HEAT TRANSFER IN EXTREME MEDIA AND SYSTEMS

NKFIH 116197-116375 PROJECT
FINAL REPORT

1. Introduction

Our research aims were divided into three parts:

(1) experimentally and theoretically investigate heat transfer properties of *supercritical fluids*,
(2) continue our previous efforts finding qualitative proofs of the appearance of *non-Fourier heat conduction*,
(3) experimentally and theoretically investigate heat conduction and thermal expansion and *dissipative mechanical (i.e. rheological) properties of fluids and solids* (fluid-solids media).

We have achieved the following research results.

2. Supercritical fluids

In this research our main focus were the influence of the superciritical part of the Organic Rankine Cycle (ORC) where we have investigated several practical and theoretical aspects and developed principles to select optimal working fluids.

The effect of the Widomanomalies were studied in various real and model working fluids for supercritical and transcritical Rankine cycles. The parts of the cycles where crossing these Widom lines upon heating or cooling can cause operational or safety (stability) problems - hence the p-T region of these crossings should be avoided [10]. Then the focus of our investigation were the working fluids of Organic Rankine Cycles. Their physical-thermodynamic criteria were studied [15]. Special emphasis was given to isentropic expansion during the thermodynamic cycle Organic Rankine Cycle (ORC) is suitable for power generation based on various heat sources including solar, geothermal, biomass or waste heat. A method to use molecular degree of freedom and isochoric heat capacity were given to find the best working fluid to avoid droplet formation upon expansion of saturated vapour. The phase structure of supercritical state were studied, first with anomalous properties, then, the existence of a special work-free process was discussed in metastable liquids, where the volume-work remains zero even after macroscopic change of volume, due to the existence of zero-pressure states in metastable liquids [22].

In the final year of the project we were focusing of the study on isentropic and isenthalpic processes proceeding in the vicinity of the Widom region. It has been shown that the stability of adiabatic expansion and compression lines are seriously affected by the vicinity of some Widom anomalies [36]. Also, isentropic and isenthalpic expansions were studied, starting in the supercritical region and intruding to the metastable liquid and vapour region. These processes were used to

Date: September 24, 2019.

model the so-called small and big LOCA processes (Loss of Coolant Accidents) of supercritical water cooled nuclear reactors [37]. In the parallel research, adiabatic expansion steps of some thermodynamic cycles (like Organic Rankine Cycle and Trilateral Flash Cycle) were studied [35]. Based on the shape of the phase envelope in temperature-entropy space, we were able to find thermodynamically optimal expansion lines. With this result, one can easily design a simple cycle of a power plant, utilizing low-temperature heat sources [36].

Related publications: [10,14,21,35,36,37,38]

3. Non-Fourier heat conduction

Here our main result is the experimental discovery of non-Fourier heat conduction at room temperature in various artificial and natural materials in heat pulse experiments (see Fig 1-2). The observed structural diversity of the samples supports the prediction of our nonequilibrium thermodynamic theory regarding the universality of the non-Fourier heat conduction. Our general numerical solution schemes played a key role in the quantitative modelling.

The discovery of Guyer-Krumhansl-type heat conduction was first reported in [5], then, after a more extensive experimental study, detailed investigations were published in [8,19,26]. In these studies, heat pulse experiments have shown a non-Fourier, Guyer-Krumhansl-type heat conduction in artificial capacitor and metal foam samples and also in various rocks. According to our theoretical analysis, the existence of parallel heat conducting channels, e.g. different phonon collision mechanisms or gradient effects in a heterogeneous material may be responsible for that an effective non-Fourier heat conduction appears. Another key element of our observations is that the otherwise expected, wave-like propagation is suppressed by various dissipation mechanisms.

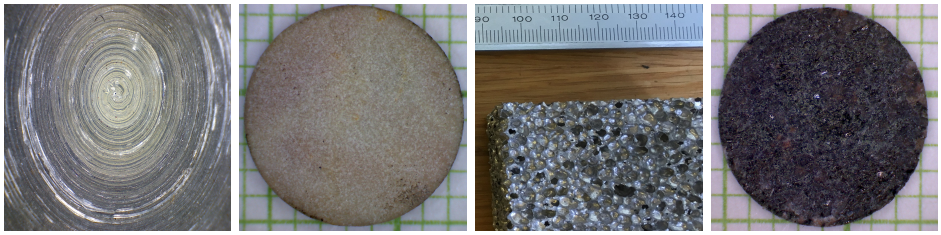

Figure 1. The heterogeneous structure of the measured materials. From left to right: capacitor, limestone from Villány, metal foam, leucocrata rock with slires.

In our theoretical investigations we partially analysed the physical and mathematical background and the alternative theories [9,15,23,25,30,31] and started to investigate the possible phenomena predicted by the next level of approximations, in particular, by ballistic heat conduction [7,24,35]. The related numerical methods were published in [27,28]. Some of our new theoretical works analysed the common aspects fo ballistic heat propagation, that is, phonon hydrodynamics and real gas dynamics in the rarefied regime [29,40]. Further project specific numerical and experimental investigations were reported in [41,45].

The related publications for experiments appeared in [5,8,19,26] for theory in [7,9,12,15,23,24,25,29,30,31,35,40] and for numerics in [27,28]. The PhD thesis of

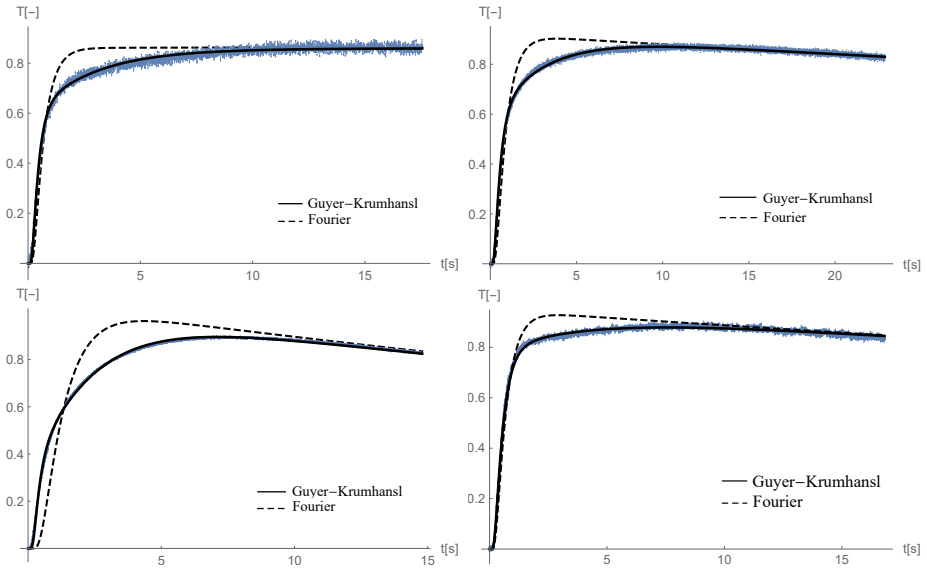

FIGURE 2. Fitted Fourier and Guyer-Krumhansl models of heat pulse experiments of the capacitor, limestone from Villány, metal foam, leucocrata rock with slires samples. The dashed line is a Fourier fit, the continuous line is the Guyer-Krumhansl fit.

Róbert Kovács was devoted to non-Fourier heat conduction and rarefied gas dynamics.

4. Rheological properties of matter

Here, we have researched the Kluitenberg-Verhás model of rheology, the basic thermodynamic building block in the family of rheological bodies. Novel analytic solutions for tunnel convergence in the presence of gravitation were calculated with a new general method [20,22] and theoretical consistency of the thermodynamic model was analysed in [46]. The thermodynamic model predicts a particular wave propagation of constitutive origin. We have started to implement the codes for a numerical investigation [47]. This is crucial from the point of view of possible experimental observations, because rheology should be distinguished from elastic and thermal expansion related phenomena [31].

Here it is worth to mention, that our experimental investigations were aimed at a particular material type, namely, andesitic rocks. Here the proper modelling of the basic rheological effects, relaxation and creep may play a role in the low-frequency sensitivity of underground gravitational wave detectors. According to the preliminary seismic investigations in the Hungarian Mátra mountains, the noise level is low and therefore characterisation measurements for a Hungarian candidate site were performed the framework of a recently started other NKFIH project (NKFIH 124366-508). At the design and interpretation of these new measurements we have considered thermal phenomena with the complete Kluitenberg-Verhás body [3,11,34,43].

Experimental reports [3,11,12,34,43] and theory [20,22,46,47].

5. General aspects of continuum thermomechanics

Without considering material frame indifference one cannot hope an objective, frame and flow independent constitutive theory [17]. The weakly nonlocal, gradient dependent theories, like our non-Fourier heat conduction model family, are particularly challenging. In this respect the nonrelativistic theories are rather instructive, [1], and may lead to unexpected and surprising fundamental results. We consider the frame independent Navier-Stokes-Fourier theory in [17,18,44] as surprising, because with the help of a third order nonrelativistic four tensor one was able to derive frame and flow independent entropy production formula and usual kinetic energy turned out to be the part of the transformation rule. The energy alone is not an objective quantity, it is not a scalar, but is a part of a four tensor and transforms accordingly.

Aspects of hierarchical structure of evolution equations were reported in [2] and the microscopic origin of viscoelasticity from first principles in [6].

The largest publication of the research period was the book of Berezovski and Ván about internal variables in thermoelasticity. In this book, the internal variables of nonequilibrium thermodynamics were applied for modeling anelastic wave propagation [12]. The common aspects of non-Fourier heat conduction and thermodynamic rheology are discussed in detail, together with further far-reaching generalisations like the thermodynamic background and origin of phase field theories and of generalized mechanics of Eringen.

Objectivity [1,17,18,33,44], other [2,4,6,12,13,32].

6. Related theoretical research

Other reported publications are indicating some background research lines seemingly without direct consequences to the reported classical research. However, the correct treatment of symmetry principles [13] in dissipative wave propagation, and the understanding of the irreversible nature of radiation-matter interaction [16] are necessary to be competitive to such massive research directions like GENERIC [A1,A2], or Rational Extended Thermodynamics [B1,B2]. We are following the ideas of Theodore von Kármán and consider theoretical clarity as the foundation of powerful technologies [C], therefore we did not want to hide these results for the sake of smoother or more uniform presentation.

Extra theory [13,16].

6.1. **Comments about publications.** This grant is a continuation of our previous research supported by the consortional OTKA grant K81161-K82024. In publications [1,2,4] only that grant number is written. However, they belong to the current research (see final report of K81161-K82024) and they appeared in this grant period. In case of publication [7] the NKFI Grant id is missing because of the adventurous past of the publication (we have received the first referee report 10 months after the submission due to administrative mistakes of the journal). In case of [41,45] the foreign coworkers acted spontaneously and the papers were promptly accepted.

7. Workplan and spending

The research was conducted basically according to the project plan. Only minimal personal changes happened (e.g. R. Kovács changed his workplace from one

consortial partner to the another) and the main publications appeared during the research period. At the end of the research we could not apply the student coworkers sooner because of the long administrative authorisation process and the extremely dense spring-summer period of the PI.

8. External references

[A1] Öttinger, H.C., Beyond Equilibrium Thermodynamics, Wiley, 2005.

[A2] Pavelka, M., Klika, V. and Grmela, M., Multiscale Thermo-Dynamics: Introduction to GENERIC, Walter de Gruyter GmbH & Co KG, 2018.

[B1] Müller, I. and Ruggeri, T., Rational Extended Thermodynamics, Springer, 1988.

[B2] Ruggeri, T., Sugiyama, M., Rational Extended Thermodynamics beyond the Monatomic Gas, Springer, 2015.

[C] Lee Edson, Örvények és repülők: Kármán Tódor élete és munkássága, Akadémiai Kiadó, 1994.