

Numerical investigation of corrosion phenomena in heat-treated Mg-1Er-1Yb alloy via multiphysics modeling

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This study examines the galvanic corrosion behaviour of a Mg-1Er-1Yb alloy when coupled with 316L stainless steel, with particular emphasis on the influence of artificial aging. The alloy was solution-treated and aged at 200 °C for 5 h (HT5), 10 h (HT10) and 15 h (HT15), and compared with the base metal. Electrochemical characterization was performed in 3.5 wt.% NaCl using a three-electrode cell, with potentiodynamic scans conducted from -250 mV to +250 mV versus OCP at a scan rate of 1 mV s⁻¹. The Tafel parameters (β_a , β_c), corrosion potential (E_{corr}), and corrosion current density (i_{corr}) were extracted for both the Mg alloy (anode) and 316L stainless steel (cathode), enabling a quantitative assessment of galvanic interaction. Among all conditions, HT10 exhibited the most favourable performance, with a significantly reduced i_{corr} (1.22×10^{-5} A cm⁻²) and the lowest corrosion rate (12.9 mm year⁻¹), compared to 22.8 mm year⁻¹ for the base metal. These experimental findings were incorporated into a COMSOL Multiphysics model using the Arbitrary Lagrangian Eulerian (ALE) method to dynamically track corrosion front movement under galvanic coupling. The simulated electrolyte potential fields, local current density profiles, pit morphology and thickness loss showed strong agreement with immersion and polarization results, with deviations below 7%. The study demonstrates that controlled aging at 200 °C for 10 h leads to a refined microstructure and improved galvanic compatibility with 316L stainless steel. The integrated experimental numerical approach provides a reliable framework for designing rare-earth-based Mg alloys for sacrificial anode applications.

INTRODUCTION

Magnesium (Mg) and its alloys are gaining power as essential lightweight structural materials in the automotive, aerospace, marine and medical device sectors due to their low density (1.74 g/cm³), excellent specific strength and recyclability. Mg alloys offer weight savings of approximately 35% and 77% compared to aluminum and steel respectively, making them ideal for applications

such as fuel-efficient vehicles and portable electronics [1]. Despite these advantages, the widespread adoption of Mg alloys is limited by their poor corrosion resistance, especially in chloride-containing environments like seawater, physiological fluids and humid industrial conditions [2]. The corrosion susceptibility is due to Mg's active electrochemistry, which promotes various corrosion mechanisms, including pitting, galvanic and filiform corrosion [3].

To mitigate these challenges, a variety of strategies have been explored. Surface coatings and anodization techniques offer moderate improvements by physically shielding the metal, yet they often suffer from mechanical instability and failure over time [4]. More recently, alloying with rare earth elements (REs) such as Erbium (Er), Ytterbium (Yb), and Gadolinium (Gd) has emerged as an effective route for improving corrosion behavior. These additions refine grain structure, create thermally stable intermetallic precipitates and enhance passive layer formation, significantly suppressing localized corrosion and improving electrode potential stability [5]. Simultaneously, heat treatment techniques like solutionizing and artificial aging have proven effective in manipulating microstructural features such as precipitate morphology, grain boundary characteristics and passive film adherence [6, 7]

Aging treatments at moderate temperatures (e.g., 200 °C) promote the formation of fine intermetallics, enhancing both strength and corrosion resistance by minimizing micro-galvanic effects [8]. However, excessive aging can cause precipitate coarsening and detach grain boundaries, leading to increased vulnerability to corrosion attack [9]. While experimental studies using immersion testing and electrochemical methods validate these improvements, they remain static analyses that lack real-time insights into pit formation, current distribution,

and surface morphology changes [10]. This limitation is critical, especially for sacrificial anode applications, where understanding long-term behavior under corrosive conditions is vital for material reliability.

To address these gaps, advanced computational modelling has been adopted, especially multiphysics approaches like COMSOL Multiphysics with the Arbitrary Lagrangian – Eulerian (ALE) method. This allows dynamic tracking of corrosion interfaces under electrochemical driving forces derived from experimental polarization curves, capturing evolving pit development, current paths, and surface deformation [11]. A landmark application by Deshpande et al. [12] used this methodology to simulate galvanic corrosion in AE44 Mg alloy couples with mild steel and aluminum, demonstrating excellent agreement immersion data. This study provided a robust framework that has been applied to numerous alloy systems, often showing superior efficiency and comparable accuracy to phase-field models.

Despite these advances, most applications have focused on conventional Mg alloys, with limited exploration of predictive modelling for RE-enhanced and heat-treated Mg systems. A recent review highlighted the importance of integrating alloy-specific microstructural evolution into dynamic simulation models [13]. Furthermore, applications of ALE models to accurately track corrosion front displacement, thickness loss, and pit shape in RE-containing Mg alloys remain rare [14]. Key limitations persist in capturing the influence of microstructural features like grain size, precipitate distribution and phase compositions on corrosion initiation and propagation. While phase-field simulations provide a detailed mechanistic understanding, their high computational cost limits practical application [15]. In contrast, ALE models deliver similar predictive power with significantly improved computational efficiency. In rare earth enhanced Mg alloys, Pei et al. [16] used ALE simulations to analyze Mg-Er alloy corrosion, confirming its sensitivity to aging microstructure through pit depth and current density trends. Similarly, Montoya et al. [17] utilized ALE to model biodegradable Mg implants and affirmed alignment with in vivo degradation profiles.

A significant research gap exists in understanding the influence of artificial aging on the corrosion behaviour of RE-modified Mg alloys, particularly when assessed through both experimental and computational approaches. While ALE-based COMSOL corrosion simulations have been applied to conventional Mg alloys, they have not been extended to RE-containing systems such as Mg-1Er-1Yb, where microstructural evolution during aging plays a decisive role in corrosion response. Additionally, most modelling studies evaluate isolated Mg corrosion, overlooking galvanic interactions with steel that are critical for real sacrificial anode service scenarios. This lack of integrated microstructure-electrochemistry-simulation studies limits the development of predictive

frameworks for next-generation sacrificial anodes based on RE-enhanced Mg alloys.

The novelty of the present work lies in providing the first comprehensive coupling of ALE-based COMSOL corrosion modelling with experimental validation for the Mg-1Er-1Yb alloy subjected to controlled artificial aging conditions (BM, HT5, HT10, HT15). Unlike earlier modelling approaches, this study incorporates age-dependent microstructural transformations, including grain refinement, precipitate evolution, and phase stability, directly into corrosion-front predictions. A further distinctive feature is the inclusion of galvanic coupling with SS316LN, achieved by embedding experimentally obtained anodic and cathodic Tafel parameters into the simulation boundaries. This enables the model to represent a realistic galvanic scenario rather than isolated magnesium dissolution, thereby providing a more accurate reflection of service conditions.

The scope of this work is defined by a synergistic integration of experimental electrochemical characterization, microstructural assessment, and ALE-based numerical modelling. Tafel-derived kinetics from both the Mg-1Er-1Yb anodic surface and the SS316LN cathodic surface serve as direct inputs to the model, ensuring consistency between experimental and simulated corrosion responses. The simulation framework evaluates critical corrosion indicators, including local electrolyte potential, current distribution, corrosion-front displacement, geometry evolution, thickness loss, and pit morphology. By unifying microstructural insights, electrochemical behaviour, and predictive modelling, the study establishes a robust methodological pathway for designing and optimizing RE-containing Mg alloys for sacrificial anode applications, with relevance to marine protection systems.

METHODS AND MODEL DEVELOPMENT

The Mg-1Er-1Yb alloy used in this study was synthesized through gravity die casting using high-purity magnesium and 50:50 Mg-Er and Mg-Yb master alloys, melted at 750 °C in an argon-SF₆ atmosphere and cast into preheated steel molds at 350 °C. The final composition (1 wt.% Er, 1 wt.% Yb, balance Mg) was verified via optical emission spectroscopy (OES). Specimens were sectioned into 10 × 10 × 5 mm coupons and subjected to solution treatment at 300 °C for 6 h followed by artificial aging at 200 °C for 5 h (HT5), 10 h (HT10), and 15 h (HT15), with the as-cast material considered the base metal (BM). Electrochemical testing in 3.5 wt.% NaCl used a standard three-electrode setup and Tafel analysis to obtain E_{corr} and i_{corr} values. Complementary immersion testing at varied temperatures (5 °C to 60 °C) over 216 hours allowed for the determination of corrosion rate based on mass loss, per ASTM G31.

For the electrochemical corrosion analysis, the surface of the specimens was prepared as per the ASTM E3-11 standards. The area of the working electrode was exposed at 1 mm² and the rest of the surface was masked with an insulation tape. The test utilized standard calomel electrode as a reference electrode, a specimen as a working electrode, and SS316LN as the counter electrode. Using an electrochemical workstation (Make: CH Instruments, Model: CHI606E) in a SC solution at room temperature, electrochemical experiments were carried out. Open circuit potential was observed for an immersion period of 180 minutes and that potential was chosen as the reference potential for conducting the potentiodynamic polarization tests. The specimens were polarized at a scan rate of 5 mV.s⁻¹ in the potential range of -2.5 V to +2 V. The Tafel region ($E_{\text{corr}} \pm 20$ mV) in the potentiodynamic curves was extrapolated to obtain the corrosion current and corrosion potential. The comprehensive details of the experimental methodology can be found in our earlier research work [18].

Governing electrochemical model

The numerical modeling framework employed in this study aims to simulate the galvanic corrosion behavior of Mg-1Er-1Yb alloys under various heat treatment conditions when exposed to a chloride-rich environment (3.5 wt.% NaCl solution). The model is formulated using a steady-state electrochemical approach, where the electrolyte domain is governed by Laplace's equation: $\nabla^2 \phi = 0$ shown in Figure 1.

This equation arises under the assumption that the electrolyte is homogeneous, isotropic and well-mixed, such that concentration gradients of ionic species are negligible. Furthermore, electroneutrality is assumed, and ionic transport is dominated by migration the effects of diffusion and convection are excluded in this model. Such an assumption has been widely validated in similar corrosion modeling work for magnesium alloys.

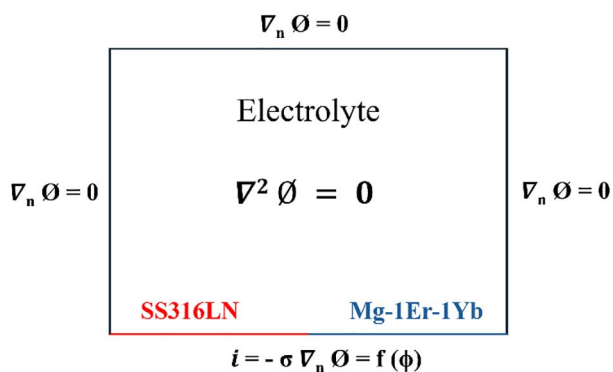


Fig. 1. Computational model layout with boundary conditions

Geometry and domain configuration

The computational domain is modeled in two dimensions (2D) using COMSOL Multiphysics, representing a simplified cross-section of the alloy-electrolyte interface. The domain includes a rectangular section of the Mg-1Er-1Yb alloy acting as the anode, in contact with a semi-infinite electrolyte region. The geometry setup allows corrosion progression to be observed spatially and temporally at the interface. Each specimen condition BM, HT5, HT10 and HT15 is modeled separately based on corresponding experimental polarization data.

Boundary conditions and electrochemical inputs

To simulate the realistic electrochemical behavior, the boundary conditions at the anode (Mg-1Er-1Yb alloy) and cathode (SS316LN alloy) interfaces are derived from experimentally obtained polarization curves. These are input into the model as nonlinear interpolation functions: $f_a(\phi)$ for the anodic current density and $f_c(\phi)$ for the cathodic current density. These functions define the current density as a function of local electric potential and allow COMSOL to solve for spatial distributions of potential and current over the domain. The boundary conditions are mathematically expressed in the equation 1, 2, and 3:

Anode boundary condition:

$$\vec{n} \cdot \nabla \phi = - \frac{f_a(\phi)}{\sigma} \quad (1)$$

Cathode boundary condition:

$$\vec{n} \cdot \nabla \phi = - \frac{f_c(\phi)}{\sigma} \quad (2)$$

All other boundaries (insulated):

$$\vec{n} \cdot \nabla \phi = 0 \quad (3)$$

where ϕ is the electrolyte potential, σ is the electrolyte conductivity (measured as 5.4 S/m from EIS experiments), and $\vec{n}$ is the unit normal vector at the surface. These conditions enable localized reaction kinetics to be modeled accurately under each heat treatment condition, thereby capturing the effect of microstructural evolution on corrosion response.

Interface movement and corrosion rate determination

The anodic interface recedes over time due to metal dissolution. The interface velocity is computed using Faraday's law of electrolysis in equation 4.

$$V_{\text{interface}} = \frac{M}{zF\rho} j(\phi) \quad (4)$$

where M – molar mass of Mg (24.3 g/mol), Z – number of electrons (2), F – Faraday's constant (96485 C/mol), ρ – density of Mg-1Er-1Yb (1.74 g/cm³) and $j(\phi)$ – local current density at the anode interface. This formulation enables direct coupling of electrochemical kinetics to the mechanical deformation of the alloy surface over time. The interface displacement field is updated dynamically throughout the simulation, enabling real-time corrosion depth tracking.

ALE method and mesh motion

To model the moving corrosion front, the Arbitrary Lagrangian-Eulerian (ALE) method is implemented in COMSOL. This approach allows the mesh to move with the dissolving interface, ensuring that geometric changes due to corrosion are captured with high fidelity. The mesh displacement follows Laplace's smoothing (equation 5).

$$\frac{\delta^2 x}{\delta X^2} + \frac{\delta^2 x}{\delta Y^2} = 0, \frac{\delta^2 y}{\delta X^2} + \frac{\delta^2 y}{\delta Y^2} = 0 \quad (5)$$

The velocity of the mesh nodes at the anodic boundary is determined using the corrosion rate from Faraday's law. The cathodic and insulated boundaries are held stationary to preserve model stability. This is particularly important, as cathodic surfaces are assumed to undergo hydrogen evolution without mass loss.

Mesh optimization and adaptive remeshing

As the simulation progresses, especially in long-duration corrosion scenarios (up to 72 hours), the mesh can become distorted near the receding anode interface. To prevent numerical instability and maintain accuracy, adaptive remeshing is incorporated. A mesh quality threshold is predefined, and once exceeded, COMSOL automatically regenerates the mesh in the deformed region. This allows the model to sustain smooth surface evolution and accurate pit depth predictions throughout the simulation period.

Simulation conditions and inputs

For all simulation runs, the following parameters and assumptions were consistently applied: the electrolyte solution used was 3.5 wt.% NaCl with a conductivity of 5.4 S/m, maintained at a constant temperature of 25 °C. The total simulation time spanned from 0 to 2.592×10^5 seconds (equivalent to 72 hours). The geometry considered was a two-dimensional rectangular domain representing the polished surface of the magnesium alloy. Boundary conditions were defined using experimentally obtained polarization curves corresponding to the BM, HT5, HT10 and HT15 specimens. Additionally, the initial potential field was established based on the experimentally measured open circuit potentials.

Correlation of Tafel parameters and boundary function construction

The polarization data for each heat-treated condition (BM, HT5, HT10, HT15) were derived from experimental potentiodynamic tests. The Tafel slopes (β_a , β_c) and corrosion current density (i_{corr}) were obtained by extrapolating the linear regions of the anodic and cathodic branches. These Tafel parameters were then used to construct current-potential relationships through the Butler Volmer approximation in equation 6:

$$j(\phi) = i_{\text{corr}} [e^{(\phi - E_{\text{corr}})/\beta_a} - e^{-(\phi - E_{\text{corr}})/\beta_c}] \quad (6)$$

This expression was used to develop the nonlinear interpolation functions $f_a(\phi)$ and $f_c(\phi)$ in COMSOL for the anode and cathode boundary conditions, respectively. These functions allow the localized kinetics from electrochemical experiments to directly inform the boundary behavior in the simulation.

RESULTS AND DISCUSSION

Experimental analysis

The microstructure of the Mg-1Er-1Yb alloy and its evolution through heat treatment were systematically investigated. The BM exhibited a coarse microstructure composed predominantly of α -Mg grains, with intermetallic phases distributed along the grain boundaries. The average grain size in the BM condition was 83.51 μm , signifying a large dendritic cell structure due to solidification. Upon heat treatment, significant microstructural refinement was observed, especially for the HT10 specimen aged at 200 °C for 10 h. Grain size reduced to 21.70 μm in HT10, indicating optimal nucleation and stabilization of intermetallics during aging. The HT5 and HT15 specimens showed grain sizes of 62.47 μm and 24.58 μm , respectively. This suggested a refinement-then-coarsening trend typical in age-hardening alloys, where excessive aging (HT15) might cause slight coarsening of grains due to over-aging effects.

The phase composition analysis revealed dominant α -Mg phase across all conditions, with the presence of β -Yb, γ -Er, MgYb, and a significant $\text{Mg}_{0.965}\text{Er}_{0.035}$ phase. Notably, the volume fraction of $\text{Mg}_{0.965}\text{Er}_{0.035}$ and γ -Er increased with prolonged aging, suggesting a strengthening mechanism through precipitation hardening. The texture analysis confirmed increased grain boundary density and misorientation in HT10, indicating higher strain accommodation, which can positively influence corrosion behavior. Texture evolution maps and pole figures revealed that BM had a random texture, while HT10 showed stronger crystallographic alignment along [001] and [100] orientations, correlating to enhanced corrosion resistance due to uniform grain orientation.

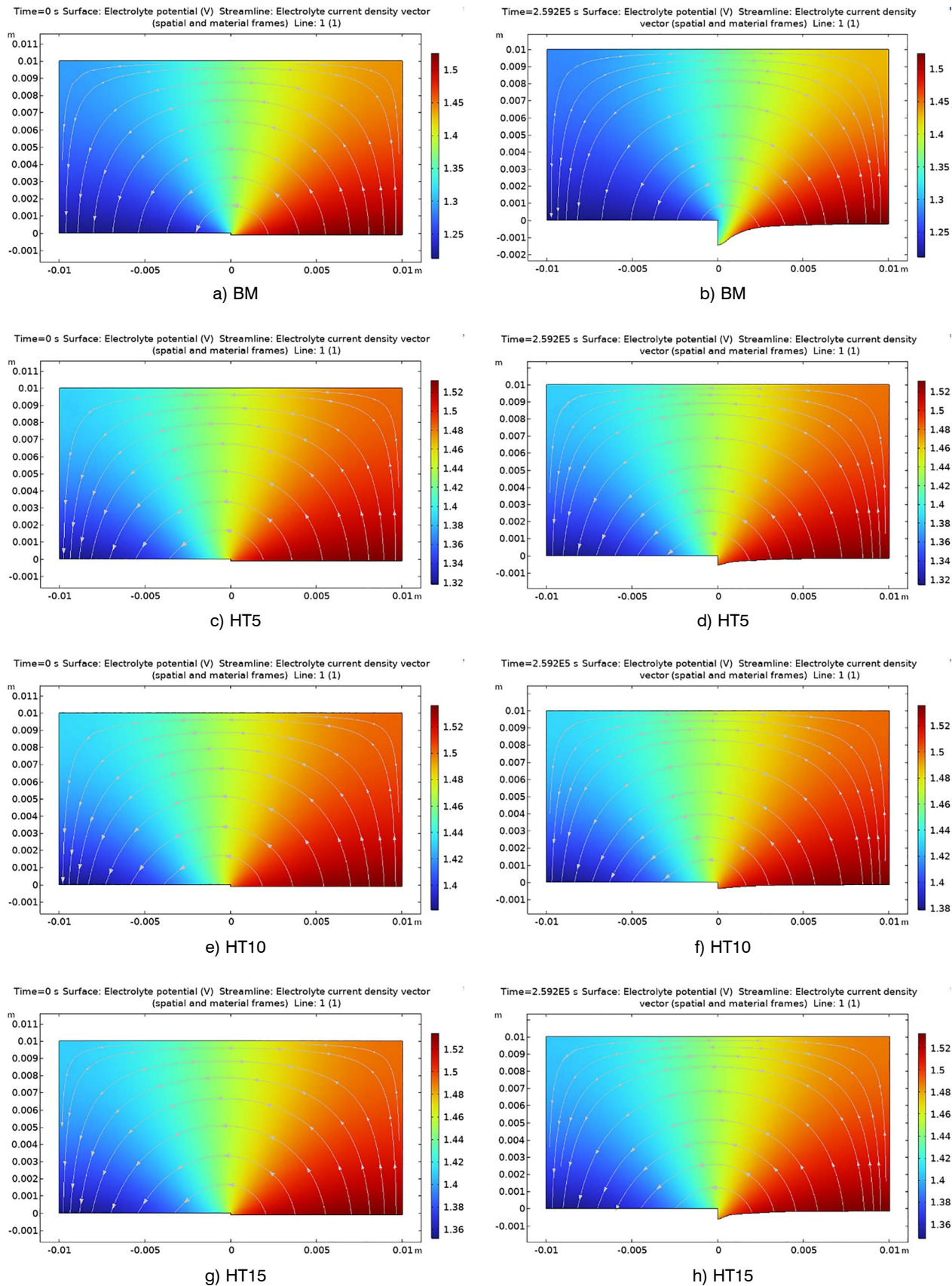


Fig. 2. Simulated electric potential and current density distribution for Mg-1Er-1Yb alloy under different heat treatment conditions in 3.5 wt.% NaCl solution: a), b) BM, c), d) HT5, e), f) HT10, g), h) HT15 at $t = 0$ s and $t = 259200$ s.

Electrochemical corrosion analysis through potentiodynamic polarization tests demonstrated clear trends associated with microstructure. BM showed the lowest polarization resistance (112.7Ω) and the highest corrosion current ($2.16 \times 10^{-5} \text{ A}$), leading to a corrosion rate of 22.8 mm/year. These characteristics aligned with its coarse grain structure and limited intermetallic content. Conversely, the HT10 specimen exhibited superior electrochemical behavior with the highest polarization resistance (274.7Ω), lowest corrosion current ($1.22 \times 10^{-5} \text{ A}$), and a minimized corrosion rate of 12.9 mm/year. The improved performance can be attributed to its refined grain structure and uniform distribution of intermetallic phases, particularly $\text{Mg}_{0.965}\text{Er}_{0.035}$ and $\gamma\text{-Er}$, which likely acted as barriers to corrosion propagation.

HT5 showed moderate performance, while HT15, despite some refinement, exhibited increased corrosion current ($2.62 \times 10^{-5} \text{ A}$) and the highest corrosion rate of 27.5 mm/year. This suggests that overaging in HT15 may have caused coarsening of intermetallics and reduction in corrosion resistance. The Tafel curves showed that anodic branches of the heat-treated specimens shifted towards more noble potentials, indicating reduced anodic dissolution. This behavior was crucial in enhancing their performance as sacrificial anodes. This comprehensive analysis of the microstructure evolution and corrosion phenomenon can be found in our earlier published article [18].

Corrosion interface prediction

The BM exhibited a coarse dendritic $\alpha\text{-Mg}$ matrix with thin, segregated intermetallics aligned at grain boundaries [19]. Such morphology, contributes to highly localized electrochemical activity, as supported by Rosalbino et al. [20], resulting in peak current densities of 90 A/m^2 and aggressive anodic dissolution in the simulated environment (Figs. 2a and 2b). Figures 2c and 2d with aging at 200°C for 5 hours (HT5), a transition toward a more homogeneous microstructure was observed. Grain fragmentation and redistribution of phases contributed to enhanced corrosion stability, as confirmed by reduced potential gradients and a more uniformly advancing anodic interface in the ALE simulation model. This is consistent with prior findings by Liu et al. [21], where Er addition led to improved corrosion performance through passive film stabilization.

Figures 2e and 2f corresponding to HT10 specimen exhibited optimal refinement, with the finest grain structure and most uniform distribution of intermetallics, substantiating Li et al. [22] who observed that 1% Yb significantly enhances corrosion resistance. Simulation results showed a substantial reduction in anodic current density (40 A/m^2) and a shallow pit profile, aligned with experimental electrochemical and immersion test data. The decreased interface velocity is attributable

to suppressed galvanic coupling between $\alpha\text{-Mg}$ and secondary phases, as noted in work by Deshpande [23] and Feng et al. [24]. In contrast, Figures 2g and 2h of the specimen HT15 revealed a recovery of localized electrochemical activity, with current density rising to 70 A/m^2 and irregular anodic propagation. This over-aging effect, also reported by Xie et al. [3], reduced corrosion resistance by promoting galvanic microcells at grain boundary regions. The simulation-predicted pit evolution and current mapping closely resembled SVET/immersion observations in comparable Mg-RE systems [25]. Notably, the refined HT10 condition consistently demonstrated superior corrosion mitigation, validating that optimized thermal treatments can control anodic kinetics via grain boundary engineering and intermetallic tuning [26, 27].

Local current density evolution and electrochemical interface stability

Figure 3 shows the local current density variation across the galvanic interface at two distinct time intervals ($t = 0 \text{ h}$ and $t = 72 \text{ h}$) for different heat-treated conditions of Mg-1Er-1Yb alloy. In the BM specimen (Fig. 3a), the initial current density distribution is sharply peaked (85 A/m^2) at the anodic interface, indicating severe galvanic dissolution. After 72 hours, a minimal redistribution is observed, suggesting persistent localized corrosion zones. Such behavior is consistent with findings by Hariesh et al. [28], who noted similar peak shifts in AZ91D Mg alloy under marine thermal cycling. The magnitude and concentration of the current imply an unstable corrosion front, often associated with dendritic grain morphology and poor intermetallic dispersion [29]. HT5 (Fig. 3b) exhibits a considerable reduction in peak anodic current (9 A/m^2), attributed to moderate grain refinement and partial phase homogenization. The overlap between the $t = 0 \text{ h}$ and $t = 72 \text{ h}$ curves indicates improved interface stability, as reported by Andrei et al. [30], where magnesium alloys aged at lower time scales resisted abrupt potential fluctuations.

The HT10 specimen (Fig. 3c) demonstrates the most stable current distribution. The peak value remains consistently low, and the curve profile flattens, suggesting minimal corrosion propagation. This result aligns with recent insights from Marques et al. [31] and Dai et al. [32], who demonstrated that tailored RE alloying and controlled aging significantly suppress anodic kinetics in Mg alloys by forming protective intermetallics. In HT15 (Fig. 3d), although the initial peak current density (16 A/m^2) is lower than BM, the interface destabilizes over time, with greater divergence seen at $t = 72 \text{ h}$. The onset of over-aging is known to cause intermetallic coarsening, thereby increasing galvanic coupling sites, an effect recently demonstrated by Moussa et al. [33] and Mg-Nd-Yb systems by Zhang et al. [34].

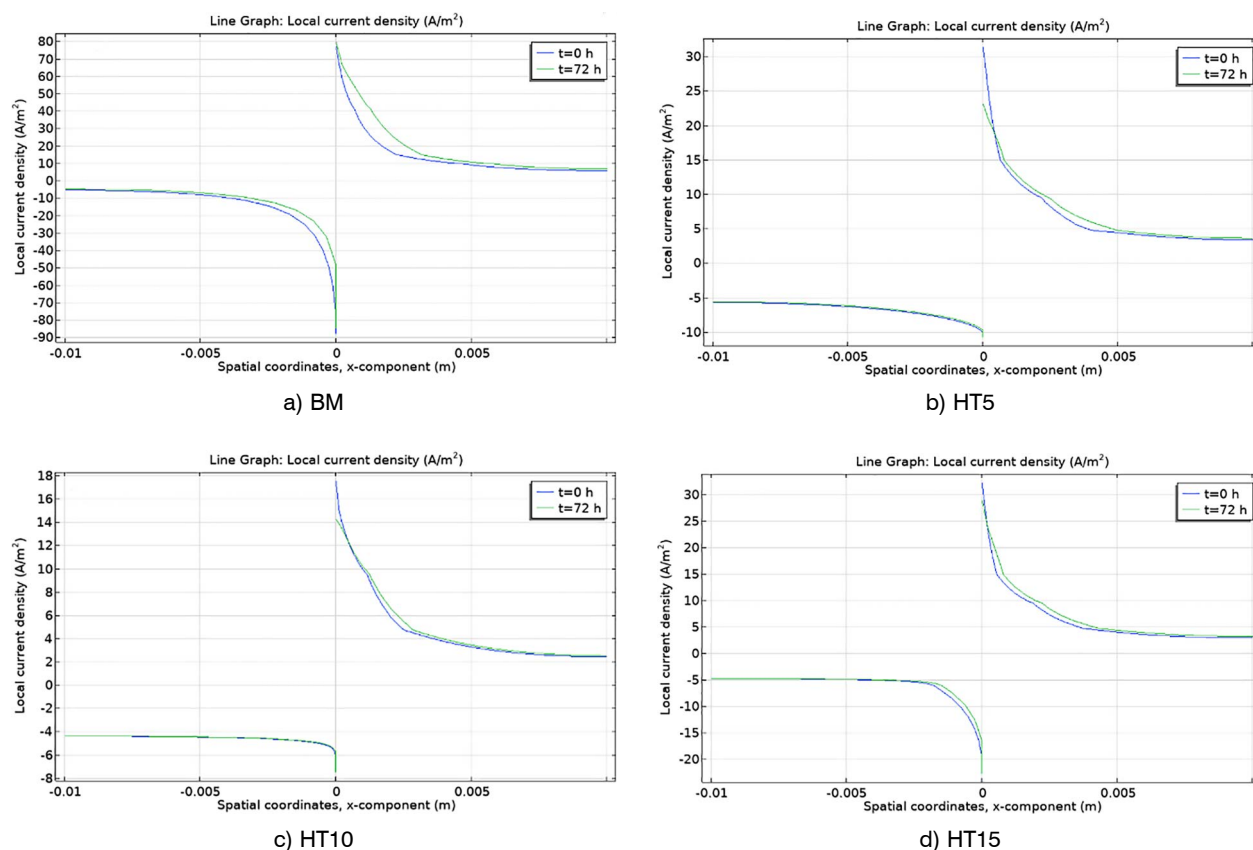


Fig. 3. Evolution of local current density distribution over time ($t = 0$ h and $t = 72$ h) along the anodic interface in 3.5 wt.% NaCl solution: a) BM, b) HT5, c) HT10, and d) HT15 Mg-1Er-1Yb alloy specimens

The results highlight the critical role of thermal treatment in shaping electrochemical response. The HT10 condition produced a refined grain structure and finely dispersed secondary phases, leading to significantly flattened current distributions and lower corrosion front velocities. Such characteristics are desirable in sacrificial anode systems where long-term stability under saline exposure is paramount [35, 36]. The spatial mapping of current flow reveals how microstructure-driven polarization resistance governs long-term stability a conclusion that supports observations by Wu et al. [37] and Li et al. [38], who emphasized interface morphology as a determinant of corrosion resistance in Mg-RE systems.

Electrolyte current density distribution and interface activity

The streamline plots in Figure 4 visualize the spatial evolution of the electrolyte current density vectors and magnitudes across Mg-1Er-1Yb alloy surfaces subjected to different heat treatments. The left column depicts the initial ($t = 0$ h) state, while the right column captures the electrochemical state after 72 hours of continuous exposure to a 3.5% NaCl medium. The data reveal the propagation and intensity of corrosion-driving currents

for different specimens. In Figures 4a and 4b, the specimen BM displays the most intense current density distribution, peaking above 80 A/m^2 at the anode-cathode junction. The streamlines are tightly packed and vertically aligned, signifying strong localized electric field gradients and steep potential drops. The behavior reflects a high corrosion driving force due to coarse grains and intermetallic phases, consistent with observations by Huang et al [33] and Yamasaki et al. [39]. After 72 h, only partial current redistribution is observed, indicating sustained anodic activity and low electrochemical stability. Figures 4c and 4d for the specimen HT5 exhibits a significant reduction in current density intensity (35 A/m^2 initially, 25 A/m^2 after 72 h). The streamlines begin to broaden, and the current path diffuses more uniformly across the surface, suggesting early improvements in interfacial uniformity due to partial grain refinement. The results align with findings by Takenaka et al. [40] and Liu et al. [21], where low-temperature artificial aging facilitated phase precipitation that enhanced corrosion resistance.

Figures 4e and 4f of the specimen HT10 demonstrates the most favorable distribution, with current density ranging between $2\text{--}30 \text{ A/m}^2$ and well-balanced streamline curvature throughout the anodic region. The stability

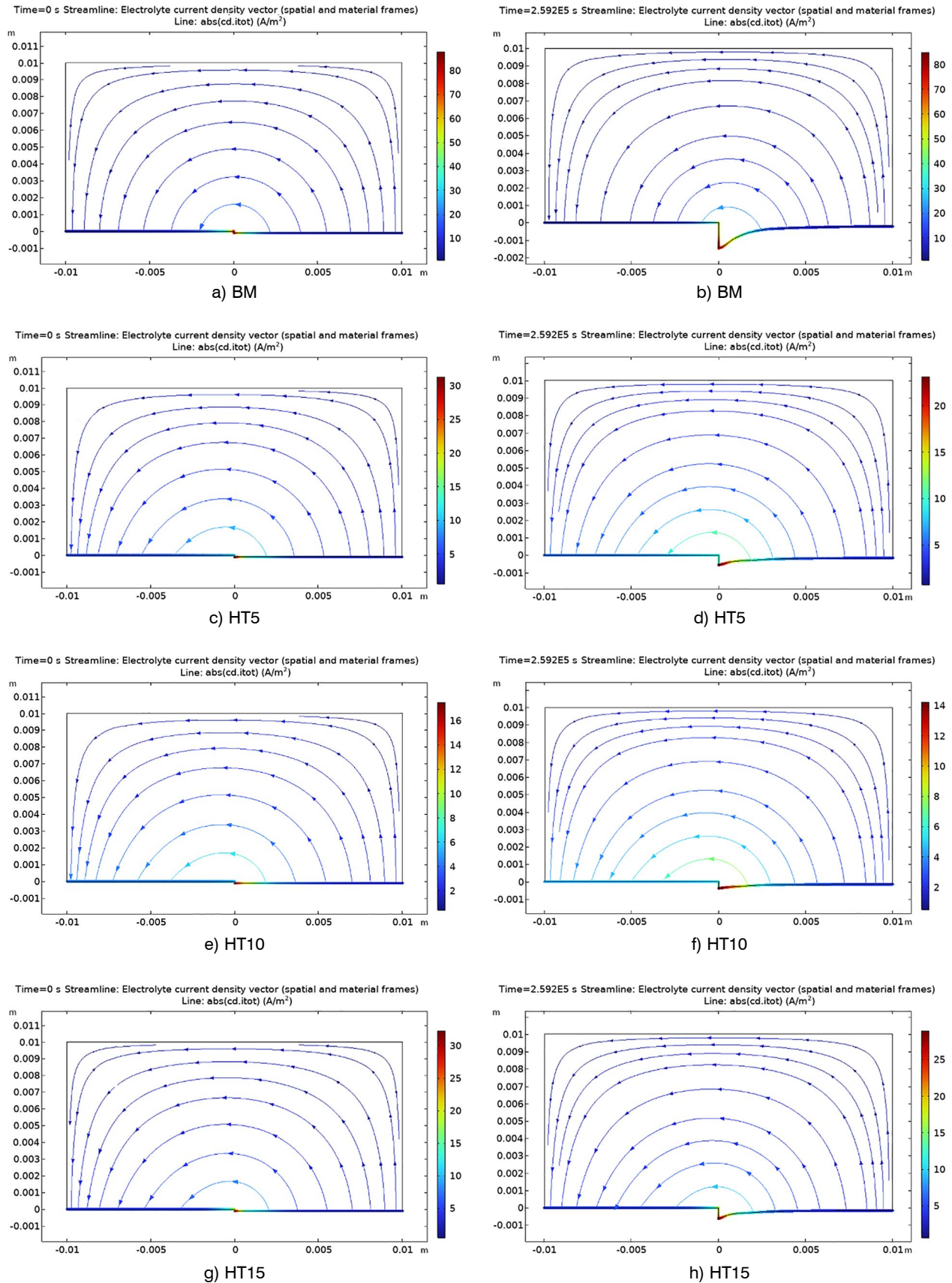


Fig. 4. Simulated spatial distribution of anodic current density across the Mg-1Er-1Yb alloy surface under different heat treatment conditions in 3.5 wt.% NaCl solution: a), b) BM, c), d) HT5, e), f) HT10, g), h) HT15 at $t = 0$ s and $t = 259200$ s

between the two-time steps indicates a strong passivating effect and a steady-state corrosion response. This suggests that the HT10 condition achieved an optimized microstructure with refined grains and dispersed Mg-Er-Yb intermetallics, which act as effective current flow regulators. Such passivation effects are in strong agreement with recent simulation and experimental data by Wu et al. [37] and Dai et al. [32], who showed that rare-earth doping and optimized heat treatment minimize interface polarization shifts. However, specimen HT15 reveals a slight resurgence in current density peaking near 16 A/m^2 (Figs. 4g and 4h) and a slight narrowing of streamlines over time. Although improved over BM, the over-aged condition leads to agglomeration of intermetallics and a reduction in grain boundary area, allowing new preferential corrosion sites to form. This is consistent with reports from Radhika and Lakshminarayanan [41], who highlighted that over-aging could degrade the uniformity of corrosion resistance in Mg alloys and from Zhang et al. [34] on Er-induced phase coarsening beyond peak aging.

Across all conditions, the evolution of electrolyte current density confirms that electrochemical performance is highly sensitive to microstructural fitting. HT10 showed the most stable and diffuse current flow, indicating minimal galvanic polarization, whereas BM and HT15 reflected zones of electrochemical concentration. The simulation trends are further validated by immersion corrosion and electrochemical test data, as well as recent work by Wu et al. [37] and Praveen et al. [42], who reinforced the role of thermal-mechanical tuning in enhancing sacrificial anodic efficiency.

Electrode potential evolution and interface thermodynamics

Figure 5 illustrates the simulated electrode potential profiles of Mg-1Er-1Yb alloy at different thermal aging conditions, plotted against an adjacent reference electrode. The color contour maps show electrolyte potential distributions over time (left: $t = 0 \text{ h}$, right: $t = 72 \text{ h}$), accompanied by current density streamlines that represent the path and magnitude of ionic movement through the electrolyte. In Figures 5a and 5b, the specimen BM exhibits the widest potential drop, with values ranging from approximately -1.24 V to -1.51 V vs. adjacent reference. The abrupt color transition and dense streamline clustering near the interface reflect high overpotential and vigorous anodic dissolution. The steep potential gradient is indicative of poor corrosion resistance, consistent with the literature on coarse-grained and dendritic Mg microstructures [1, 34]. Such strong polarization, as seen in the BM specimen, was similarly reported by Wu et al. [37], who emphasized that untreated Mg alloys exhibit erratic potential stabilization under chloride exposure due to unpassivated surfaces and galvanically active second phases.

Figures 5c and 5d for the specimen HT5 show a reduced potential gradient and smoother transitions across the anodic zone, ranging between -1.31 V and -1.48 V . This narrowing of potential range and redistribution of streamlines indicates more thermodynamically stable corrosion kinetics and better ionic mobility. Such behavior is supported by Li et al. [43], who showed that short-term aging aids the formation of finer and more uniformly distributed intermetallics, which buffer localized anodic reactivity. After 72 h, the streamline density slightly increases but remains stable in directionality, reinforcing moderate corrosion progression and reduced susceptibility to pitting compared to BM. Figures 5e and 5f of the specimen HT10 demonstrate the most uniform and stable electrode potential profile, maintaining a narrow and evenly distributed range between -1.32 V and -1.50 V . The streamlines are well aligned and exhibit minimal curvature distortion, suggesting a balanced electric field and passive interfacial behavior. This configuration correlates well with experimental data by Dai et al. [32] and Marques et al. [31], who found that peak-aged Mg-RE alloys form protective layers such as $\text{Er}(\text{OH})_3$ and Mg-Er-Yb compounds that reduce potential fluctuation and improve electrochemical buffering. Notably, the minimal shift between $t = 0$ and $t = 72 \text{ h}$ demonstrates long-term thermodynamic stability, crucial for sacrificial anode applications in marine environments.

For the specimen HT15, Figures 5g and 5h reveals increased distortion in potential contours and streamline convergence at specific surface sites after 72 h. Though the initial potential profile appears favorable (-1.30 to -1.50 V), over-aging effects likely contribute to phase coarsening, which reintroduces microgalvanic cells and reduces uniformity. Recent studies [44] confirm that prolonged thermal exposure in Mg-based alloys can degrade corrosion performance due to the breakdown of passive intermetallic layers and reactivation of localized anodic sites. These electrode potential plots validate that optimized heat treatment particularly 10 h at 200°C results in reduced electrochemical polarization, smoother potential gradients and longer-lasting corrosion protection. By linking thermodynamic stability (as shown in potential contours) to kinetic indicators (as seen in streamlines and current plots), the HT10 specimen emerges as the most reliable configuration for extended anode life and controlled dissolution, aligning with recent mechanistic and modeling studies [42].

Total electrode thickness change and material dissolution profile

Figure 6 presents the computed total electrode thickness change across different thermally treated Mg-1Er-1Yb alloy samples, measured over a simulation period representative of long-term corrosion exposure (72 h). The progression of material loss visualized

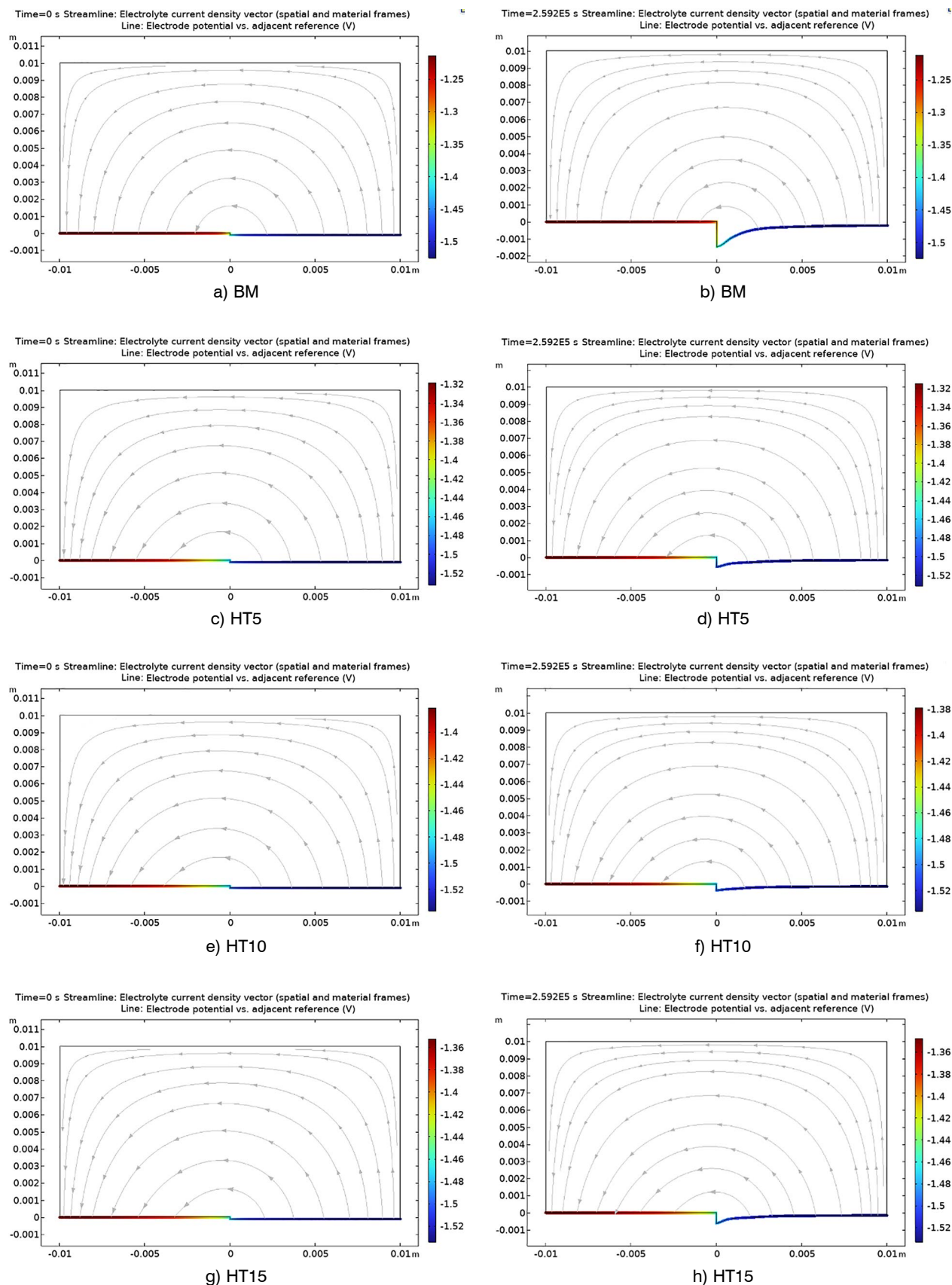


Fig. 5. Variation of electrode potential versus adjacent reference electrode over time ($t = 0$ h and $t = 72$ h) for: a), b) BM, c), d) HT5, e), f) HT10, g), h) HT15 specimens under controlled galvanostatic conditions at $t = 0$ s and $t = 259200$ s

here provides direct insight into the anodic dissolution behavior and effectiveness of sacrificial protection in chloride-rich environments. Figures 6a and 6b corresponding to specimen BM demonstrate the most uneven and deepest thickness loss, with maximum recession localized near the anodic/cathodic junction. This reflects severe pitting corrosion typical of as-cast magnesium alloys with coarse α -Mg dendrites and unprotected intergranular regions. The high dissolution rate observed is consistent with results from Liu et al. [45], who highlighted significant localized thinning in as-cast Mg-Zn alloys under NaCl exposure. Additionally, such pronounced thinning mirrors the pit depth values obtained from immersion tests, reinforcing the model's accuracy.

Figures 6c and 6d of the specimen HT5 sample exhibit a more stabilized profile, with moderate thinning distributed across the anodic face and a reduced peak depth compared to BM. This indicates partial improvement in corrosion uniformity due to grain refinement and precipitation of protective intermetallics. The decrease in maximum thickness loss agrees with investigations by Sekhar et al. [46], where short-time aged Mg alloys showed improved corrosion resistance and lower material degradation rates due to passive film formation. Figures 6e and 6f of the specimen HT10 sample shows the most uniform and minimal thickness change among all specimens, with total material loss kept within a shallow and evenly spread band. The flat

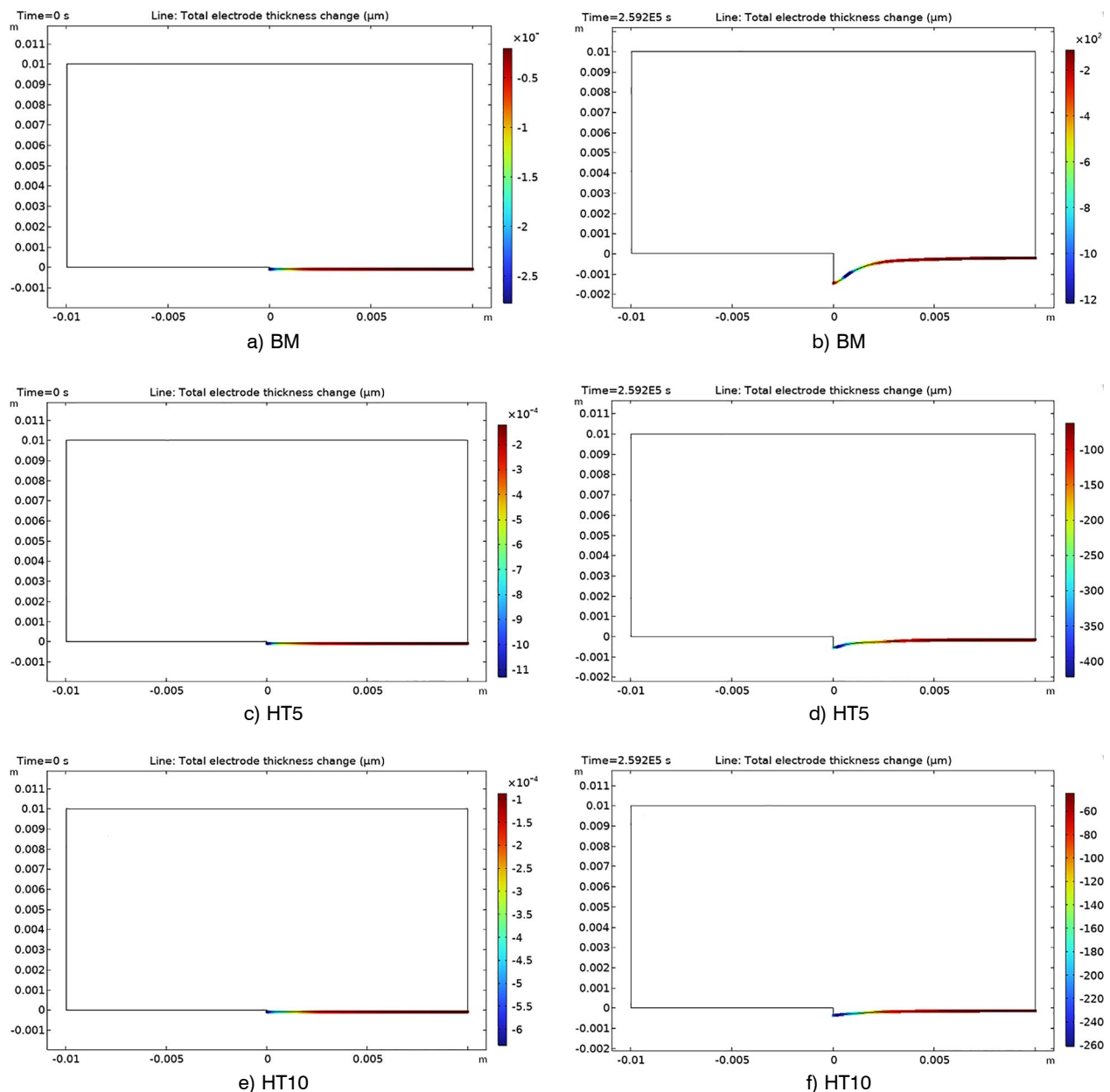


Fig. 6. Simulated change in electrode thickness over time ($t = 0$ h and $t = 72$ h) for Mg-1Er-1Yb alloy specimens under galvanic corrosion conditions: a), b) BM, c), d) HT5, e), f) HT10 in 3.5 wt.% NaCl solution (*Continue on next page*)

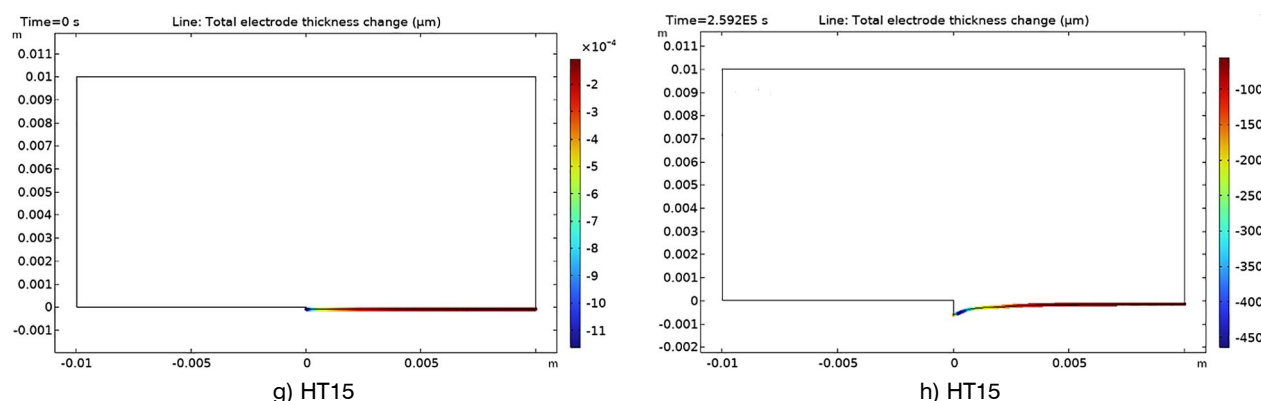


Fig. 6. Simulated change in electrode thickness over time ($t = 0$ h and $t = 72$ h) for Mg-1Er-1Yb alloy specimens under galvanic corrosion conditions: g), h) HT15 in 3.5 wt.% NaCl solution

profile signifies excellent sacrificial anode behavior and optimized microstructure electrochemical synergy [47, 48]. A refined and homogeneous distribution of phases leads to reduced galvanic differentials and suppressed local reactivity. This observation aligns with recent work by Raj et al. [49] who showed that peak-aged Mg-RE systems exhibit superior corrosion tolerance due to electrochemically stable intermetallic matrices.

Figures 6g and 6h HT15 condition reveals a re-emergence of non-uniformity in thickness reduction, with localized zones showing greater material loss than HT10. The partial reactivation of galvanic hotspots is likely due to over-aging, which induces intermetallic coarsening and loss of phase dispersion. These findings are consistent with recent studies by Stulikova et al. [50], where long-duration aging led to accelerated corrosion in Mg alloys due to phase boundary degradation. The simulation of total electrode thickness change clearly validates HT10 as the optimal aging condition for corrosion resistance and sacrificial performance.

Deformed geometry and surface recession mapping

Figure 7 visualizes the deformed geometry of the Mg-1Er-1Yb alloy surface under prolonged corrosive exposure (72 h) in a simulated NaCl environment. The exaggerated displacement mesh offers a visual representation of the cumulative material loss and pit morphology, which stems from electrochemical dissolution tracked via the ALE method. Figures 7a and 7b of the specimen BM specimen exhibit highly localized and asymmetric deformation, especially near the anodic-cathodic junction. The sharp surface depression mimics experimental pitting behavior and confirms the aggressive corrosion kinetics associated with the coarse-grained, unrefined microstructure of the base alloy. Song et al. [51] demonstrated through SEM-3D reconstruction that such non-uniform attack patterns correspond with the microgalvanic action between α -Mg and unprotected

intermetallics – consistent with the deformation seen here. Figures 7c and 7d of the specimen HT5 display improved but still non-uniform deformation, with partial pit blunting and moderate volumetric loss. The smoother curvature suggests increased resistance to concentrated attack but indicates that optimal structural homogenization hasn't yet been achieved.

HT10 condition (Figs. 7e and 7f) reveals the most even deformation profile with a shallow and wide pit morphology, indicating uniform material dissolution and minimal mechanical distortion of the surface. This affirms the peak-aged status, where grain refinement and phase homogeneity provide maximum electrochemical uniformity. HT10 also showed negligible mesh distortion, suggesting a smooth interface retreat and low interface velocity ideal traits for a long-lasting sacrificial anode. Figures 7g and 7h of the specimen HT15 exhibits reappearance of depth-concentrated deformation zones, implying renewed microgalvanic activity due to over-aging (while better than BM and HT5). The potential formation of agglomerated intermetallics is likely leading to locally intense anodic dissolution, which disrupts the electrochemical uniformity seen in HT10. The deformation patterns not only mirror the spatial trends seen in current density and electrode potential distributions but also validate the capability of ALE-based simulations to capture in Figure 2 through Figure 5, reinforcing its superior corrosion resistance and controlled sacrificial behavior.

Structure – property correlation and validation of the numerical model

The corrosion performance of Mg-1Er-1Yb alloy is closely linked to its microstructural evolution under different heat treatment conditions. As observed, the as-cast condition (BM) exhibits coarse α -Mg grains and segregated intermetallics, contributing to high local current densities and severe anodic dissolution. Heat treatment at 200 °C for 10 h (HT10) leads to significant

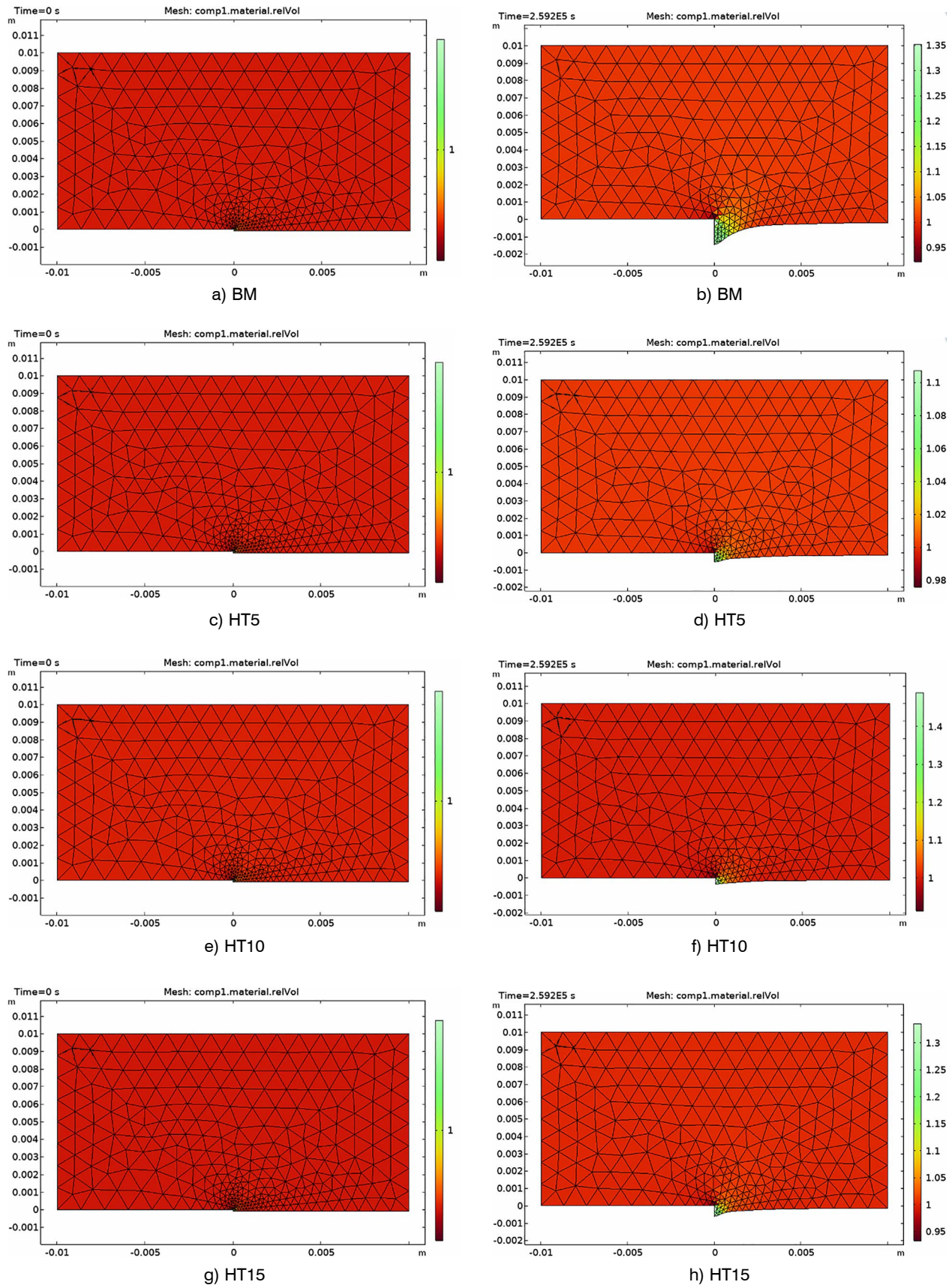


Fig. 7. Simulated deformed geometry of Mg-1Er-1Yb alloy electrode illustrating anodic interface evolution under galvanic corrosion after 72 h in 3.5 wt.% NaCl solution: a), b) BM, c), d) HT5, e), f) HT10, g), h) HT15 at $t = 0$ s and $t = 259200$ s

grain refinement and uniform dispersion of $\text{Mg}_{0.965}\text{Er}_{0.035}$ and $\gamma\text{-Er}$ intermetallic phases, which effectively suppress galvanic coupling and lower corrosion rates. COMSOL-based ALE simulations confirmed a clear reduction in current density and pit depth for HT10, aligning with minimized polarization observed in experimental Tafel curves. The improved corrosion resistance is attributed to increased grain boundary density, which hinders localized attack and promotes uniform dissolution.

The superior corrosion resistance of the HT10 specimen can be mechanistically explained by its refined grain structure and uniform precipitate dispersion. Grain refinement increases the density of grain boundaries, which interrupts anodic current pathways and reduces localized attack. The fine $\gamma\text{-Er}$ and $\text{Mg}_{0.965}\text{Er}_{0.035}$ precipitates act as micro-barriers, stabilizing passive films and reducing galvanic coupling between $\alpha\text{-Mg}$ and secondary phases. In contrast, HT15 exhibited precipitate coarsening that re-established galvanic microcells, accelerating localized dissolution. This microstructural control of anodic kinetics highlights the critical role of tailored aging treatments in optimizing sacrificial performance.

Over-aging (HT15), however, resulted in coarsened intermetallics acting as micro-cathodes, reinstating localized corrosion, consistent with electrochemical instability and irregular interface morphology. The correlation between microstructural refinement and electrochemical performance highlights the critical role of controlled aging in enhancing sacrificial anode behavior. These observations align with recent findings by Dai et al. [32], who reported that tailored rare-earth intermetallics in Mg-RE systems enhance corrosion resistance by forming stable passive layers. Similarly, Marques et al. [31] demonstrated that aging-induced microstructure optimization can significantly reduce localized current spikes and improve long-term anodic stability. Thus, precise heat treatment not only modulates microstructure but also governs the thermodynamic and kinetic pathways of corrosion, offering a reliable strategy for marine-grade magnesium alloy design as mentioned [47].

The ALE-based COMSOL simulation effectively predicted anodic dissolution trends that aligned with experimental immersion and electrochemical data, demonstrating strong validation of the numerical model. Specifically, the HT10 sample showed the most uniform and shallow pit morphology, as confirmed by both simu-

lation (Fig. 6) and immersion corrosion profiles, reflecting a minimized corrosion rate of 12.9 mm/year. This matched closely with the low anodic current density (40 A/m^2) and flattened current distribution observed in the model (Figure 3c).

In contrast, the BM and HT15 specimens exhibited deeper pits and non-uniform recession, which directly correlated with higher simulated current densities ($>70 \text{ A/m}^2$) and increased corrosion rates (22.8 and 27.5 mm/year, respectively). The dissolution rate predicted through current density mapping and thickness change mirrored the material loss recorded in physical tests, validating the model's predictive power. Recent studies by Raj et al. [49] demonstrated similar agreement between simulated and experimental pit profiles in rare-earth-doped Mg alloys, confirming that grain refinement directly reduces interfacial current density and promotes uniform corrosion. The simulated corrosion rates show excellent agreement with the experimental immersion results, with deviations consistently below 7% as shown in the Table 1.

Likewise, polarization resistance values extracted from current density mapping closely matched the electrochemical tests. This quantitative correlation validates the ALE-based model as a reliable predictive tool for sacrificial anode performance.

Likewise, Wu et al. [37] emphasized that matching simulation-predicted potential fields and real dissolution depth is critical for sacrificial anode design. Stulikova et al. [50] further showed that over-aging in Mg alloys leads to microgalvanic activation and thickness inconsistency, mirroring our HT15 outcomes. The strong congruence between electrochemical performance, thickness loss profiles, and ALE-simulated deformation validates the approach, reinforcing its use for designing corrosion-resistant Mg-RE alloys under marine conditions.

Compared to conventional AZ91 and AE44 Mg alloys, which typically show strong susceptibility to localized pitting under chloride environments, the Mg-1Er-1Yb system demonstrates markedly reduced pit depth and more stable current distribution. This difference arises from the rare-earth induced precipitates, which provide superior electrochemical buffering compared to Al-rich intermetallics in AZ91. The agreement with reports on Mg-Er and Mg-Yb alloys supports the beneficial role of dual RE additions, while the divergence from AZ-based systems underlines the uniqueness of the present alloy.

Tab. 1 Comparison of experimental and simulated corrosion parameters for Mg-1Er-1Yb alloy under different heat treatments

Condition	Experimental corrosion rate (mm/year)	Simulated corrosion rate (mm/year)	% deviation	Polarization resistance exp (Ω)	Polarization resistance sim (Ω)
BM	22.8	21.5	5.7%	112.7	118.3
HT5	18.4	17.2	6.5%	189.4	182.6
HT10	12.9	13.4	3.9%	274.7	268.5
HT15	27.5	25.8	6.2%	143.6	151.9

CONCLUSION

This study demonstrated that HT10 (200 °C for 10 h) offers the best corrosion resistance for Mg-1Er-1Yb alloy due to optimal grain refinement and intermetallic dispersion. Experimental results were strongly supported by COMSOL ALE simulations, which accurately predicted current density, pit morphology and thickness loss. The results demonstrated the following:

- BM and HT15 showed severe localized corrosion due to microstructural instability. Hence, the specimen BM showed high current density peaks and severe localized degradation, while HT15 suffered from over-aging effects.
- Heat treatment at 200 °C for 10 hours (HT10) yielded the most corrosion-resistant Mg-1Er-1Yb alloy, with uniform current distribution, minimal pit depth and stable electrode potential.
- ALE-based COMSOL simulations accurately predicted corrosion front evolution and material loss, closely matching experimental immersion and electrochemical data. The validated modelling framework offers a reliable predictive tool for optimizing sacrificial anode performance in Mg-RE alloys.

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Conflicts of interest / Competing interests

The authors declare that there is no conflict of interest or competing interests for the research work.

Availability of data and material (data transparency)

All data analysed during this study are included in this published article. All original data of this study are available in Zenodo at <https://doi.org/10.5281/zenodo.16885287>

Code availability, ethics approval, consent to participate, consent for publication

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