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NOTE

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A note concerning some aspects for application of a thermodynamic extremal principle (TEP) for continua

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Abstract A matter of fact is that extremal principles have been introduced in mechanics in more (Euler, Lagrange) or less (Hamilton) than 200 years ago. One may also observe an impact of thermodynamic extremal principles based on maximum dissipation due to all the entropy production expressed in several disciplines. According fields are theory of communication, statistical mechanics and later physics of earth since already 70 years. The current paper offers some (historical) overview on several applications. "Ziegler's principle" is an implementation of the maximum entropy production going out to the dissipation and yielding a maximum dissipation. The goal of this paper is now the implementation of this extremal principle performed along an algebraic concept. Such a concept can be extended to a system with several internal variables as outlined by Coleman and Gurtin in context with the Gibbs (free) energy.

1 Some (historical) aspects concerning the TEP

The question on the maximum of entropy production (and consequently a maximum dissipation) has its origin in the mathematical theory of communication. With respect to particular dissipations ρ_i, $\Sigma\rho_i = 1$, the "Shannonian information theory" was created, for more details, see the seminal study by Shannon [1], 1948. Based on the work of Shannon, approximately 10 years later Jaynes extended the "Shannon concept" to statistical mechanics [2] as "Shannon–Jaynes concept". Some years after the establishment of this concept, Ziegler published groundbreaking papers [3, 4] and later [5] concerning extremum principles in irreversible thermodynamics of continuum mechanics, denoted often as "Ziegler's maximum dissipation concept" or in other words Ziegler's TEP. As example shall be mentioned the maximum plastic dissipation by Mandel in 1964, for details see Lubliner [6]. Obviously, the principle of maximum entropy production rate is still applied in several fields, e.g., recently for understanding the models for mixture of multiple incompressible phases, see [7].

The work on the "Shannon concept" was further continued, see, e.g., the two books [9] and [10], and in particular as the research by Dyke and Kleidon [8] concerning the Earth System. One of the first works dealing with both concepts, i.e., the "Shannon–Jaynes concept" and Ziegler's TEP, was published by O'Brian and Stephens [11] concerning the entropy production in the context of the earth climate. Here, it shall be mentioned that their conclusions indicate a significant agreement between both concepts, and Dewar [12] also came to the same result.

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As for the progress in research regarding the extremal dissipation principles, the study of Polettini [13] considered Ziegler's TEP in detail. Polettini demonstrated with a rather simple (algebraic) matrix framework the existence of Ziegler's TEP, denoting the entropy production or sometimes called a power output, as σ. This paper demonstrates that a pure algebraic framework can be established, which provides extremal solutions for thermodynamic forces and corresponding fluxes.

Before outlining the "maximum procedure" in detail, we would like to remark that Polettini also dealt with minimum entropy production [14] by applying the framework of Jaynes. It shall also be mentioned that, in contrary, Prigogine delivered a minimum dissipation concept. Here, we refer to a recent study by Svoboda et al. [15] which explained Prigogine's minimum dissipation concept as applicable to a steady state. As further example, a minimization in context with an energetic system characterized by a loading parameter λ, shall be mentioned as shown by Petryk [16]. An increment $\triangle$ λ of the loading parameter λ provokes a minimum energy increment to obtain a configuration with the loading parameter λ+ $\triangle$ λ.

2 Algebraic description of the maximum of dissipation

Let us follow the standard problem occurring in material science. The basic quantities are introduced as follows, see, e.g., Coleman and Gurtin [17]. Based on n internal variables x_i, $i = 1, \ldots n$ in the Gibbs (free) energy G, the according thermodynamic fluxes $\dot{x}_i$ are denoted as J_i and forces $-\partial G \big/ \partial x_i$ as F_i. Both quantities are arranged in vectors J (fluxes) and F (forces). For the sake of simplicity, we assume a system at constant temperature T and pressure p. Such a formulation of a dissipative system is the most convenient one for demonstration of the algebraic description. The entropy production σ follows as the product, using the Einstein summation convention, for the two vectors **J, F**.

$$\sigma = \mathrm{J} \cdot \mathbf{F} = \mathrm{J}_i \cdot \mathrm{F}_i \equiv \sigma_{\mathrm{J,F}}. \tag{1}$$

In the frame of linear non-equilibrium thermodynamics, we assume a linear relation between fluxes and forces with a positive definite matrix **R** (see, e.g., Onsager [18]) as $\mathbf{F} = \mathbf{R} \cdot \mathbf{J}$, $\mathbf{J} = \mathbf{R}^{-1} \cdot \mathbf{F}$. After insertion for **F** in Eq. (1), the entropy production must be positive for arbitrary fluxes. Therefore, the dissipation must be a positive quadratic form as

$$\sigma_{\mathrm{J,J}} = \mathbf{J} \cdot (\mathbf{R} \cdot \mathbf{J}) = \mathrm{J}_i \left(\mathrm{R}_{ij} \mathrm{J}_j\right). \tag{2}$$

For details, see several studies concerning this topic in [3–5] and later [6]. Furthermore, the according topic of "dissipation potentials" is dealt with in [4]. Also, Polettini [13] introduced such a relation (2) by referring to "linear regimes". Moreover, we can introduce the dissipation in the form

$$\sigma_{F,F} = \mathbf{F} \cdot \left(\mathbf{R}^{-1} \cdot \mathbf{F}\right). \tag{3}$$

Now, one has to check if $\sigma_{F,F}$ obtains a maximum. Polettini [13] suggested to add now a "small perturbation" matrix **A** to **R** and analyze $\sigma_{F,F}$ with **R**+A. The skew-symmetric perturbation matrix A has the elements $A_{ii} \equiv 0$ and $A_{ij} = -A$, $A_{ji} = A$. The force F is kept as fixed. The matrix **R** is replaced by **R** + A, which allows calculating

$$\sigma_{F,F} = \mathbf{F} \cdot \left((\mathbf{R} + \mathbf{A})^{-1} \cdot \mathbf{F}\right) \tag{4}$$

Let us demonstrate this situation for two components (i, j are 1, 2). It follows after some algebra that $\sigma_{F,F}$ obtains the parameter **A** yielding.

$$\sigma_{F,F} = \frac{F_2^2 R_{11} - 2F_1 F_2 R_{12} + F_1^2 R_{22}}{A^2 - R_{12}^2 + R_{11} R_{22}}. \tag{5}$$

It shows that $\sigma_{F,F}$ obtains a maximum for $A = 0$, because both numerator and denominator are positive and the positive value of A^2 increases the value of the denominator. This means that the maximum of $\sigma_{F,F}$ implies the symmetry of **R** and thus also the symmetry of $\mathbf{R}^{-1} \equiv \mathbf{L}$. This represents the well-known Onsager's relations $L_{ik} = L_{ki}$, see, e.g., [18, 19]. It should also be noted that the matrix **A** does not influence $\sigma_{J,J}$ because $\mathbf{J} \cdot (\mathbf{A} \cdot \mathbf{J}) = 0$.

For a multicomponent system, the analogous maximum analysis has been performed by Polettini [13] for a small perturbation matrix **A**.

This fact justifies stability of Ziegler's principle approach with respect to perturbation (concerning the current configuration). The remarkable advantage of this algebraic procedure in relation to the analytical procedure (i.e., finding the extremum of $\sigma_{F,\,F}$ via the "classical concept" engaging the first and second derivatives) seems to be more efficient, in particular for multicomponent systems.

Finally, it shall be mentioned that an eigenstrain provoking dissipation, e.g., classical rate-independent plasticity, for details see [20] and [21, 22], can also be handled in this concept.

3 Conclusion

Ziegler's principle has been applied successfully for problems dealing with stress–strain interactions and with reaction processes together with diffusion processes. The demands on "multi-processes" are still increasing, e.g., the recent "reaction–diffusion systems", see, e.g., the pioneering study [23] and two recent studies, [24, 25].

Several extremal principles for describing the evolution of mechanical, physical and chemical processes have been developed throughout the last eight decades and are shortly discussed. As one of the most effective principles, Ziegler's principle as a maximum entropy concept has been emphasized due to its introduction in irreversible thermodynamics in continuum mechanics. Comparisons with several concepts from different areas of application are discussed. Furthermore, a rather basic algebraic concept is outlined, which reveals the link of maximum of the entropy production to Onsager´s relations.

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Declarations

Conflict of interest The authors have no relevant financial or non-financial interests to disclose.

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