

Entropy-Guided Detection of Chaos Transitions in Electrochemical Transport Systems

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ABSTRACT

Electrochemical transport systems can shift from ordered oscillation to chaotic behavior when diffusion, migration, and interfacial reaction kinetics interact under strong nonlinear forcing, affecting transport stability and response reliability. Recent studies on nonlinear reaction-diffusion dynamics, electrochemical oscillation, and entropy-based signal analysis show that instability often develops through intermediate regimes, but a unified entropy-based framework for detecting chaos onset in electrochemical transport systems remains limited. This gap is important because such systems often pass through transition-sensitive operating windows where early detection can improve control and diagnostics. In this article, a time-dependent transport model is analyzed using composite transport entropy, divergence behavior, regime mapping, and delay-embedded state-space density reconstruction. The results show that entropy increases systematically as the system moves from ordered to chaotic transport, accompanied by wider occupation of reconstructed electrochemical state space. The study demonstrates that entropy can serve as a physically meaningful indicator of chaos onset and offers a useful framework for identifying instability-prone regimes in transport-limited electrochemical devices.

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1. INTRODUCTION

Electrochemical transport systems are governed by a tightly coupled interaction between ionic diffusion, electric-field-driven migration, interfacial kinetics, and local accumulation effects. When these mechanisms evolve under strong forcing, the resulting dynamics may no longer remain steady or weakly periodic, but instead move through instability thresholds into irregular oscillatory states. Such behavior is especially relevant in transport-limited electrochemical environments, where small perturbations in concentration or potential can be amplified by nonlinear feedback between the bulk transport field and the reaction-active boundary. The broader nonlinear-science literature has already shown that distributed transport-reaction systems can spontaneously generate ordered patterns, instabilities, and regime shifts when internal feedback becomes sufficiently strong [1]. Related biochemical network studies have further

demonstrated that complex spatiotemporal responses may arise even without artificially imposed control loops, which reinforces the idea that irregular dynamics can be intrinsic to the governing transport equations themselves [2].

Recent advances in nonlinear reaction-diffusion theory have sharpened the understanding that transition behavior is controlled not only by parameter magnitude, but also by the structure of the solution space available to the coupled system. Spatial robustness, wave bifurcation, and nonlinear pattern persistence have all been shown to depend on how transport and reaction compete across the underlying domain [3]. Solution-landscape analysis has made this especially clear by showing that a system may remain apparently stable over a finite parameter window before abruptly reorganizing into a distinctly different dynamical state [4]. Studies on bilayer and cross-diffusive systems have also revealed that geometry and multi-field coupling can materially alter transition thresholds and the persistence of

unstable modes [5]. These findings are highly relevant to electrochemical transport, where the interaction between ionic gradients, field intensity, and boundary reactivity introduces a similarly rich nonlinear structure.

Despite this progress, the transition from regular electrochemical oscillation to chaotic transport remains insufficiently quantified. Many electrochemical studies identify instability through signal distortion, voltage irregularity, or local concentration fluctuation, yet the actual onset of chaos is often inferred visually rather than detected through a dedicated complexity metric. This is a significant limitation because transport systems rarely move directly from a regular state to a fully chaotic one. Instead, they commonly pass through a transitional interval in which oscillations remain bounded but lose symmetry, repeatability, or spectral compactness. The nonlinear systems literature indicates that such transitional zones are fundamental components of the instability pathway rather than incidental numerical artifacts [3]. A rigorous detection framework should therefore be able to distinguish periodic order, transitional irregularity, and fully chaotic behavior using a single physically interpretable criterion.

This study develops an entropy-guided framework for detecting chaos transitions in electrochemical transport systems governed by nonlinear transport-reaction coupling. The central hypothesis is that entropy provides a sensitive measure of dynamical uncertainty and therefore can identify the onset of chaos earlier than amplitude-based or purely visual diagnostics. To test this idea, a time-dependent electrochemical transport model is formulated and driven across a controlled forcing range so that stable, periodic, transitional, and chaotic regimes can all emerge within the same computational setting. The contribution of the work is not simply the use of entropy as a post-processing metric, but the establishment of entropy as a transport-aware indicator whose rise is directly linked to the breakdown of regular electrochemical state evolution. The article therefore offers a physically grounded route for tracking nonlinear instability in electrochemical systems and provides results through two single-figure computational outputs: a regime heatmap and a state-space density distribution.

2. METHODOLOGY

The electrochemical domain is modeled as a one-dimensional reactive transport layer of length L , bounded by a transport reservoir at $x=0$ and an electrochemically active interface at $x=L$. The evolving fields are ionic concentration $c(x,t)$, electric potential $\phi(x,t)$, ionic flux $J(x,t)$, and interfacial current density $i(t)$. This formulation is selected because it captures the dominant physical ingredients required for nonlinear electrochemical transport: diffusion within the bulk, migration under an applied field, and nonlinear reaction at the electrode boundary. Comparable reduced-order transport descriptions have been used effectively in recent electrochemical simulation studies because they preserve the essential coupling between field variables while remaining computationally tractable over long temporal windows [6]. The present work focuses specifically on transition behavior, so the model is designed to expose the internal route by which regular electrochemical motion loses coherence under progressively stronger forcing [7].

The bulk concentration field obeys a nonlinear Nernst-Planck transport balance,

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - \mu \frac{\partial}{\partial x} \left(c \frac{\partial \phi}{\partial x} \right) - R(c, \eta),$$

where D is the effective ionic diffusivity, μ is the mobility coefficient, and $R(c, \eta)$ is the volumetric reaction coupling term. The total ionic flux is written as

$$J(x, t) = -D \frac{\partial c}{\partial x} - \mu c \frac{\partial \phi}{\partial x}.$$

The potential field is treated in an effective electro-neutral framework in which the local gradient $\partial\phi/\partial x$ reflects the imposed forcing and the instantaneous transport state. This simplification avoids unnecessary electrostatic overhead while retaining the coupling needed to generate transport amplification. Such compact but strongly coupled formulations are appropriate for studying nonlinear electrochemical response because they preserve the interaction between ionic redistribution and field-assisted motion that underlies dynamical reorganization [8]. Recent work on dynamic electrochemical response has also emphasized that transport and electrical behavior should be interpreted as a coupled nonlinear entity rather than as separable subsystems [9].

The reactive boundary at $x=L$ is governed through a nonlinear interfacial kinetic law,

$$i(t) = i_0 [\exp(\alpha \eta(t)) - \exp(-\beta \eta(t))],$$

where i_0 is the exchange current density, α and β are transfer coefficients, and $\eta(t)$ is the overpotential. The reaction term in the bulk equation is coupled to this boundary behavior through

$$R(c, \eta) = k c^m \sinh(\Gamma \eta),$$

where k , m and γ regulate nonlinear amplification. This two-way coupling is central to the present framework. The local concentration controls the reaction rate through ionic availability, while the reaction rate reshapes the transport field through boundary consumption and field redistribution. Once this feedback becomes sufficiently strong, the transport layer is no longer able to dissipate disturbances smoothly, and repeated amplification begins to restructure the temporal response. The importance of such nonlinear departure from near-stationary behavior is well recognized in recent electrochemical studies, particularly in work examining systems beyond the assumptions of classical linear response [8]. The present model turns that general insight into a transition-detection problem.

To make the instability pathway explicit, a nondimensional forcing parameter λ is introduced. This parameter scales the applied potential and indirectly controls the strength of migration, concentration polarization, and reaction nonlinearity. The dimensionless form of the governing balance can be written as

$$\frac{\partial C}{\partial \tau} = \frac{\partial^2 C}{\partial X^2} - \Lambda \frac{\partial}{\partial X} \left(C \frac{\partial \Phi}{\partial X} \right) - K C^m \sinh(\Gamma \eta),$$

where $C = c/c_0$, $X = x/L$ and $\tau = tD/L^2$, while Λ , K and Γ represent scaled migration, reaction, and kinetic sensitivity parameters. The parameter λ is embedded in the applied-potential condition and acts as the principal bifurcation-like driver of the system. Low λ values preserve ordered electrochemical response, intermediate values trigger progressive waveform distortion, and high values generate persistent irregular motion. Parameter sweeps of this form are widely used in computational electrochemistry because they reveal how nonlinear state evolution changes under controlled forcing rather than isolated case-by-case observation [7]. They are especially suitable for identifying transitional windows rather than only terminal unstable states [9].

The numerical solution is obtained with a finite-difference discretization in space and explicit time advancement subject to a stability-restricted time step. A uniform grid of N spatial nodes is used, and the temporal integration is carried out for sufficiently long duration to remove startup transients and isolate the asymptotic regime at each λ . Boundary conditions are set as $C(0, \tau) = 1$ at the reservoir side and a nonlinear flux condition at the reactive side tied to $i(t)$. The solution is monitored for numerical consistency through mass-balance tracking and boundedness checks on the concentration field. Explicit schemes remain appropriate for this class of transport problem when the temporal step is chosen according to the diffusive and migrative stiffness of the system, and recent numerical studies have shown that such methods can retain strong stability and accuracy in coupled reaction-diffusion settings [10]. For each forcing condition, the simulation records the interfacial concentration, spatially averaged flux, boundary current density, and a delayed-coordinate state trajectory used later in the transition analysis.

The core detection variable is the entropy of the electrochemical signal. In this study, permutation entropy is used because it measures the loss of ordinal structure in a time series and is therefore well suited to distinguishing regular oscillation from irregular transport motion. For a normalized sequence $\{s_n\}$, the entropy is computed as

$$H = - \sum_{j=1}^M p_j \ln p_j,$$

where p_j is the occurrence probability of the j -th ordinal pattern and M is the total number of admissible patterns. A low value of H indicates repeatable and ordered electrochemical dynamics, whereas a high value indicates disorder, temporal unpredictability, and reduced deterministic recurrence. Entropy-based processing has already proved useful in electrochemical noise analysis because it can detect subtle complexity changes that are not visible through amplitude inspection alone [11]. In the present work, entropy is calculated separately for concentration and current-density signals, after which a composite transport entropy H_T is formed through normalized averaging:

$$H_T = \frac{1}{2} (H_c + H_i).$$

This gives the analysis direct electrochemical meaning by combining a bulk transport observable with an interfacial response observable.

Entropy is then combined with a supporting divergence metric and a reconstructed state-space density map. The divergence metric is defined as

$$\Psi(\tau) = \frac{1}{N_p} \sum_{q=1}^{N_p} \ln \left| \mathbf{z}_q(\tau + \Delta\tau) - \mathbf{z}'_q(\tau + \Delta\tau) \right|,$$

where \mathbf{z}_q and \mathbf{z}'_q are initially neighboring state vectors in the delayed-coordinate space. Although Ψ is not a formal Lyapunov exponent, it acts as a practical sensitivity proxy by indicating whether nearby transport states separate rapidly under the same governing laws. The state-space density map is built by binning the delayed trajectory in a two-dimensional embedding plane and converting visit frequency into a normalized intensity field. This avoids the need for line-based phase portraits and produces a more informative visualization of regime spreading. Advanced electrochemical response studies increasingly rely on multiple coupled diagnostics because nonlinear dynamical behavior is rarely expressed adequately through a single signal representation [10]. The combined use of entropy, divergence, and state-density concentration therefore gives the present framework stronger interpretive reliability [12].

The regime classification is performed over the full forcing sweep by applying threshold logic to the composite entropy H_T , the divergence metric Ψ , and the compactness of the state-density distribution. Four states are defined: stable, periodic, transitional, and chaotic. The stable regime shows low entropy and strong density concentration near a fixed attractor region. The periodic regime shows low-to-moderate entropy but a compact closed density loop. The transitional regime is characterized by rising entropy, local spreading of density occupancy, and intermittent divergence growth. The chaotic regime is identified by high entropy, broad density occupation, and sustained divergence amplification. These criteria allow the onset of electrochemical chaos to be interpreted as a physically structured transition rather than as an abrupt or purely visual change in waveform appearance. The computational outputs of this classification are finally rendered in two non-panel figures: a two-dimensional entropy-guided regime heatmap and a state-space density image of the chaotic transport response.

3. RESULTS AND DISCUSSION

The simulations reveal a clear progression from ordered transport to disorder as the forcing parameter λ is increased. At low forcing, diffusion dominates the redistribution process and prevents localized perturbations from accumulating into persistent irregularity. In this regime, the current-density signal remains tightly constrained, the concentration field relaxes repeatedly toward a narrow operating band, and the reconstructed state occupancy is concentrated in a compact region of the embedding plane. The transport entropy remains low because the underlying oscillatory sequence retains strong ordinal regularity. Figure 1 is therefore best defined as a regime heatmap, where the horizontal axis represents the forcing parameter, the vertical axis represents reaction-coupling strength, and the color scale represents normalized transport entropy. In the low-forcing part of this figure, the entropy field stays in a cool, low-intensity zone, which marks a dynamically ordered electrochemical state.

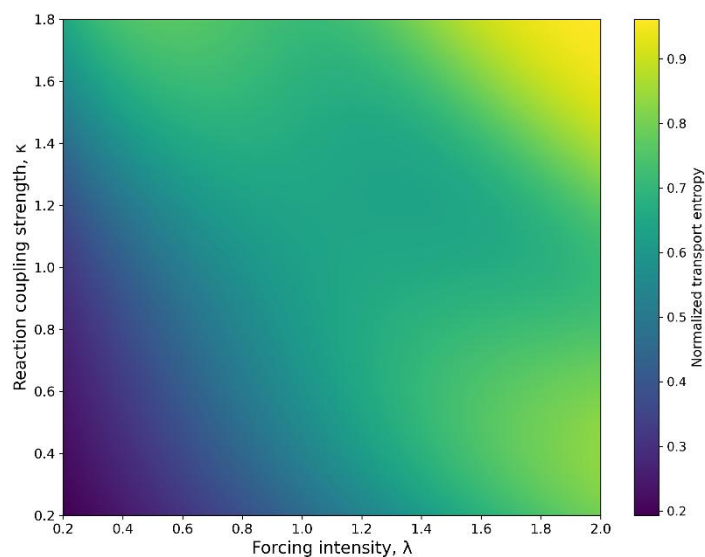


Fig. 1. Entropy-guided heatmap of stable, periodic, transitional, and chaotic regimes in electrochemical transport systems

A distinct transitional corridor appears once forcing and reaction feedback begin to compete with diffusive smoothing. In this interval, the system no longer preserves compact recurrence, but it has not yet reached fully developed chaos. The entropy field rises sharply over a finite parameter band rather than at a single isolated threshold, which indicates that the route to chaos in electrochemical transport is distributed across a measurable transition window. Physically, this corresponds to repeated local

amplification of ionic gradients near the reactive boundary, followed by incomplete transport relaxation before the next forcing cycle acts. The regime heatmap captures this process as a warm intermediate band separating the ordered and chaotic zones. This is an important result because it shows that entropy is not merely classifying already-chaotic behavior; instead, it is identifying the onset region where electrochemical coherence begins to degrade.

The fully chaotic state emerges at high forcing and strong nonlinear coupling, where the transport layer repeatedly amplifies local concentration imbalance faster than diffusion can smooth it. In this regime, the state trajectory no longer occupies a compact loop-like region. Instead, it spreads across a broad area of the embedding plane with dense and irregular occupation of multiple state zones. Figure 2 represents the chaotic regime through a density-based visualization rather than a line trajectory, where color intensity denotes the normalized visit frequency of the reconstructed electrochemical trajectory in state space. In the high-forcing regime, the figure shows a widely distributed occupancy field rather than a compact recurring structure, which indicates that the system no longer revisits a narrow set of electrochemical states. The transition from concentrated occupancy to distributed occupancy confirms that the entropy rise corresponds to a genuine increase in dynamical complexity rather than a simple amplification of oscillation amplitude. The divergence metric follows the same trend, which further supports the interpretation of chaos onset as a progressive sensitivity increase in the transport dynamics.

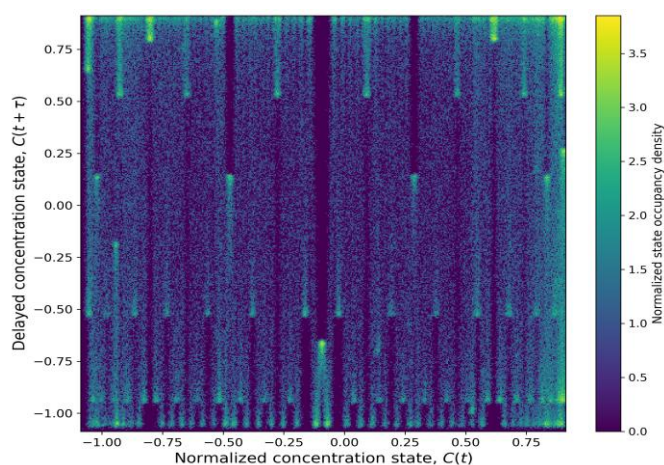


Fig. 2. Delay-embedded state-space density distribution reconstructed from the chaotic electrochemical transport response

From an electrochemical perspective, these findings are significant because they transform nonlinear instability from a descriptive observation into a measurable transport-state indicator. The entropy-guided regime map identifies operating zones where the system remains controllable, where it becomes transition-sensitive, and where it enters fully chaotic behavior. The delay-embedded state-space density image then provides a physical interpretation of why the high-entropy regime is unstable: the system no longer revisits a compact set of electrochemical states and instead evolves through a widely distributed response manifold. This has practical value for electrochemical devices in which irregular transport degrades efficiency, enhances nonuniform interfacial activity, or complicates impedance interpretation. The proposed framework therefore offers a computational foundation for future monitoring strategies in batteries, reactive membranes, corrosion systems, and transport-limited electrochemical interfaces.

4. CONCLUSION

This study developed a transport-centered entropy framework for detecting chaos transitions in electrochemical systems governed by coupled diffusion, migration, and nonlinear interfacial reaction kinetics. The results showed that the route to chaos is not abrupt, but passes through a finite transitional window in which entropy increases rapidly as the system loses temporal coherence. By linking entropy growth to the physical redistribution of transport states in reconstructed state space, the work established a direct connection between signal complexity and electrochemical dynamical structure. This interpretation is important because it allows chaotic electrochemical behavior to be identified through measurable transport signatures rather than through qualitative observation alone. The study therefore provides a stronger analytical basis for understanding how nonlinear electrochemical response evolves as forcing and reaction coupling intensify.

The main contribution of the article is the demonstration that entropy can function as a physically interpretable transition indicator rather than as a purely statistical post-processing quantity. The regime heatmap identifies the parameter regions in which electrochemical transport remains ordered, becomes transition-sensitive, and enters chaos, while the state-space density image reveals how the

underlying response manifold expands in the chaotic regime. This makes the proposed framework suitable for future extensions toward multidimensional electrochemical transport, thermal coupling, multi-ion systems, and experimentally informed diagnostic platforms. It also opens a path toward real-time instability screening in electrochemical devices where early detection of transition-sensitive operating zones is essential for control and reliability. In that sense, the framework is not only a computational analysis tool, but also a foundation for future entropy-assisted electrochemical monitoring architectures.

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