Dynamic Symmetry, Information Entropy, and Boundary Dissipation in Open Chemical Reaction Networks

Abstract: Dynamic symmetry theory proposes that adaptive systems persist not by minimising disorder or maximising rigidity, but by maintaining a workable relation between stabilising and exploratory tendencies. This note develops a concrete mathematical version of that claim for open chemical reaction networks. Using the standard nonequilibrium thermodynamics of chemostatted networks, it defines a Dynamic Symmetry Index directly in terms of two established quantities: Shannon information entropy over the internal state distribution and entropy production rate generated by boundary-maintained chemical affinities. A numerical illustration in a minimal open network shows the expected pattern: the dissipation-based order variable increases with driving, the information-theoretic diversity variable eventually declines, and the Dynamic Symmetry Index reaches an interior maximum at intermediate forcing.

1. Introduction

One of the central ambitions of dynamic symmetry theory is to move beyond a metaphorical account of the edge of chaos and to supply a mathematical language capable of comparing adaptive regimes across domains. The underlying intuition is simple: systems that persist and remain responsive appear to occupy a region between rigidity and dissolution. Yet this intuition becomes scientifically valuable only when it can be expressed within established formalisms rather than merely described alongside them.

Nowhere is this challenge sharper than in nonequilibrium thermodynamics. Open networks survive by exchanging matter and energy with their environments, and their organised behaviour is inseparable from the dissipation that those exchanges entail. The conceptual difficulty is that the relevant quantities do not collapse into a single variable. Thermodynamic entropy production tracks irreversibility and boundary-maintained throughput, while information-theoretic entropy tracks uncertainty or diversity over internal states. Neither can simply be substituted for the other.

This note argues that dynamic symmetry theory can nevertheless forge a bridge between them. The bridge is not a universal identity. It is a structured relation. In a standard open chemical reaction network, informational diversity and boundary dissipation can be treated as complementary variables and combined into a Dynamic Symmetry Index. The proposal is that regimes of high adaptive potential occur not where either variable is extreme, but where both are appreciable and neither dominates.

2. Thermodynamic setting

The nonequilibrium thermodynamics of open chemical reaction networks provides a rigorous framework for the analysis of driven, chemostatted systems. In this setting, selected species are held at fixed concentrations or chemical potentials by reservoirs, while the remaining internal species evolve according to mass-action kinetics or a chemical master equation. Because the reservoirs impose persistent constraints, the internal system may settle into a nonequilibrium steady state rather than relaxing to detailed balance.

A key insight of this framework is that entropy production is not an incidental by-product but a constitutive feature of open nonequilibrium organisation. In elementary reaction networks, the entropy production rate can be written as a sum of flux-affinity products. Reaction topology matters because broken conservation laws and emergent cycles determine the independent thermodynamic forces available to the system. Nonequilibrium free-energy functionals also acquire an information-theoretic interpretation, since relative entropy measures the distance between the actual state and an equilibrium reference state.

3. Minimal open network

Consider the elementary chemostatted network

$$A \rightleftharpoons X, X \rightleftharpoons Y, Y \rightleftharpoons B.$$

Species A and B are maintained at fixed concentrations by large reservoirs, while species X and Y are internal. The concentrations or chemical potentials of A and B are externally maintained, so the internal subsystem remains open and may sustain a nonequilibrium steady state whenever the chemical-potential difference

$$\Delta\mu = \mu_A - \mu_B$$

is nonzero.

At the deterministic level, mass-action kinetics defines forward and backward fluxes for each reaction. At steady state, a single net throughput J passes through the internal chain from A to B. At the stochastic mesoscopic level, the system is described by a chemical master equation over the copy numbers of X and Y, yielding a stationary distribution $p^*_{n_X,n_Y}$.

4. Information entropy and boundary dissipation

For the internal state distribution of the open network, define the stationary Shannon entropy

$$H^* = -\sum_{n_X, n_Y} p^*_{n_X, n_Y} \ln p^*_{n_X, n_Y}.$$

Define the normalised disorder variable

$$D = \frac{H^*}{H_{\max}},$$

where $H_{\max}$ is the maximal entropy over the sampled support. Next define the order-like thermodynamic variable using the entropy production rate,

$$O = \frac{\dot{S}_{\mathrm{tot}}}{\dot{S}_{\mathrm{tot}} + K},$$

with $K > 0$ a characteristic dissipation scale. In open nonequilibrium networks, sustained entropy production maintains organised currents and persistent chemical transformations. In that specific dynamic sense, it is reasonable to treat dissipation as an order-like quantity.

5. Dynamic Symmetry Index for open CRNs

A suitable open-network form of the Dynamic Symmetry Index is

$$\mathrm{DSI}_{\mathrm{CRN}} = 4OD(1 - |O - D|).$$

This index vanishes when either organised throughput or informational diversity vanishes, and it is suppressed when one component overwhelms the other. It is high only when both variables are substantial and approximately balanced.

6. Numerical methods

A finite-state birth-death version of the minimal open network was simulated on the triangular state space (n_X, n_Y) with $n_X + n_Y \leq N$, using $N = 30$, $[B] = 1$, and symmetric rate constants $k_1 = k_2 = k_3 = k_{-1} = k_{-2} = k_{-3} = 1$. The external driving was varied by changing $[A]$ over a geometric range from 1 to 40, corresponding to $\Delta\mu = \ln([A]/[B])$. For each value of $[A]$, the stationary distribution was obtained from the null space of the Markov generator, Shannon entropy was computed from that stationary distribution, and the entropy production rate was computed from the stationary bidirectional probability currents. The normalised variables D, O, and $\mathrm{DSI}_{\mathrm{CRN}}$ were then evaluated across the forcing range.

7. Results

Figure 1 (below) shows the numerical behaviour of the three key variables across the forcing range. The dissipation-based variable O rises monotonically with forcing, reflecting the steady increase in nonequilibrium throughput and entropy production as the chemical-potential difference grows. The information-based variable D remains high at low forcing and then declines at stronger driving as the stationary distribution becomes more concentrated on a narrower set of high-throughput states.

Most importantly, $\mathrm{DSI}_{\mathrm{CRN}}$ exhibits a clear interior maximum at intermediate forcing rather than at either extreme. In the present simulation, the maximum occurs at $\Delta\mu \approx 3.381$, where the simultaneous presence of substantial dissipation and substantial informational diversity yields the highest dynamic-symmetry score. This is the signature expected of a dynamically symmetric regime: it is absent near equilibrium, where dissipation is too weak, and it declines again at strong forcing, where diversity is eroded by canalisation.

8. Discussion

This construction does not collapse Shannon entropy, thermodynamic entropy production, relative entropy, and nonequilibrium free energy into one quantity. Instead, it reframes the problem by treating informational diversity and dissipation as complementary variables whose relation matters more than either variable alone. In that respect, dynamic symmetry theory does not replace open-network thermodynamics; it supplements it with a criterion for locating adaptive regimes.

The numerical illustration does not by itself prove a general theorem. It does, however, show that the proposed bridge can be made operational in a concrete open-network model. That is enough to move the theory beyond metaphor and toward a testable research programme.

9. Conclusion

By defining a Dynamic Symmetry Index for a minimal chemostatted reaction network in terms of Shannon entropy and entropy production rate, and by illustrating its behaviour numerically in a finite-state open network, this note proposes a concrete mathematical bridge between information entropy and boundary dissipation. The bridge is neither an identity nor a replacement for thermodynamics. It is a relation: a way of identifying intermediate nonequilibrium regimes in which internal diversity and organised dissipative throughput are jointly sustained.

Appendix A. Notation

Symbol	Meaning
A, B	Chemostatted boundary species
X, Y	Internal species
$\Delta\mu$	Chemical-potential difference between reservoirs
J	Net steady throughput through the internal chain
$\dot{S}_{\mathrm{tot}}$	Entropy production rate
$p^*_{n_X,n_Y}$	Stationary probability distribution
H^*	Stationary Shannon entropy
D	Normalised informational diversity
O	Normalised dissipation-based order variable
$\mathrm{DSI}_{\mathrm{CRN}}$	Dynamic Symmetry Index for open CRNs

Figure 1

The numerical figure provided with this note plots O, D, and $\mathrm{DSI}_{\mathrm{CRN}}$ against $\Delta\mu$. The key empirical signature is the interior peak of $\mathrm{DSI}_{\mathrm{CRN}}$ at intermediate forcing.