

Entropy Production in Synthetic MC

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Abstract—In this abstract, we investigate synthetic molecular communication (SMC) systems in terms of non-equilibrium thermodynamics. By analyzing entropy production for different molecule release dynamics, we demonstrate that the release process at the transmitter (TX) significantly influences the thermodynamics of the receiver (RX). This study serves as a foundation for developing a general thermodynamic framework for SMC systems, with future work focusing on the minimization of entropy production and noise characterization.

I. INTRODUCTION

SMC is a nature-inspired communication paradigm, where information is encoded into the properties of molecules. SMC facilitates communication in environments where conventional EM-based approaches cannot be applied. The envisioned applications of SMC range from medical applications, such as in-body communication and health monitoring, to agricultural applications such as smart pest control [1].

One major challenge is developing efficient and reliable SMC systems. For instance, the TX should release signaling molecules as efficiently as possible, and the RX should optimize their detection. Moreover, since many SMC systems operate in sensitive environments (e.g., inside the body), they must neither interfere with nor be disrupted by surrounding processes. Current optimization approaches are largely scenario-specific, and a general framework is still lacking.

An important yet largely unexplored approach in the molecular communication (MC) community for developing a general, system-independent framework to characterize and optimize SMC systems is the use of non-equilibrium thermodynamics. This discipline provides a foundation for analyzing systems that continuously exchange matter, energy, and information with their surroundings. For instance, [2], [3] introduced fundamental equations for non-equilibrium thermodynamic processes and the concept of minimal energy dissipation. [4] explored entropy production, suggesting that a system in a steady state should minimize its entropy generation. [5] extended these concepts to entropy production in heat transfer and fluid flow. To date, only [6] has examined the thermodynamic energy costs of MC systems.

This abstract introduces entropy production and minimization as a framework for characterizing and optimizing SMC systems. Lowering entropy production can enhance energy and resource efficiency, reducing heat dissipation and improving information transmission. Additionally, minimizing entropy could support the mitigation of noise and interference at the RX. We first outline a general SMC framework based on entropy production, followed by a simple example investigating how the molecule release influences the entropy production at the RX. Finally, we discuss the potential of entropy production minimization for the optimization of SMC systems.

II. GENERAL FRAMEWORK

In order to analyze an SMC system, as shown in Fig. 1, in terms of non-equilibrium thermodynamics, a general description has to be based on the constant exchange of matter caused, e.g., by the release, propagation or reaction of molecules.

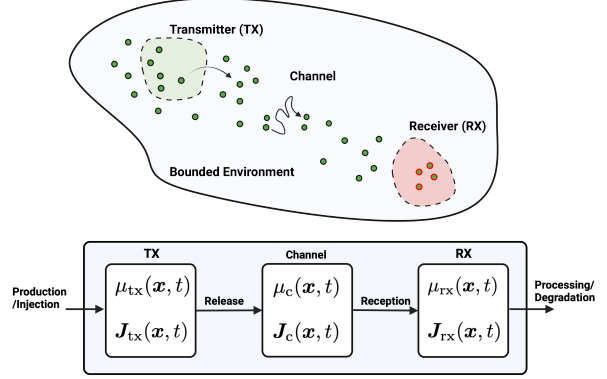


Fig. 1. Top: General structure of an SMC system consisting of a TX, channel and RX. Bottom: Schematic representation of an SMC system in terms of fluxes and chemical potentials.

Therefore, we describe the dynamics of each block of an SMC system (see the block diagram in Fig. 1) in terms of a flux $\mathbf{J}_\chi(\mathbf{x}, t)$ in $\text{mol m}^{-2} \text{s}^{-1}$, where $\chi \in \{\text{tx}, \text{c}, \text{rx}\}$ and $\mathbf{x} \in \mathbb{R}^3$ is a space coordinate. By the flux $\mathbf{J}_\chi(\mathbf{x}, t)$, we can describe the production, reaction, propagation of signaling molecules, in TX, channel and RX, and their exchange between these blocks representing release and reception.

Chemical Potentials: According to [2], every flux $\mathbf{J}_\chi(\mathbf{x}, t)$ is driven by a chemical potential gradient as follows

$$\mathbf{J}_\chi(\mathbf{x}, t) = -L_\chi \nabla \mu_\chi(\mathbf{x}, t), \quad (1)$$

where ∇ is the gradient operator, and L_χ is a phenomenological transport coefficient in $\text{mol J}^{-1} \text{s}^{-1} \text{m}^{-1}$ which is related, e.g., to a diffusion coefficient or a permeability. The chemical potential μ_χ in (1) describes how the free energy of the system changes when molecules flow through a point \mathbf{x} under constant thermodynamic conditions. Therefore, μ_χ can be defined as the partial derivative of the Gibbs free energy G with respect to the number of molecules N , keeping temperature T , pressure P , and other relevant variables constant. Similarly, it can be expressed in terms of the concentration c_χ of molecules at \mathbf{x}

$$\mu_\chi(\mathbf{x}, t) = \left(\frac{\partial G(\mathbf{x}, t)}{\partial N} \right)_{T, P} = \mu_{\chi, 0} + RT \ln c_\chi(\mathbf{x}, t), \quad (2)$$

where $\mu_{\chi, 0}$ (J mol^{-1}) is an initial potential, R is the gas constant ($\text{J mol}^{-1} \text{K}^{-1}$) and T is the temperature (K).

Entropy Production: Based on the description in terms of fluxes and chemical potentials, the entropy production rate σ in $\text{J K}^{-1} \text{s}^{-1}$ in each block χ of an SMC system is defined as follows [2]

$$\sigma_\chi(t) = \frac{1}{T} \int_{V_\chi} \mathbf{J}_\chi(\mathbf{x}, t) \cdot (-\nabla \mu_\chi(\mathbf{x}, t)) d\mathbf{x}. \quad (3)$$

The entropy production rate (3) describes how thermodynamic entropy increases due to irreversible processes such as diffusion, reaction, or transport across membranes. Therefore,

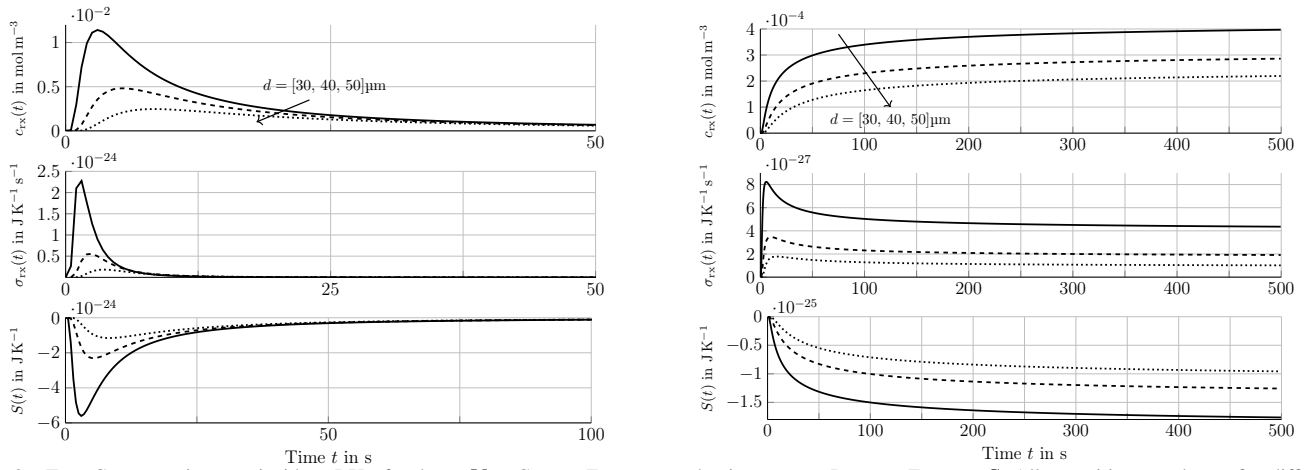


Fig. 2. Top: Concentration c_{rx} inside a RX of volume V_{rx} . Center: Entropy production rate σ . Bottom: Entropy S . All quantities are shown for different distances d between TX and RX and for an instantaneous (left column) and a constant release of molecules (right column).

minimizing the entropy production can help to reduce the energy, wasted by the TX.

Entropy: The change of entropy S (J K^{-1}) can be derived either from the production rate (3) or directly via

$$S_{\chi}(t) = -k_b \int_{V_{\chi}} c_{\chi}(\mathbf{x}, t) \ln \frac{c_{\chi}(\mathbf{x}, t)}{C_0} d\mathbf{x}, \quad (4)$$

where c_{χ} is the concentration in block χ , k_b is the Boltzman constant, and C_0 is a scaling factor typically chosen as the equilibrium concentration. In SMC systems, the entropy can be interpreted as a measure of how dispersed the energy in the form of molecules is in the system. Therefore, the largest entropy in a system is achieved when all molecules are uniformly distributed and the system is in equilibrium.

III. EXAMPLE

In the following, we investigate the entropy production in SMC systems. To that end, we consider a simple example SMC system with a point TX located at $\mathbf{x} = [0, 0, 0]$ and a transparent RX with volume V_{rx} in distance d , in an unbounded diffusive environment with diffusion coefficient D . We compare an instantaneous release of $N = 1000$ molecules at $t = 0$, and a constant release with release rate $q = N/t_{sim}$ ($t_{sim} = 500\text{s}$). The default parameters are $D = 5 \cdot 10^{-11} \text{m}^2 \text{s}^{-1}$, $V_{rx} = 4/3\pi r_{rx}^3$, $r_{rx} = 1\mu\text{m}$. Figure 2 shows the concentration c_{rx} in the receiver (top plots), entropy production rate σ_{rx} according to (3) (center plots), and entropy S_{rx} according to (4) (bottom plots), for an instantaneous release (left) and a constant release of molecules (right).

Instantaneous Release: As expected, the received signal c_{rx} peaks when molecules enter the RX, with amplitude and spread varying depending on distance d . Inspecting σ_{rx} , we observe that entropy production also peaks upon molecular arrival at the RX. However, since σ_{rx} is related to the chemical potential gradient, it decays to zero once all molecules have left the RX volume. With increasing distance, σ_{rx} decreases as molecules spread out and fewer reach the RX. A similar trend is seen for the entropy S_{rx} in the RX, where a negative peak occurs upon molecular arrival. While global entropy is always ≥ 0 and non-decreasing (due to diffusion), the entropy in the RX exhibits a transient negative peak. This is due to the large $\nabla\mu_{rx}$ when molecules arrive, while $S_{rx} \rightarrow 0$ for $t \rightarrow \infty$ as the system returns to equilibrium.

Constant Release: For the constant release, we observe that c_{rx} increases as molecules arrive at the RX and eventually stabilizes at a constant value. Inspecting σ_{rx} , we see that entropy production peaks when molecules enter the RX volume. Unlike the instantaneous release, σ_{rx} does not return to zero but instead remains negative over the entire simulation time. This is due to the continuous exchange of matter in the RX, while J_{rx} and $\nabla\mu_{rx}$ remain constant. A similar trend is observed for the entropy S_{rx} , which decreases but also stabilizes. From a thermodynamic perspective, the system attains a new quasi-equilibrium state due to the constant molecular release.

IV. DISCUSSION

In this abstract, we introduced a preliminary description of SMC systems through the lens of non-equilibrium thermodynamics and demonstrated that communication in SMC systems can be characterized by chemical potentials and entropy. By comparing two extreme molecule release scenarios (instantaneous vs. constant release), we observed that the release dynamics significantly impact entropy production at the RX. Thus, to minimize entropy production at the RX, the release process at the TX must be carefully designed.

This study serves as an initial investigation to establish a general framework for representing SMC systems within non-equilibrium thermodynamics, bridging the gap to methodologies commonly used in chemical engineering. Nonetheless, this approach holds great potential for analyzing and optimizing SMC systems. Moving forward, we will explore strategies to minimize entropy production by optimized release patterns at the TX and careful RX design. Additionally, we will examine noise in SMC systems and its role in entropy production.

REFERENCES

- [1] T. Nakano, A. W. Eckford, and T. Haraguchi, *Molecular Communication*, 2nd ed. Cambridge University Press, 2024.
- [2] L. Onsager, "Reciprocal relations in irreversible processes I," *Phys. Rev.*, vol. 38, no. 12, 1931.
- [3] —, "Reciprocal relations in irreversible processes II," *Phys. Rev.*, vol. 38, no. 12, 1931.
- [4] I. Prigogine, *Introduction to Thermodynamics of Irreversible Processes*, 1962.
- [5] A. Bejan and J. Kestin, *Entropy Generation through Heat and Fluid Flow*, 1983.
- [6] A. W. Eckford, B. Kuznets-Speck, M. Hinczewski, and P. J. Thomas, "Thermodynamic properties of molecular communication," in *IEEE Int. Symp. Inf. Theory*, 2018, pp. 2545–2549.