FINAL REPORT
The development of mathematical and experimental methods in non-equilibrium thermodynamics

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1 Introduction

Our research consists of two main branches. The first one is about the experimental analysis of heat conduction in heterogeneous materials. The second one is the theoretical investigation of the thermodynamic background of constitutive equations, focusing on the physical and mathematical aspects. Thus in the following, we are separately discussing them in detail.

2 Experimental results

Previously, we reported about the following results related to our room temperature experiments.

- We managed to design and produce multiple 3D printed samples.
- We measured seven types of rock samples, each having at least three different thicknesses.

We performed measurements on each rock and steel samples, repeated several times. We observed the size dependence of thermal diffusivity, and in some cases, we also found the non-Fourier phenomenon with its size dependence, too. Regarding the 3D printed steel samples, the measured data is unfortunately proved to be too noisy, which makes it difficult to evaluate. We developed and tested several ideas to eliminate that high uncerainty from the data, but with no success. Therefore, merely the results related to the rock samples are published so far in this respect in the EUROCK Proceedings.

The pandemic situation had a serious impact on that part of the research. Due to closure of the university, we also had to close our laboratory and no measurements had been conducted until September 2020. At that time, we had only two months to achieve a progression. During this two months period, we built in a new temperature measurement point on the front surface in order to improve the evaluation procedure, but here, the thermal radiation from the flash lamp made it difficult to use this data.

All these difficulties together made us to change our research plan. First, during the quarantine period, we found a new analytical solution for the generalized heat equation, called Guyer-Krumhansl equation, used for the evaluations. It results in a more handy, simpler expression than the one found in 2018 [A]. Second, we managed to develop a new, automatic evaluation procedure based on this analytical solution, and we re-evaluated all the existing measured data with this procedure. It confirmed the size-dependence of the thermal parameters and non-Fourier behavior, and fine tuned the parameters. This is the reason why we did not continue immediately with an impact factor journal paper after having the experimental results. At this moment, we are preparing two papers for international journals.

1. This first paper is on the analytical solution and its utilization on the experimental data. The main result is that we found closed form relations between the data and the thermal parameters.
2. Exploiting the previously mentioned results, we reformulate the evaluation of the existing data, showing the size-dependence of the thermal diffusivity and the non-Fourier behavior.

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Both papers are planned to be submitted until January 2021.

In our previous report, we mentioned the collaboration with Federico Vázquez and Péter Ván in which we found the size-scaling effects to be important in nano-sized layered objects. One paper is published regarding this research. Also, in parallel, we continued this collaboration and we developed the idea of spectral thermal diffusivity, based on specific dispersion relations, and it would be helpful to characterize the heterogeneous materials. A manuscript is currently under preparation, and planned to submitted in February 2021.

Regarding the rarefied gas experiments, one paper was published in 2019, and we have one manuscript under review in International Journal of Engineering Science. In that one, we managed to find and evaluate an experiment, which shows the change in speed of sound between the pressures of 2 to 100000 Pa, using the internal variable theory. Also, we compared that model to another one from Extended Irreversible Thermodynamics [B].

3 Theoretical results

We reported previously the results on the compatibility conditions between non-equilibrium thermodynamics and the approach of GENERIC. This investigation indeed revealed several physical and mathematical aspects, especially about the dissipation potentials, internal variables, hiearchy of tensorial variables and current multipliers. This research is conducted in collaboration with Michal Pavelka. However, due to the pandemic, we had to modify our plan and this research has been delayed but the manuscript is planned to be submitted about February 2021.

We managed to achieve advancements on the solution methods. First, as it is mentioned in regard the experimental results, we developed the Galerkin approximation for generalized heat equations and rheological models, which serves as an efficient numerical method and also offers a simpler analytical solution. On the other hand, we continued our research on simplectic integration and two papers are published. These together cover a 1, 2 and a 3D numerical algorithm for modeling elastic and rheological wave propagation. The comparison with a finite element method provided by a commercial software (COMSOL), it turned out that our algorithm is significantly faster and more accurate, especially in the sense of respecting the physical expectations (e.g., conservation of energy during the time stepping).

In 2015, we started to investigate low-temperature heat conduction problems, especially the ballistic heat conduction [B], appearing in extremely pure crystals around 10-20 K. In [C], in collaboration with Péter Ván, the so-called ballistic-conductive equation was derived. In the present project, we achieved two results in this respect.

1. We found an analytical solution for this system of partial differential equations, which allowed a deeper insight into the definition of boundary conditions, and their time evolutions.

2. In collaboration with Patrizia Rogolino, we developed a thermo-mechanical model, consisting a coupling between the non-Fourier part and the thermal expansion. It revealed that the simplest extension of the Fourier equation is enough, but should be coupled to the Duhamel-Neumann-type thermo-mechanical model. This is tested on the experimental data available from the literature.

The manuscript presenting these results is currently under review, and available here [D]. For the sake of completeness, we mention again briefly the results presented in our previous report:

- In collaboration with Patrizia Rogolino, we analyzed the thermodynamic background of nonlinear non-Fourier models such as the Maxwell-Cattaneo-Vernotte equation. We also developed a numerical scheme for such equations. We proved that in a particular nonlinearity (e.g., considering the temperature dependence of material parameters), a nonlinear stability analysis is not necessary and can be substituted with the linear one, with some apriori assumptions about the temperature field.

- With Péter Ván, we have shown that the second law of thermodynamics can reproduce the Euler-Lagrange equations, and can be a good alternative to derive evolution equations. We developed some examples, e.g., mass point mechanics, phase fields, and gravitational fields.

- Thirdly, in collaboration with Srboljub Simic and Damir Madjarevic, we made an in-depth comparison between different thermodynamic approaches regarding rarefied gas models. We derived the compatibility relations that connect these models.

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- There are advancements in the analytical solutions for rheological models as well. We are currently reformulating an earlier work [E] with extending the analysis with finite element validation and fine tuning the discussion in the light of our recent findings about the 2 and 3D numerical solutions.

All these have been published in 3 journals. Moreover, together with Srboljub Simic, we published a review paper about the open mathematical questions in non-equilibrium thermodynamics.

4 The consequences of pandemic

It has been almost a year since we had to adapt to the current situations and to re-schedule our research plan. It has a serious impact on the experimental work what we conduct in our research. Since it was not possible to attend on conferences and all the other visiting programs were deleted, we decided to re-allocate the financial resources.

As an outcome, beyond our original plans, we managed to significantly improve the IT background of the research group. Besides, we started to prepare for the improvement of the flash device. Our new project (NKFIH FK 134277), started on 01. December 2020, is partially devoted to that task, and some of our resources has been spent in a way to improve the temperature measurement, change the sample holder, and we want to have a new flash lamp as well. Hopefully, it will allow us to obtain a uniquely detailed set of experimental data about the thermal behavior of heterogeneous materials, and being capable to conduct measurements on various 3D printed samples and fluids, too, extending our research in the direction of nanofluids and biological materials.

5 Personal changes

During the project, only a minor change happened: an MSc student, Anna Fehér has joined to the project. Her work was especially helpful in the experimental research, sample preparation and improving the evaluation methods. She is devoted to this research and plans to be a Ph.D. student in 2021.

6 Fulfillment of the workplan

Besides the pandemic situation, we managed to follow our workplan as much as it was possible. According to our original research schedule, we planned to publish 6 journal papers, 1 review paper, 8 presentations on international conferences and 2 on national conferences. In this respect, we achieved our goals. Here, you can find the complete list of the presentations and posters. Unfortunately, there is no conference participation in the second year of the project.

- R. Kovács: Generalizing constitutive laws: the role of non-equilibrium thermodynamics. GAMM2019, Berlin.
- R. Kovács, T. Fülöp, M. Szücs, P. Ván: A numerical solution method for noise calculations. Vacuum Fluctuations *at Nanoscale and Gravitation: theory and experiments, Sardegna, 2019.*
- R. Kovács, P. Ván, S. Simic, D. Madjarevic: Non-equilibrium thermodynamics of ballistic propagation, 80th Jubilee of Miroslav Grmela, Prague, 2019.
- R. Kovács, P. Ván, S. Simic, D. Madjarevic: Non-equilibrium thermodynamics of rarefied gases, JETC2019, Barcelona.
- R. Kovács, P. Ván, S. Simic, D. Madjarevic: Challenges in modeling rarefied gases, HEEP2019, Mátrafüred.
- Kovács R.: Ballisztikus transzport: elméleti és kísérleti eredmények. ELFT Vándorgyűlés, Sopron, 2019.
- Kovács R., Fülöp T., Szücs M.: Szimplektikus módszerek alkalmazása numerikus feladatokban. Magyar Mechanikai Konferencia, Miskolc, 2019.
- F. Vázquez, *P. Ván, R. Kovács: Heat transport regimes in superlattices, JETC2019, Barcelona.*
- Á. Rieth, R. Kovács: On the numerical solutions of generalized heat equations, JETC2019, Barcelona. Poster presentation.

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- T. Fodor, D. Hermann, R. Kovács: Non-Fourier heat conduction: numerical and experimental study, JETC2019, Barcelona. Poster presentation.
- Á. Rieth, R. Kovács: *Numerical methods for heat conduction, HEEP2019, Mátrafüred.*
- R. Kovács, Á. Rieth, T. Fülöp, M. Szücs: Numerical method for generalized constitutive laws, ICCHMT, Róma, 2019.
- Szücs M., Fülöp T.: A GENERIC nemegyensúlyi termodinamikai keretrendszer, avagy a Hamilton-féle kanonikus egyenletek disszipatív általánosítása, Magyar Mechanikai Konferencia, Miskolc, 2019.
- T. Fülöp, *M. Szücs, R. Kovács: Time dependence in thermodynamics – theory and engineering applications,* HEEP2019, Mátrafüred. Poster presentation.
- M. Szücs, T. Fülöp: Irreversible thermodynamics in the GENERIC (General Equation for the Non-equilibrium Reversible Irreversible Coupling) framework, HEEP2019, Mátrafüred.
- T. Fülöp, M. Szücs: Temporal Thermodynamics I. Theory. JETC2019, Barcelona.
- T. Fülöp, M. Szücs: Temporal Thermodynamics II. Applications. JETC2019, Barcelona.

7 References

[A] R. Kovács: Analytic solution of Guyer-Krumhansl equation for laser flash experiments. International Journal of Heat and Mass Transfer (127), 631-636, 2018.

[B] R. Kovács, P. Rogolino, D. Jou: When theories and experiments meet: rarefied gases as a benchmark of non-equilibrium thermodynamic models. Under review. arXiv: 1912.02158

[C] R. Kovács, P. Ván: Generalized heat conduction in heat pulse experiments International Journal of Heat and Mass Transfer (83), 613-620, 2015.

[D] G. Balassa, P. Rogolino, Á. Rieth, R. Kovács: Analytical and numerical modelling of ballistic heat conduction observed in heat pulse experiments. Under review. arXiv: 2004.06659

[E] Fülöp Tamás; Szücs Mátyás: Analytical solution method for rheological problems of solids. Under preparation. arXiv: 1810.06350

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