A CHARACTERISTIC GALERKIN METHOD WITH ADAPTIVE ERROR CONTROL FOR THE CONTINUOUS CASTING PROBLEM

ZHIMING CHEN* RICARDO H. NOCHETTO† ALFRED SCHMIDT‡

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Abstract. The continuous casting problem is a convection-dominated nonlinearly degenerate diffusion problem. It is discretized implicitly in time via the method of characteristics, and in space via continuous piecewise linear finite elements. A posteriori error estimates are derived for the L^1L^1 norm of temperature which exhibit a mild explicit dependence on velocity. The analysis is based on special properties of a linear dual problem in non-divergence form with vanishing diffusion and strong advection. Several simulations with realistic physical parameters illustrate the reliability of the estimators and the flexibility of the proposed adaptive method.

Keywords. a posteriori error estimates, continuous casting, method of characteristics, convection dominated diffusion, degenerate parabolic equations

1991 Mathematics subject classification: 65N15, 65N30, 35K60

1 Introduction

Let the ingot occupy a cylindrical domain Ω with large aspect ratio. Let $0 < L < +\infty$ be the length of the ingot and $\Gamma \subset \mathbf{R}^d$ for $d = 1$ or 2 be its (polygonal) cross section. We show $\Omega = \Gamma \times (0, L)$ in Figure 1, and hereafter write $x = (y, z) \in \Omega$ with $y \in \Gamma$ and $0 < z < L$.

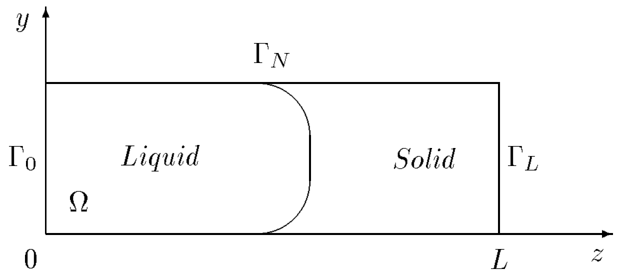

Figure : The domain Ω

*Institute of Mathematics, Academia Sinica, Beijing 100080, PR China. Partially supported by the National Natural Science Foundation of China under the grant No.19771080 and China National Key Project "Large Scale Scientific and Engineering Computing".

†Department of Mathematics and Institute for Physical Science and Technology, University of Maryland, College Park, MD 20742, USA. Partially supported by NSF Grant DMS-9623394 and NSF SCREMS 9628467.

‡Institut für Angewandte Mathematik, Universität Freiburg, 79104, Germany. Partially supported by DFG.

We study the following *convection-dominated nonlinearly degenerate diffusion* problem

$$\partial_t u + v(t)\partial_z u - \Delta\theta = 0 \quad \text{in} \quad Q_T, \tag{1.1}$$

$$\theta = \beta(u) \quad \text{in} \quad Q_T, \tag{1.2}$$

$$\theta = g_D \quad \text{on} \quad \Gamma_0 \times (0,T), \tag{1.3}$$

$$\partial_\nu\theta + p(\theta - \theta_{\text{ext}}) = 0 \quad \text{on} \quad \Gamma_N \times (0,T), \tag{1.4}$$

$$u(x,0) = u_0(x) \quad \text{in} \quad \Omega, \tag{1.5}$$

where

$$\Gamma_0 = \Gamma \times \{0\}, \quad \Gamma_L = \Gamma \times \{L\}, \quad \Gamma_N = \partial\Gamma \times (0,L), \quad Q_T = \Omega \times (0,T), \tag{1.6}$$

and $\theta + \theta_c$ is the absolute temperature, θ_c is the melting temperature, u is the enthalpy, $v(t) > 0$ is the extraction velocity of the ingot, ν is the unit outer normal to $\partial\Omega$, and θ_{ext} is the external temperature. The mapping $\beta : \mathbf{R} \to \mathbf{R}$ is Lipschitz continuous and monotone increasing; since β is not strictly increasing, (1.1) is *degenerate* parabolic. The missing *outflow* boundary condition on Γ_L is unclear because the ingot moves at the casting speed and is cut shorter from time to time. It is thus evident that any standard boundary condition could only be an approximation. We impose either a Neumann

$$\partial_\nu\theta = g_N \le 0 \quad \text{on} \quad \Gamma_L \times (0,T), \tag{1.7}$$

or a Dirichlet outflow condition

$$\theta = g_D < 0 \quad \text{on} \quad \Gamma_L \times (0,T). \tag{1.8}$$

Enforcing (1.7) with $g_N = 0$ is equivalent to assuming that the normal heat flux on Γ_L is entirely due to advection, which turns out to be an excellent approximation. Both boundary conditions lead to artificial boundary layers, with the second being more pronounced. In our simulations of §7 with real physical parameters, we take $g_N = 0$ and adjust g_D to minimize this effect. It is convenient to denote by Γ_D the Dirichlet part of $\partial\Omega$, that is Γ_0 for (1.7) and $\Gamma_0 \cup \Gamma_L$ for (1.8). The linear Robin condition (1.4) on that part of Γ_N in contact with air is just an approximation of the actual nonlinear Stefan-Boltzmann radiation law condition ($\sigma > 0$)

$$-\partial_\nu\theta = \sigma\big((\theta + \theta_c)_+^4 - \theta_{\text{ext}}^4\big) \quad \text{on} \quad \Gamma_N \times (0,T). \tag{1.9}$$

We see that linearizing (1.9) around a constant temperature leads to (1.4).

The importance of simulating and controlling the continuous casting process in the production of steel, copper, and other metals is recognized in industry. The extraction velocity $v(t)$ as well as the cooling conditions on the mold and water spray region are known to be decisive in determining material properties of the ingot. Avoiding excessive thermal stresses and material defects is an essential, and rather empirical, aspect of the continuous casting process.

If the extraction velocity $v(t)$ is assumed constant, and diffusion in the extraction direction z is ignored, then the resulting steady-state problem can be reformulated as a standard Stefan problem with a fictitious time $t = z/v$ [16], [23]. However, changes in the casting velocity v as well as in the cooling conditions are not only expected during a cycle of several hours of operation but are also desirable to handle late-arriving ladle, ladle or pouring problems, temporary malfunctions, etc. The casting machine must adjust to these demands and maintain production without degrading quality. The full non-stationary model (1.1)-(1.5) is thus more realistic than the steady state model in practical simulations and online control of continuous casting processes.

The system (1.1)-(1.5) is a special case of general Stefan problems with prescribed convection [25]. An outflow Dirichlet condition together with an inflow Neumann condition is assumed in [25] to guarantee uniqueness of weak solutions; our more realistic boundary data (1.3) and (1.7)-(1.8) violate this restriction. Under the additional assumption that the free boundary does not touch the inflow boundary Γ_0, uniqueness of weak solutions to (1.1)-(1.5) and (1.8) is shown in [24].

A posteriori error estimates are computable quantities that measure the actual errors without knowledge of the limit solution. They are instrumental in devising algorithms for mesh and time-step modification which equidistribute the computational effort and so optimize the computations. Ever since the seminal paper [1] on elliptic problems, adaptivity has become a central theme in scientific and engineering computations. In particular, a posteriori error estimators have been derived in [8], [9] for linear and mildly nonlinear parabolic problems, and in [20], [3] for degenerate parabolic problems of Stefan type. Duality is the main tool in the analysis of [8],[9],[20], and so is in the present paper. We stress that the techniques of [19],[3] circumvent duality and thus apply to non-Lipschitz nonlinearities.

The purpose of this paper is twofold: we first introduce and analyze an *adaptive* method with error control, and second we apply it to steel casting, a concrete engineering application. We combine the method of characteristics for time discretization [7],[17],[22], with continuous piecewise linear finite elements for space discretization [5]. We derive a posteriori error estimators which provide the necessary information to modify the mesh and time step according to varying external conditions and corresponding motion of the solid-liquid interface. Our estimates exhibit a mild dependence on an upper bound V for the casting velocity $v(t)$, depending on the outflow conditions (1.7) and (1.8), which results from a novel and rather delicate analysis of a linearized dual problem - a convection-dominated degenerate parabolic with non-divergence form and a Dirichlet outflow condition. We stress that this mild as well as explicit dependence on V is a major improvement with respect to previous L^2-based a priori analyses of [2] for the continuous casting problem and of [7],[22] for parabolic PDE with large ratio advection/diffusion; they lead to an exponential dependence on V, unless $\Omega = \mathbf{R}^d$ or the characteristics do not intercept $\partial\Omega$ [17], which is not the case in Figure 1. We finally remark that convergence of a fully discrete finite element scheme for (1.9) is proved [4]; error estimates cannot in general be expected due to lack of compactness except on special cases [18].

The paper is organized as follows. In §2 we state the assumptions and set the problem. In §3 we discuss the fully discrete scheme, which combines the method of characteristics and finite elements. In §4 we introduce the concept of parabolic duality and prove several crucial stability estimates. In §5 we prove the a posteriori error estimates. In §6 we discuss an example with exact solution and document the method's performance. We conclude in §7 with applications to casting of steel with realistic physical parameters.

2 Setting

We start by stating the hypotheses concerning the data.

(H1) $\beta(s) = 0$ for $s \in [0, \lambda]$ and $0 < \beta_1 \le \beta'(s) \le \beta_2$ for a.e. $s \in \mathbf{R}\backslash[0, \lambda]$; $\lambda > 0$ is the latent heat.

(H2) $0 < v_0 V \le v(t) \le V$ for $t \in [0, T]$ and $|v'(t)| \le v_1 V$ a.e. $t \in [0, T]$, with $v_0, v_1 > 0$ constants.

(H3) $\theta_0 = \beta(u_0) \in W^{1,\infty}(\Omega)$, and the initial interface $F_0 := \{x \in \Omega : \ \theta_0(x) = 0\}$ is Lipschitz.

(H4) $p \in H^1(0, T; W^{1,\infty}(\Gamma_N))$; $p \ge 0$.

(H5) $\theta_{\text{ext}} \in H^1(0, T; C(\bar\Gamma_N))$.

(H6) $g_D \in H^1(0, T; C(\bar\Gamma_D))$; $g_D(x, 0) = \theta_0(x)$ on Γ_D.

(H7) $g_N \in H^1(0, T; C(\bar\Gamma_L))$.

(H8) Uniqueness condition: $\exists\ \varepsilon_0, \rho_0 > 0$ such that $\theta \ge \rho_0$ a.e. in $\Gamma \times [0, \varepsilon_0] \times [0, T]$.

(H9) Solidification condition: $\exists\ \varepsilon_1, \rho_1 > 0$ such that $\theta \le -\rho_1$ a.e. in $\Gamma \times [L - \varepsilon_1, L] \times [0, T]$ and $\beta'(s) = \alpha > 0$ for $\beta(s) \le -\rho_1$.

(H10) $V \ge 1$.

We remark that (H8) is reasonable since it is satisfied for Stefan problems with $v = 0$ due to the continuity of θ and positivity of $\theta|_{\Gamma_0}$; heuristically the larger v, and so V, the larger the width ε_0. The condition (H9) is an implicit assumption on data which corresponds to the ingot being solid in the vicinity of Γ_L, where it is to be cut, as well as having a constant conductivity β'. (H9) is only needed to handle (1.7). In addition, (H10) is not restrictive in that we are interested in the convection-dominated case. In view of (H4)-(H7) we may consider $p, \theta_{\text{ext}}, g_D, g_N$ extended to Ω in such a way that $\theta_{\text{ext}}, g_D, g_N \in H^1(0, T; C(\bar\Omega))$, $p \in H^1(0, T; W^{1,\infty}(\Omega))$.

Let $\mathbf{V}_0 = \{v \in H^1(\Omega) : v = 0 \text{ on } \Gamma_D\}$ and $\mathbf{V}^*$ the dual space of $\mathbf{V}_0$. The weak formulation of (1.1)-(1.8) then reads as follows.

Continuous Problem. *Find u and θ such that*

$$\theta \in L^2(0, T; H^1(\Omega)), \quad u \in L^\infty(0, T; L^\infty(\Omega)) \cap H^1(0, T; \mathbf{V}^*),$$

$$\theta(x, t) = \beta(u(x, t)) \quad a.e.\ (x, t) \in Q_T,$$

$$\theta(x, t) = g_D(x, t) \quad a.e.\ (x, t) \in \Gamma_D \times (0, T),$$

$$u(\cdot, 0) = u_0,$$

and for a.e. $t \in (0, T)$ and all $\phi \in \mathbf{V}_0$ the following equation holds

$$\langle \partial_t u, \phi \rangle + v(t) \langle \partial_z u, \phi \rangle + \langle \nabla \theta, \nabla \phi \rangle + \langle\langle p\theta, \phi \rangle\rangle_{\Gamma_N} = \langle\langle p\theta_{\text{ext}}, \phi \rangle\rangle_{\Gamma_N} + \langle\langle g_N, \phi \rangle\rangle_{\Gamma_L}. \tag{2.1}$$

Hereafter, $\langle \cdot, \cdot \rangle$ stands for either the inner product in $L^2(\Omega)$ or the duality pairing between $\mathbf{V}^*$ and $\mathbf{V}_0$, and $\langle\langle \cdot, \cdot \rangle\rangle_E$ denotes the inner product in $L^2(E)$ with $E \subset \partial\Omega$; if $E = \partial\Omega$ we omit the subscript. We stress that the last term in (2.1) is absent when (1.8) is imposed. Existence and uniqueness of solutions (u, θ) to this problem satisfying $\theta \in C(\bar Q_T)$ are known [24].

3 Discretization

We now introduce the fully discrete problem, which combines continuous piecewise linear finite elements in space with characteristic finite differences in time. In fact, we use the method of characteristics to discretize the convection [7],[17],[22]. We denote by τ_n the n-th time step and set

$$t^n := \sum_{i=1}^{n} \tau_i, \quad \varphi^n(\cdot) := \varphi(\cdot, t^n)$$

for any function φ continuous in $(t^{n-1}, t^n]$. Let N be the total number of time steps, that is $t^N \geq T$. If e_z denotes the unit vector in $\mathbf{R}^d$ in the z-direction, then $\frac{dx}{dt} = v(t)e_z$ defines the forward characteristics, and $U(t) = u(x(t), t)$ satisfies

$$\frac{dU}{dt} = \partial_t u + v\partial_z u. \tag{3.1}$$

The characteristic finite difference method is based on writing

$$\bar{x}^{n-1} = x - v^{n-1}\tau_n e_z, \quad \bar{u}^{n-1}(x) = u(\bar{x}^{n-1}, t^{n-1}),$$

for $n \geq 1$ and discretizing (3.1) by means of backward differences as follows:

$$\frac{dU^n}{dt} \approx \frac{U^n - U^{n-1}}{\tau_n} \quad \Rightarrow \quad \partial_t u^n + v^n \partial_z u^n \approx \frac{u^n - \bar{u}^{n-1}}{\tau_n}.$$

Therefore the discretization in time of (1.1)-(1.2) reads

$$\frac{u^n - \bar{u}^{n-1}}{\tau_n} - \Delta\beta(u^n) = 0 \;\text{ in } \Omega. \tag{3.2}$$

As $\bar{u}^{n-1}(x)$ is well defined only for $\bar{x}^{n-1} \in \bar{\Omega}$, one has to either restrict the time step size τ_n (at least locally) or extend u^{n-1} beyond the inflow boundary Γ_0.

We denote by $\mathcal{M}^n$ a uniformly regular partition of Ω into simplexes [5]. The mesh $\mathcal{M}^n$ is obtained by refinement/coarsening of $\mathcal{M}^{n-1}$, and thus $\mathcal{M}^n$ and $\mathcal{M}^{n-1}$ are *compatible*. Given a triangle $S \in \mathcal{M}^n$, h_S stands for its diameter and ρ_S for its sphericity and they satisfy $h_S \leq 2\rho_S/\sin(\alpha_S/2)$, where α_S is the minimum angle of S; h denotes the mesh density function $h|_S = h_S$ for all $S \in \mathcal{M}^n$. Uniform regularity of the family of triangulations is equivalent to $\alpha_S \geq \alpha^* > 0$, with α^* independent of n. We also denote by $\mathcal{B}^n$ the collection of boundaries or sides e of $\mathcal{M}^n$ in Ω; h_e stands for the size of $e \in \mathcal{B}^n$.

Let $\mathbf{V}^n$ indicate the usual space of C^0 piecewise linear finite elements over $\mathcal{M}^n$ and $\mathbf{V}_0^n = \mathbf{V}^n \cap \mathbf{V}_0$. Let $\{x_k^n\}_{k=1}^{K^n}$ denote the interior nodes of $\mathcal{M}^n$. Let $I^n : C(\bar{\Omega}) \to \mathbf{V}^n$ be the usual Lagrange interpolation operator, namely $(I^n\varphi)(x_k^n) = \varphi(x_k^n)$ for all $1 \leq k \leq K^n$. Finally, let the discrete inner products $\langle\cdot,\cdot\rangle^n$ and $\langle\!\langle\cdot,\cdot\rangle\!\rangle_E^n$ be the sum over $S \in \mathcal{M}^n$ of the element scalar products

$$\langle\varphi,\chi\rangle_S^n = \int_S I^n(\varphi\chi)dx, \quad \langle\!\langle\varphi,\chi\rangle\!\rangle_S^n = \int_{S\cap E} I^n(\varphi\chi)d\sigma,$$

for any piecewise uniformly continuous functions φ, χ. It is known that for all $\varphi, \chi \in \mathbf{V}^n$ [20]

$$\Big|\int_S \varphi\chi dx - \int_S I^n(\varphi\chi)dx\Big| \leq \frac{1}{8}h_S^2 \|\nabla\varphi\|_{L^2(S)} \|\nabla\chi\|_{L^2(S)} \;\; \forall S \in \mathcal{M}^n, \tag{3.3}$$

$$\Big|\int_e \varphi\chi d\sigma - \int_e I^n(\varphi\chi)d\sigma\Big| \leq \frac{1}{8}h_S^2 \|\nabla\varphi\|_{L^2(e)} \|\nabla\chi\|_{L^2(e)} \;\; \forall e \in \mathcal{B}^n. \tag{3.4}$$

for any $S \in \mathcal{M}^n$ and $e \in \mathcal{B}^n$.

The discrete initial enthalpy $U^0 \in \mathbf{V}^0$ is defined at nodes x_k^0 of $\mathcal{M}^0 = \mathcal{M}^1$ to be

$$U^0(x_k^0) := u_0(x_k^0) \quad \forall\ x_k^0 \in \Omega \backslash F_0, \quad U^0(x_k^0) := 0 \quad \forall\ x_k^0 \in F_0.$$

Hence, U^0 is easy to evaluate in practice.

Discrete Problem. *Given $U^{n-1}, \Theta^{n-1} \in \mathbf{V}^{n-1}$, then $\mathcal{M}^{n-1}$ and τ^{n-1} are modified as described below to get $\mathcal{M}^n$ and τ_n and thereafter $U^n, \Theta^n \in \mathbf{V}^n$ computed according to the following prescription*

$$\Theta^n = I^n\beta(U^n), \quad \Theta^n - I^n g_D^n \in \mathbf{V}_0^n, \quad \bar{U}^{n-1} := U^{n-1}(\bar{x}^{n-1}),$$

$$\frac{1}{\tau_n}\langle U^n - I^n\bar{U}^{n-1}, \varphi\rangle^n + \langle\nabla\Theta^n, \nabla\varphi\rangle + \langle\!\langle p^n(\Theta^n - \theta_{\text{ext}}^n), \varphi\rangle\!\rangle_{\Gamma_N}^n = \langle\!\langle g_N^n, \varphi\rangle\!\rangle_{\Gamma_L}^n \quad \forall\varphi \in \mathbf{V}_0^n. \tag{3.5}$$

We stress that the right-hand side of (3.5) vanishes in case $\Gamma_D = \Gamma_0 \cup \Gamma_L$, and $p, \theta_{\text{ext}}, g_N$ need only be piecewise smooth. In view of the constitutive relation $\Theta^n = I^n\beta(U^n)$ being enforced only at the nodes, and the use of mass lumping, the discrete problem yields a monotone operator in $\mathbf{R}^{K^n}$ which is easy to implement and solve via either nonlinear SOR [20] or monotone multigrid [12].

We conclude this section with some notation. Let the jump of $\nabla\Theta^n$ across $e \in \mathcal{B}^n$ be

$$[\![\nabla\Theta^n]\!]_e := (\nabla\Theta^n_{|S_1} - \nabla\Theta^n_{|S_2}) \cdot \nu_e. \tag{3.6}$$

Note that with the convention that the unit normal vector ν_e to e points from S_2 to S_1, the jump $[\![\nabla\Theta^n]\!]_e$ is well defined. Let U and $\hat{U}$ denote the piecewise constant and piecewise linear extensions of $\{U^n\}$, that is $U(\cdot, 0) = \hat{U}(\cdot, 0) = U^0(\cdot)$ and, for all $t^{n-1} < t \le t^n$,

$$U(\cdot, t) := U^n(\cdot) \in \mathbf{V}^n, \quad \hat{U}(\cdot, t) := \frac{t^n - t}{\tau_n}U^{n-1}(\cdot) + \frac{t - t^{n-1}}{\tau_n}U^n(\cdot).$$

Finally, for any $\gamma > 0, k \ge 0$ and $\omega \subset \Omega$ we introduce the mesh dependent norms

$$|\!|\!|\, h^\gamma\varphi \,|\!|\!|_{H^k(\omega)} := \Big(\sum_{e \subset \omega, e \in \mathcal{B}^n} h_e^{2\gamma} \|\, \varphi \,\|^2_{H^k(e)}\Big)^{1/2}, \quad \|\, h^\gamma\varphi \,\|_{H^k(\omega)} := \Big(\sum_{S \subset \omega, S \in \mathcal{M}^n} h_S^{2\gamma} \|\, \varphi \,\|^2_{H^k(S)}\Big)^{1/2}.$$

4 Parabolic Duality

In this section we study a linear backward parabolic problem in non-divergence form, which can be viewed as the adjoint formal derivative of (1.1). For any $U \in BV(0, T; L^2(\Omega))$, we define

$$b(x,t) = \begin{cases} \dfrac{\beta(u) - \beta(U)}{u - U} & \text{if } u \neq U, \\ \beta_1 & \text{otherwise.} \end{cases} \tag{4.1}$$

It is clear from (H1) that $0 \le b(x,t) \le \beta_2$, for a.e. $(x,t) \in Q_T$. Let $b_\delta \in C^2(\bar{Q}_T)$ be a regularization of b satisfying

$$b_\delta \ge \delta > 0, \quad 0 \le b_\delta - b \le \delta \quad \text{a.e. in } Q_T, \tag{4.2}$$

where $0 < \delta \leq 1$ is a parameter to be chosen later. For arbitrary $t_* \in (0, T]$ and $\chi \in L^\infty(Q_T)$, let ψ be the solution of the following linear backward parabolic problem

$$\mathcal{L}_\delta(\psi) := \partial_t \psi + v(t)\partial_z \psi + b_\delta \Delta \psi = -b^{1/2}\chi \quad \text{in} \quad \Omega \times (0, t_*), \tag{4.3}$$

$$\psi = 0 \quad \text{on} \quad \Gamma_D \times (0, t_*), \tag{4.4}$$

$$\partial_\nu \psi + p\psi = 0 \quad \text{on} \quad \Gamma_N \times (0, t_*), \tag{4.5}$$

$$\psi(x, t_*) = 0 \quad \text{in} \quad \Omega, \tag{4.6}$$

and

$$\partial_\nu \psi + \frac{v(t)}{b_\delta}\psi = 0 \quad \text{on} \quad \Gamma_L \times (0, t_*) \tag{4.7}$$

provided (1.7) is enforced; we set $Q_* = \Omega \times (0, t_*)$. Existence of a unique solution $\psi \in W_q^{2,1}(Q_*)$ for any $q \geq 2$ of (4.3)-(4.6) follows from the theory of nonlinear strictly parabolic problems [13]. Note that we impose a Dirichlet outflow boundary condition on Γ_0, which yields a boundary layer for ψ.

We now embark in the derivation of a priori estimates for the regularity of ψ. It turns out that such a technical endeavor depends on the boundary condition on Γ_L, which becomes inflow for (4.3). Consequently we distinguish the two cases on $\Gamma_L \times (0, t_*)$

$$\partial_\nu \psi + \frac{v(t)}{b_\delta}\psi = 0 \qquad \textit{Robin inflow condition,} \tag{4.8}$$

$$\psi = 0 \qquad \textit{Dirichlet inflow condition,} \tag{4.9}$$

corresponding to (1.7) and (1.8): the former is more realistic but leads to worse stability bounds. We start with a simple, but essential, non-degeneracy property first proved in [2, Lemma 3.2].

Lemma 4.1 *Let $\xi, \rho \in \mathbf{R}$ satisfy $|\beta(\xi)| \geq \rho > 0$. Then we have*

$$|\xi - \eta| \leq \Big(\frac{1}{\beta_1} + \frac{\lambda}{\rho}\Big)|\beta(\xi) - \beta(\eta)|, \quad \forall\ \eta \in \mathbf{R}. \tag{4.10}$$

Proof. We only show the case $\beta(\xi) \geq \rho$ because the other $\beta(\xi) \leq -\rho$ is similar. In view of (H1) we see that $\xi > \lambda$ since $\beta(\xi) > 0$. If $\eta > \lambda$ the assertion follows directly from $\beta' \geq \beta_1$. For any $\eta \in [0, \lambda]$, we have $\beta(\eta) = 0$ and

$$\begin{aligned} |\xi - \eta| \leq |\xi - \lambda| + \lambda \ &\leq \ \frac{1}{\beta_1}|\beta(\xi) - \beta(\lambda)| + \frac{\lambda}{\rho}\rho \\ &\leq \ \frac{1}{\beta_1}|\beta(\xi)| + \frac{\lambda}{\rho}|\beta(\xi)| \\ &= \ \Big(\frac{1}{\beta_1} + \frac{\lambda}{\rho}\Big)|\beta(\xi) - \beta(\eta)|. \end{aligned}$$

Finally, if $\eta < 0$, we use the previous inequality with $\eta = 0$ together with $\beta(\xi), -\beta(\eta) > 0$, to get

$$\begin{aligned} |\xi - \eta| \leq |\xi - 0| + |0 - \eta| \ &\leq \ \Big(\frac{1}{\beta_1} + \frac{\lambda}{\rho}\Big)|\beta(\xi)| + \frac{1}{\beta_1}|\beta(\eta)| \\ &\leq \ \Big(\frac{1}{\beta_1} + \frac{\lambda}{\rho_0}\Big)|\beta(\xi) - \beta(\eta)|. \end{aligned}$$

This completes the proof of (4.11). ■

The following result is a trivial consequence of (4.1) and Lemma 4.1.

Corollary 4.1 *There exists $r > 0$ depending on ρ_0 of* (H8) *and ρ_1 of* (H9) *such that*

$$b(x,t) \geq r \quad \text{in } \Gamma \times \big([0,\varepsilon_0] \cup [L-\varepsilon_1, L]\big) \times [0,T]. \tag{4.11}$$

We observe that Corollary 4.1 only guarantees non-degeneracy of b but not its differentiability. If, in addition, $\beta(U) \leq -\rho_1$ on $\Gamma \times [L-\varepsilon_1, L] \times [0,T]$, which can be verified a posteriori, then (H9) leads to

$$b(x,t) = \alpha > 0 \quad \text{in } \Gamma \times [L-\varepsilon_1, L] \times [0,T]. \tag{4.12}$$

This property will also be assumed for b_δ whenever it is valid for b.

4.1 Robin Inflow Condition

Throughout this section we assume that (4.8) is enforced. To motivate the estimates below consider the simplified PDE obtained from (4.3) by setting $b_\delta = 0, v(t) = V$ and $b\chi = 1$, namely,

$$\partial_t \Lambda + V \partial_z \Lambda = -1, \tag{4.13}$$

with terminal condition (4.6). If the inflow condition were $\partial_\nu \Lambda = 0$ then the method of characteristics would yield the solution $\Lambda(z,t) = t_* - t$ for the resulting transport problem. Such a Λ is an upper bound for the actual solution $\psi \geq 0$ of (4.13) satisfying $\partial_\nu \psi \leq 0$ on Γ_L. We then see that ψ is bounded uniformly in V, and expect a boundary layer of size $1/V$ due to the outflow Dirichlet condition on Γ_0 and the presence of non-vanishing diffusion (4.11) near Γ_0; so $|\partial_\nu \psi| \leq CV$ on Γ_0. We now set $A = \| \chi \|_{L^\infty(Q_*)}$, and proceed to justify these heuristic arguments.

Lemma 4.2 *The following a priori bound is valid*

$$\| \psi \|_{L^\infty(Q_*)} \leq \beta_2^{1/2} t_* \| \chi \|_{L^\infty(Q_*)}.$$

Proof. Consider the barrier function $\Lambda(t) = \beta_2^{1/2} A (t_* - t)$. In view of (H1), we easily get

$$\mathcal{L}_\delta(\Lambda \pm \psi) = -\beta_2^{1/2} A \mp b^{1/2} \chi \leq 0.$$

Since $\Lambda \pm \psi \geq 0$ on $\Gamma_0 \times (0,t_*)$ and $\Omega \times \{t_*\}$, along with

$$\partial_\nu(\Lambda \pm \psi) + q(\Lambda \pm \psi) = q\Lambda \geq 0,$$

where $q = \frac{v}{b_\delta}$ on $\Gamma_L \times (0,t_*)$ and $q = p$ on $\Gamma_N \times (0,t_*)$, the strong maximum principle yields the desired estimate

$$\Lambda \pm \psi \geq 0 \quad \text{in } Q_*. \quad ■$$

To obtain a bound for $\partial_z \psi$ on Γ_0 we modify a barrier technique in [24] to allow for variable velocity $v(t)$. We also explicitly trace the dependence on V and t_*.

Lemma 4.3 *There exists C independent of V and T such that the following a priori bound is valid for all $0 \le t_* \le T$*

$$|\partial_\nu \psi| \le CVt_* \|\,\chi\,\|_{L^\infty(Q_*)} \quad on\ \Gamma_0 \times (0, t_*). \tag{4.14}$$

Proof. For $k > 0$ to be chosen later consider the barrier function

$$\sigma(z) = k\Big(1 - e^{-Vz/r}\Big) - \Big(\frac{\beta_2^{1/2} A}{v_0 V}\Big) z, \quad 0 \le z \le \varepsilon_0.$$

Since (4.2) and (4.11) imply $r \le b \le b_\delta$, and (H2) thus leads to $v(t) - b_\delta \frac{V}{r} \le 0$, a simple calculation yields

$$\mathcal{L}_\delta(\sigma) = -v(t)\Big(\frac{\beta_2^{1/2} A}{v_0 V}\Big) + \frac{V}{r}\, k e^{-Vz/r}\Big(v(t) - b_\delta \frac{V}{r}\Big) \le -\beta_2^{1/2} A.$$

Hence

$$\mathcal{L}_\delta(\sigma \pm \psi) \le 0 \quad \text{in } \Gamma \times (0, \varepsilon_0) \times (0, t_*).$$

Upon taking

$$k = \frac{\beta_2^{1/2} A (v_0 V t_* + \varepsilon_0)}{v_0 V (1 - e^{-V\varepsilon_0/r})},$$

and using Lemma 4.2, we deduce the boundary conditions

$$\begin{aligned}
&\sigma \pm \psi \ge 0 \quad \text{on } \Gamma_0 \times (0, t_*) \cup \Omega \times \{t_*\},\\
&\sigma \pm \psi \ge k(1 - e^{-V\varepsilon_0/r}) - \frac{\beta_2^{1/2} A \varepsilon_0}{v_0 V} - \beta_2^{1/2} t_* A = 0 \quad \text{on } (\Gamma \times \{\varepsilon_0\}) \times (0, t_*),\\
&\partial_\nu(\sigma \pm \psi) + p(\sigma \pm \psi) = p\sigma \ge 0 \quad \text{on } \Gamma_N \times (0, t_*).
\end{aligned}$$

Now the strong maximum principle implies that

$$\sigma \pm \psi \ge 0 \quad \text{in } \Gamma \times [0, \varepsilon_0] \times [0, t_*].$$

Since $\sigma(0) = 0$, we immediately obtain the asserted estimate

$$|\partial_z \psi| \le \sigma'(0) = \frac{Vk}{r} - \frac{\beta_2^{1/2} A}{v_0 V} \le \frac{Vk}{r} = \frac{\beta_2^{1/2} (v_0 V t_* + \varepsilon_0)}{v_0 r (1 - e^{-V\varepsilon_0/r})} A \quad \text{on } \Gamma_0 \times (0, t_*). \quad \blacksquare$$

It turns out that we also need a bound on the tangential derivative $\partial_y \psi$ on Γ_L, which cannot be derived with a barrier technique. To this end we first prove a local gradient estimate in the vicinity of Γ_L, namely on the sets $\omega_1 := \Gamma \times (L - \varepsilon_1, L), \omega_0 := \Gamma \times (L - \varepsilon_1/2, L)$. Let $\zeta \in C^\infty(\mathbf{R})$ be a cut-off function satisfying

$$0 \le \zeta \le 1, \qquad \zeta(s) = 0 \quad \forall\ -\infty < s \le L - \varepsilon_1, \qquad \zeta(s) = 1 \quad \forall\ L - \frac{\varepsilon_1}{2} \le s < \infty.$$

Lemma 4.4 *Let (4.12) hold for both b and b_δ. We then have the gradient estimate*

$$\int_0^{t_*} \int_{\omega_1} \zeta^2 |\nabla \psi|^2 + \int_0^{t_*} \int_{\Gamma_L} v\psi^2 \le C t_*^3 \|\,\chi\,\|^2_{L^\infty(Q_*)}. \tag{4.15}$$

Proof. Multiply (4.3) by the admissible test function $-\zeta^2\psi$ and integrate in space and time. In light of (4.12), integration by parts leads to

$$\frac{1}{2}\int_{\omega_1}\zeta^2\psi^2(\cdot,t) \quad + \quad \int_t^{t_*}\int_{\omega_1} -\frac{v}{2}\partial_z(\zeta^2\psi^2)+\frac{v}{2}\psi^2\partial_z\zeta^2+\alpha\zeta^2|\nabla\psi|^2+2\alpha\zeta\nabla\psi\cdot\psi\nabla\zeta$$
$$- \quad \int_t^{t_*}\int_{\partial\omega_1}\alpha\zeta^2\psi\partial_\nu\psi = \int_t^{t_*}\int_{\omega_1} b^{1/2}\chi\zeta^2\psi.$$

The second term can be rewritten as

$$\int_t^{t_*}\int_{\omega_1} -\frac{v}{2}\partial_z(\zeta^2\psi^2) = \int_t^{t_*}\int_{\Gamma_L} -\frac{v}{2}\zeta^2\psi^2,$$

whereas the third term is non-negative. Applying Cauchy-Schwarz inequality, the fifth term is bounded above by

$$2\alpha\int_t^{t_*}\int_{\omega_1}\zeta|\nabla\psi||\psi\nabla\zeta| \le \frac{\alpha}{2}\int_t^{t_*}\int_{\omega_1}\zeta^2|\nabla\psi|^2 + 2\alpha\int_t^{t_*}\int_{\omega_1}\psi^2|\nabla\zeta|^2.$$

In view of (4.5) and (4.7), the boundary term becomes

$$-\int_t^{t_*}\int_{\partial\omega_1}\alpha\zeta^2\psi\partial_\nu\psi = \int_t^{t_*}\int_{\Gamma_N}\alpha p\zeta^2\psi^2 + \int_t^{t_*}\int_{\Gamma_L} v\zeta^2\psi^2.$$

Collecting all these estimates, and discarding some non-negative terms, we end up with the asserted result

$$\frac{\alpha}{2}\int_t^{t_*}\int_{\omega_1}\zeta^2|\nabla\psi|^2 + \frac{1}{2}\int_t^{t_*}\int_{\Gamma_L} v\zeta^2\psi^2 \le \int_t^{t_*}\int_{\omega_1} 2\alpha\psi^2|\nabla\zeta|^2 + b^{1/2}|\chi\psi|\zeta^2 \le Ct_*^3A^2. \quad \blacksquare$$

Lemma 4.5 *Let* (4.12) *hold for both* b *and* b_δ. *Then there exists* $C>0$ *independent of* V *and* t_* *such that the following a priori bounds are valid for all* $0\le t_*\le T$

$$\max_{0\le t\le t_*}\|\nabla\psi(\cdot,t)\|^2_{L^2(\Omega)} + \int_t^{t_*}\!\!\int_\Omega b_\delta|\Delta\psi|^2dxdt + \int_t^{t_*}\!\!\int_{\Gamma_L} v|\nabla\psi|^2d\sigma dt \le CV^3t_*^3\|\chi\|^2_{L^\infty(Q_*)}.$$

Proof. We multiply (4.3) by $\Delta\psi$ and integrate over $\Omega\times(t,t_*)$ to get

$$\int_t^{t_*}\!\!\int_\Omega \partial_t\psi\Delta\psi + \int_t^{t_*}\!\!\int_\Omega v\partial_z\psi\Delta\psi + \int_t^{t_*}\!\!\int_\Omega b_\delta|\Delta\psi|^2 = \int_t^{t_*}\!\!\int_\Omega -b^{1/2}\chi\Delta\psi.$$

The rest of the proof consists of estimating each term separately. We examine them in turn.
1. Integrating by parts and using the boundary conditions (4.4), (4.5), and (4.7), as well as the terminal condition (4.6), we obtain

$$\int_t^{t_*}\!\!\int_\Omega \partial_t\psi\Delta\psi = \frac{1}{2}\|\nabla\psi(\cdot,t)\|^2_{L^2(\Omega)} - \int_t^{t_*}\!\!\int_{\Gamma_N} p\psi\partial_t\psi - \int_t^{t_*}\!\!\int_{\Gamma_L}\frac{v}{\alpha}\psi\partial_t\psi.$$

Since

$$-\int_t^{t_*}\!\!\int_{\Gamma_N} p\psi\partial_t\psi = \frac{1}{2}\int_{\Gamma_N} p\psi(\cdot,t)^2 + \frac{1}{2}\int_t^{t_*}\!\!\int_{\Gamma_N}\psi^2\partial_t p,$$

and

$$-\int_t^{t_*}\!\!\int_{\Gamma_L} \frac{v}{\alpha}\psi\partial_t\psi = \frac{1}{2\alpha}\int_{\Gamma_L} v\psi^2(\cdot,t) + \frac{1}{2\alpha}\int_t^{t_*}\!\!\int_{\Gamma_L} \psi^2\partial_t v,$$

according to (H2), (H4), and Lemma 4.2 we readily arrive at

$$\int_t^{t_*}\!\!\int_\Omega \partial_t\psi\Delta\psi \geq \frac{1}{2}\| \nabla\psi(\cdot,t) \|^2_{L^2(\Omega)} - Ct_*^3 VA^2.$$

2. Integrating again by parts and using (4.5) and (4.7), we have

$$\int_t^{t_*}\!\!\int_\Omega v\partial_z\psi\Delta\psi = -\int_t^{t_*}\!\!\int_\Omega \frac{v}{2}\partial_z|\nabla\psi|^2 - \int_t^{t_*}\!\!\int_{\Gamma_N} vp\psi\partial_z\psi - \int_t^{t_*}\int_{\Gamma_0} v|\partial_z\psi|^2 + \int_t^{t_*}\!\!\int_{\Gamma_L} v|\partial_z\psi|^2.$$

Making use of (4.4) and (4.7), the first term on the right-hand side gives rise to

$$-\int_t^{t_*}\!\!\int_\Omega \frac{v}{2}\partial_z|\nabla\psi|^2 = -\frac{1}{2}\int_t^{t_*}\!\!\int_{\Gamma_L} v|\partial_y\psi|^2 + v|\partial_z\psi|^2 + \frac{1}{2}\int_t^{t_*}\int_{\Gamma_0} v|\partial_z\psi|^2,$$

whereas, in view of (H4), the second term of the right-hand side yields

$$-\int_t^{t_*}\!\!\int_{\Gamma_N} vp\psi\partial_z\psi = \int_t^{t_*}\!\!\int_{\Gamma_N} -\frac{v}{2}\partial_z(p\psi^2) + \frac{v}{2}\psi^2\partial_z p \geq -CVt_*^3A^2.$$

These estimates, together with Lemma 4.3, lead to the expression

$$\begin{aligned}\int_t^{t_*}\!\!\int_\Omega v\partial_z\psi\Delta\psi &\geq -CVt_*^3A^2 - \frac{1}{2}\int_t^{t_*}\int_{\Gamma_0} v|\partial_z\psi|^2 - \frac{1}{2}\int_t^{t_*}\!\!\int_{\Gamma_L} v|\partial_y\psi|^2 + \frac{1}{2}\int_t^{t_*}\!\!\int_{\Gamma_L} v|\partial_z\psi|^2\\ &\geq -CV^3t_*^3A^2 - \frac{1}{2}\int_t^{t_*}\int_{\Gamma_L} v|\partial_y\psi|^2 + \frac{1}{2}\int_t^{t_*}\!\!\int_{\Gamma_L} v|\partial_z\psi|^2.\end{aligned}$$

To proceed any further we thus must bound the tangential derivative $|\partial_y\psi|$ on Γ_L.
3. We now invoke the well known trace inequality

$$\| \nabla\psi \|^2_{L^2(\Gamma_L)} \leq C\| \nabla\psi \|_{L^2(\omega_0)}\Big(\| \nabla\psi \|_{L^2(\omega_0)} + \| D^2\psi \|_{L^2(\omega_0)}\Big) \qquad \forall\ 0 < t < t_*.$$

To estimate $\| D^2\psi \|_{L^2(\omega_0)}$ we resort to elliptic regularity theory. Since $\zeta^2\psi$ satisfies in ω_1

$$\Delta(\zeta^2\psi) = \zeta^2\Delta\psi + 4\zeta\nabla\psi\nabla\zeta + \psi\Delta\zeta^2, \tag{4.16}$$

together with non-homogeneous boundary conditions

$$\partial_z(\zeta^2\psi) = -\frac{v}{\alpha}(\zeta^2\psi) \quad \text{on } \Gamma_L, \qquad \zeta^2\psi = 0 \quad \text{on } \Gamma_{L-\varepsilon_1}, \qquad \partial_\nu(\zeta^2\psi) + p(\zeta^2\psi) = 0 \quad \text{on } \Gamma_N,$$

computing the right-hand side of (4.16) in $L^2(\Omega)$ and $\frac{v}{\alpha}\zeta^2\psi$ in $H^1(\Omega)$, we deduce for all $0 < t < t_*$

$$\| D^2\psi \|_{L^2(\omega_0)} \leq \| D^2(\zeta^2\psi) \|_{L^2(\omega_1)} \leq C\| \Delta\psi \|^2_{L^2(\omega_1)} + CV^2\| \zeta\nabla\psi \|^2_{L^2(\omega_1)} + CV^2\| \psi \|^2_{L^2(\omega_1)}.$$

If we next integrate in time and use Lemmas 4.2 and 4.4 in conjunction with the Cauchy-Schwarz inequality, we thus obtain

$$\begin{aligned}\int_t^{t_*} \| \partial_y \psi \|^2_{L^2(\Gamma_L)} &\leq \eta \int_t^{t_*} \| \Delta\psi \|^2_{L^2(\omega_1)} + \frac{C}{\eta} V^2 \int_t^{t_*} \| \zeta \nabla \psi \|^2_{L^2(\omega_1)} + \| \psi \|^2_{L^2(\omega_1)} \\ &\leq \frac{C}{\eta} V^2 t_*^3 A^2 + \eta \int_t^{t_*} \| \Delta\psi \|^2_{L^2(\omega_1)} \qquad \forall\ 0 < \eta \leq 1, \end{aligned} \tag{4.17}$$

whence

$$\int_t^{t_*} \int_\Omega v \partial_z \psi \Delta \psi \geq -CV^2 \Big(V + \frac{1}{\eta} \Big) t_*^3 A^2 - \frac{\eta}{2} V \int_t^{t_*} \| \Delta\psi \|^2_{L^2(\omega_1)}.$$

4. We finally collect all previous estimates to arrive at

$$\begin{aligned}\| \nabla \psi \|^2_{L^2(\Omega)} &+ \int_t^{t_*} \int_\Omega b_\delta |\Delta\psi|^2 + \int_t^{t_*} \int_{\Gamma_L} v |\partial_z \psi|^2 \\ &\leq CV^2 \Big(V + \frac{1}{\eta} \Big) t_*^3 A^2 + \eta V \int_t^{t_*} \| \Delta\psi \|^2_{L^2(\omega_1)} + \int_t^{t_*} \int_\Omega |\chi|^2. \end{aligned}$$

We see that choosing $\eta = \frac{\alpha}{2V}$, and using the crucial fact (4.12), we infer all the asserted estimates except for that of the tangential derivative on Γ_L. This estimate follows from (4.17). ■

Corollary 4.2 *Let* (4.12) *hold for both* b *and* b_δ. *Then there exists* $C > 0$ *independent of* V *and* t_* *such that the following a priori bounds are valid for all* $0 \leq t_* \leq T$

$$\int_0^{t_*} \int_\Omega |\partial_t \psi + v(t) \partial_z \psi|^2 dx dt \leq CV^3 t_*^3 \| \chi \|^2_{L^\infty(Q_*)}.$$

Proof. This is a direct consequence of Lemma 4.5 and (4.3). ■

Corollary 4.3 *Let* (4.12) *hold for both* b *and* b_δ. *Then there exists* $C > 0$ *independent of* V *and* t_* *such that the following a priori bounds are valid for all* $0 \leq t_* \leq T$

$$\int_0^{t_*} \delta \| D^2 \psi \|^2_{L^2(\Omega)} dt \leq CV^3 t_*^3 \| \chi \|^2_{L^\infty(Q_*)}.$$

Proof. Since $b_\delta \geq \delta$, we deduce from Lemma 4.5 that

$$\int_0^{t_*} \delta \| \Delta \psi \|^2_{L^2(\Omega)} dt \leq CV^3 t_*^3 \| \chi \|^2_{L^\infty(Q_*)}.$$

We use again the argument of step 3 in Lemma 4.5, but now in Ω. Since Ω is a rectangle and ψ satisfies the Dirichlet condition $\psi = 0$ on Γ_0, together with the Neumann conditions $\partial_\nu \psi = -\frac{v}{\alpha} \psi$ on Γ_L and $\partial_\nu \psi = -p\psi$ on Γ_N, elliptic regularity theory [10], [11] yields

$$\| D^2 \psi \|^2_{L^2(\Omega)} \leq C \| \Delta \psi \|^2_{L^2(\Omega)} + CV \| \nabla \psi \|^2_{L^2(\Omega)}.$$

Consequently, with the aid of the interpolation estimates [10, p.173]

$$\| \nabla \psi \|^2_{L^2(\Omega)} \leq \eta \| D^2 \psi \|^2_{L^2(\Omega)} + \frac{1}{C\eta} \| \psi \|^2_{L^2(\Omega)}$$

we realize that choosing $\eta = \frac{1}{2CV}$ leads to the desired bound. ■

4.2 Dirichlet Inflow Condition

Throughout this section we assume that (1.8) is enforced. As in §4.1, we first examine the behavior of the simplified PDE (4.13) with inflow boundary condition $\psi = 0$ on Γ_L. If we allow $t_* = \infty$, then the method of characteristics gives the solution $\psi(z,t) = (L-z)/V$. Due to the effect of the terminal condition $\psi = 0$ at $t = t_* < \infty$, such a solution is larger than the actual one, and both exhibit an outflow boundary layer of size $1/V$ near Γ_0. Since the size of the solution is also about $1/V$, we expect $\partial_z \psi$ to be bounded uniformly in V on Γ_0. This heuristic reasoning is made rigorous below. We set again $A = \| \chi \|_{L^\infty(Q_*)}$.

Lemma 4.6 *The following a priori bound is valid for all $x \in \bar{\Omega}$ and $0 \leq t \leq t_* \leq T$*

$$|\psi(x,t)| \leq \frac{\beta_2^{1/2} L}{v_0 V} \| \chi \|_{L^\infty(Q_*)}.$$

Proof. We consider the barrier function $\Lambda(z) = (\beta_2^{1/2} A / v_0 V)(L - z)$ for $0 \leq z \leq L$. A simple calculation using (H2) implies

$$\mathcal{L}_\delta(\Lambda \pm \psi) = -v(t)\Big(\frac{\beta_2^{1/2} A}{v_0 V}\Big) \pm (-b^{1/2}\chi) \leq -\beta_2^{1/2} A \pm b^{1/2}\chi \leq 0.$$

With respect to boundary conditions, we see that (4.4) and (4.6) yield

$$\Lambda \pm \psi \geq 0 \quad \text{on } \Gamma_D \times (0, t_*) \cup \Omega \times \{t_*\},$$

and (4.5) gives

$$\partial_\nu(\Lambda \pm \psi) + p(\Lambda \pm \psi) = p\Lambda \geq 0 \quad \text{on } \Gamma_N \times (0, t_*).$$

Therefore, applying the strong maximum principle results in the desired bound

$$\Lambda \pm \psi \geq 0 \quad \text{in } \bar{\Omega} \times [0, t_*]. \quad \blacksquare \tag{4.18}$$

A direct consequence of (4.18) and $\Lambda = 0$ on $\Gamma_L \times (0, t_*)$ is that

$$|\partial_\nu \psi| \leq -\Lambda'(L) = \frac{\beta_2^{1/2}}{v_0 V} \| \chi \|_{L^\infty(Q_*)} \quad \text{on } \Gamma_L \times (0, t_*). \tag{4.19}$$

We now prove a similar bound on the outflow boundary Γ_0.

Lemma 4.7 *There exists $C > 0$ independent of V and t_* such that for all $0 \leq t_* \leq T$*

$$|\partial_\nu \psi| \leq C \| \chi \|_{L^\infty(Q_*)} \quad \textit{on } \Gamma_0 \times (0, t_*). \tag{4.20}$$

Proof. We proceed as in Lemma 4.3, with the same barrier function $\sigma(z)$ and $k = \frac{\beta_2^{1/2} A (L + \varepsilon_0)}{v_0 V (1 - e^{-V\varepsilon_0/r})}$. $\blacksquare$

Lemma 4.8 *There exists $C > 0$ independent of V and t_* such that for all $0 \leq t_* \leq T$*

$$\max_{0 \leq t \leq t_*} \| \nabla \psi(\cdot, t) \|^2_{L^2(\Omega)} + \int_0^{t_*} \int_\Omega b_\delta |\Delta \psi|^2 dx dt \leq C V t_* \| \chi \|^2_{L^\infty(Q_*)}.$$

Proof. We proceed as in Lemma 4.5, that is we first multiply (4.3) by $\Delta\psi$ and integrate by parts over Q_*. The only difference arises in treating the convection term, which now reads

$$\int_t^{t_*}\!\!\int_\Omega v\partial_z\psi\Delta\psi = \frac{1}{2}\int_t^{t_*}\int_{\Gamma_L} v|\partial_z\psi|^2 - \frac{1}{2}\int_t^{t_*}\int_{\Gamma_0} v|\partial_z\psi|^2 - \int_t^{t_*}\int_{\Gamma_N}\frac{vp}{2}\partial_z|\psi|^2.$$

The first term on the right-hand side, which was problematic before, can now be eliminated because it is ≥ 0. The proof concludes as in Lemma 4.5. $\blacksquare$.

Corollary 4.4 *There exists $C > 0$ independent of V and t_* such that for all $0 \leq t_* \leq T$*

$$\int_0^{t_*}\int_\Omega \Big(|\partial_t\psi + v(t)\partial_z\psi|^2 + \delta|D^2\psi|\Big)dxdt \leq CVt_*\|\,\chi\,\|^2_{L^\infty(Q_*)}.$$

4.3 Discontinuous p

We investigate the effect in 2d of a finite number of discontinuities of p along Γ_N; this corresponds to abrupt changes in the cooling conditions as in the examples of §7. The estimates above remain all valid except for those in Corollaries 4.3 and 4.4, which involve second derivatives of ψ.

Using the intrinsic definition of fractional Sobolev spaces, together with the fact that p is piecewise $W^{1,\infty}$ over Γ_N, results in $\partial_\nu\psi = -p\psi \in H^{1/2-\epsilon}$ in a vicinity of such discontinuities for $\epsilon > 0$. Elliptic regularity theory implies [15, p.188], [11]

$$\int_0^{t_*}\delta\|\psi\|^2_{H^{2-\epsilon}(\Omega)}dt \leq C_\epsilon V^k {t_*}^k\|\,\chi\,\|^2_{L^\infty(Q_*)} \quad \forall\ \epsilon > 0, \tag{4.21}$$

where $k = 3, 1$ for the Neumann and Dirichlet conditions, respectively. There is thus a slight loss of regularity with respect to the smooth case for both boundary conditions.

4.4 Error Representation Formula

We now derive an explicit representation formula for the error $\|\,\beta(u) - \beta(U)\,\|_{L^1(Q_*)}$ based on the linear backward parabolic problem (4.3)-(4.7). We only assume that $U(\cdot, t)$ is piecewise constant, so the derivation below applies to the solution U of (3.5).

We first multiply (4.3) by $-(u - U)$, and integrate in space and time from 0 to $t_* = t^m$. We examine the various contributions in turn. Since U is piecewise constant in time, we have

$$-\int_0^{t^m}\langle\partial_t\psi, u - U\rangle = \int_0^{t^m}\Big(\langle\psi, \partial_t(u - \hat{U})\rangle + \langle\partial_t\psi, U - \hat{U}\rangle\Big)dt + \langle\psi^0, u_0 - U^0\rangle.$$

Integrating by parts we get

$$-\int_0^{t^m}\langle v(t), \partial_z\psi(u - U)\rangle = \int_0^{t^m} v(t)\langle\psi, \partial_z(u - U)\rangle - \int_0^{t^m} v(t)\langle\!\langle\psi, u - U\rangle\!\rangle_{\Gamma_L},$$

and using (4.1) we also obtain

$$\begin{aligned}
-\int_0^{t^m}\langle b_\delta\Delta\psi, u - U\rangle \;&=\; \int_0^{t^m}\langle\nabla\psi, \nabla(\beta(u) - \beta(U))\rangle \\
&-\; \int_0^{t^m}\langle\!\langle\partial_\nu\psi, \beta(u) - \beta(U)\rangle\!\rangle + \int_0^{t^m}\langle(b - b_\delta)\Delta\psi, u - U\rangle.
\end{aligned}$$

Since

$$b^{1/2}|u-U| = |\beta(u)-\beta(U)|^{1/2}|u-U|^{1/2} \geq \beta_2^{-1/2}|\beta(u)-\beta(U)|,$$

collecting these estimates, and making use of (2.1), we easily end up with

$$\|\,\beta(u)-\beta(U)\,\|_{L^1(Q^m)} \leq \beta_2^{1/2} \sup_{\chi\in L^\infty(Q^m)} \frac{|\mathcal{R}(\psi)|}{\|\chi\|_{L^\infty(Q^m)}}, \tag{4.22}$$

where $\mathcal{R}$, the *parabolic residual*, is the following distribution

$$\begin{aligned}\mathcal{R}(\psi) = \langle u_0 - U^0, \psi^0\rangle &+ \int_0^{t^m} \langle U-\hat{U}, \partial_t\psi\rangle dt + \int_0^{t^m} \langle u-U, (b-b_\delta)\Delta\psi\rangle dt \\ &- \int_0^{t^m} \Big(\langle \partial_t\hat{U} + v(t)\partial_z U, \psi\rangle + \langle\nabla\beta(U), \nabla\psi\rangle\Big) dt \\ &- \int_0^{t^m} \Big(\langle\!\langle p(\beta(U)-\theta_{\text{ext}}), \psi\rangle\!\rangle_{\Gamma_N} + \langle\!\langle \partial_\nu\psi, g_D - \beta(U)\rangle\!\rangle_{\Gamma_0} - \langle\!\langle g_N, \psi\rangle\!\rangle_{\Gamma_L}\Big) dt.\end{aligned}$$

We conclude that an estimate of the error solely depending on discrete quantities and data may be obtained upon evaluating $\mathcal{R}$ in suitable negative Sobolev norms. The latter are dictated by the a priori bounds of §§4.1 and 4.2. This program is carry out in §5.1 for the fully discrete solution U of (3.5).

5 A Posteriori Error Analysis

We first introduce the interior residual R^n and boundary residual B^n:

$$R^n := \frac{U^n - I^n\bar{U}^{n-1}}{\tau_n}, \quad B^n := \begin{cases} \partial_\nu\Theta^n + I^n p^n(\Theta^n - I^n\theta^n_{\text{ext}}) & \text{on } \Gamma_N, \\ \partial_\nu\Theta^n - I^n g_N^n & \text{on } \Gamma_L. \end{cases}$$

Theorem 5.1 (Neumann Outflow) *Let (1.7) be enforced and $\Theta^n \leq -\rho_1$ in $\Gamma\times[L-\varepsilon_1, L]$ for any $n \geq 1$. Then there exists a constant $C>0$ independent of V and t^m such that the following a posteriori error estimate holds for all $t^m \in [0,T]$,*

$$\int_0^{t^m} \|\,\beta(u)-\beta(U)\,\|_{L^1(\Omega)} dt \leq C(Vt^m)^{3/2}\Big(\mathcal{E}_0 + \sum_{i=5}^{10}\mathcal{E}_i + \Big(\Lambda_m\sum_{i=1}^{4}\mathcal{E}_i\Big)^{1/2}\Big), \tag{5.1}$$

where

$$\Lambda_m = \Big(\sum_{n=1}^{m}\tau_n\big(1+\lambda|\Omega| + \|\,\Theta^n\,\|^2_{L^2(\Omega)}\big)\Big)^{1/2} \tag{5.2}$$

and the error indicators $\mathcal{E}_i$ are given by

$$
\begin{aligned}
\mathcal{E}_0 &:= (V^3 t^m)^{-1/2} \| \, u_0 - U^0 \, \|_{L^1(\Omega)} && \textit{initial error,} \\
\mathcal{E}_1 &:= \Big(\sum_{n=1}^{m} \tau_n ||| \, h^{3/2} [\![\nabla \Theta^n]\!] \, |||^2_{L^2(\Omega)} \Big)^{1/2} && \textit{jump residual,} \\
\mathcal{E}_2 &:= \Big(\sum_{n=1}^{m} \tau_n \| \, h^2 R^n \, \|^2_{L^2(\Omega)} \Big)^{1/2} && \textit{interior residual,} \\
\mathcal{E}_3 &:= \Big(\sum_{n=1}^{m} \tau_n ||| \, h^{3/2} B^n \, |||^2_{L^2(\partial\Omega \setminus \Gamma_D)} \Big)^{1/2} && \textit{boundary residual,} \\
\mathcal{E}_4 &:= \Big(\sum_{n=1}^{m} \tau_n \| \, \beta(U^n) - I^n \beta(U^n) \, \|^2_{L^2(\Omega)} \Big)^{1/2} && \textit{constitutive relation,} \\
\mathcal{E}_5 &:= \Big(\sum_{n=1}^{m} \tau_n \| \, U^n - I^n U^{n-1} \, \|^2_{L^2(\Omega)} \\
&\quad + \sum_{n=1}^{m} \frac{\tau_n}{V^2} \| \, U^n - I^n U^{n-1} \, \|^2_{L^2(\Gamma_L)} \Big)^{1/2} && \textit{time residual,} \\
\mathcal{E}_6 &:= \Big(\sum_{n=1}^{m} \tau_n \| \, U^{n-1} - I^n U^{n-1} \, \|^2_{L^2(\Omega)} \\
&\quad + \sum_{n=1}^{m} \frac{\tau_n}{V^2} \| \, U^{n-1} - I^n U^{n-1} \, \|^2_{L^2(\Gamma_L)} \Big)^{1/2} && \textit{coarsening,} \\
\mathcal{E}_7 &:= (V^3 t^m)^{-1/2} \sum_{n=1}^{m} \tau_n \| \, R^n - (\partial_t \hat{U} + v(t) \partial_z \hat{U}) \, \|_{L^1(\Omega)} && \textit{characteristic residual,} \\
\mathcal{E}_8 &:= \sum_{n=1}^{m} \tau_n \| \, h^2 \nabla R^n \, \|_{L^2(\Omega)} && \textit{interior quadrature,} \\
\mathcal{E}_9 &:= \sum_{n=1}^{m} \tau_n ||| \, h^{3/2} (\Theta^n - I^n \theta^n_{\text{ext}}) \, |||_{H^1(\Gamma_N)} \\
&\quad + \Big(\sum_{n=1}^{m} \frac{\tau_n}{V} ||| \, h^2 \partial_y (I^n g_N^n) \, |||^2_{L^2(\Gamma_L)} \Big)^{1/2} && \textit{boundary quadrature,} \\
\mathcal{E}_{10} &:= (V^3 t^m)^{-1/2} \sum_{n=1}^{m} \int_{t^{n-1}}^{t^n} \| \, \theta_{\text{ext}} - I^n \theta^n_{\text{ext}} \, \|_{L^1(\Gamma_N)} \\
&\quad + (V^3 t^m)^{-1/2} \sum_{n=1}^{m} \int_{t^{n-1}}^{t^n} \| \, p - I^n p^n \, \|_{L^\infty(\Gamma_N)} \| \, \Theta^n - \theta_{\text{ext}} \, \|_{L^1(\Gamma_N)} \\
&\quad + (V^3 t^m)^{-1/2} \sum_{n=1}^{m} \int_{t^{n-1}}^{t^n} \| \, g_N - I^n g_N^n \, \|_{L^1(\Gamma_L)} \\
&\quad + (V t^m)^{-1/2} \sum_{n=1}^{m} \int_{t^{n-1}}^{t^n} \| \, g_D - I^n g_D^n \, \|_{L^1(\Gamma_0)} && \textit{boundary discretization.}
\end{aligned}
$$

Theorem 5.2 (Dirichlet Outflow) *Let (1.8) be satisfied. Then there exists a constant $C > 0$ independent of V and t^m such that the following a posteriori error estimate holds for all $t^m \in [0, T]$,*

$$
\int_0^{t^m} \| \, \beta(u) - \beta(U) \, \|_{L^1(\Omega)} dt \le C (V t^m)^{1/2} \Big(\mathcal{E}_0 + \sum_{i=5}^{10} \mathcal{E}_i + \Big(\Lambda_m \sum_{i=1}^{4} \mathcal{E}_i \Big)^{1/2} \Big), \tag{5.3}
$$

where Λ_m is defined in (5.2) and the error indicators $\mathcal{E}_i$ are given by

$$\begin{aligned}
\mathcal{E}_0 &:= (V^3 t^m)^{-1/2} \| u_0 - U^0 \|_{L^1(\Omega)} && \textit{initial error,}\\
\mathcal{E}_1 &:= \Big(\sum_{n=1}^m \tau_n \||\, h^{3/2} [\![\nabla \Theta^n]\!] \,\||^2_{L^2(\Omega)} \Big)^{1/2} && \textit{jump residual,}\\
\mathcal{E}_2 &:= \Big(\sum_{n=1}^m \tau_n \| h^2 R^n \|^2_{L^2(\Omega)} \Big)^{1/2} && \textit{interior residual,}\\
\mathcal{E}_3 &:= \Big(\sum_{n=1}^m \tau_n \||\, h^{3/2} B^n \,\||^2_{L^2(\partial\Omega\setminus\Gamma_D)} \Big)^{1/2} && \textit{boundary residual,}\\
\mathcal{E}_4 &:= \Big(\sum_{n=1}^m \tau_n \| \beta(U^n) - I^n \beta(U^n) \|^2_{L^2(\Omega)} \Big)^{1/2} && \textit{constitutive relation,}\\
\mathcal{E}_5 &:= \Big(\sum_{n=1}^m \tau_n \| U^n - I^n U^{n-1} \|^2_{L^2(\Omega)} \Big)^{1/2} && \textit{time residual,}\\
\mathcal{E}_6 &:= \Big(\sum_{n=1}^m \tau_n \| U^{n-1} - I^n U^{n-1} \|^2_{L^2(\Omega)} \Big)^{1/2} && \textit{coarsening,}\\
\mathcal{E}_7 &:= (V^3 t^m)^{-1/2} \sum_{n=1}^m \tau_n \| R^n - (\partial_t \hat{U} + v(t) \partial_z \hat{U}) \|_{L^1(\Omega)} && \textit{characteristic residual,}\\
\mathcal{E}_8 &:= \sum_{n=1}^m \tau_n \| h^2 \nabla R^n \|_{L^2(\Omega)} && \textit{interior quadrature,}\\
\mathcal{E}_9 &:= \sum_{n=1}^m \tau_n \||\, h^{3/2} (\Theta^n - I^n \theta^n_{\text{ext}}) \,\||_{H^1(\Gamma_N)} && \textit{boundary quadrature,}\\
\mathcal{E}_{10} &:= (V^3 t^m)^{-1/2} \sum_{n=1}^m \int_{t^{n-1}}^{t^n} \| \theta_{\text{ext}} - I^n \theta^n_{\text{ext}} \|_{L^1(\Gamma_N)} \\
&+ (V^3 t^m)^{-1/2} \sum_{n=1}^m \int_{t^{n-1}}^{t^n} \| p - I^n p^n \|_{L^\infty(\Gamma_N)} \| \Theta^n - \theta_{\text{ext}} \|_{L^1(\Gamma_N)} \\
&+ (V^3 t^m)^{-1/2} \sum_{n=1}^m \int_{t^{n-1}}^{t^n} \| g_D - I^n g^n_D \|_{L^1(\Gamma_L)} \\
&+ (V t^m)^{-1/2} \sum_{n=1}^m \int_{t^{n-1}}^{t^n} \| g_D - I^n g^n_D \|_{L^1(\Gamma_0)} && \textit{boundary discretization.}
\end{aligned}$$

Remark 5.1. We note that the quantity Λ_m in the estimates involves the L^2 norm of the discrete temperature which is difficult to localize in practical computations. This bound, clearly achieved experimentally, can be proved by an a priori stability analysis which incorporates mesh changes.

Remark 5.2. If the meshes $\mathcal{M}^n$ are of weakly acute type, or equivalently the stiffness matrix $(\nabla\phi_i, \nabla\phi_j)_{i,j}$ is an M-matrix, then the discrete maximum principle holds and guarantees the uniform boundedness of Θ^n; thus $\Lambda_m \le C\sqrt{t^m}$. If for all interelement sides e and corresponding pair of adjacent simplexes, the sum of angles opposite to e does not exceed π, then $\mathcal{M}^n$ is weakly acute in 2D. Such a condition is not very restrictive in practice since it can be enforced with automatic mesh generators as long as the initial mesh exhibits this property.

5.1 Residuals

The error analysis hinges on the crucial estimate (4.22). To express the oscillatory character of $\mathcal{R}$ in (4.4), we resort to Galerkin orthogonality. This replaces the evaluation of $\mathcal{R}$ in negative Sobolev spaces but that on positive spaces plus weights depending on the mesh size h and the regularity of ψ. We first rewrite the discrete problem (3.5), for $t^{n-1} < t \le t^n$, $\phi \in \mathbf{V}_0$, and $\varphi \in \mathbf{V}_0^n$, as follows:

$$
\begin{aligned}
&\langle \partial_t \hat{U} + v(t)\partial_z U, \phi\rangle + \langle \nabla\Theta, \nabla\phi\rangle + \langle\!\langle p(\Theta - \theta_{\text{ext}}), \phi\rangle\!\rangle_{\Gamma_N} - \langle\!\langle g_N, \phi\rangle\!\rangle_{\Gamma_L} \\
&\quad = \Big\langle \partial_t \hat{U} + v(t)\partial_z \hat{U} - \tau_n^{-1}(U^n - I^n \bar{U}^{n-1}), \phi \Big\rangle \\
&\quad + v(t)\langle \partial_z (U - \hat{U}), \phi\rangle \\
&\quad + \langle R^n, \phi - \varphi\rangle \\
&\quad + \langle \nabla\Theta^n, \nabla(\phi - \varphi)\rangle + \langle\!\langle I^n p^n(\Theta^n - I^n\theta^n_{\text{ext}}), \phi - \varphi\rangle\!\rangle_{\Gamma_N} - \langle\!\langle I^n g^n_N, \phi - \varphi\rangle\!\rangle_{\Gamma_L} \\
&\quad + \Big(\langle R^n, \varphi\rangle - \langle R^n, \varphi\rangle^n\Big) \\
&\quad + \Big(\langle\!\langle I^n p^n(\Theta^n - I^n\theta^n_{\text{ext}}), \varphi\rangle\!\rangle_{\Gamma_N} - \langle\!\langle I^n p^n(\Theta^n - I^n\theta^n_{\text{ext}}), \varphi\rangle\!\rangle^n_{\Gamma_N}\Big) \\
&\quad + \Big(\langle\!\langle I^n g^n_N, \varphi\rangle\!\rangle^n_{\Gamma_L} - \langle\!\langle I^n g^n_N, \varphi\rangle\!\rangle_{\Gamma_L}\Big) \\
&\quad + \langle\!\langle (p - I^n p^n)(\Theta^n - \theta_{\text{ext}}) + I^n p^n(I^n\theta^n_{\text{ext}} - \theta_{\text{ext}}), \phi\rangle\!\rangle_{\Gamma_N} + \langle\!\langle I^n g^n_N - g_N, \phi\rangle\!\rangle_{\Gamma_L}.
\end{aligned}
\tag{5.4}
$$

This is the so-called Galerkin orthogonality, and reflects the essential property that the left-hand side is small in average. We next take $\phi = \psi$ and realize that to define φ we need to interpolate ψ under minimal regularity assumptions. We thus resort to the Clément interpolation operator $\Pi^n : L^2(\Omega) \to \mathbf{V}_0^n$, which satisfies the following local approximation properties [6], for $k = 1, 2$,

$$\|\psi - \Pi^n\psi\|_{L^2(S)} + h_S\|\nabla(\psi - \Pi^n\psi)\|_{L^2(S)} \le C^* h_S^k \|\psi\|_{H^k(\tilde{S})}, \tag{5.5}$$

$$\|\psi - \Pi^n\psi\|_{L^2(e)} \le C^* h_e^{k-1/2} \|\psi\|_{H^k(\tilde{S})}, \tag{5.6}$$

where $\tilde{S}$ is the union of all elements surrounding $S \in \mathcal{M}^n$ or $e \in \mathcal{B}^n$. The constant C^* depends solely on the minimum angle of the mesh $\mathcal{M}^n$. An important by-product of shape regularity of $\mathcal{M}^n$ is that the number of adjacent simplexes to a given one is bounded by a constant A independent of n, mesh-sizes and time-steps. Hence

$$\sum_{S \in \mathcal{M}^n} \|\xi\|^2_{L^2(\tilde{S})} \le A\|\xi\|^2_{L^2(\Omega)} \quad \forall\, \xi \in L^2(\Omega).$$

This, in conjunction with (5.6) for $k = 1$, yields the H^1-stability bound

$$\|\nabla\Pi^n\psi(\cdot, t)\|_{L^2(\Omega)} \le (1 + C^* A^{1/2})\|\nabla\psi(\cdot, t)\|_{L^2(\Omega)}. \tag{5.7}$$

Consequently, we select φ in (5.4) to be

$$\varphi(\cdot, t) = \Pi^n\psi((\cdot, t)) \quad \forall t^{n-1} < t \le t^n.$$

Since $\beta(U^n) = \alpha U^n = I^n\beta(U^n)$ on Γ_L, we then obtain an explicit expression for the residual $\mathcal{R}(\psi) = \sum_{i=0}^{12} \mathcal{R}_i(\psi)$ of (4.4), where

$$
\begin{aligned}
\mathcal{R}_0(\psi) &= \langle u_0 - U_0, \psi^0\rangle, \\
\mathcal{R}_1(\psi) &= \sum_{n=1}^{m} \int_{t^{n-1}}^{t^n} \langle \nabla\Theta^n, \nabla(\Pi^n\psi - \psi)\rangle dt, \\
\mathcal{R}_2(\psi) &= \sum_{n=1}^{m} \int_{t^{n-1}}^{t^n} \langle R^n, \Pi^n\psi - \psi\rangle dt, \\
\mathcal{R}_3(\psi) &= \sum_{n=1}^{m} \int_{t^{n-1}}^{t^n} \langle\!\langle B^n - \partial_\nu\Theta^n, \Pi^n\psi - \psi\rangle\!\rangle dt, \\
\mathcal{R}_4(\psi) &= \sum_{n=1}^{m} \int_{t^{n-1}}^{t^n} \Big(\langle \nabla(I^n\beta(U^n) - \beta(U^n)), \nabla\psi\rangle - \langle\!\langle I^n\beta(U^n) - \beta(U^n)), \partial_\nu\psi\rangle\!\rangle\Big) dt, \\
\mathcal{R}_5(\psi) &= \sum_{n=1}^{m} \int_{t^{n-1}}^{t^n} \Big(\langle U - \hat{U}, \partial_t\psi\rangle - v(t)\langle \partial_z(U - \hat{U}), \psi\rangle\Big) dt, \\
\mathcal{R}_6(\psi) &= \sum_{n=1}^{m} \int_{t^{n-1}}^{t^n} \langle \tau_n^{-1}(U^n - I^n\bar{U}^{n-1}) - \partial_t\hat{U} - v(t)\partial_z\hat{U}, \psi\rangle dt, \\
\mathcal{R}_7(\psi) &= \sum_{n=1}^{m} \int_{t^{n-1}}^{t^n} \Big(\langle R^n, \Pi^n\psi\rangle^n - \langle R^n, \Pi^n\psi\rangle\Big) dt, \\
\mathcal{R}_8(\psi) &= \sum_{n=1}^{m} \int_{t^{n-1}}^{t^n} \Big(\langle\!\langle I^n p^n(\Theta^n - I^n\theta_{\text{ext}}^n), \Pi^n\psi\rangle\!\rangle_{\Gamma_N}^n - \langle\!\langle I^n p^n(\Theta^n - I^n\theta_{\text{ext}}^n), \Pi^n\psi\rangle\!\rangle_{\Gamma_N}\Big) dt, \\
\mathcal{R}_9(\psi) &= \sum_{n=1}^{m} \int_{t^{n-1}}^{t^n} \Big(\langle\!\langle I^n g_N^n, \Pi^n\psi\rangle\!\rangle_{\Gamma_L} - \langle\!\langle I^n g_N^n, \Pi^n\psi\rangle\!\rangle_{\Gamma_L}^n\Big) dt, \\
\mathcal{R}_{10}(\psi) &= \sum_{n=1}^{m} \int_{t^{n-1}}^{t^n} \langle\!\langle (I^n p^n - p)(\Theta^n - \theta_{\text{ext}}) + I^n p^n(\theta_{\text{ext}} - I^n\theta_{\text{ext}}^n), \psi\rangle\!\rangle_{\Gamma_N} dt, \\
\mathcal{R}_{11}(\psi) &= \sum_{n=1}^{m} \int_{t^{n-1}}^{t^n} \Big(\langle\!\langle g_N - I^n g_N^n, \psi\rangle\!\rangle_{\Gamma_L} + \langle\!\langle I^n g_D^n - g_D, \partial_\nu\psi\rangle\!\rangle_{\Gamma_0}\Big) dt, \\
\mathcal{R}_{12}(\psi) &= \int_0^{t^m} \langle u - U, (b - b_\delta)\Delta\psi\rangle dt.
\end{aligned}
\tag{5.8}
$$

The rest of the argument consists of estimating each term $\mathcal{R}_i(\psi)$ separately. We rely on the regularity results of §4.1.

We decompose the integral $\langle \nabla\Theta^n, \nabla(\Pi^n\psi - \psi)\rangle$ over all elements $S \in \mathcal{M}^n$ and next integrate by parts to obtain the equivalent expression

$$\langle \nabla I^n\Theta^n, \nabla(\Pi^n\psi - \psi)\rangle = \sum_{e\in\mathcal{B}^n} \langle\!\langle [\![\nabla\Theta^n]\!]_e, \psi - \Pi^n\psi\rangle\!\rangle_e + \langle\!\langle \partial_\nu\Theta^n, \Pi^n\psi - \psi\rangle\!\rangle, \tag{5.9}$$

where $\langle\!\langle\cdot,\cdot\rangle\!\rangle_e$ denotes the L^2-scalar product on $e \in \mathcal{B}^n$, and $[\![\nabla\Theta^n]\!]_e$ is defined in (3.6). In view of

(5.6), we obtain

$$\sum_{n=1}^{m}\int_{t^{n-1}}^{t^n}\sum_{e\in\mathcal{B}^n}\langle\!\langle[\![\nabla\Theta^n]\!]_e,\psi-\Pi^n\psi\rangle\!\rangle_e\le C\sum_{n=1}^{m}\int_{t^{n-1}}^{t^n}\||\, h^{3/2}[\![\nabla\Theta^n]\!]_e\,\||_{L^2(\Omega)}\| D^2\psi\,\|_{L^2(\Omega)}.$$

Since the last term in (5.9) cancels out with a similar one in $\mathcal{R}_3(\psi)$, adding $\mathcal{R}_1(\psi)$ and $\mathcal{R}_3(\psi)$ and using (5.6) with $k=2$ again, in conjunction with Corollary 4.3, we get

$$|\mathcal{R}_1(\psi)+\mathcal{R}_3(\psi)|\le C(Vt^m)^{3/2}\delta^{-1/2}\|\,\chi\,\|_{L^\infty(Q^m)}\Big(\mathcal{E}_1+\mathcal{E}_3\Big).$$

For $\mathcal{R}_2(\psi)$ we employ (5.5) with $k=2$ and Corollary 4.3 to arrive at

$$|\mathcal{R}_2(\psi)|\le C\sum_{n=1}^{m}\int_{t^{n-1}}^{t^n}\|\,h^2R^n\,\|_{L^2(\Omega)}\|\,D^2\psi\,\|_{L^2(\Omega)}\le C(Vt^m)^{3/2}\delta^{-1/2}\|\,\chi\,\|_{L^\infty(Q^m)}\mathcal{E}_2.$$

To estimate $\mathcal{R}_4(\psi)$, we integrate by parts and then use Lemma 4.5. We have

$$|\mathcal{R}_4(\psi)|\le\sum_{n=1}^{m}\int_{t^{n-1}}^{t^n}\|\,I^n\beta(U^n)-\beta(U^n)\,\|_{L^2(\Omega)}\|\,\Delta\psi\,\|_{L^2(\Omega)}\le C(Vt^m)^{3/2}\delta^{-1/2}\|\,\chi\,\|_{L^\infty(Q^m)}\mathcal{E}_4.$$

These are all the terms involving $\delta^{-1/2}$. The remaining terms require lower regularity of ψ and are thus independent of δ, except for $\mathcal{R}_{12}$ which is also of different character.

If $l(t)$ is the piecewise linear function $l(t):=\tau_n^{-1}(t^n-t)$, then $U-\hat{U}=l(t)(U^n-U^{n-1})$. Consequently, integration by parts and the fact that $\psi=0$ on Γ_0 yield

$$-v(t)\langle\partial_z(U-\hat{U}),\psi\rangle=l(t)\langle U^n-U^{n-1},v(t)\partial_z\psi\rangle-l(t)\langle\!\langle U^n-U^{n-1},v(t)\psi\rangle\!\rangle_{\Gamma_L}.$$

Coupling the first term on the right-hand side with the remaining one in $\mathcal{R}_5(\psi)$, and writing $U^n-U^{n-1}=(U^n-I^nU^{n-1})+(I^nU^{n-1}-U^{n-1})$, we obtain with the aid of Corollary 4.2

$$\begin{aligned}\sum_{n=1}^{m}&\int_{t^{n-1}}^{t^n}l(t)\langle U^n-U^{n-1},\partial_t\psi+v(t)\partial_z\psi\rangle dt\\&\le C(\mathcal{E}_5+\mathcal{E}_6)\Big(\int_0^{t^m}\|\,\partial_t\psi+v(t)\partial_z\psi\,\|_{L^2(\Omega)}^2\Big)^{1/2}\le C(Vt^m)^{3/2}\|\,\chi\,\|_{L^\infty(Q^m)}(\mathcal{E}_5+\mathcal{E}_6).\end{aligned}$$

This is an essential step because neither $\partial_t\psi$ nor $\partial_z\psi$ are smooth alone, but rather their special combination above. In light of Lemma 4.4, the remaining boundary term in $\mathcal{R}_5(\psi)$ gives rise to

$$\begin{aligned}-\sum_{n=1}^{m}&\int_{t^{n-1}}^{t^n}l(t)\langle\!\langle U^n-U^{n-1},v(t)\psi\rangle\!\rangle_{\Gamma_L}\\&\le\Big(\sum_{n=1}^{m}\frac{\tau_nV}{2}\|\,U^n-U^{n-1}\,\|_{L^2(\Gamma_L)}^2\Big)^{1/2}\Big(\int_0^{t^m}\|\,v^{1/2}\psi\,\|_{L^2(\Gamma_L)}^2\Big)^{1/2}\\&\le C(Vt^m)^{3/2}\|\,\chi\,\|_{L^\infty(Q^m)}(\mathcal{E}_5+\mathcal{E}_6).\end{aligned}$$

The term $\mathcal{R}_6(\psi)$ is easy to handle by Lemma 4.2, namely,

$$\begin{aligned}|\mathcal{R}_6(\psi)| &\le \sum_{n=1}^{m} \int_{t^{n-1}}^{t^n} \| \tau_n^{-1}(U^n - I^n\bar{U}^{n-1}) - \partial_t \hat{U} - v(t)\partial_z \hat{U} \|_{L^1(\Omega)} \| \psi \|_{L^\infty(\Omega)} \\ &\le C(Vt^m)^{3/2} \| \chi \|_{L^\infty(Q^m)} \mathcal{E}_7.\end{aligned}$$

The next three terms $\mathcal{R}_7(\psi)$ to $\mathcal{R}_9(\psi)$ represent the effect of quadrature, and can be treated via (3.3) and (3.4). Hence, (5.7) and Lemma 4.5 imply

$$\begin{aligned}|\mathcal{R}_7(\psi)| &\le C \sum_{n=1}^{m} \int_{t^{n-1}}^{t^n} \| h^2 \nabla R^n \|_{L^2(\Omega)} \| \nabla \psi \|_{L^2(\Omega)} \le C(Vt^m)^{3/2} \| \chi \|_{L^\infty(Q^m)} \mathcal{E}_8, \\ |\mathcal{R}_8(\psi)| &\le C \sum_{n=1}^{m} \int_{t^{n-1}}^{t^n} \| I^n p^n \|_{W^{1,\infty}(\Gamma_N)} ||| h^{3/2}(\Theta^n - I^n \theta^n_{\text{ext}}) |||_{H^1(\Gamma_N)} \| \psi \|_{H^1(\Omega)} \\ &\le C(Vt^m)^{3/2} \| \chi \|_{L^\infty(Q^m)} \mathcal{E}_9.\end{aligned}$$

Moreover, if we modify the boundary values of $\Pi^n\psi$ by using the L^2 local projection over the sets $\text{supp}(\phi_k) \cap \partial\Omega$ instead of $\text{supp}(\phi_k)$, where $\{\phi_k\}_k$ is the canonical basis of $\mathbf{V}^n$, we achieve optimal approximability over $\partial\Omega$. If we now use Lemma 4.5, we obtain

$$|\mathcal{R}_9(\psi)| \le CV^{-1/2} \sum_{n=1}^{m} \int_{t^{n-1}}^{t^n} ||| h^2 \partial_y (I^n g_N^n) |||_{L^2(\Gamma_L)} \| v^{1/2} \partial_y \psi \|_{L^2(\Gamma_L)} \le C(Vt^m)^{3/2} \| \chi \|_{L^\infty(Q^m)} \mathcal{E}_9.$$

In addition, Lemma 4.2 yields

$$\begin{aligned}|\mathcal{R}_{10}(\psi)| \le \| \psi \|_{L^\infty(Q_m)} \sum_{n=1}^{m} \int_{t^{n-1}}^{t^n} \Big(&\| I^n p^n - p \|_{L^\infty(\Gamma_N)} \| \Theta^n - \theta_{\text{ext}} \|_{L^1(\Gamma_N)} \\ &+ \| I^n p^n \|_{L^\infty(\Gamma_N)} \| \theta_{\text{ext}} - I^n \theta^n_{\text{ext}} \|_{L^1(\Gamma_N)} \Big) dt \le C(Vt^m)^{3/2} \| \chi \|_{L^\infty(Q^m)} \mathcal{E}_{10},\end{aligned}$$

and

$$\begin{aligned}|\mathcal{R}_{11}(\psi)| &\le \sum_{n=1}^{m} \int_{t^{n-1}}^{t^n} \Big(\| g_N - I^n g_N^n \|_{L^1(\Gamma_L)} \| \psi \|_{L^\infty(\Gamma_L)} + \| g_D - I^n g_D^n \|_{L^1(\Gamma_0)} \| \partial_\nu \psi \|_{L^\infty(\Gamma_0)} \Big) dt \\ &\le C(Vt^m)^{3/2} \| \chi \|_{L^\infty(Q^m)} \mathcal{E}_{10}.\end{aligned}$$

The last residual $\mathcal{R}_{12}(\psi)$ is of different nature from those above. We notice that (H1) and the a priori bound $\| \theta \|_{L^2(Q^m)} \le C$ imply

$$\| u - U^n \|^2_{L^2(\Omega)} \le C\Big(\lambda|\Omega| + \| \Theta^n - \theta \|^2_{L^2(\Omega)} \Big) \le C\Big(1 + \lambda|\Omega| + \| \Theta^n \|^2_{L^2(\Omega)} \Big) =: C\Xi_n^2,$$

whence Lemma 4.5 yields

$$|\mathcal{R}_{12}(\psi)| \le C\delta^{1/2} \Big(\sum_{n=1}^{m} \tau_n \Xi_n^2 \Big)^{1/2} \Big(\int_0^{t^m} \| b_\delta^{1/2} \Delta\psi \|^2_{L^2(\Omega)} dt \Big)^{1/2} \le C\delta^{1/2} (Vt^m)^{3/2} \Lambda_m \| \chi \|_{L^\infty(Q^m)}.$$

5.2 Proof of Theorem 5.1

Collecting the above estimates for $\mathcal{R}_i(\psi)$, and inserting them back into (4.22), we obtain

$$\int_0^{t^m} \| \beta(u) - \beta(U) \|_{L^1(\Omega)} dt \leq C(Vt^m)^{3/2}\Big(\mathcal{E}_0 + \sum_{i=5}^{10} \mathcal{E}_i + q(\delta)\Big),$$

where

$$q(\delta) = \delta^{-1/2} \sum_{i=1}^{4} \mathcal{E}_i + \delta^{1/2}\Lambda_m.$$

The asserted estimate follows from optimizing $q(\delta)$, namely from choosing $\delta = \Lambda_m^{-1} \sum_{i=1}^4 \mathcal{E}_i$.

5.3 Proof of Theorem 5.2

We first notice that the residual $\mathcal{R}(\psi)$ of (4.4) remains unaltered provided we remove $\langle\!\langle g_N, \psi\rangle\!\rangle_{\Gamma_L}$ and change Γ_0 by $\Gamma_D = \Gamma_0 \cap \Gamma_L$. The equality (5.4), expressing Galerkin orthogonality, is also valid provided all terms containing g_N are eliminated. We proceed as in §§5.1 and (5.1), but now using the regularity results of §4.2. The assertion follows immediately.

5.4 Discontinuous p

We examine now the case where p is piecewise Lipschitz as in §§4.3 and 7. In view of (4.21), the estimators in Theorems 5.1 and 5.2 which depend on second derivatives of ψ change as follows:

$$\mathcal{E}_1 := \Big(\sum_{n=1}^{m} \tau_n \||\, h^{3/2-\epsilon}[\![\nabla\Theta^n]\!] \,\||^2_{L^2(\Omega)}\Big)^{1/2},$$

$$\mathcal{E}_2 := \Big(\sum_{n=1}^{m} \tau_n \| h^{2-\epsilon} R^n \|^2_{L^2(\Omega)}\Big)^{1/2},$$

$$\mathcal{E}_3 := \Big(\sum_{n=1}^{m} \tau_n \||\, h^{3/2-\epsilon} B^n \,\||^2_{L^2(\partial\Omega\setminus\Gamma_D)}\Big)^{1/2},$$

for all $\epsilon > 0$. Moreover, the constants $C > 0$ in Theorems 5.1 and 5.2 depend also on ϵ, whereas the other estimators do not change.

6 Performance

In this section we explain how the estimators from §5 can be used for mesh and time-step modification, and document the performance of the resulting adaptive method.

6.1 Localization

The error estimators $\mathcal{E}_i$ of both Theorems 5.1 and 5.2 can be split into element contributions $E_i^n(S)$ at each time t^n, as explained in [20]; we omit this here. We use them to equidistribute the space contributions by refinement/coarsening of the mesh $\mathcal{M}^n$ and the time contributions by modifying the time step τ^n. Except for the time and characteristic residuals $\mathcal{E}_5$ and $\mathcal{E}_7$, which serve to adjust τ_n, all other estimators provide information for space adaptation of $\mathcal{M}^n$. The latter is performed via bisection; we refer to [21] for a brief summary of these techniques.

6.2 Example: Travelling wave

An explicit solution for the nonlinearity $\beta(u) = \min(u, 0) + \max(u - 1, 0)$ is given by the travelling wave

$$\beta(u(x, y, t)) = \begin{cases} (1 - \exp(s)) & \text{if } s \le 0 \text{ (liquid)}, \\ 2(1 - \exp(s)) & \text{if } s > 0 \text{ (solid)}, \end{cases} \qquad \text{where } s = (\nu \cdot v - V)(\nu \cdot (x, y) - Vt),$$

with $\nu = (\cos(\alpha), \sin(\alpha))$ and parameters $v = (2, 0)$, $V = 0.4$, $\alpha = \pi/6$; V is the interface velocity in the normal direction ν. We solve the problem in the domain $\Omega = (0.0, 1.0) \times (0.0, 0.2)$ for time $t \in (1, 2)$ with Dirichlet boundary condition on $\partial\Omega$. To avoid any mesh effects, the interface normal ν is rotated from the horizontal direction by α. This way ν is never parallel to any mesh edge. As the domain in the applications of Section 7 has a very large aspect ratio, we explore here the use of elongated elements. We thus compare simulations with meshes of aspect ratios 1 and 5 originated from the macro triangulations of Figure 1, for the explicit travelling wave solution.

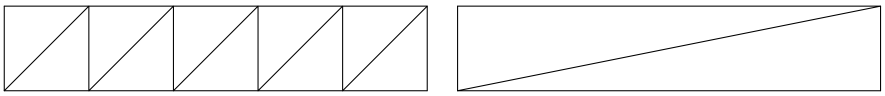

Figure 1: Example 6.2. Macro triangulations with aspect ratios 1 and 5.

Figures 2 and 4 show adaptive meshes at time $t = 1.1$, generated with error tolerances tol $= 0.5$ and tol $= 0.25$, while Figure 3 depicts isothermal lines at the same time; the latter look the same for all simulations. Figure 5 displays the error $||e_{\beta(u)}(t)||_{L^1(\Omega)}$ and Figure 6 the mesh element counts for simulations with both aspect ratios. Finally, Figure 7 shows the total error for different given tolerances and mesh aspect ratios. Even though the triangle counts are larger for simulations with larger aspect ratio, the estimators and the adaptive method behave well. It is thus reasonable to use elongated elements in the following application. In any event, we do not employ specialized estimators or adaptive methods for anisotropic meshes such as [26]. The application of such methods to degenerate parabolic equations is still to be investigated.

7 Applications to Casting of Steel

We study the casting of a slab in 2D. This problem was proposed in [14], and a similar problem with time dependent parameters was studied in [16]. In order to derive non-dimensional equations (1.1)-(1.8), we first rescale the physical equations with the material parameters.

7.1 Scaling

In this section, we mark all physical quantities by a tilde. The original equations with physical coefficients for temperature $\tilde{\theta}$ (in units [$^\circ K$]) and energy density (or enthalpy) $\tilde{u}$ (in units [kg/ms^2])

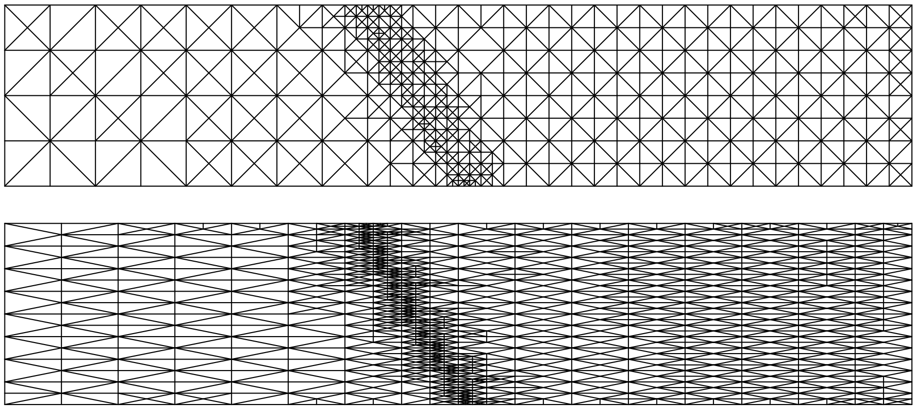

Figure 2: Example 6.2. Meshes with aspect ratios 1 and 5 for tol $= 0.5$ at $t = 1.1$.

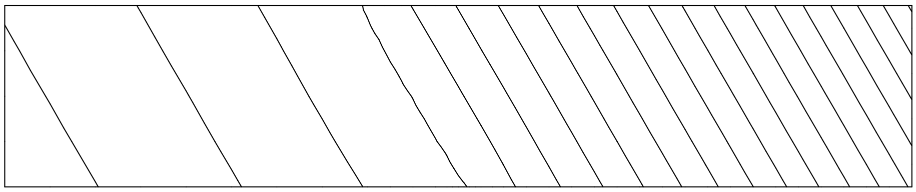

Figure 3: Example 6.2. Isothermal lines at $\beta(u) = k/8$, $k = -16 \ldots 3$, at $t = 1.1$.

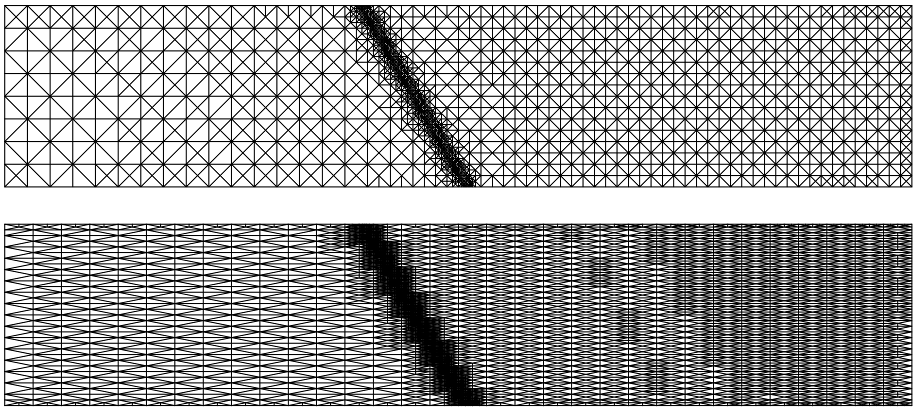

Figure 4: Example 6.2. Meshes with aspect ratios 1 and 5 for tol $= 0.25$ at $t = 1.1$.

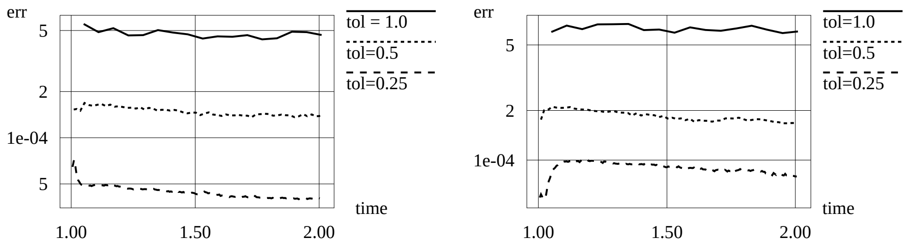

Figure 5: Example 6.2. $||e_{\beta(u)}(t)||_{L^1(\Omega)}$ for meshes with aspect ratios 1 (left) and 5 (right).

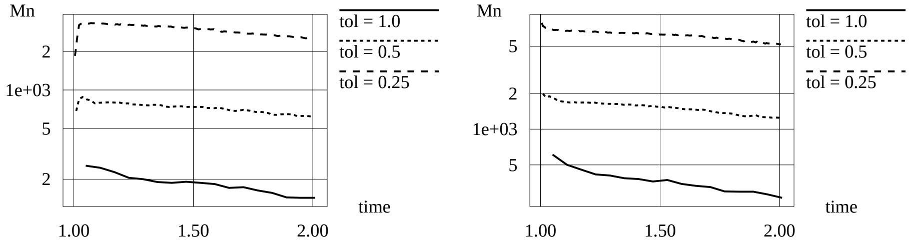

Figure 6: Example 6.2. Triangle counts for meshes with aspect ratios 1 (left) and 5 (right).

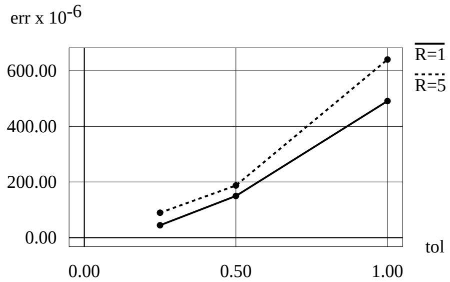

Figure 7: Example 6.2. $||e_{\beta(u)}(t)||_{L^1(L^1)}$ for meshes with aspect ratios $R = 1, 5$.

read

$$\begin{aligned}
\partial_{\tilde{t}}\tilde{u} + \tilde{v}\partial_{\tilde{z}}\tilde{u} &= \tilde{\nabla}\cdot(\tilde{k}\tilde{\nabla}\tilde{\theta}) && \text{in } \tilde{\Omega}\times(0,\tilde{T}),\\
\tilde{u} &= \tilde{\rho}(\tilde{c}\tilde{\theta} + \tilde{\chi}\tilde{\lambda}) && \text{in } \tilde{\Omega}\times(0,\tilde{T}),\\
\tilde{\theta} &= \tilde{g}_D && \text{on } \tilde{\Gamma}_0\times(0,\tilde{T}),\\
\tilde{k}\partial_{\tilde{\nu}}\tilde{\theta} + \tilde{p}(\tilde{\theta} - \tilde{\theta}_{\text{ext}}) &= 0 && \text{on } \tilde{\Gamma}_N\times(0,\tilde{T}),\\
\tilde{u}(\cdot,0) &= \tilde{u}_0 && \text{in } \tilde{\Omega},\\
\tilde{k}\partial_{\tilde{\nu}}\tilde{\theta} &= \tilde{g}_N && \text{on } \tilde{\Gamma}_L\times(0,\tilde{T})\\
\text{or}\quad \tilde{\theta} &= \tilde{g}_D && \text{on } \tilde{\Gamma}_L\times(0,\tilde{T}).
\end{aligned}$$

The physical coefficients and their units are: casting speed $\tilde{v}\,[m/s]$, heat conductivity $\tilde{k}\,[kg\,m/s^3\,°K]$, density $\tilde{\rho}\,[kg/m^3]$, specific heat $\tilde{c}\,[m^2/s^2\,°K]$, latent heat $\tilde{\lambda}\,[m^2/s^2]$, melting temperature $\tilde{\theta}_m\,[°K]$, heat transfer coefficient $\tilde{p}\,[kg/s^3\,°K]$, and external cooling temperature $\tilde{\theta}_{\text{ext}}\,[°K]$. Here $\tilde{\chi}$ stands for the characteristic function of the liquid phase. In the remainder of this section, subscripts s and l indicate the corresponding coefficients for the solid and liquid phase.

The simulations are done over a slab of length $\tilde{L} = 25\,m$ and height $0.21\,m$. We use material parameters for steel with 0.09% carbon content. Temperature–dependent data provided in [14] are approximated by piecewise constant data for the liquid and solid phase: $\tilde{k}_{\text{s}} = 30\,kg\,m/s^3\,°K$, $\tilde{k}_{\text{l}} = 180\,kg\,m/s^3\,°K$, $\tilde{c}_{\text{s}} = 660\,m^2/s^2\,°K$, $\tilde{c}_{\text{l}} = 830\,m^2/s^2\,°K$, $\tilde{\rho} = 7400\,kg/m^3$, $\tilde{\lambda} = 276\,000\,m^2/s^2$, and $\tilde{\theta}_{\text{m}} = 1733\,°K$.

The boundary condition on $\tilde{\Gamma}_N$ depends on the position along the slab; the model has a mold cooling zone ($1.15m$) and three water spray zones which include radiation. The (nonlinear) radiation condition (1.9) is linearized by using

$$(\tilde{\theta}^4 - \tilde{\theta}^4_{\text{ext}}) \approx (\tilde{\theta} - \tilde{\theta}_{\text{ext}})(\tilde{\theta}_m + \tilde{\theta}_{\text{ext}})(\tilde{\theta}^2_m + \tilde{\theta}^2_{\text{ext}}).$$

The (linear) Robin conditions on $\tilde{\Gamma}_N$ in the mold and spray regions are then

$$-\tilde{k}\partial_{\tilde{\nu}}\tilde{\theta} = \begin{cases} \tilde{p}(\tilde{\theta} - \tilde{\theta}_{\mathrm{mold}}) & \text{if } \tilde{z} < 1.15m, \\ \tilde{p}(\tilde{\theta} - \tilde{\theta}_{\mathrm{H2O}}) + \tilde{\sigma}\epsilon(\tilde{\theta} - \tilde{\theta}_{\mathrm{rad}})(\tilde{\theta}_m + \tilde{\theta}_{\mathrm{rad}})(\tilde{\theta}_m^2 + \tilde{\theta}_{\mathrm{rad}}^2) & \text{if } \tilde{z} > 1.15m. \end{cases}$$

Casting and boundary parameters are given in Table 1. In this model, the quantities p and θ_{ext} exhibit discontinuities along Γ_N, which results in hypotheses (H4) and (H5) not being satisfied. But, as stated in Remark 5.3, the estimates are still valid in the case of piecewise smooth boundary data. On the other hand, a refined model might include some mollifying effect of water spraying, which removes these discontinuities.

Quantity	Value	Unit	Description
$\tilde{v}$	0.0225	$\frac{m}{s}$	casting speed
$\tilde{g}_D$	1818	$^{\circ}K$	on $\tilde{\Gamma}_0$: inflow temperature
$\tilde{g}_D$	1250	$^{\circ}K$	on $\tilde{\Gamma}_L$: outflow temperature
$\tilde{g}_N$	0	$\frac{kg}{s^3}$	on $\tilde{\Gamma}_L$: outflow temperature flux
$\tilde{p}$	1500	$\frac{kg}{s^3\,^{\circ}K}$	on $\tilde{\Gamma}_N$, $\tilde{z} \in (0, 1.15)m$: heat transfer in mold
$\tilde{\theta}_{\mathrm{mold}}$	353	$^{\circ}K$	mold external temperature
$\tilde{p}$	700	$\frac{kg}{s^3\,^{\circ}K}$	on $\tilde{\Gamma}_N$, $\tilde{z} \in (1.15, 4.4)m$: heat transfer in first spray region
$\tilde{p}$	350	$\frac{kg}{s^3\,^{\circ}K}$	on $\tilde{\Gamma}_N$, $\tilde{z} \in (4.4, 14.6)m$: heat transfer in second spray region
$\tilde{p}$	50	$\frac{kg}{s^3\,^{\circ}K}$	on $\tilde{\Gamma}_N$, $\tilde{z} \in (14.6, 25)m$: heat transfer in third spray region
$\tilde{\theta}_{\mathrm{H2O}}$	300	$^{\circ}K$	cooling water temperature
$\tilde{\sigma}$	5.67 E−8	$\frac{kg}{s^3\,^{\circ}K^4}$	Stefan–Boltzmann constant
ϵ	0.8		emission factor
$\tilde{\theta}_{\mathrm{rad}}$	370	$^{\circ}K$	$\tilde{z} \in (1.15, 14.6)m$: air temperature
$\tilde{\theta}_{\mathrm{rad}}$	710	$^{\circ}K$	$\tilde{z} \in (14.6, 25)m$: air temperature in third spray region

Table 1: Casting and boundary parameters.

Using a length scale $\bar{X}\,[m]$ and a time scale $\bar{T}\,[s]$, the physical quantities can be transformed into dimensionless ones as follows:

$$x := \frac{\tilde{x}}{\bar{X}}, \qquad t := \frac{\tilde{t}}{\bar{T}}, \qquad u := \frac{\tilde{u}}{\tilde{\rho}\tilde{\lambda}} - \frac{\tilde{c}_{\mathrm{s}}\tilde{\theta}_{\mathrm{m}}}{\tilde{\lambda}}, \qquad \theta := \begin{cases} \frac{\tilde{c}_{\mathrm{s}}}{\tilde{\lambda}}(\tilde{\theta} - \tilde{\theta}_{\mathrm{m}}) & \text{if } \tilde{\theta} \le \tilde{\theta}_{\mathrm{m}}, \\ \frac{\tilde{c}_{\mathrm{l}}}{\tilde{\lambda}}(\tilde{\theta} - \tilde{\theta}_{\mathrm{m}}) & \text{if } \tilde{\theta} \ge \tilde{\theta}_{\mathrm{m}}, \end{cases}$$

$$v := \frac{\tilde{v}\bar{T}}{\bar{X}}, \qquad k := \frac{\tilde{k}\bar{T}}{\tilde{\rho}\tilde{c}\bar{X}^2}, \qquad p := \frac{\tilde{p}\bar{T}}{\tilde{\rho}\tilde{c}\bar{X}}, \qquad g_D := \frac{\tilde{c}}{\tilde{\lambda}}(\tilde{g}_D - \tilde{\theta}_{\mathrm{m}}), \qquad g_N := \frac{\tilde{g}_N\bar{T}}{\tilde{\rho}\tilde{\lambda}\bar{X}}.$$

Using these new quantities, the dimensionless equation reads

$$u_t + v\,\partial_z u - \Delta\beta(u) \;=\; 0 \quad \text{in } \Omega \times (0,T), \quad \text{with } \beta(u) = \begin{cases} k_{\mathrm{s}} u & \text{if } u < 0, \\ 0 & \text{if } u \in [0,1], \\ k_{\mathrm{l}}(u-1) & \text{if } u > 1. \end{cases}$$

Dirichlet boundary conditions are transformed into

$$\beta(u) = k\,g_D \qquad \text{on } \Gamma_0 \times (0,T),$$

and the scaled Robin and Neumann conditions are

$$k\,\partial_\nu\theta + p(\theta-\theta_{\text{ext}}) \;=\; 0 \quad\Leftrightarrow\quad \partial_\nu\beta(u) + \frac{p}{k}(\beta(u)-k\theta_{\text{ext}}) \;=\; 0 \quad \text{on } \Gamma_N\times(0,T),$$
$$\partial_\nu\beta(u) \;=\; g_N \quad \text{on } \Gamma_L\times(0,T).$$

After scaling with $\bar{X} = 10\,m$, $\bar{T} = 10^5\,s \approx 28\,h$, the non-dimensional domain is of size 0.021×2.5 and the slopes of β are $k_s = 0.006$, $k_l = 0.029$. A temperature range $\tilde{\theta} \in (1000, 1800)\,°K$ leads to scaled values $|\beta(u)| = O(10^{-2})$, while the scaled latent heat is $\lambda = 1$. The scaled convection speed is $v = 225$, so convection is *dominant*. The simulations run for $t \in (0, 0.1)$, which is equivalent to a final time $\tilde{T} = 10000s \approx 2\frac{3}{4}h$. Initial conditions are chosen piecewise linear in z direction, with a prescribed initial position of the interface at $z = L/10$. This is a convenient but totally unphysical initial condition: there is liquid in contact to water/air. The long–time behavior does not depend on the actual choice of initial conditions though.

Figure 8: Domain aspect ratio.

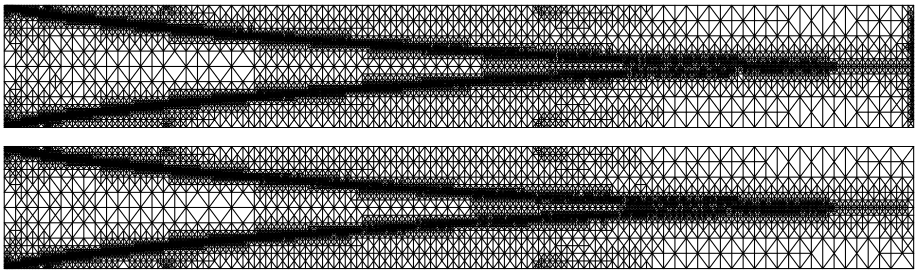

Figure 9: Adapted mesh for stationary solution, Dirichlet (top) and Neumann (bottom) outflow; vertical scale = 16.

Figure 10: Graph of temperature for stationary solution with Dirichlet (top) and Neumann (bottom) outflow.

The actual aspect ratio of the domain is depicted in Figure 8; so for visualization purposes, the height of all subsequent domains is scaled by a factor 16. The numerical simulations start from a macro triangulation of Ω into 20 triangles with aspect ratio ≈ 12. Figures 9 and 10 compare adapted meshes and graphs of the temperature for Dirichlet and Neumann outflow conditions with error tolerances tol $= 2$ and tol $= 45$, respectively. It can be easily seen that the Dirichlet outflow condition generates a sharp boundary layer at Γ_L but no oscillations elsewhere; both solutions are indeed very similar away from Γ_L. To avoid this unphysical boundary layer, the following simulations were all done with a vanishing Neumann outflow condition. We conclude this paper with two simulations with time-dependent parameters.

7.2 Example: Oscillating Velocity

First, we prescribe a variable casting speed

$$\tilde{v}(\tilde{t}) = 0.0175 + 0.005 * \sin(0.00175\,\tilde{t})\ [m/s],$$

which has a strong influence on the length of the liquid pool inside the slab. The largest velocity is chosen equal to the constant velocity in the problem with stationary casting speed; all other parameters are left unchanged. This guarantees that the liquid pool will not reach the outflow boundary. The variable velocity is shown in Figure 11, together with the number of elements in the adapted meshes $M(t^n) = \#(\mathcal{M}^n)$ and time step sizes. Due to a longer liquid pool (and interface), there are more mesh elements when the velocity is larger and a smaller time step size is needed. Figures 12 and 13 display adaptive meshes and temperature graphs for $t = 0.05$ and $t = 0.07$, corresponding to large and small velocity values. Some spurious oscillations can be seen in the temperature graphs near jumps of Robin boundary conditions. They are created by the method of characteristics which transport such cusps in the z direction. Therefore, an upper bound of 0.00025 ($= 25\,s$) is imposed in this simulation.

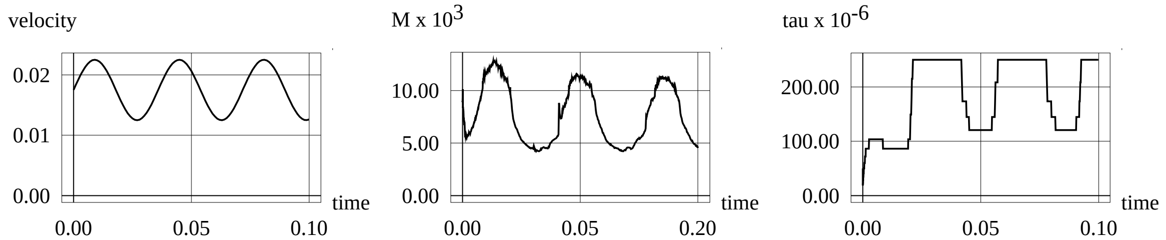

Figure 11: Variable casting speed. Velocity $\tilde{v}(t)$, element count, and time step sizes.

7.3 Example: Oscillating Cooling

For constant casting velocity $\tilde{v} = 0.0225\,m/s$, we model a varying cooling water flow rate in the second spray region by a time dependent heat transfer coefficient:

$$\tilde{p}(\tilde{t}) = 550 + 200\sin(0.00175\,\tilde{t})\ [kg/s^3\,{}^\circ K] \quad \text{on } \Gamma_L,\ \tilde{z} \in (4.4, 14.6)\,m.$$

Again, this has an influence on the length of the liquid pool inside the slab, which gets longer when the cooling coefficient is smaller, thereby representing a reduced water flow.

Figure 14 shows the varying parameter $\tilde{p}(t)$ and the corresponding mesh element counts. Adaptive meshes and temperature graphs for $t = 0.05$ and $t = 0.07$ are displayed in Figures 15 and 16.

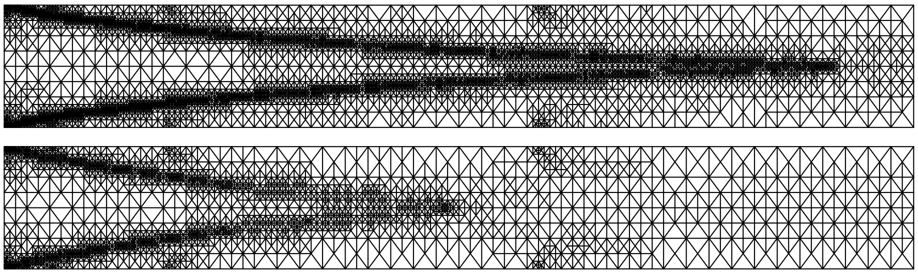

Figure 12: Variable casting speed. Adaptive meshes for $t = 0.05$ (top) and $t = 0.07$ (bottom).

Figure 13: Variable casting speed. Temperature graphs for $t = 0.05$ (top) and $t = 0.07$ (bottom).

As the liquid pool length does not depend so strongly on $\tilde{p}(t)$ as it did on $\tilde{v}(t)$, the mesh element count changes only slightly in this example; the larger changes for $t < 0.02$ are due to the given initial conditions. The time step size is not shown but equals the given upper bound 0.00025 for $t > 0.02$. The oscillations in Figure 16 near jumps of Robin boundary conditions along Γ_N uncover the undesirable condition $v\tau \gg h$ for the method of characteristics. We show the beneficial effect of reducing the time step in the botton picture of Figure 16. This graph corresponds to $t = 0.05$ for a simulation with smaller tolerance for the time error estimate, which leads to a time step size $\tau = 0.00006$ $(= 6\,s)$ for $t > 0.025$: $v\tau < h$ holds and the oscillations are removed.

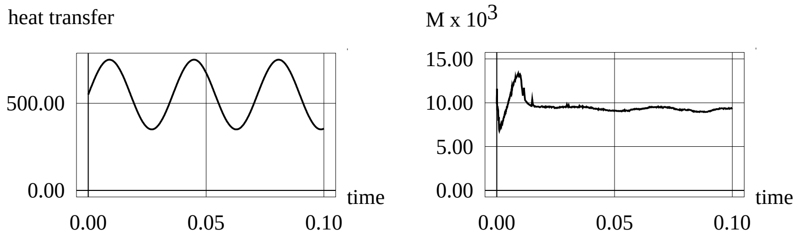

Figure 14: Variable cooling. Heat transfer coefficient $\tilde{p}(t)$ and element counts.

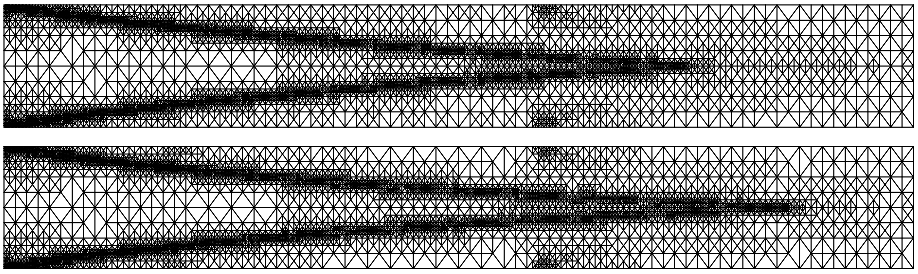

Figure 15: Variable cooling. Adaptive meshes for $t = 0.05$ (top) and $t = 0.07$ (bottom).

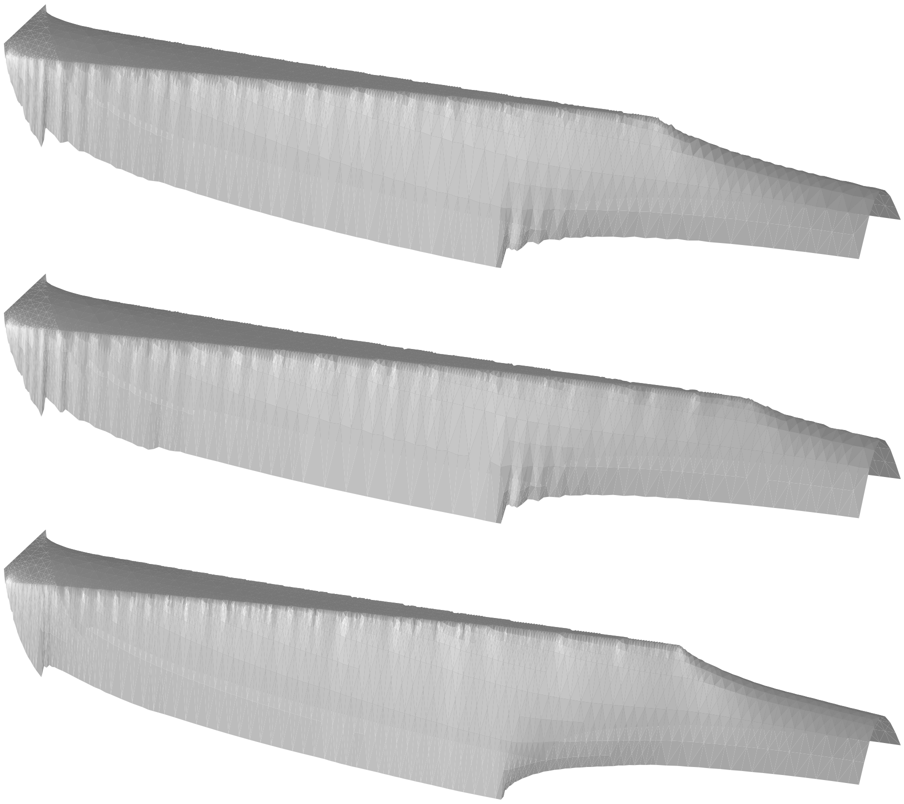

Figure 16: Variable cooling. Temperature graphs for $t = 0.05$ (top) and $t = 0.07$ (middle); Simulation with smaller time step size for $t = 0.05$ (bottom).

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