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Calculation of entropy balance equations in a nested system

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A viewpoint of non-equilibrium thermodynamics is useful for the investigation of environmental phenomena such as climate changes and the oceanic circulation [1,2]. Especially, the entropy production is a useful quantity because it works as a potential function for the system of our concern under certain conditions [1,2]. It is defined as the time derivative of entropy produced inside the system. We have been investigating the change in entropy production and the flow of entropy in a nested reaction-diffusion system in order to seek for a universal rule for the time evolution of non-equilibrium dynamic systems.

We firstly examined the relation between the entropy production and the pattern dynamics in a simple reaction-diffusion system [3-5], and revealed that the entropy production can be used as an index of self-organized patterns. Then, by introducing a newly defined chemical potential, we showed the way to calculate the entropy flow [5]. The entropy flow is the time derivative of the entropy that is produced through the interaction between the system and its environment. Concomitantly, the sum of the entropy production and the entropy flow can be calculated as well. This sum is called the entropy change.

We applied this method to calculate these thermodynamic quantities when a reaction-diffusion system sustained self-replicating pulses. The result indicated that the entropy change depends on the dynamics of the system. The entropy change converges to zero when the pattern in the system looks quiescent (i.e., a quasi steady state is achieved), whereas it moves away from zero while the pulse self-replicates. Consequently, the entropy change varies proportional to the speed of the pattern development. Therefore it might be regarded as the thermodynamic distance from a steady state. This property is coincident with an intrinsic property of entropy as a state function of a system.

Next, we considered a nested open system. Dealing with a nested system is important for better understanding of nature, even through mathematical models, because of the following reason. We used to introduce a steady assumption for the environment of a mathematical model. However, this is a rough approximation of nature. In an environmental system or in a biological system, for example, both the system of our concern and its environment have their own dynamics and interact each other through the open boundary of the system. Sometimes biological systems seem to make their profits of such interactions, and this could be expected similarly in a dynamical geo-system.

Our nested system consists of two subsystems: a bath and a one-dimensional reaction-diffusion medium. The bath is a continuously-stirred tank reactor which is connected with its environment. We assume that only one of chemical species (the substrate) flows into the bath from its environment, and all chemical species can flow out from the bath to the environment. The one-dimensional medium is immersed in the bath and all the chemical species in the bath can diffuse in and out from the medium across its surface. In the presentation, we will show that mutual interactions between the medium and the bath causes in the medium a new quasi-stable state that cannot be realized when the dynamics of the bath is stable. We will also refer to the relation among the dynamics and thermodynamic quantities and revisit the meaning of the 2nd thermodynamic law.

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