FINAL REPORT
Coupled problems in nonequilibrium thermodynamics

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1 Introduction

Our research consists of two primary branches. The first one is about investigating open questions in experimental heat conduction, particularly related to heterogeneous materials. The second one, the theoretical investigation, is based on both thermodynamic analysis and improving solution methods, focusing on the physical and mathematical aspects. Thus, in the following, we are separately discussing them in detail.

2 The consequences of pandemic

The pandemic affected only the first year of the project due to the strongly limited possibilities about conference participation and the experiments conducted at the university. The research work was optimized accordingly, and therefore the PI reports no further disadvantage.

3 Experimental results

During the project, several collaborations are formed:

- Dr. Attila Géczy (BME): the focus is placed on biologically degradable printed circuit boards. Due to the innovative material composition, investigating the thermal behavior was inevitable.
- Dr. Krisztina László (BME): her research group provided several metal-organic frameworks, particularly designed for gas storage, thus these materials are highly porous.
- We have also started a collaboration with the ALICE group of CERN in which work we thermally characterized highly porous carbon foams, serving as a structural basis for the new generation ITS3 detector. Our contact person is Dr. Gergely Barnaföldi (HUN-REN Wigner RCP).
- Prof. Imre Orbulov (BME) and his PhD student, János Maróti: our focus is on the thermal behavior of composite metal foams (including particle reinforcement too). This collaboration is extended with involving the Germany-based company NETZSCH Gmbh. NETZSCH has invited our research group and we developed a consistent experimental plan related to metal foams, consisting of several static and dynamic mechanical and thermal analysis. The PI also managed to involve the research group of Prof. Éva Lublóy, and her expertise in CT scanning.
- Additionally, micro-capsuled phase changing materials are also investigated in collaboration with Dr. Tivadar Feczkó (HUN-REN TTK), applied for highly heat resistant building insulation.

All these collaboration present the wide applicability of the developed thermodynamic theory for heat conduction of heterogeneous materials. We managed to publish WoS papers almost in all these topics. Interestingly, many of these materials showed a transient thermal behavior beyond Fourier, thus in proper material characterization, it was crucial to apply an alternative heat conduction model.

In regard to these alternative heat conduction equations, the PI and his PhD student, Anna Fehér, came to the conclusion that the two-temperature model is not applicable to determine the thermal transport parameters since the resulting parameter set is not unique. Furthermore, we found that there are only two viable alternatives to model heterogeneous materials, the so-called Guyer–Krumhansl (GK) and Jeffreys heat equations. We also found that we can distinguish between static and dynamic thermal conductivity (Jeffreys) and thermal diffusivity (GK), depending on the model. These models can provide an equivalent temperature history, both have a consistent thermodynamic background, thus both can be a practically useful alternative in describing multicomponent heat conducting systems. With Anna Fehér, numerous advancements are achieved which all will be included in her PhD thesis.

The PI wishes to highlight that a new flash equipment is designed and built during the project period. This task is primarily based on the work of Dr. Krisztián Sztankó who is involved in the project from 2023. That new test bench consists of a chamber with controllable temperature in the range of -20 °C to 120 °C. It required the thorough thermal analysis of the chamber, insulation and the design of Peltier cooling system. Furthermore, we already have a programmable xenon lamp with which we can test the sensitivity for the boundary conditions, utilize a frequency sweep, and due to the controllable temperature, we also will be able to investigate material nonlinearities. The test phase is expected during the spring of 2025.

The role of material nonlinearities has been became more and more important in our research. In this regard, we are focusing on the behavior of supercritical fluids and phase changing processes. We have initiated the preparation of a heat transfer test equipment for supercritical CO2, but most of our current investigation remained on a theoretical level, see later. However, in regard to the phase changing processes, a test bench is designed and built in order to study the transient behavior of the phase changing, the Bénard cells, serving as a basis for simulations, and the utilized setting is also useful to study heat storage systems. Two paraffin-filled containers are prepared, one of them, however, consists of a 3D printed aluminum lattice to mimic the presence of an open-cell metal foam but avoiding numerous difficulties. A temperature control system, insulation and data acquisition are designed and utilized for these experiments. A master student, Dávid Illés, was also involved and he presented the work on a scientific student conference and he is also preparing his final project on these results.

Last but not least, the PI also mentions the work related to the modeling of droplet evaporation. Single droplet evaporation measurements are used to validate vaporization models. The analysis clearly showed that continuum models are required to properly evaluate the evaporation phenomenon due to the significant temperature gradient in the suspension. However, lumped parameter models do have relevance when heat and mass transfer in sprays containing a large number of droplets. Furthermore, our previous studies focused on combustion applications. However, other engineering applications in refrigeration, drying, and agriculture also exist. Therefore, our motivation was to compare the results of a one-dimensional model with the results of the previous lumped parameter modeling approach to map the limitations. To deduce general conclusions, evaporating water droplets were considered and no fiber suspension was taken into account. Droplet lifetime and surface temperature values were used as indicators for the comparison. The varied parameters were ambient pressure and temperature, droplet size, and relative velocity between the droplet and ambient gas. A manuscript is under preparation.

4 Theoretical results

Our primary focus was placed on the improvement of analytical and numerical solution methods, keeping the material nonlinearities and coupled problems as a central question.

From this point of view, the behavior of supercritical fluids is particularly interesting. On the one hand, utilizing Liu's procedure on the Navier–Stokes—Fourier equation showed that even in the classical irreversible thermodynamic framework, gradient-dependent transport properties can emerge. Adding that nonlinearities become strong in the supercritical regime, such findings can have significant influence, even on the experimental design and its evaluation. Our group, particularly Dr. Mátyás Szücs, developed a numerical scheme utilizing operator splitting. It means that the reversible-irreversible parts, or fields with notably different time scales can be separately discretized. Therefore, while convective terms introduce numerical difficulties in diffusive systems, one can easily obtain a reliable numerical solution in this way. This was also advantageous in the simulation of the so-called piston effect, a thermal expansion-induced pressure wave, a thermo-acoustic phenomenon. It is worth mentioning that the so-called GENERIC thermodynamic framework is also investigated in detail, and the most common heat conduction models are derived with the help of this particular thermodynamic approach. It also separates the reversible and irreversible parts, and therefore provides a suitable basis for the operator splitting as well.

Also motivated originally by development of reliable numerical schemes for challenging thermodynamical phenomena, we started to explore the Widom region of supercritical fluids where material nonlinearities are remarkable and time-dependent processes are strongly sensitive to these nonlinearities. We have found a universal leading elliptic relationship between material quantities analytically, and demonstrated it numerically. Power laws for the pressure dependence of the parameters of the ellipse have been identified.

We have generalized our extended symplectic numerical scheme for viscoelastic processes, to incorporate coupling to heat conduction via thermal expansion. The scheme is explicit, is second-order accurate, runs fast and produces reliable results, as monitoring total energy conservation and positive definite entropy production rate also demonstrated. Earlier, we showed that COMSOL produces solutions with significant dispersion and dissipation errors, therefore this step now allows to fully simulate a detailed thermo-mechanical viscoelastic process with notably different time scales.

Utilizing the Backward Error Analysis approach, we explored how the Newmark numerical method distorts the transient structural dynamics equation (with damping allowed). Using this, we provided appropriate slight tuning of the stiffness and damping matrices of the system via which numerically induced artificial damping was eliminated. Also, with the same compensation technique we succeeded in making the traditionally second-order Newmark method fourth-order accurate. These improvements are achieved with the same time step and with the original Newmark method – the only aspect adjusted is the coefficient matrices of the model. Accordingly, existing – e.g., proprietary – software like Ansys and Abaqus can conveniently be used for the Newmark method. We have demonstrated superior performance compared to the generalized-alpha method and the 4th-order Runge–Kutta scheme as well.

Continuing with the solution methods, the PI wants to mention the advancements in regard to the finite element methods for non-Fourier heat conduction models. The PI and Dr. Balázs Tóth together worked on a mixed hp-type finite element approach that can properly take into account the boundary conditions on contrary to COMSOL. Our analysis also revealed the reason why COMSOL provides a false (but somehow convergent) solution to the GK equation: the second-order spatial derivative term requires particular attention, it requires additional integralibility conditions which are not satisfied by COMSOL. Furthermore, a multi-field variational formalism is developed in which the flux of the heat flux is also treated as a separate, independent field variable. Based on these variational approaches as mathematical background, a family of mixed hp-version FEMs, which is capable of reliably and efficiently modeling the temperature responses, is designed. The robustness of the hp-FE framework constructed is tested on the following two heat pulse experiments as benchmark problems: (i) sinusoid laser pulse heating process and (ii) rectangular (step-like) laser pulse train. It is verified that uniformly stable, exponentially increasing p-convergences and fast algebraic h-convergences can be obtained. As expected, the p-convergence rates are much faster than the h-convergence rates and it has outstandingly high precision in each thermodynamic model and test problem.

The PI also mentions the research done regarding the development of the theory of nonequilibrium thermodynamics, incorporating gravity and quantum effects. The research group made advancements towards the derivation of a single component weakly nonlocal fluid, deriving the family of generalized Korteweg fluids. It has consequences on thermodynamic methodological perspectives, on nonrelativistic self-gravitating fluids, and interestingly, showing analogies with quantum mechanics. Based on the results found so far, the second law of thermodynamics has a crucial role in the holographic property of classical fluids. In regard thermodynamic originated gravity modeling, extensive simulations are performed, and several galactic rotational curves are investigated, and compared to observations. The accuracy of the thermodynamic fit is comparable to the MOND-EFE parameterizations and the Dark Matter models.

Overall, the PI's research group achieved several, practice-oriented results from both an experimental and a theoretical point of view, significantly extending the capabilities of the thermodynamic modeling.

5 Fulfillment of the workplan

Despite the initial difficulties due to pandemic, the research group fulfilled all the planned goals. Although several minor results could not be mentioned here, the extensive publication record and conference attendance clearly show the PI's group activity. During the project, about 30 conference presentations, 15 posters, and more than 50 papers are published, both on national and international journals and conferences. During this period, 2 ERC Starting proposals are submitted by the PI, one of them selected into the interview round as well. Furthermore, the PI also submitted 2 MTA Lendület proposals, both are evaluated with excellent reviews, but unfortunately could not be funded. Besides, in 2024, two additional NKKP proposals are submitted by the PI, one Starting and one Excellence in order to ensure the continuation of the research project. On the top of that, Dr. Péter Ván also submitted 2 ERC Andvanced, 3 OTKA and 1 NKKP Advanced proposals.

6 Personal changes and further project info

During the project, Dr. Gábor Balassa, Dr. Mátyás Szücs, Dr. Dávid Csemány are obtained their PhD degree. Furthermore, Anna Fehér and Donát Takács made significant steps forward their PhD degree with the help of this research fund, and it is expected that they finish their studies in 2025. Additionally, Réka Somogyfoki and Máté Pszota started their PhD studies in 2022, and supported by this grant. Dr. Tamás Fülöp and the PI both started the preparations for their DSc degree. It is expected that the PI will submit his DSc thesis in the beginning of 2025.

Furthermore, Dr. Krisztián Sztankó joined to the project, and he was responsible for the experimental equipments, and notably helped us to make further advancements in the project.

Dr. Mátyás Szücs and the PI have taken part in the organization of the 19th European Meeting on Supercritical Fluids (EMSF 2023, May 21-24. Budapest, emsf2023.com). At this conference, L. Schaul (MSc student) and Donát Takács had an oral presentation about the piston effects, supercritical fluids, and related numerical techniques. Furthermore, Dr. Péter Ván, Dr. Tamás Fülöp and Dr. Balázs Vásárhelyi organized a national conference at BME dedicated to the memory of Csaba Asszonyi, called "Mérnökgeológia-Kőzetmechanika Konferencia 2023" (in Hungarian), where five of us had an oral presentation related to rock mechanics, rheology and heat conduction. Furthermore, the PI has been invited to the Messina University (Italy) and held a 12 hours long PhD course "Physical and mathematical aspects of Non-Fourier heat conduction" during June-July, 2022, in the program of PhD in Mathematics and Computational Sciences. In 2024, besides the PI, Dr. Péter Ván and Dr. Mátyás Szücs were invited to the Salerno University (Italy) by Prof. Vincenzo Tibullo.

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