_0$, for $0 \leq t \leq T$, where c_0 is a positive constant.

A_2. The initial function $g \geq 0$ is sufficiently smooth and satisfies certain compatibility conditions like $g(0) = 0$.

A_3. The function f in (1.5) belongs to $C^1(0,\infty)$ with its derivative $f'(r) \geq 0$, for $r > 0$, and $f(0) = 0$. Further, it is assumed that $f'(r)$ is bounded for bounded r like $|f'(r)| \leq K(r)$, where K is an increasing function of r.

With respect to A_1, the global existence and regularity results have been established by Fasano *et al.*[4] for the Problem $\tilde{\mathrm{P}}$ with a degenerate free boundary condition that satisfies $s(0) = 0$. Thus, for the present problem, with non-degenerate free boundary and appropriate compatibility condition on g, the global existence, uniqueness and regularity conditions (given below in (2.8)) can be proved using Fasano *et al.*[4]. Conrad *et al.*[**2**] have discussed the well-posedness of a similar problem arising in a dissolution–growth process. Further, the restriction $s(t) \geq c_0$, based on physical considerations, precludes the disappearance of any phase in [0,T]. The assumptions A_2 and A_3 apply even when the problem is well-posed. We note that on the free boundary $s(t)$, U is taken to be positive. This can be motived on physical grounds (see Fasano *et al.*[4] or Conrad *et al.*[**2**]) and therefore, f is differentiable on $s(t)$.

For numerical methods, Fasano *et al.*[4] have discussed a convergent finite difference numerical algorithm based on a shooting method for a time discretization of Problem $\tilde{\mathrm{P}}$ with $s(0) = 0$. Quite recently, Murray and Carey [**5**] have developed a moving finite element method using a predictor-corrector scheme and have examined the numerical accuracy and stability numerically. The present contribution developes error estimates for the finite element Galerkin method using fixed domain techniques.

2. THE FIXED DOMAIN AND GALERKIN METHODS.

The major difficulty with solving Problem $\tilde{\mathrm{P}}$ numerically is the moving free boundary. The obvious solution is to transform the problem to an appropriate fixed domain formulation (Crank [**3**]). However, such formulations are not achieved without a trade-off which, in one way or another, complicates the underlying pde structure by introducing additional non-linearity to compensate for fixing the moving free boundary. For Problem $\tilde{\mathrm{P}}$, a fixed domain formulation is derived using the Landau-type transformation

$$y = xs(t). \tag{2.1}$$

In this way, on setting $u(x,t) = U(y,t)$, Problem $\tilde{\mathrm{P}}$ is replaced by the following fixed domain formulation, Problem P, which consists of a coupled system of a parabolic equation in u with a typical nonlinearity and an ordinary differential equation in s.

Problem P. Find $\{u(x,t), s(t)\}$ such that

$$s(t)^2 u_t - u_{xx} = xu_x s(t) f(u(1,t)), \quad (x,t) \in I \times (0,T], \tag{2.2}$$

$$u(x,0) = g(x), \quad x \in I, \tag{2.3}$$

$$u(0,t) = 0, \quad 0 < t \leq T, \tag{2.4}$$

$$u_x(1,t) = -s\frac{ds}{dt}[u(1,t) + q(t)], \tag{2.5}$$

$$\frac{ds}{dt} = f(u(1,t)), \quad 0 < t \leq T, \tag{2.6}$$

with $s(0) = 1$.

Using (2.6), equation (2.5) can be rewritten as

$$u_x(1,t) = -sf(u(1,t))[u(1,t) + q(t)], \quad 0 < t \leq T. \tag{2.7}$$

Let $u, v \in L^2(I)$, $(u,v) = \int_I u\,v\,dx$ and $\|u\|^2 = (u,u)$. Let $H^k = H^k(I)$ denote the corresponding Sobolev space $W^{k,2}(I)$ with norm denoted by $\|.\|_k$. If X is a normed linear space with norm $\|.\|_X$, and the mapping $\phi : (a,b) \mapsto X$ is strongly measurable and p-th integrable, then

$$\|\phi\|_{L^p(a,b;X)} = (\int_a^b \|\phi\|_X^p \,dt)^{1/p}, \quad 1 \leq p < \infty,$$

and, for $p = \infty$,

$$\|\phi\|_{L^\infty(a,b;X)} = \sup_{a \leq t \leq b} \|\phi(t)\|_X.$$

Let us further assume that the following regularity conditions hold for the pair{u,s}

$$u \in W^{1,2}(0,T; H^{r+1}), \quad s \in W^{1,\infty}(0,T). \tag{2.8}$$

The function u and s in the above mentioned spaces are bounded by a common constant say K_1.

The Weak Formulation. Set $H_0^1(I) = \{v \in H^1 : v(0) = 0\}$. Multiply both the sides of (2.2) by $v \in H_0^1$ and integrate the second term in the left hand side by parts to obtain

$$(s^2 u_t, v) + (u_x, v_x) = sf(u(1))(xu_x, v) - sf(u(1))[u(1) + q], \quad t > 0 \tag{2.9}$$

with

$$(u(0), v) = (g, v), \quad v \in H_0^1.$$

Here, the notation $u(1)$ is used in place of $u(1,t)$.

The Galerkin Procedure. Let S_h^0 be a finite dimensional subspace of H_0^1 with the following properties:

(i) Approximation property. There is a positive constant K_0, independent of h, such that for $v \in H^m \cap H_0^1$

$$\inf_{\chi \in S_h^0} \|v - \chi\|_j \leq K_0 h^{m-j} \|v\|_m, \quad 0 \leq j \leq 1,\, 1 \leq m \leq r+1.$$

(ii) Inverse property. For $\chi \in S_h^0$,

$$\|\chi\|_{L^\infty} \leq K_0\, h^{-\frac{1}{2}} \|\chi\|.$$

The continuous time Galerkin approximation u^h of u is now defined to be the mapping $u^h \colon [0,T] \mapsto S_h^0$ such that

$$\begin{aligned} (s_h^2 u_t^h, \chi) + (u_x^h, \chi_x) &= s_h f(u^h(1))(x u_x^h, \chi) \\ &\quad - s_h f(u^h(1))(u^h(1) + q)\chi(1), \quad \chi \in S_h^0,\ t > 0, \end{aligned} \tag{2.10}$$

with

$$(u^h(0), \chi) = (P_h g, \chi),$$

where P_h denotes an appropriate projection onto S_h^0 to be defined below.

Further, the continuous time Galerkin approximation s_h of s is given by

$$\frac{ds_h}{dt} = f(u^h(1)), \quad t \in (0,T] \tag{2.11}$$

with $s_h(0) = 1$.

For a given $u^h(0)$ as well as $s_h(0)$, (2.10) and (2,11) together yield a system of nonlinear ordinary differential equations. Because of the conditions on f, this system has at least a unique local solution by Picard's existence theorem. The global existence of a unique pair $\{u^h, s_h\}$ on the whole of [0,T] has been examined by Pani *et al.* [**6**].

3. AUXILIARY PROJECTION AND RELATED ESTIMATES.

Define

$$(3.1)\qquad a(s,u;v,w)=(v_x,w_x)-sf(u(1))(xv_x,w),\quad u\in L^\infty,\quad v,\,w\in H^1.$$

This operator satisfies the following properties:

(i) There is a constant $K_2=K_2(K_0,K_1)$ such that

$$|a(s,u;v,w)|\le K_2\|v\|_1\|w\|_1,\quad v,w\in H_0^1.$$

(ii) {Gärding inequality} There exist positive constants α and ρ, with ρ depending on K_0 and K_1, such that

$$a(s,u;v,v)\ge\alpha\|v\|_1-\rho\|v\|^2,\quad v\in H_0^1.$$

For $t\ge 0$, let $\tilde{u}\in S_h^0$ be the projection of u defined by

$$(3.2)\qquad a(s,u;u-\tilde{u},\chi)=0,\quad \chi\in S_h^0.$$

The existence of a unique $\tilde{u}\in S_h^0$ can be shown using the analysis of Schatz [**7**].

Setting $\eta=u-\tilde{u}$, we state below in Theorem 3.1 some estimates for η, η_t and $\eta(1)$ which will be required in the sequel. A proof can be found in Pani *et al.* [**6**].

Theorem 3.1. *For $t\in[0,T]$, the error η satisfies*

$$\|\eta\|_j+\|\eta_t\|_j\le K_4h^{m-j},\quad 0\le j\le 1,\,1\le m\le r+1,$$

and

$$|\eta(1)|\le K_4h^{2m-2},\quad 1\le m\le r+1,$$

where the generic constant K_4 may depend on K_0,K_1 and K_2.

4. A PRIORI ERROR ESTIMATES.

Let $\xi = u^h - \tilde{u}$ and $e = u - u^h = \eta - \xi$ with $e_1 = s - s_h$. In order to maintain a uniform degree of approximation, we define $P_h g = \tilde{u}(\cdot, 0)$, where $\tilde{u}$ is the projection of u on to S_h^0,defined in (3.2). Thus $\xi(x, 0) = 0$. Before we compare u^h and $\tilde{u}$, we introduce the following additional assumptions about u^h; namely, there exists a positive constant $K^* \geq 2K_1$ such that

$$|||u^h||| \leq K^*, \tag{4.1}$$

where

$$|||u^h||| = \|u_t^h\|_{L^2(L^2)} + \|u^h\|_{L^\infty(H^1)}.$$

Since we shall show that

$$|||e||| = O(h^r), \quad r > 0,$$

the bound in (4.1) is indeed not a restriction on u^h. As a consequence of (4.1), we have

$$|s_h(t)| \leq 1 + \int_0^t |f(t', u^h(1))|\, dt',$$

and hence

$$\|s_h\|_{L^\infty(0,T)} \leq K(K^*, T). \tag{4.2}$$

We now turn to estimate ξ.

Theorem 4.1. *Assume that (4.1) holds along with the regularity conditions (2.8). Then there exists a constant $K_5 = K_5(K_1, K_4, K^*)$ such that*

$$\|\xi\|_{L^\infty(L^2)} + \|e_1\|_{L^\infty(0,T)} + \beta\|\xi\|_{L^2(H^1)} \leq K_5 h^m, \tag{4.3}$$

for $2 \leq m \leq r + 1$.

Proof: From (2.9) with $v = \chi$ and (3.2), it follows that

$$s^2(\tilde{u}_t, \chi) + (\tilde{u}_x, \chi_x) - sf(u(1))(x\tilde{u}_x, \chi) = -s^2(\eta_t, \chi) - sf(u(1))[u(1) + q]\chi(1).$$

Substracting this last result from (2.10), we obtain

$$
\begin{aligned}
s^2(\xi_t,\chi)+(\xi_x,\chi_x) &= sf(u(1))(x\xi_x,\chi)+s[f(u^h(1)-f(u(1))](xu_x^h,\chi)\\
&\quad - e_1 f(u^h(1))(xu_x^h,\chi)+e_1(s+s_h)(u_t^h,\chi)+s^2(\eta_t,\chi)\\
&\quad + s[f(u^h(1))-f(u(1))](u^h(1,t)+q)\chi(1)+e_1 f(u^h(1))(u^h(1,t)+q)\chi(1)\\
&\quad + sf(u(1))(\eta(1)-\xi(1))\chi(1).
\end{aligned}
\tag{4.4}
$$

In addition, subtraction of (2.11) from (2.6) and multiply the resulting equation by e_1 yields

$$
\frac{1}{2}\frac{d}{dt}|e_1|^2=[f(u^h(1)-f(u(1))]e_1. \tag{4.5}
$$

From (4.4) with $\chi=\xi$ and (4.5), it follows that

$$
\begin{aligned}
\frac{1}{2}\frac{d}{dt}[|s|^2\|\xi\|^2+|e_1|^2]+\|\xi_x\|^2 &\le K(K_1,K^*,\varepsilon)[\|\xi\|^2+|e_1|^2]+3\varepsilon\|\xi_x\|^2\\
&\quad + K(K_1,K^*,\varepsilon)[\|\eta_t\|^2+|\eta(1)|^2]+K(K^*,K_1)|\xi(1)|^2.
\end{aligned}
$$

Here, we have used Poincáre's inequality and the obvious inequality that $ab\le\frac{1}{2\varepsilon}a^2+\frac{\varepsilon}{2}b^2$, where $a,b\ge 0$ with $\varepsilon>0$. To estimate the last two terms, we shall use the inequality $|\xi(1)|^2\le 2\|\xi\|\,\|\xi_x\|$, since $\xi\in H_0^1$. This yields

$$
\begin{aligned}
\frac{1}{2}\frac{d}{dt}[|s|^2\|\xi\|^2+|e_1|^2]+(1-5\varepsilon)\|\xi_x\|^2 &\le K(K_1,K^*,\varepsilon)[\|\eta_t\|^2+|\eta(1)|^2]\\
&\quad + K(K_1,K^*,\varepsilon)[\|\xi\|^2+|e_1|^2].
\end{aligned}
$$

Choosing ε so that $2(1-5\varepsilon)=\beta_1>0$, we obtain after integration with respect to t

$$
\begin{aligned}
|s(t)|^2\|\xi(t)\|^2+|e_1(t)|^2+\beta_1\int_0^t\|\xi_x(t')\|^2\,dt' &\le K(K_1,K_4,K^*)[h^{2m}+h^{4m-4}]\\
&\quad + K(K_1,K^*)\int_0^t[\|\xi(t')\|^2+|e_1(t')|^2]\,dt'.
\end{aligned}
$$

Here, we have used the estimates for η_t and $\eta(1)$ given in Theorem 3.1. On using Gronwall's Lemma with $s(t)\ge c_0$, for $t\in[0,T]$, we obtain the required result for $r\ge 1$.

Remark 4.1. If higher regularity is assumed for the elliptic problem associated with (3.1), negative norm estimate for η_t can be derived such as

$$
\|\eta_t\|_{-1}=O(h^{m+1}),\quad 3\le m\le r+1. \tag{4.6}
$$

Consequently, the L^2 estimates for ξ can be improved to be of order h^{r+2} for $r \geq 2$. A subsequent application of the inverse property gives an estimate for ξ in $L^\infty(L^\infty)$.

For an H^1 estimate, we have the following result.

Theorem 4.2. *Let all the assumptions in Theorem 4.1 hold. Then there exists a constant* $K_6 = K_6(k_1, K_4, K_5, K^*)$ *such that*

$$|||\xi||| \leq K_6 h^{m-1}, \tag{4.7}$$

for $2 \leq m \leq r+1$.

Proof: Choose $\chi = \xi_t$ in (4.4) and use Schwartz inequality to obtain

$$\begin{aligned} |s|^2\|\xi_t\|^2 + \frac{1}{2}\frac{d}{dt}\|\xi_x\|^2 \leq\ & K_1(\|\xi_x\| + \|\eta_t\|)\|\xi_t\| + 3K(K_1, K^*)|e_1|\|\xi_t\| \\ & + K(K_1, K^*)(|\eta(1)| + |\xi(1)|)\|\xi_t\| \\ & + K(K_1, K^*)(|\eta(1)| + |\xi(1)| + |e_1|)|\xi_t(1)|. \end{aligned}$$

Appealing to the inverse property for the term contain in $|\xi(1)||\xi_t(1)|$, it follows that

$$\begin{aligned} |s|^2\|\xi_t\|^2 + \frac{1}{2}\frac{d}{dt}\|\xi_x\|^2 \leq\ & 5\varepsilon\|\xi_t\|^2 + K(K_1, K^*, \varepsilon)\|\xi_x\|^2 + K(K_1, K^*, \varepsilon)[\|\eta_t\|^2 \\ & + |e_1|^2 + |\eta(1)|^2 + h^{-1}(|\eta(1)|^2 + \|\xi\|^2 + |e_1|^2)]. \end{aligned}$$

Since $s \geq c_0$, choose ε so that $2(c_0^2 - 5\varepsilon) = \tilde{\beta}_1 > 0$ and integrate with respect to t. Using the estimates in Theorem 3.1, it follows that

$$\int_0^t \|\xi(t')\|^2\,dt' + \|\xi_x(t)\|^2 \leq K(K_1, K^*, \tilde{\beta}_1)[h^{m-1} + \int_0^t \|\xi_x(t')\|^2\,dt'].$$

Therefore an application of Gronwall's Lemma gives the desired results for $m \geq 2$.

Since $\|e\| \leq \|\xi\| + \|\eta\|$, it follows from Theorems 3.1,4.1 and 4.2 that:

Theorem 4.3. *Let* $\{u, s\}$ *be a smooth solution pair of Problem P satisfying the regularity conditions (2.8). Further, let the Galerkin approximation* $\{u^h, s_h\}$ *satisfy (4.1) and (4.2). Then the following estimates hold, for* $2 \leq m \leq r+1$,

$$\|e\|_{L^\infty(H^j)} \leq K_7 h^{m-j}, j = 0, 1, \tag{4.8}$$

$$\|e_1\|_{L^\infty(0,T)} \leq K_7 h^m, \tag{4.9}$$

where $K_7 = K_7(K_0, K_1, K_4, K_5, K_6, K^*)$. In addition, for sufficiently small h and $m \geq 2$,

$$|||u^h||| \leq 2K_1 \leq K^*, \tag{4.10}$$

and consequently, K_7 can be chosen independently of K^*.

Proof: The estimates (4.8) and (4.9) follow from Theorems 3.1, 4.1 and 4.2 using the triangle inequality. For the second part,

$$\begin{aligned} |||u^h||| &\leq |||u||| + |||e||| \\ &\leq K_1 + K_7 h^{m-1}. \end{aligned}$$

Consequently, for sufficiently small h and for $m \geq 2$,

$$|||u^h||| \leq 2K_1 \leq K^*,$$

which completes the proof.

Remark 4.2. It follows from Remark 4.1 that

$$\|e\|_{L^\infty(L^\infty)} = O(h^{r+1}), \quad r \geq 2,$$

and

$$\|e\|_{L^\infty(H^{-1})} = O(h^{r+2}), \quad r \geq 2.$$

We note that, for the above estimates, higher regularity conditions are needed for the pair $\{u, s\}$ than the regularity conditions (2.8). Further, using superconvergent result for $\eta_t(1)$, it is possible to improve the H^1 estimates of ξ to be

$$\|\xi\|_{L^\infty(H^1)} = O(h^{r+1}), \quad r \geq 1.$$

In this way, an optimal error estimate for $\|e\|_{L^\infty(L^\infty)}$ is obtained without using the inverse property.

Now, the Galerkin approximation of $U(y,t)$ is defined to be

$$U^h(y,t) = u^h(x,t),$$

where $y = s_h x$ with s_h as in (2.11).

Finally, we state below the error estimates in terms of $U - U^h$.

Theorem 4.4. *For a suitably smooth solution pair* $\{U, s\}$,

$$\|U - U^h\|_{L^\infty(0,T;H^j(\tilde{\Omega}(t)))} = O(h^{r+1-j}), \quad j = 0, 1,$$

and

$$\|s - s_h\|_{L^\infty(0,T)} = O(h^{r+1}),$$

where $\tilde{\Omega}(t) = \big(0, \min(s(t), s_h(t))\big)$, *and* $r \geq 1$.

Remark 4.3. In this paper, we have only discussed the continuous time Galerkin method. Details about fully discrete schemes and numerical experimentation can be found in Pani *et al.* [**6**].

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