Heat conduction beyond Fourier’s Law: theoretical predictions and experimental validation

Ph.D. Thesis by
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Abstract

This dissertation discusses the physical and experimental background behind the extension of classical heat conduction equation, the Fourier’s law. From the theoretical point of view, the framework of non-equilibrium thermodynamics with internal variables is used to obtain a powerful generalization, the ballistic-conductive equation. The non-equilibrium thermodynamical framework is compared to the kinetic theory based Rational Extended Thermodynamical one. It is shown that the modeling of a real rarefied gas and a rarefied phonon gas is similar in our framework.

The ballistic-conductive model is tested in different fields of heat conduction. The chapter of low temperature heat conduction discusses the modeling challenge of NaF experiments where one may observe various wave propagation forms of heat. The results are compared to the Rational Extended Thermodynamical approach and to Y. Ma’s hybrid phonon gas model.

The chapter of room temperature experiments is devoted to the work conducted in the Department of Energy Engineering, BME. Here, the deviation from Fourier’s law is observed in inhomogeneous materials such as rocks and metal foams. The realization of the Fourier hierarchy of Guyer-Krumhansl equation led to the physical interpretation of the observed phenomenon.

In the chapter about biological heat conduction the popular models are discussed with their relation to thermodynamics. Then a series of heat pulse experiment by Tang et al. is modeled. It highlights the main misunderstandings related to non-Fourier heat conduction in this field.

In this work, the same modeling framework is applied to low and room temperature heat propagation phenomena, to artificial and natural test samples and also to living tissues. This is a strong argument that the non-equilibrium thermodynamics with internal variables is universal, like Fourier’s law for local equilibrium phenomenon.

Keywords: Non-equilibrium thermodynamics, ballistic propagation, heat pulse experiments, heat conduction
Declaration

Undersigned, Róbert Kovács, author of this Thesis, hereby, I declare that I prepared this Thesis myself, and I used only the referred sources. All parts of the Thesis, which are either cited verbatim or with the same content but rephrased as in the original source, are referred unambiguously and with providing the sources used.

Budapest, May 1, 2017

Alulírott Kovács Róbert kijelentem, hogy ezt a doktori értekezést magam készítettem, és abban csak a megadott forrásokat használtam fel. Minden olyan részt, amelyet szó szerint, vagy azonos tartalomban, de átfogalmazva más forrásból átvettem, a forrás megadásával egyértelműen megjelölttem.

Budapest, 2017. május 1.

Róbert Kovács
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Summary and Theses

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Chapter 1

Introduction

The evolution of science is like individual human evolution. At the beginning the world seems to be perfect and a child is chasing this perfection. A slow understanding of the true, lovely but less complete reality is like the birth of thermodynamics. The world is not ideal, there is no reversibility, there is no equilibrium, losses and dissipation are everywhere. However, it is hard to face such a reality and also hard to deal with it. Idealization is useful and in certain cases it is necessary. It serves as a stepping stone for a human mind to approaching the real understanding of a phenomenon step by step.

Nevertheless, most of the processes which relevant for engineers can be treated as static or quasi-static and the notion of equilibrium can be exploited. Thanks to technological developments, the age of nano-scale devices has begun. The characteristic time and length of processes become very short. This is the adolescent age of science, where humanity starts to discover the core of nature. From the side of experiments, it turned out many years ago that the classical laws, such as Fourier’s law of heat conduction, could be wrong under certain circumstances. It is high time to explain phenomena beyond classical laws. Some of the researchers are surprised by the fact that thermodynamics as a framework to extend the classical equations can be used in this sense. The classical side of thermodynamics enables to calculate the temperature of a gas, or predict the pressure as the function of temperature or the time, etc.

Moreover, the second law is expected to be universal and general. One needs to understand its role for processes, for non-locality, for material models of physics: for constitutive equations.

However, the world continues.

During the last few decades, different branches of thermodynamics evolved to extend the validity of the classical theory. In this thesis, the so-called non-equilibrium thermodynamics with internal variables is discussed. As we will see, non-equilibrium thermodynamics is simple, constructive and universal. These characteristics are not trivial and not evident. Why would it be universal? Why would it be constructive? The answer is short but not simple: everything is up to entropy. Here comes the universality: all processes let them be mechanical, chemical or anything else, produce entropy. As Albert Einstein wrote [1]:

“A theory is the more impressive, the greater the simplicity of its premises is, the more different kinds of things it relates, and the more extended is its area of applicability. Therefore the deep impression that classical thermodynamics made upon me. It is the only physical theory of universal content, which I am convinced that, within the framework of applicability of its basic concepts, will never be overthrown.”
In this work, we demonstrate the simplicity, universality and constructive property of the theory in the example of an effective description of non-Fourier heat conduction. Our approach is universal because it is independent of the material structure. It is constructive and simple because one needs only minimal assumptions to derive such extensions independently from exact knowledge about the material. This background serves as a backbone to all other chapters.

Further parts of this dissertation discuss the applications of the presented thermodynamical framework. The chapter 'Heat conduction at low temperature' devoted to present one of the most extraordinary heat conduction problems in the corresponding literature. It is the wave nature of heat conduction and the ballistic propagation of heat. This chapter presents briefly the experimental background of low temperature phenomena and discusses the questions of modeling.

The fourth chapter is devoted to room temperature experiments using inorganic materials. The deviation from Fourier’s law occurs in a different way than in the case of low temperatures. This statement could be trivial. One may think that the propagation mechanisms depend on the applied temperature range. Considering both experiments and the literature it is not trivial at all how this deviation should be experienced and in what kind of material could be observed. As we will see, the inhomogeneity of the structure leads to deviation from Fourier’s law. Nevertheless, what kind of heterogeneities leads to what kind of deviation? What is the appropriate extension of Fourier’s law? This chapter will answer the questions; furthermore, it presents our series of experiments both with natural and artificial materials. Our goal was to find the deviation and model it.

The last chapter is about biological heat conduction. It is useful to present the modeling techniques on non-artificial materials. The questions of modeling a piece of skin could be really complicated due to anatomical reasons. Through a few orders of magnitude the human body consists of fractal structures such as the vascular system. It is hard to decide during the modeling of a piece of skin how to treat effectively the medium. Can it be simplified? How do the biological models work and how can our extended model be used? This chapter is devoted to answer these questions.

In order to summarize the motivation of my research:

- There is no continuum theory in the literature that is able to model all propagation modes.

- The existing and leading theories are mostly based on kinetic theory, adapting the phonon hydrodynamic background. The advantages and disadvantages of phonon based models are discussed later.

- My goal was to derive a continuum model and develop a framework to unify the phenomena of non-Fourier heat conduction. Moreover, this unifying model should be compatible with the kinetic theory.

- The theoretical modeling of existing experiments is insufficient.

I carried out the following steps in my work:

- In chapter two, I applied the theory of internal variables and Nyiri-multipliers to develop the necessary theoretical background and derived the ballistic-conductive model. It is applied to model all the presented experiments and it unifies the different propagation modes. I compared this continuum thermodynamic background to the relevant ones from kinetic theory.
- I developed a numerical scheme to solve the ballistic-conductive model for heat pulse experiments.

- In chapter three, I tested the ballistic-conductive model on NaF experiments and compared these results to literature. The emphasis is on the modeling of ballistic propagation.

- In chapter four, I present a series of room temperature experiments where my role was to prepare the samples and evaluate the measurements.

- In chapter five, I extended my research to the field of biology. I criticized the existing biologically inspired heat conduction models and I evaluated a series of heat pulse experiments from literature.

Seemingly, these fields can look different but they have a common point: non-equilibrium thermodynamics. I believe that it connects everything and not only within this dissertation.
Chapter 2
Non-equilibrium thermodynamics

There are several theories that extend the validity of Fourier’s law by additional terms in the constitutive equation. Some of them are consistent with thermodynamics, others are not. Many different derivations exist in the literature. In this chapter we show our version. This continuum thermodynamic model covers all generalizations of the Fourier’s law. It is a unified theory of heat conduction which is universal in the following sense. It is based on general principles and not on microscopic or structural peculiarities of the material. Therefore it is expected to be valid as long as these general principles are valid. It allows us to use the same model in different problems.

Remark: My related publications are [2,3]. These papers cover the derivation of ballistic-conductive model, the developed numerical method and the comparison with the kinetic theory concerning heat conduction. In the section related to rarefied gases I present my latest unpublished results.

2.1 Physics behind the generalization

Heat conduction is based on the energy balance and on the constitutive equation, describing material properties. In this case, the generalization means the extension of the constitutive equation. The extension can be done in the direction of time and in the direction of space. The first one is called memory extension when the history of the material is considered. The second one is called nonlocal extension, there the state of neighboring space points are accounted as well. In our case the extension is weakly nonlocal, while it is represented by extra time and space derivatives in the constitutive equation.

Several methods exist to obtain generalizations of the Fourier’s law. A mathematical approach focuses on the final result, what is the form of the equation but not necessarily interested in the physical meaning of the terms or the coefficients. E.g. it is customary to modify the original – physical – coefficients in order to obtain something interesting from a mathematical point of view. For example, a heat diffusion problem is analyzed by Meissner and Spitzmann [4], where a heat pulse experiment is conducted in vitreous silica at low temperature, below 2K. These experiments are based on the fact that anomalous thermal conductivity is measured in such material by Anderson et al. [5] and discussed in the framework of quantum mechanics [6]. According to Meissner, it can be explained explicitly by time dependent specific heat [4]. In fact, mathematically this time dependent thermal diffusivity in Fourier equation is equivalent with a non-time dependent thermal diffusivity in Maxwell-Cattaneo-Vernotte equation. A further example is presented by Barna and Kersner [7]. In this work, the Maxwell-Cattaneo-Vernotte
equation becomes non-autonomous and an explicit time dependency is introduced. Non-equilibrium thermodynamics excludes models like these.

It is popular to assume a delay, a time lag and then obtain a simpler weakly non-local equation with Taylor series expansion. This may lead to inconsistent models that contradict elementary expectations and basic principles. A single time lag is obvious from this point of view, because it destroys the time translation invariance of the equation. However, the investigation of such questions is beyond this thesis, therefore it is not analyzed. The variety of the methods and aspects is wide. In general, we expect compatibility with the second law of thermodynamics and with spacetime evolution, and the micro-scale background. The second law offers a complete system of conditions to obtain asymptotically stable equilibrium. In this work, a non-equilibrium thermodynamic model is compared to a kinetic theory based one.

In classical irreversible thermodynamics (CIT) for heat conduction, the entropy density $s$ is the function of the internal energy only. The assumption of local equilibrium of thermal interaction leads to Fourier’s equation in the continuum case. Non-equilibrium thermodynamics can characterize deviation from local equilibrium both in the entropy density and in the entropy current by introducing internal variables. The existence of internal variables assumes the non-classical behavior of the material, it represents an internal property. However, one needs to derive an evolution equation for them. In this respect, two ways are possible to derive an evolution equation [8–10]. The first one applies a Hamiltonian variational principle, and the variable is called dynamical degrees of freedom and it is typical for continuum mechanics. For instance, the microstructural inhomogeneity (e.g. dislocations in the crystal) is modeled by a dynamical degree of freedom. Usually, the free energy is assumed to depend on that. The introduction of dissipation requires the existence of a dissipation pseudo-potential which depends on an internal variable. It leads to a separation between intrinsic and thermal dissipation [11].

On the other hand, the evolution equation for the dynamic internal variables of state can be derived from the inequality of entropy production. Its first thermodynamical theory and framework is presented by Coleman and Gurtin [12]. In the case of classical theory of irreversible processes, the entropy density is extended by an internal variable, one example is given by de Groot and Mazur to model sound absorption [13]. In this case, the entropy current remains the classical one. There the entropy density is extended with a second order tensor as internal variable to generalize the Navier-Stokes equation by obtain coupling between the pressure tensor and internal variable. In this work, we use the entropy inequality to derive the evolution equation. Furthermore, beyond the extension of entropy density, the entropy current density is also extended. Its role is discussed later. Further example is discussed by Verhás for rheology [14].

These theories can be unified. With dual, weakly nonlocal internal variables one can derive the Hamiltonian structures of the non-dissipative theories of mechanics from thermodynamic principles. This theory covers most of the known models from continuum mechanics and thermodynamics. For example, it consists of the concept of microtemperature from A. Berezovski and M. Berezovski [15]. The properties of such framework is discussed in detail by Berezovski et al. [16].

2.1.1 Derivation of the ballistic-conductive model

Let us consider a rigid heat conductor, where the mass density $\rho$ is constant and the velocity field is uniform, hence the material time derivatives are identical to partial time
derivatives. It simplifies the physics of the model. Our starting point is the conservation of internal energy:

\[ \rho \partial_t e + \partial^i q^i = 0, \]  

(2.1)

where \( \partial_t \) is the partial time derivative, \( q^i \) is the heat flux, \( e \) denotes the density of internal energy and it can be expressed as \( e = cT \) in case of constant specific heat \( c \) and \( T \) is the temperature. The summation convention of Einstein is used; nevertheless, the co- and contravariant quantities are not distinguished here. It is still an open question and requires further considerations of Galilean relativistic thermodynamics [17].

The second law of thermodynamics is exploited in this framework. However, the second law can be formulated in different ways. Matolcsi enumerate four different definitions of the literature to demonstrate that none of them is complete and one must define the second law in a mathematically correct and physically sound manner [18]. For classical continua the physical content of the second law of thermodynamics is the asymptotic stability of homogeneous equilibrium solutions of the field equations. The well-known particular requirements in non-equilibrium thermodynamics are

1. The entropy density is a concave function of the corresponding state variables. This is thermodynamic stability.

2. The entropy is increasing in an insulated system, that is the entropy production is nonnegative.

Therefore the balance of entropy is an inequality:

\[ \sigma_s = \rho \partial_t s + \partial^i J^i \geq 0, \]  

(2.2)

where \( s \) denotes entropy density and \( J^i \) is the entropy current density. In non-dissipative case the entropy production \( \sigma_s \) is zero. For heat conduction the state variable in local equilibrium is the internal energy density. Here we introduce two additional basic fields, i.e. internal variables: a vectorial \( \xi^i \) and a symmetric tensor \( Q_{ij} \). This choice of field variables allows comparison with theories of Extended Thermodynamics and they have a particular clear interpretation in a phonon hydrodynamics.

Thermodynamic stability is preserved by assuming a quadratic deviation in the entropy density [14],

\[ s(e, \xi^i, Q^{ij}) = s_{eq}(e) - \frac{m_1}{2} \xi^i \xi^i - \frac{m_2}{2} Q^{ij} Q^{ij} - \frac{\hat{m}_2}{2} (Q^{ij} - (Q^{kk}/3) \delta^{ij})^2, \]  

(2.3)

where \( m_1 \), \( m_2 \) and \( \hat{m}_2 \) are positive scalar material parameters and \( \delta^{ij} \) stands for the Kronecker symbol. In our case, this general isotropic entropy density can be simplified to

\[ s(e, \xi^i, Q^{ij}) = s_{eq}(e) - \frac{m_1}{2} \xi^i \xi^i - \frac{m_2}{2} Q^{ij} Q^{ij}, \]  

(2.4)

and this form will be used in further calculations. In case of heat conduction, it is customary to choose heat flux, \( q^i \), as internal variable [19,20] in order to accommodate kinetic theory derivation of continuum equations. Then one can calculate the entropy production with using the following Gibbs relation for partial derivatives of the entropy density:

\[ de = Tds - A^i d\xi^i - A^{ij}_2 dQ^{ij}, \]  

(2.5)
where $A^i_1$ and $A^i_j$ are called affinities. The corresponding partial derivatives are:

$$
\frac{\partial s}{\partial e} = \frac{1}{T}; \quad \frac{\partial s}{\partial \xi^i} = \frac{A^i_1}{T} = -m_1\xi^i; \quad \frac{\partial s}{\partial Q^{ij}} = \frac{A^i_j}{T} = -m_2Q^{ij}.
$$

(2.6)

The classical entropy current is

$$
J^i = \frac{q^i}{T}.
$$

(2.7)

There are several generalizations, Müller [21] was the first who assumed the existence of a vector $K^i$ as an extension for classical entropy current but he did not considered that it is a constitutive quantity,

$$
J^i = \frac{q^i}{T} + K^i.
$$

(2.8)

It is discussed by Verhás [22,23] that $K^i$ should disappear when all the internal variables vanish and therefore must have the following form [24]:

$$
K^i = \sum_{L=1}^{N} F^i_L \xi_L,
$$

(2.9)

where $\xi^i_L$ is the $L^{th}$ internal variable and $F^i_L$ is a multiplier, a constitutive quantity. This thread is followed here by introducing the so-called Nyíri multipliers [24]. These are also constitutive functions but they can be eliminated from the system. The entropy current is considered as

$$
J^i = b^{ij} \xi^j + B^{ijk} Q^{jk},
$$

(2.10)

where $b^{ij}$ is a 2nd order tensor and $B^{ijk}$ is a 3rd order tensor. These quantities are called current multipliers. Further example of the application of current multipliers can be found in [25]. Here the constitutive equations are derived with the help of Liu procedure [26]. In what follows, the mentioned identification between $\xi^i$ and $q^i$ is made and exploited.

Furthermore, let us simplify the notation of partial derivatives such as $\frac{\partial s}{\partial e} := \partial_e s$. Then the entropy production $\sigma_s$ is calculated as follows:

$$
\sigma_s = \rho \partial_t s + \partial^i J^i = \\
\rho \left( \partial_t s \partial_t e + \partial_q s \partial_t q^i + \partial_Q^{ij} s \partial_t Q^{ij} \right) + \partial^i \left( b^{ij} q^j + B^{ijk} Q^{jk} \right) = \\
\rho \left( \frac{1}{T} \partial_t e - m_1 q^i \partial_t q^i - m_2 Q^{ij} \partial_t Q^{ij} \right) + \\
(\partial^i b^{ij}) q^j + b^{ij} (\partial^i q^j) + (\partial^i B^{ijk}) Q^{jk} + B^{ijk} (\partial^i Q^{jk}) = \\
q^j (\partial^i b^{ij} - \rho m_1 \partial_t q^j) + \partial^i q^j \left( b^{ij} - \frac{1}{T} \delta^{ij} \right) + \\
Q^{ij} (\partial^i B^{ijk} - \rho m_2 \partial_t Q^{ij}) + B^{ijk} \partial^i Q^{jk} \geq 0.
$$

(2.11)

The balance equation of internal energy (2.1) is exploited. In order to solve this inequality, the entropy production is written as a sum of product of thermodynamic forces ($X_L$) and fluxes ($J_L$) [14]:

$$
\sigma_s = \sum_L X_L J_L.
$$

(2.12)

In our case the separation can be done according to Table 2.1, and linear relationship is assumed between the forces and fluxes:

$$
J_L = \sum_C C_L X_L,
$$

(2.13)
where \( C_L \) are Onsager’s conductivity coefficients \([27,28]\). In the following they are considered as constant. The separation of fluxes and forces in case of Nyíri multipliers is not straightforward and not unique. The mathematical background is treated in more detail in \([29,30]\).

<table>
<thead>
<tr>
<th>Fluxes</th>
<th>Thermal</th>
<th>Extended thermal</th>
<th>Internal</th>
<th>Extended internal</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \partial^b b^j - m_1 \partial_t q^i )</td>
<td>( b^i - \frac{1}{T} \delta^{ij} )</td>
<td>( \partial^i B^{ijk} - m_2 \partial_t Q^{ijk} )</td>
<td>( B^{ijk} )</td>
<td></td>
</tr>
<tr>
<td>( q^i )</td>
<td>( \partial^i q^i )</td>
<td>( Q^{ij} )</td>
<td>( \partial^i Q^{ijk} )</td>
<td></td>
</tr>
</tbody>
</table>

Table 2.1: Thermodynamic fluxes and forces

Let us consider an isotropic material and one dimensional propagation. Then the linear solution of inequality (2.11) is

\[
\begin{align*}
  m_1 \partial_t q - \partial_x b &= -l_1 q, \quad (2.14) \\
  m_2 \partial_t Q - \partial_x B &= -k_1 Q + k_{12} \partial_x q, \quad (2.15) \\
  b - \frac{1}{T} &= -k_{21} Q + k_2 \partial_x q, \quad (2.16) \\
  B &= n \partial_x Q. \quad (2.17)
\end{align*}
\]

Here the following conditions are required for the coefficients \( l_1, k_1, k_2, k_{12}, n \):

\[
  l_1 \geq 0, \quad k_1 \geq 0, \quad k_2 \geq 0, \quad n \geq 0, \quad K = k_1 k_2 - k_{12} k_{21} \geq 0. \quad (2.18)
\]

Eliminating the current multipliers \( b \) and \( B \) by substitution, evolution equations for \( q \) and \( Q \) are obtained. The \( Q \) can be also eliminated and one obtains:

\[
\begin{align*}
  m_1 m_2 \partial_t u q + (m_2 l_1 + m_1 k_1) \partial_t q - (m_1 n + m_2 k_2) \partial_x q + nk_2 \delta_x^j q - & (l_1 n + K) \partial_x q + k_1 l_1 q = m_2 \partial_x q \frac{1}{T} + k_1 \partial_x q \frac{1}{T} - n \delta_x^j \frac{1}{T}. \quad (2.19)
\end{align*}
\]

At this point one may wonder the physical role of \( Q \) in this model. In general, the internal variables can be eliminated in the same way as the current multipliers. It leads to an equation where only the temperature is a variable. However this form has some disadvantages from the point of view of boundary conditions. It will be discussed in the section where the applied numerical method is introduced. Anyway, the exact physical role of such variable is not necessarily important or for higher order terms even does not exists. In this model, it has a clear physical role and it will be discussed soon. **Ballistic-conductive equation (BC):** Taking \( n = k_2 = 0 \), entropy production requires \( K = -k_{12} k_{21} \geq 0 \) which means that one of the coefficients is smaller than zero. More accurately, this is the antisymmetric part of the Onsager’s conductivity matrix, i.e. the Casimir-relation is applied here and \( |k_{12}| = |k_{21}| \). One obtains the following system:

\[
\begin{align*}
  m_1 \partial_t q - \partial_x B &= -l_1 q, \quad (2.20) \\
  m_2 \partial_t Q &= -k_1 Q + k_{12} \partial_x q, \\
  B - \frac{1}{T} &= -k_{21} Q.
\end{align*}
\]

If one eliminates the current multiplier \( B \) from the system (2.20), it yields

\[
\begin{align*}
  m_1 \partial_t q + l_1 q - k_{21} \partial_x Q &= 0, \\
  m_2 \partial_t Q + k_1 Q - k_{12} \partial_x q &= 0. \quad (2.21)
\end{align*}
\]
then one can identify the parameters as \( \tau_q = \frac{m_1}{l_1}, \lambda = \frac{1}{l_1 T}, \kappa_{21} = \frac{k_{21}}{l_1}, \tau_Q = \frac{m_2}{k_1}, \kappa_{12} = k_{12}, \)
in its final form:

\[
\begin{align*}
\tau_q \partial_t q + q + \lambda \partial_x T + \kappa_{21} \partial_x Q &= 0, \\
\tau_Q \partial_t Q + Q - \kappa_{12} \partial_x q &= 0,
\end{align*}
\]

(2.22)

where \( \lambda \) is the Fourier thermal conductivity, \( \tau_q \) and \( \tau_Q \) are called thermal relaxation times.

Eliminating \( Q \) one obtains:

\[
\tau_Q \partial_t (\tau_q \partial_t q + q + \lambda \partial_x T) + (\tau_q \partial_t q + q + \lambda \partial_x T) + \kappa^2 \partial_{xx} q = 0.
\]

(2.23)

This model has a central role in this work. It incorporates the known deviations from Fourier’s law, namely the second sound and ballistic propagation. For further analysis it is essential to prove that the system (2.22) is hyperbolic and to calculate the characteristic propagation speed of the system. The hyperbolic property can be proved easily, i.e. by definition we need to rewrite the system into the canonical form and calculate the eigenvalues of coefficient matrix \( A^{ab} \in \mathbb{R}^{n \times n} \) [31]. The canonical form reads as

\[
\partial_t u^a + A^{ab} \partial_x u^b + B^{ab} u^b = F,
\]

(2.24)

where \( u^a \in \mathbb{R}^n \) denotes the vector of variables and \( F(t, x) : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}^n \) is an arbitrary piecewise continuous function. If the coefficient matrix \( A^{ab} \) can be diagonalized and its eigenvalues are real then the system is hyperbolic. If all of the eigenvalues are different then the system is strictly hyperbolic; if the matrix \( A^{ab} \) is symmetric, the system is called symmetric hyperbolic. If any of the eigenvalues are infinite, the system is parabolic. Here \( u^a = (T, q, Q) \), \( F = 0 \) and the non-zero eigenvalues of matrix \( A \) are

\[
\zeta_{1,2} = \pm \frac{-\rho c \kappa_{12} \kappa_{21} + \lambda \tau_Q}{\rho c \tau_q \tau_Q},
\]

(2.25)

if these are finite, therefore the system (2.22) is hyperbolic. The \( \zeta_{1,2} \) values are identical to the characteristic propagation speeds described by (2.22).

### 2.1.2 Lower order models

Here, beside the introduction of other extended models I present the characteristic solutions of each heat conduction equation for a heat pulse experiment. The detailed description of such experiment will be shown later. Nevertheless, the main features of these models can be demonstrated. These results are based on my previous work [3]. The following assumptions lead us to well-known constitutive equations.

- **Fourier equation** [32]: The simplest and most widely used model in engineering applications; \( n = m_1 = m_2 = k_2 = 0 \) and \( k_{12} = 0 \) yields:

\[
l_1 q = \partial_x \frac{1}{T}.
\]

(2.26)

By the differentiation of the reciprocal temperature on the right-hand side and division by \( l_1 \) yields

\[
q = -\frac{1}{l_1 T^2} \partial_x T,
\]

(2.27)
where one can define the Fourier thermal conductivity coefficient as \( \lambda = \frac{1}{l_T} \). Substitution into the energy balance (2.1) leads to

\[
\partial_t T = \alpha \partial_{xx} T, \tag{2.28}
\]

where \( \alpha = \frac{\lambda}{\rho c} \) stands for the thermal diffusivity, \( \rho \) is the mass density and \( c \) is the specific heat. Here we have assumed that \( \lambda, \rho \) and \( c \) are constants. The most often mentioned problem of Fourier’s law is its parabolic property, physically related to the infinite speed of signal propagation. It can be demonstrated by following the reasoning of Fichera [33]. Let us assume an infinite one dimensional space with a unit disturbance\(^1\) at \( x = 0 \) and \( t = 0 \). Then one can find a solution for \( t > 0 \) at any space and time as

\[
T(x,t) = \frac{1}{2\sqrt{\pi \alpha t}} e^{-\frac{x^2}{4\alpha t}}, \tag{2.29}
\]

where for any \( |x| \) and \( t > 0 \) the \( T(x,t) > 0 \) follows. That is the temperature changes immediately after an initial disturbance at any distance. This property seems contradictory against our physical sense but this law is still working in most of the engineering tasks. Fichera also emphasizes as a concluding remark that Fourier’s theory has a limited validity and also the sensitivity of a thermometer is limited, too [33].

It is worth to mention that this solution can be found by a simple observation of self-similarity which leads to this fundamental solution of Fourier equation [35]. One can notice also, this is a Gaussian function, the normalization is required to satisfy the conservation of energy and further solutions with given initial data \( T(x,0) \) can be calculated by a convolution with this Gaussian kernel.

**Remark 1:** In physics, such solution corresponds to Brownian motion or random walk which is interesting because the heat equation is deterministic but the random walk is stochastic. Einstein also analyzed this problem in this respect [36,37]. Its further analysis points far beyond the topic of this thesis.

**Remark 2:** The special relativistic reformulation of the Fourier equation is still parabolic; therefore the signal propagation speed remains infinite in the previous sense. Moreover, in hyperbolic models it is always finite but can be higher than the speed of light. The causality is not related to the propagation speed [38]. The relativistic physics, introducing energy-momentum does not help, the special relativistic extension of the classical Navier-Stokes-Fourier system, called Eckart theory [39] is unstable and the stability problem comes from the Fourier part. Therefore, higher order theories like Maxwell-Cattaneo-Vernotte one, must be applied in relativistic framework. Such theory is the Israel-Stewart theory [40,41], but its mathematical structure makes it difficult to prove the stability and the hyperbolicity of the system. In this respect, it is easier to deal with divergence type models such as one by Liu et al. [42] and Ruggeri [43]. This model is analyzed further and extended by Geroch and Lindblom [44].

**Remark 3:** According to P. M. Mariano, a strict mathematical treatment of microstructural processes can lead to an extension of balance equation of internal energy and results finite speed of signal propagation [45,46].

\(^1\)In a more general way, this disturbance can be represented by a Dirac distribution and its solution corresponds to the Green function of (2.28) [34].
Characteristic solution: Figure 2.1 shows the expected temperature history from a heat pulse experiment. Such curve is used to determine the thermal diffusivity of a material, for details see [47].

Figure 2.1: A typical solution for Fourier equation [3].

- Maxwell–Cattaneo–Vernotte equation (MCV): This model is the simplest extension of Fourier’s law and at very low temperature – at the order of 10 K – it can model the phenomenon of second sound, i.e. the wave nature of heat propagation. This model appears already in [48], and proposed by Cattaneo [49] and Vernotte [50] on different grounds. From the point of view of non-equilibrium thermodynamics the fundamental assumption to obtain MCV equation is the quadratic extension of the entropy density (2.4). It was proposed by Gyarmati [51, 52]. If

\[ n = k_2 = m_2 = k_{12} = 0 \]

in (2.19) the MCV equation follows:

\[ m_1 \partial_t q + l_1 q = \partial_x \frac{1}{T}. \]  

(2.30)

Compared to the Fourier case, there is a new parameter, the relaxation time for the heat flux, i.e. \( \tau_q = \frac{m_1}{l_1} \):

\[ \tau_q \partial_t T + \partial_x T = \alpha \partial_{xx} T. \]  

(2.31)

While equation (2.30) can be derived on various ways without a complete thermodynamic theory, it is paradoxical. E.g. Barletta, Zanchini, Dedeurwaerdere et al. show that the MCV equation with local equilibrium is controversial, because approaching the equilibrium, entropy is decreasing [53-55]. Nevertheless, this problem can be solved by using the generalized entropy (2.4) [52, 56]. A related observation is due to Taitel who considered wave like temperature equilibration looking paradoxical [57]. These aspects are analyzed by Barletta and Zanchini [53]. This form of the paradox is not solved [58, 59]. It must be noted here that Taitel himself in [57] derive the MCV equation with Taylor series expansion.
For (2.31), \( u^i = (T, q) \) and the eigenvalues of \( A \) are \( \zeta_{1,2} = \pm \sqrt{\frac{\alpha}{\tau_q}} \), i.e. the signal propagation speed is finite and it depends on the relaxation time and thermal diffusivity. It can be greater than the speed of light [38]. When \( \tau_q \) tends to zero then (2.31) tends to Fourier equation and the propagation speed also goes to infinite.

**Characteristic solution:** The figure 2.2 shows a wave front in the solution. The peak is not always apparent. It can be predicted directly with the characteristic propagation speed.

![Rear side temperature](image)

**Figure 2.2:** A typical solution for MCV equation [3].

- **Guyer–Krumhansl equation** (GK): This equation is used for evaluating our measurements, discussed in chapter 4. The GK equation can be obtained when \( n = m_2 = 0 \):\[
-K \partial_{xx} q + m_1 k_1 \partial_t q + k_1 l_1 q = k_1 \partial_x \frac{1}{T}, \quad (2.32)
\]
\[
- \kappa^2 \partial_{xx} q + \tau_q \partial_t q + q = -\lambda \partial_x T. \quad (2.33)
\]

After the same steps of the rearrangement of parameters, one can define the dissipation coefficient as \( \kappa^2 = \frac{\kappa}{k_1 l_1} \), it is nonnegative due to (2.18). In the theory of extended thermodynamics, in the particular case of rarefied gases with a particular micromechanism of heat conduction, this dissipation coefficient is related to the mean free path by the Knudsen number \( Kn = \frac{l}{L} \), where \( l \) is the mean free path and \( L \) is the reference length of the sample. Then the differential equation for temperature (2.31) is extended by a mixed derivative,

\[
\tau_q \partial_{tt} T + \partial_t T = \alpha \partial_{xx} T + \kappa^2 \partial_{txx} T. \quad (2.34)
\]

**Characteristic solution:** Figure 2.3 shows the unique feature of GK equation: it covers the transition from under-damped (MCV-like region) to over-damped (over-diffusive region, see chapter 4 and 5 later) solutions through the classical one.
Jeffreys-type thermodynamical equation (JE): if \( n = m_1 = k_2 = k_{12} = 0 \), then:

\[
m_2 l_1 \partial_t q + l_1 k_1 q = k_1 \partial_x \frac{1}{T} + m_2 \partial_{xt} \frac{1}{T}.
\]  

(2.35)

It should be noted that the relaxation time in this case is different from the previous one, because \( \tau = \frac{m_2}{k_1} \) is not identical to \( \tau_q \) considering that background, that is

\[
\tau \partial_t q + q = -\lambda \partial_x T - \chi^2 \left( \partial_{xt} T - \frac{2}{T} \partial_x T \partial_t T \right),
\]  

(2.36)

where \( \chi^2 = \frac{m_2}{k_1 k_{12}} > 0 \) because of (2.18). This is a nonlinear equation but the last term may be neglected and the obtained equation is

\[
\tau \partial_t q + q = -\lambda \partial_x T - \lambda \tau \partial_{xt} T.
\]  

(2.37)

This is similar to the so-called dual phase lag (DPL) model, except that there the two relaxation times are not identical. We considered equation (2.36) as a thermodynamic consistent version of DPL. When \( \lambda \) and \( \tau \) are constants one can easily obtain the differential equation for the temperature. This is identical to (2.34) in one spatial dimension.

The DPL model is popular because of its simple derivation. Tzou [61] proposed it in order to account time delay effect. The goal is to generalize the single phase lag concept and introduce two phase lags both in the temperature gradient and heat flux. As we have mentioned above the single phase lag theory contradicts basic principles. DPL equation in 1+1 D is derived by Taylor series expansion, taking the constitutive equation

\[
q(x, t + \tau_q) = -\lambda \partial_x T(x, t + \tau_T),
\]  

(2.38)

where \( \tau_q > 0 \) and \( \tau_T > 0 \) represent the relaxation times of the heat flux and temperature gradient and \( \lambda \) is the thermal conductivity. Then a Taylor series expansion gives:

\[
q(x, t) + \tau_q \partial_t q(x, t) \approx -\lambda \left( \partial_x T(x, t) + \tau_T \partial_{xt} T(x, t) \right).
\]  

(2.39)
The higher order terms are simply neglected. In this case, there is no relation between the relaxation times. There exists other versions of DPL, too, namely the "type 2 DPL" (DPL2) and "type 3 DPL" (DPL3). In these extensions the Taylor series expansion is continued. In case of DPL2, the constitutive equation according to [62,63] reads as

\[ q(x,t) + \tau_q \partial_t q(x,t) = -\lambda \left( \partial_x T(x,t) + \tau_T \partial_{xx} T(x,t) + \frac{\tau_T^2}{2} \partial_{tx} T(x,t) \right). \] (2.40)

The DPL3 model is extended by the second order time derivative of the heat flux:

\[ q(x,t) + \tau_q \partial_t q(x,t) + \frac{\tau_q^2}{2} \partial_{tt} q = -\lambda \left( \partial_x T(x,t) + \tau_T \partial_{xx} T(x,t) + \frac{\tau_T^2}{2} \partial_{tx} T(x,t) \right). \] (2.41)

The higher order terms are not able to improve the model because they are not based on the second law and lead to inconsistencies [64–66]. Moreover, instead of improvement with these terms, it is more difficult to solve the model. Examples are demonstrated in chapter 5.

In the literature DPL-type constitutive equations are analyzed in order to prove the uniqueness and well-posedness of a process driven by such constitutive equations. It is found by Fabrizio et al. [67–69] that there are mathematical conditions beyond the physical ones to obtain an exponentially stable equilibrium solution for DPL equation. That is, the DPL equation is a wrong model without any further ado. However, such condition requires negative time delay (called as retarded effect) between the heat flux and temperature gradient, i.e. \( \tau_q - \tau_T \leq 0 \) which excludes the opposite case. It is important because Tzou in [70] directly interprets both case with the cause – effect concept, i.e. the quantity with the higher relaxation time is the effect caused by the other one. As Fabrizio states [67], the DPL model can be rewritten with the time delay difference \( \tau_d := \tau_q - \tau_T \) which leads to a single phase lag model but here the temperature gradient have a relaxation time, with \( \tau_d < 0 \). The opposite case is mathematically ill-posed which enlightens the validity of MCV equation but excludes equations based on arbitrary Taylor series expansion. Quintanilla et al. [71,72] obtains the same conclusion regarding the relaxation times and the ill-posedness.

- **Green–Naghdhi equation** (GN): Two variations exist, the general one and the simple one. The common feature is that both require to assume Casimir-type reciprocity relation (antisymmetric conductivity matrix) in our framework. Here the simple GN equation is discussed only which can be derived with the parameters of \( n = m_2 = l_1 = 0 \),

\[-K \partial_{xx} q + m_1 k_1 \partial_t q = k_1 \partial_x \frac{1}{T},\] (2.42)

\[-\kappa^2 \partial_{xx} q + \tau_q \partial_t q = -\lambda \partial_x T.\] (2.43)

The parameters are the same as in the GJ equation. A further interesting feature is that in reversible case – when entropy production is zero – it can produce heat propagation when using the \( J^i = \frac{\partial q}{\partial T} \) classical formula for the entropy flux. It leads to a particular dissipative wave equation for the temperature:

\[ \tau_q \partial_t T = \alpha \partial_{xx} T + \kappa^2 \partial_{txx} T. \] (2.44)
**Characteristic solution:** Figure 2.4 shows the clear sign of wave propagation. The damping influence of the mixed derivative term in (2.44) appears in the solution as decreasing wave amplitude.

![Figure 2.4: The typical solutions for GN equation [3].](image)

- **Cahn–Hilliard type extension:** if \( n = m_1 = m_2 = 0 \) holds, we obtain:
  
  \[
  k_1 l_1 q - K \partial_{xx} q = k_1 \partial_x \frac{1}{T},
  \]

  \[
  q - \kappa^2 \partial_{xx} q = -\lambda \partial_x T.
  \]

  This is similar to the hypertemperature model of Forest and Amestoy except a sign [73]. This model is not discussed further.

- **Generalized equation:** if \( n = m_1 = 0 \) holds and \( Q \) is eliminated, one obtains the generalized equation:
  
  \[
  m_2 l_1 \partial_t q - m_2 k_2 \partial_{xt} q - K \partial_{xx} q + l_1 k_1 q = k_1 \partial_x \frac{1}{T} + m_2 \partial_{xt} \frac{1}{T}.
  \]

  Ván and Fülöp have derived the same equation without \( Q \) [74].

We mention here two other theories due to their different point of view. Wang and Guo derived a non-Fourier equation with the help of thermomass theory [66, 75, 76]. It is inspired by Tolman’s theory, which states the existence of heat - mass duality in the frame of general relativity, which means that heat propagation also has some kind of inertia [77].

The second one is connected to the work of Cimmelli and Kosiński [78–80]. A scalar internal variable, \( \beta \), is introduced there, which is connected to the absolute temperature \( \Theta \) by the following kinetic equation:

\[
\tau \dot{\beta} + \beta = \Theta,
\]
where $\tau$ is the relaxation time, $\Theta$ is the absolute temperature and the Fourier’s law is modified as

$$q = -k(\Theta, \beta)\nabla\beta,$$

(2.49)

here the thermal conductivity is a function of these different temperatures. It leads to a hyperbolic evolution equation to the non-equilibrium temperature and $\beta$ is called semi-empirical temperature. This approach is used to calculate low temperature phenomena such as second sound by Frischmuth and Cimmelli [81–83]. Later a coupled thermo-mechanical model is constructed with using this semi-empirical equation [84].

### 2.2 Relation to the kinetic theory

Non-equilibrium thermodynamics is expected to be compatible with kinetic theory. This compatibility is not trivial when considering the complete hierarchy of the moment series, and usually considered from the point of view of kinetic theory only: how could we construct a viable set of continuum evolution equations from the known phase field evolution. Interestingly, these attempts failed to give a satisfactory result. Higher than second-order levels the different series expansions turn out to be unstable [85, 86]. In this work we start from the other way around. What are the particular restrictions in a non-equilibrium thermodynamic framework that lead to a hierarchical system of evolution equations? The thermodynamic approach can warrant stability. In this section we investigate the problem in single component fluids, but first focus on the particular case of heat conduction. The kinetic theory of heat conduction is presented and compared to the ballistic-conductive model. Then the kinetic theory based extended thermodynamical (ET) theory is presented in case of dense gases according to [87–89]. In the following, in our non-equilibrium thermodynamic theory, the same generalizations and extensions from the ballistic-conductive model will be used to obtain the rarefied gas model from kinetic theory.

There are two theories of continua that extend the validity of classical irreversible thermodynamics and propose a system of equations which is expected to be compatible with kinetic theory. The first one is called Extended Irreversible Thermodynamics (EIT), the second one is called Rational Extended Thermodynamics (RET). For EIT, the relation to kinetic theory is weak. The compatibility is not strictly required, e.g. the material coefficients are not calculated. The state space is extended with the fluxes, these are treated as independent variables. It is in agreement with Grad’s 13-moment theory [90]. The classical entropy current is not extended. For RET, the compatibility with kinetic theory is strict and continuum evolution equations are derived including all coefficients.

The theory of internal variables is more general than the EIT and the compatibility can be easily achieved by choosing the heat flux for an internal variable as it is already suggested [8, 9, 91]. Here we generalized the entropy flux with Nyíri multipliers which is more general than the one used in EIT or RET.

**Remark:** In the following, my goal was to investigate the role of Nyíri multipliers, how they influence the constitutive equations regarding the coupling between different tensorial order quantities. Furthermore, I used the same generalization of entropy density and entropy current density as in the ballistic-conductive model to derive a model of rarefied gases.
2.2.1 Heat conduction in the framework of kinetic theory

It is surprisingly complicated to model heat conduction with particles. The first reasonable model was a system consisting of point-like masses which are connected by springs. However, ideal springs lead to wavelike propagation. The numerical solution [92,93] of such system with nonlinear springs gives non-dissipative description with solitons. It is also analyzed by Zabusky, Kruskal and Rosenau [94–96]. Moreover, Michel et al. can present a diffusive type energy transport solution for a 1D quantum system [97]. Landau call attention to the anharmonical vibrations of an atom in crystal lattice, particularly these kinds of vibrations should be considered in the description of heat conduction [98]. According to Ashcroft and Mermin, the strictly harmonic crystals have infinite thermal conductivity and the anharmonic vibrations cause finite speed of energy propagation [99].

There is another approach with phonons, quasi-particles of lattice vibrations that emphasizes statistical physics, this approach leads to phonon hydrodynamics [100]. The interactions between phonons can be classified as [19,101]:

- Normal (N) processes: the total momentum of phonons is conserved during the interaction,
- Resistive (R) processes: the opposite of N processes, total momentum is not conserved.

Common in both cases is that the energy is conserved during the interactions. A third type, called as Umklapp process also exists where neither the energy nor the momentum is conserved [19]. The thermal conductivity $\lambda$ is expected to be in connection with R processes and their frequencies $\frac{1}{\tau_R}$, i.e.

$$\lambda = \frac{c^2}{3} c_v \tau_R,$$

(2.50)

where $c$ is the Debye speed of phonons, $c_v$ is the isochoric specific heat, and $\tau_R$ is the characteristic time of the R processes. The Debye speed is calculated in the following way [101]:

$$\frac{3}{c^3} = \sum_{\alpha=1}^{3} \frac{1}{c_{\alpha}^3},$$

(2.51)

where $\alpha$ is related to the different propagation modes as $\alpha = 1$ means longitudinal propagation and $\alpha = 2; 3$ stands for the two transversal propagation modes; $c_{\alpha}$ is the corresponding propagation speed. In this approach, Fourier’s law can be applied only when the R processes are significantly dominant which results the diffusive kind of heat propagation. However, if one decreases the temperature then N processes become dominant and the wave nature of heat conduction reveals itself. The Fourier’s law is modified and one can derive the MCV equation [101]:

$$\frac{\partial Q_i}{\partial t} + \frac{c^2}{3} c_v \frac{\partial T}{\partial x_i} = -\frac{1}{\tau_R} Q_i,$$

(2.52)

where $Q_i$ is the heat flux. There is a third mechanism of heat transport, the energy transport by ballistic phonons. In case of ballistic propagation there is no interaction between phonons, these particles just go through the sample without colliding. In order to include these propagation modes into phonon hydrodynamics, one needs to distinguish
between the phase density for the R and N processes. The resistive processes tend to the function \( f_R \) and the normal processes tend to the distribution function \( f_N \):

\[
\begin{align*}
    f_R &= \frac{y}{\exp\left(\frac{\hbar k}{k_B T} - 1\right)}, \\
    f_N &= \frac{y}{\exp\left\{\frac{\hbar k}{k_B T} \left(1 - \frac{3}{4} \frac{c p_i n}{4 \pi T^4}\right)\right\} - 1},
\end{align*}
\]

where \( \hbar \) is the Planck constant, \( k_B \) is the Boltzmann constant, \( k \) denotes the wavenumber, \( n_i \) is the unit vector in the direction of \( k \), \( p_i \) is the momentum, \( y \) is a constant \( y = 3/(8\pi^3) \), \( a \) is also a constant, see below. The temperature \( T \) is defined as the energy density by Debye law for phonons \([101]\):

\[
e = a T^4; \quad a = \frac{4\pi^5}{5} \frac{k_B^4}{\hbar^3 c^3}.
\]

The phase density \( f \) evolves according to the Boltzmann equation,

\[
\partial_t f + c n_i \partial_i f = \hat{S},
\]

where \( \hat{S} \) is the production of phase density, the so-called collision integral. In the Callaway model these different distributions \( f_R \) and \( f_N \) are considered and combined in relaxation terms:

\[
\hat{S} = -\frac{1}{\tau_R} (f - f_R) - \frac{1}{\tau_N} (f - f_N).
\]

This assumption implies that two different equilibrium distributions exist in this system. Instead of solving the Boltzmann equation, one can approximate the solution by momentum series expansion. It leads to a system of momentum equations and introduce new quantities this way:

\[
u_{\langle i_1 i_2 \ldots i_N \rangle} = \int k n_{\langle i_1 \ldots i_n \rangle} f dk. \tag{2.58}
\]

Here \( \langle \cdot \rangle \) denotes the traceless symmetric part of a tensor. The first momentum is the energy density, the second one is the momentum density, the third one is the energy flux and the fourth one is the deviatoric part of the pressure tensor \([19]\), i.e.

\[
e = h c u; \quad p_i = h u_i; \quad Q_i = h c^2 u_i; \quad N_{ij} = h c u_{ij}. \tag{2.59}
\]

Let us note that this method leads to a system with infinite number of equations. One of the central problems of kinetic theory is how to close this system. Several techniques exist both for the expansion and also for the closure \([102]\). For heat conduction one applies the simplest one, neglecting the highest order flux, truncating the series, i.e. the new highest order \( \sim N + 1^{th} \) quantity is considered as zero. One obtains the following system of partial differential equations in 1+1 dimensions:

\[
\frac{\partial u_{\langle n \rangle}}{\partial t} + \frac{n^2}{4n^2 - 1} c \frac{\partial u_{\langle n-1 \rangle}}{\partial x} + c \frac{\partial u_{\langle n+1 \rangle}}{\partial x} = \begin{cases} 
0, & n = 0 \\
-\frac{1}{\tau_R} u_{\langle 1 \rangle}, & n = 1 \\
-\left(\frac{1}{\tau_R} + \frac{1}{\tau_N}\right) u_{\langle n \rangle}, & 2 \leq n \leq N
\end{cases} \tag{2.60}
\]

One has to apply \( N \approx 30 \) equations to obtain a good approximation of the ballistic propagation speed of phonons. Naturally, it is difficult to solve (2.60) for practical problems,
but \( N = 3 \) equations give an acceptable approximation, while one accepts that the predicted value of the ballistic propagation speed is not correct. For \( N = 3 \) we obtain a 3 field theory:

\[
\begin{align*}
\partial_t e + c^2 \partial_x p &= 0, \\
\partial_t p + \frac{1}{3} \partial_x e + \partial_x N &= -\frac{1}{\tau_R} p, \\
\partial_t N + \frac{4}{15} c^2 \partial_x p &= -\left( \frac{1}{\tau_R} + \frac{1}{\tau_N} \right) N.
\end{align*}
\]

(2.61)

If one considers \( n = k_2 = 0 \) in our general continuum model, when most of the dissipative terms are zero, the ballistic-conductive system (2.22) is obtained with equivalent structure. The relation of kinetic theory parameters and the phenomenological ones are [2]:

\[
q = c^2 p; \quad Q = N; \quad \frac{1}{\tau} = \left( \frac{1}{\tau_R} + \frac{1}{\tau_N} \right) \rightarrow \tau_q = \tau_R; \quad \tau_Q = \tau,
\]

(2.62)

\[
\lambda = \frac{\tau_R}{3} \rho c_v c^2 \rightarrow c^2 = \frac{3 \lambda \kappa_{12} \kappa_{21}}{\tau_q \rho c_v}; \quad -\kappa_{12} \kappa_{21} = \frac{4}{15} \tau_q \tau_Q c^2,
\]

(2.63)

Comparing the coefficients and variables of the two models, one can identify the internal variable \( Q \) as the current density of the heat flux. The “\( N=3 \)” case contains two parameters, i.e. the relaxation times can be fitted to a particular experiment. In the ballistic-conductive equation, there are three parameters. However, the parameter \(|k_{21}|\) can be calculated directly to obtain the measured ballistic propagation speed thus two parameters remain to fit.

### 2.2.2 Generalization of classical fluid mechanics

The goal of the generalization is to study the irreversible processes that are coupled to the propagation of sound, especially close to a shock wave. The mass density \( \rho \) is not constant any more. In the following, the extended thermodynamical background of Meixner’s theory [103] is presented.

**Remark:** These are my latest results, the manuscript is under preparation. Although this section is mostly based on the literature, I used only the corresponding ideas and basic equations and I have performed all the connected calculations except the subsection regarding the RET theory of rarefied gases.

**Meixner’s theory**

The balance equation of the mass density:

\[
\dot{\rho} + \rho \partial^i v^i = 0,
\]

(2.64)

where the upper dot denotes the material time derivative. The balance equation of the total energy:

\[
\rho \dot{e}_T + \partial^i \dot{q}^i = 0,
\]

(2.65)

where \( e_T \) is the total energy, i.e. \( e_T = e + \rho v^2 / 2 \), \( v \) is the velocity and \( e \) is the internal energy and the caloric equation of state is \( e = cT \). Here the flux of the total energy is

\[
\dot{q}^i = q^i + v^i P^{ij},
\]

(2.66)
where $P^{ij}$ denotes the pressure tensor and $q^i$ is the flux of the internal energy. The balance of internal energy is

$$\rho \dot{e} + \partial^i q^i = -P^{ij} \partial^j v^j.$$  \hfill (2.67)

We need also the balance of momentum:

$$\rho \dot{v}^i + \partial^j P^{ij} = 0,$$  \hfill (2.68)

where the pressure tensor can be decomposed to static and dynamic parts as

$$P^{ij} = \Pi^{ij} + p \delta^{ij},$$  \hfill (2.69)

where $p$ is the hydrostatic pressure. Meixner’s theory [13,103] is also based on an internal variable. The goal is to generalize the Navier-Stokes equation with a tensorial internal variable $\xi^{ij}$ in entropy density. After simplifying the isotropic form it is

$$s(e, \rho, \xi^{ij}) = s_{eq}(e, \rho) - \frac{m_1}{2} \xi^{ij} \xi^{ij},$$  \hfill (2.70)

where $s_{eq}$ corresponds to term of local equilibrium, beside the classical form of entropy current $J^i = q^i / T$, one can calculate the entropy production. The corresponding Gibbs relation is:

$$de = T ds - pdv - A^{ij} d\xi^{ij} = T ds + \frac{p}{\rho^2} d\rho - A^{ij} d\xi^{ij},$$  \hfill (2.71)

where $v = 1/\rho$ is used and $A^{ij} = T \partial_{\xi^{ij}} s = -T m_1 \xi^{ij}$ is the affinity of the internal variable.

$$\sigma_s = \rho s + \partial^i J^i = \rho \left( \partial^i s e^i + \partial^i \rho \dot{\rho} + \partial^i \xi^{ij} s \xi^{ij} \right) + \left( \partial^i \frac{1}{T} q^i + \frac{1}{T} \partial^i q^i \right) \geq 0.$$  \hfill (2.72)

The separation of thermodynamic fluxes and forces are given in Table 2.2.

<table>
<thead>
<tr>
<th>Fluxes</th>
<th>Thermal</th>
<th>Fluid</th>
<th>Internal</th>
</tr>
</thead>
<tbody>
<tr>
<td>$q^i$</td>
<td>$\Pi^{ij}$</td>
<td>$-\rho m_1 \dot{\xi}^{ij}$</td>
<td></td>
</tr>
</tbody>
</table>

| Forces | $\partial^i \frac{1}{T}$ | $-\frac{1}{T} \partial^i v^j$ | $\xi^{ij}$ |

Table 2.2: Thermodynamic fluxes and forces

Here the evolution equation of the internal variable is to be constructed according to thermodynamic requirements. After the elimination of internal variable the linear solution of the entropy inequality (2.72) in 1 spatial dimension [14]:

$$q + \lambda \partial_x T = 0,$$

$$\tau_{\Pi} \dot{\Pi} + \nu \partial_x v + \dot{\phi} \partial_x \dot{v} = 0,$$  \hfill (2.73)

where $\nu$ is the viscosity, $\phi$ is a material parameter, $\tau_{\Pi}$ is the relaxation time corresponding to the viscous dynamic pressure $\Pi$ and the heat conduction equation is preserved in its classical - parabolic - form and there is no coupling between the dynamic pressure and the heat flux. The Navier-Stokes equation is extended to a JE-type form. For comparison,
let us apply the ideal gas thermal equation of state i.e. \( p = a \rho T \) and putting down the corresponding 1+1 D balances (2.64), (2.67) and (2.68), too:

\[
\begin{align*}
\dot{\rho} + \rho \partial_x v &= 0, \\
\rho \dot{v} + \partial_t \Pi + a\rho \partial_x T + aT \partial_x p &= 0, \\
\rho cT + \partial_x q + (\Pi + a\rho T) \partial_x v &= 0, \\
q + \lambda \partial_x T &= 0, \\
\tau \dot{\Pi} + \Pi + \nu \partial_x v + \phi \partial_x \dot{v} &= 0,
\end{align*}
\]

(2.74) where \( a \) is the ratio of the Boltzmann constant and the mass of the molecule, i.e. \( a = k_B/m \) in a single component ideal gas. System (2.74) consists of the equations of Meixner’s theory in 1 spatial dimension.

**Extension of Meixner’s theory by Rational Extended Thermodynamics**

In the following, the calculation of Arima et al. [87–89] is presented with preserving their notation regarding the indices. Rational Extended Thermodynamics introduces a parallel hierarchy of energy and momentum, namely "F-series" and "G-series" as balance laws of dense gases:

\[
\begin{align*}
\partial_t F + \partial_k F_k &= 0, \\
\partial_t F_i + \partial_k F_{ik} &= 0, \\
\partial_t F_{ij} + \partial_k F_{ijk} &= P_{ij}, \\
\partial_t G_{ii} + \partial_k G_{iik} &= 0, \\
\partial_t G_{ppi} + \partial_k G_{ppik} &= Q_{ppi},
\end{align*}
\]

(2.75) where \( F(=\rho) \) is the mass density, \( F_i(=\rho v_i) \) is the momentum density, \( F_{ij} \) is the momentum flux (the total pressure), \( G_{ii} \) is the energy density and \( G_{ppi} \) stands for the energy flux. The quantities \( F_{ijk} \) and \( G_{ppik} \) are the fluxes of the corresponding density, \( P_{ij} \) and \( Q_{ppi} \) are the production terms. According to [87,104], this structure fulfills the conditions of material frame indifference (objectivity), entropy balance and causality; furthermore, the provided 14-field theory cannot be obtained by a theory with multiple internal variables.

The derivation of the constitutive equations is omitted here due to its complexity. The obtained system reads as

\[
\begin{align*}
\dot{\rho} + \rho \partial_k v_k &= 0, \\
\rho \dot{v} + \partial_t p + \partial_t \Pi - \partial_j S_{(ij)} &= 0, \\
\rho (\partial_T \varepsilon)_p \dot{T} + \left[p + \Pi - \rho^2 (\partial_T \varepsilon)_T \right] \partial_k v_k - \partial_k v_i S_{(ik)} + \partial_k q_k &= 0, \\
S_{(ij)} - 2p \partial_{(j} v_{i)} + S_{(ik)} \partial_k v_k - 2\Pi \partial_{(j} v_{i)} + 2\partial_{(j} v_{i)} S_{(j)k} - q_{(i} \partial_{(j)} K - K \partial_{(j} q_{i)} = -\frac{1}{\tau_S} S_{(ij)}, \\
\dot{\Pi} - \frac{2\hbar^2}{T} \partial_k v_k + \left(\frac{5}{3} - \frac{\partial_T p}{\rho \partial_T \varepsilon}\right) \Pi \partial_k v_k - \left(\frac{2}{3} - \frac{\partial_T p}{\rho \partial_T \varepsilon}\right) \partial_{(k} v_{i)} S_{(ik)} + \\
+ q_k \partial_k L + \left(L - \frac{\partial_T p}{\rho \partial_T \varepsilon}\right) \partial_k q_k = -\frac{1}{\tau_H} \Pi,
\end{align*}
\]
\[ \dot{q}_j + \left( 1 + \frac{K}{2} \right) q_j \partial_k v_k + \frac{K}{2} q_k \partial_j v_k + \left( 1 + L - \frac{K}{3} \right) q_k \partial_k v_j - \]
\[ - \frac{h_4}{27 T^2} \partial_j T + \frac{h_4}{2 h_2} \left( L - \frac{\partial_T p}{\rho T \varepsilon} \right) \partial_j \Pi - \frac{h_4}{4 h_3} K \partial_k S_{(jk)} + \]
\[ + \Pi \left[ \left\{ \partial_j \varepsilon - \frac{p}{\rho^2} - \partial_j \left( \frac{h_4}{4 h_2} \left( L - \frac{\partial_T p}{\rho T \varepsilon} \right) \right) \right\} \partial_j \rho \right] + \]
\[ \Pi \left[ \left\{ \partial_j \varepsilon + \partial_T \left( \frac{h_4}{4 h_2} \left( L - \frac{\partial_T p}{\rho T \varepsilon} \right) \right) \right\} \partial_j T - \frac{1}{\rho} \partial_j \Pi + \frac{1}{\rho} \partial_k S_{(jk)} \right] - \]
\[ - S_{(jk)} \left[ \left\{ \partial_j \varepsilon - \frac{p}{\rho^2} + \partial_j \left( \frac{h_4}{4 h_3} K \right) \right\} \partial_k \rho + \left\{ \partial_T \varepsilon + \partial_T \left( \frac{h_4}{4 h_3} K \right) \right\} \partial_k T \right] - \]
\[ + S_{(jk)} \left[ -\frac{1}{\rho} \partial_k \Pi + \frac{1}{\rho} \partial_i S_{(ik)} \right] = -\frac{1}{\tau_q} q_j, \quad (2.76) \]

where the notation around the indexes ( ) denotes the deviatoric part of a tensor, upper dot denotes the material time derivative, \( \tau_S, \tau_\Pi \) and \( \tau_q \) are the relaxation times, the coefficients \( h_2, h_3, h_4, L, K \) are functions of \( \rho \) and \( T \) and introduced during the derivation. Furthermore, \( S_{ij} \) is the viscous stress tensor and \( \Pi \) denotes the dynamic pressure, \( \Pi = -P/3 \varepsilon \) is the density of internal energy. The relationship between ET and the classical Navier-Stokes-Fourier can be analyzed by Maxwellian iteration and the material parameters from classical equations can be obtained. Thus, the independent variables are \( \rho, v_i, T, S_{(jk)}, \Pi, q_i \). As one can see, the resulted system is complicated. A simplified theory is constructed with 6 fields (ET6) by Arima et al. [104] where the viscous stress tensor \( S_{ij} \) is neglected as a variable. The ET6 model is compared to Meixner’s theory and found to be fully compatible [104], moreover the non-equilibrium temperature and internal variable from Meixner’s theory can be expressed explicitly with the given macroscopic variables from ET. The 6-field theory provides the simplest hyperbolic system which takes in account the dissipation phenomena. In (2.76) the different nonlinearities are mixed from the point of view of a continuum approach. E.g. several terms are due to the explicit expression of thermostatic state functions and several other terms are not interpreted \( (h_2, h_3, h_4, L, K) \). Moreover, only the linear approximation of the theory is compared to experiment. Therefore, we also restrict this comparative study to the linear version.

Let us consider the linearized form of the system (2.76) around the equilibrium state \( \rho = \rho_0, v_i = 0, T = T_0, S_{(jk)} = 0, \Pi = 0, q_i = 0 \). System (2.76) is reduced to the form below,

\[ \dot{\rho} + \rho_0 \partial_k v_k = 0, \]
\[ \rho_0 \dot{v}_i + a T_0 \partial_i \rho + a \rho_0 \partial_i T - \partial_j S_{(jk)} + \partial_i \Pi = 0, \]
\[ a \rho_0 c_v^* T + a \rho_0 T_0 \partial_k v_k + \partial_k q_k = 0, \]
\[ \dot{S}_{(ij)} - 2a \rho_0 T_0 \partial_j (v_i) - \frac{2}{1 + c_v^*} \partial_j q_i = -\frac{1}{\tau_S} S_{(ij)}, \]
\[ \dot{\Pi} + \left( \frac{2}{3} - \frac{1}{c_v^*} \right) a \rho_0 T_0 \partial_k v_k + \frac{2 \rho_0 T_0}{3 c_v^* (1 + c_v^*)} \partial_k q_k = -\frac{1}{\tau_\Pi} \Pi, \]
\[ \dot{q}_i + (1 + c_v^*) a^2 \rho_0 T_0 \partial_i T - a T_0 \partial_k S_{(jk)} + a T_0 \partial_i \Pi = -\frac{1}{\tau_q} q_i, \quad (2.77) \]

where \( c_v^* \) is the dimensionless specific heat, defined as \( c_v^* := c_v a / \rho; \) here \( c_v a / \rho \) is the specific heat corresponding the equilibrium state.
The system (2.77) can be rewritten in 1 spatial dimension:

\[
\dot{\rho} + \rho_0 \partial_x v = 0, \\
\rho_0 \dot{v} + aT_0 \partial_x \rho + \rho_0 \partial_x T + \partial_x \Pi = 0, \\
ap\rho_0 c_v^* \dot{T} + \rho_0 \partial_x v + \partial_x q = 0, \\
\tau_\Pi \dot{\Pi} + \Pi + \nu \partial_x v + \nu \frac{\nu}{1 + c_v^*} \partial_x q = 0, \\
\tau_\varphi \dot{q} + q + \lambda \partial_x T - aT_0 \partial_x \Pi = 0.
\]  

(2.78)

The material parameters, namely the bulk viscosity \(\nu\) and thermal conductivity \(\lambda\) are given as

\[
\nu = \left(\frac{2}{3} - \frac{1}{c_v^*}\right) a\rho_0 T_0 \tau_\Pi; \quad \lambda = (1 + c_v^*) a^2 \rho_0 T_0 \tau_\varphi.
\]

It is clear that in one spatial dimension this theory leads to a more complex and coupled system of equations than it is presented for Meixner’s theory (2.74).

**Extension of Meixner’s theory by Extended Irreversible Thermodynamics**

As it is mentioned, the theory of EIT operates with extending the entropy density only. In Meixner’s theory, there is an internal variable in tensorial order and it does not lead to a generalization of the heat conduction equation. It must be kept in mind that the theory of EIT uses fluxes as extension in the entropy density. Naturally, the result cannot be the same as Meixner’s theory. If one applies an internal variable, a new coupled evolution equation is used as it is presented. The following choice with fluxes leads to hyperbolic type extensions. In order to also generalize the heat equation, the heat flux \(q^i\) is introduced into the entropy density (simplified isotropic form) along with \(\Pi^{ij}\):

\[
s(e, \rho, q^i, \Pi^{ij}) = s_{eq}(e, \rho) - \frac{m_1}{2} q^i q^i - \frac{m_2}{2} \Pi^{ij} \Pi^{ij}.
\]

(2.79)

The extended Gibbs relation reads as

\[
de = T ds + \frac{P}{\rho^2} d\rho - A^i_1 dq^i - A^i_2 d\Pi^{ij},
\]

(2.80)

where \(A^i_1 = T \partial_q s, A^i_2 = T \partial_{\Pi^{ij}} s\) are the affinities. The entropy current is the classical one, furthermore, the balance equations (2.64), (2.65), (2.67) and (2.68) are the same. For entropy production one obtains:

\[
\sigma_s = \rho \dot{s} + \partial^i J^i = \]

\[
-\frac{1}{T} \Pi^{ij} - \rho m_2 \Pi^{ij} \Pi^{ij} - \rho m_1 q^i q^i + q^i \partial_i \frac{1}{T} =
\]

\[
-\Pi^{ij} \left(\frac{1}{T} \partial^i v^j + \rho m_2 \Pi^{ij}\right) + q^i \left(\partial_i \frac{1}{T} - \rho m_1 q^j\right) \geq 0.
\]

(2.81)

The separation of thermodynamic fluxes and forces are given in Table 2.3.

<table>
<thead>
<tr>
<th>Fluxes</th>
<th>Thermal</th>
<th>Fluid</th>
</tr>
</thead>
<tbody>
<tr>
<td>Forcés</td>
<td>(\partial_i \frac{1}{T} - \rho m_1 q^i)</td>
<td>(\frac{1}{T} \partial^i v^j + \rho m_2 \Pi^{ij})</td>
</tr>
</tbody>
</table>

Table 2.3: Thermodynamic fluxes and forces
It results the system below in 1 spatial dimension:

\[ \dot{\rho} + \rho \partial_x v = 0, \]
\[ \rho \dot{v} + \partial_x \Pi + a \rho \partial_x T + aT \partial_x \rho = 0, \]
\[ \rho c \dot{T} + \partial_x q + (\Pi + a \rho T) \partial_x v = 0, \]
\[ \tau_q \dot{q} + q + \lambda \partial_x T = 0, \]
\[ \tau_\Pi \dot{\Pi} + \Pi + \nu \partial_x v = 0, \]

(2.82)

where the MCV-type extensions are obtained for classical constitutive equations. Furthermore, the variable choice for entropy density determines the separation of the thermodynamic fluxes and forces later. There is no coupling between the heat conduction and fluid mechanics, in isotropic materials, according to Curie principle [90].

**Non-equilibrium thermodynamics with internal variables**

As it is demonstrated, the extension of entropy density itself is not enough to obtain coupling between the heat flux and pressure tensor. However, the Nyiri-multipliers open further possibilities within a generalized entropy current. It is analogous with the heat conduction theory leading to the ballistic-conductive equation, where the vectorial internal variable is identified as the heat flux. Let us choose the same set of extension of the state space:

\[ s(e, \rho, q^i, \xi_{ij}) = s_{eq}(e, \rho) - \frac{m_1}{2} q^i q^i - \frac{m_2}{2} \xi_{ij} \xi_{ij}, \]

(2.83)

and the entropy current is

\[ J^i = B^{ij} q^j + C^{ijk} \xi_{jk}. \]

(2.84)

Here \( B^{ij} \) and \( C^{ijk} \) are the current multipliers. A second-order tensorial quantity can be coupled to a vectorial one through the entropy current. It results a similar but richer system of equations: it consists of the same terms as in (2.82) by EIT but also adds extra terms. Hence the hyperbolic equations becomes parabolic GK-type, moreover to obtain the same terms, the resulted system must be simplified. The main difference between hyperbolic and parabolic models is the dissipation. It can be analyzed by dispersion relations and it will be discussed in the chapter of low temperature heat conduction. The Gibbs relation reads as

\[ de = T ds + \frac{p}{\rho^2} d\rho - A_1^i dq^i - A_2^i d\xi^i, \]

(2.85)

where \( A_1^i = T \partial_q s, A_2^i = T \partial_\xi s \) are the affinities corresponding to the heat flux and internal variable, respectively. One can calculate the entropy production:

\[ \sigma_s = \rho \dot{s} + \partial^i J^i = \]

\[ -\frac{1}{T} \Pi^{ij} \partial^i v^j + \partial^i q^j \left( B^{ij} - \frac{1}{T} \delta^{ij} \right) + q^j \left( \partial^i B^{ij} - \rho m_2 q^i \right) + \]
\[ \xi_{jk} \left( \partial^i C^{ijk} - m_1 \rho \dot{\xi}_{jk} \right) + C^{ijk} \left( \partial^i \dot{\xi}^{jk} \right) \geq 0. \]

(2.86)

The separation of thermodynamic fluxes and forces is given in Table 2.4.

<table>
<thead>
<tr>
<th></th>
<th>Thermal</th>
<th>Fluid</th>
<th>Internal I</th>
<th>Internal II</th>
<th>Extended internal</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fluxes</td>
<td>( \partial^i B^{ij} - \rho m_2 q^i )</td>
<td>( \Pi^{ij} )</td>
<td>( B^{ij} - \frac{1}{T} \delta^{ij} )</td>
<td>( \partial^i C^{ijk} - m_1 \rho \dot{\xi}_{jk} )</td>
<td>( C^{ijk} )</td>
</tr>
<tr>
<td>Forces</td>
<td>( q^i )</td>
<td>( -\frac{1}{T} \partial^i v^i )</td>
<td>( \partial^i q^i )</td>
<td>( \dot{\xi}^{ik} )</td>
<td>( \partial^i \dot{\xi}^{jk} )</td>
</tr>
</tbody>
</table>

Table 2.4: Thermodynamic fluxes and forces
Assuming linear relations between the thermodynamic fluxes and forces one realizes coupling between the quantities of same tensorial order:

\[ \partial^i B^{ij} - \rho m_2 \dot{q}^j = k_1 q^j, \]
\[ \Pi^{ij} = l_{11} \xi^{ij} - \frac{l_{12}}{T} \partial^i \xi^j + l_{13} \partial^i q^j, \]
\[ B^{ij} - \frac{1}{T} \delta^{ij} = l_{21} \xi^{ij} - \frac{l_{22}}{T} \partial^i \xi^j + l_{23} \partial^i q^j, \]
\[ \partial^i C^{ijk} - m \rho \dot{\xi}^{jk} = l_{31} \xi^{jk} - \frac{l_{32}}{T} \partial^j \xi^k + l_{33} \partial^j q^k, \]
\[ C^{ijk} = n \partial^i \xi^{jk}. \]

One can eliminate the internal variables easily. In one spatial dimension we obtain:

\[ \dot{\rho} + \rho_0 \partial_x v = 0, \]
\[ \rho \dot{v} + \partial_x (\Pi + p) = 0, \]
\[ \rho c \dot{T} + \partial_x q + (\Pi + p) \partial_x v = 0, \]
\[ \tau_q \dot{q} + q + \lambda \partial_x T - \kappa^2 \partial^2_x q - \delta \partial_x^2 v - \varepsilon \partial_x \Pi = 0, \]
\[ \tau_\Pi \dot{\Pi} + \Pi + \nu \partial_x v - \gamma \partial_x^2 \Pi + \eta \partial_x q = 0, \]

where the coupling is obtained not even between the dynamic pressure and heat flux but between the heat flux and velocity field, too. For direct comparison to the results of Arima et al., let us consider \( \kappa = \delta = \gamma = 0 \) beside the thermal and caloric equation of states. The additional terms in (2.88) compared to (2.78) are second order spatial derivatives of the field variables and are dissipative, they all contribute to the entropy production. The reduced system of equations is:

\[ \dot{\rho} + \rho_0 \partial_x v = 0, \]
\[ \rho \dot{v} + \partial_x (\Pi + p) = 0, \]
\[ \rho c \dot{T} + \partial_x q + \lambda \partial_x T + a \rho_0 T_0 \partial_x v = 0, \]
\[ \tau_q \dot{q} + q + \lambda \partial_x T - \kappa^2 \partial^2_x q - \delta \partial_x^2 v - \varepsilon \partial_x \Pi = 0, \]
\[ \tau_\Pi \dot{\Pi} + \Pi + \nu \partial_x v - \gamma \partial_x^2 \Pi + \eta \partial_x q = 0, \]

which system is exactly the same as (2.78). The parameters between the systems (2.89) and (2.78) can be compared directly to each other and one can find that

\[ \eta = \frac{\nu}{1 + c_v^2}; \quad \varepsilon = a T_0. \]

However, this correspondence is arbitrary. In the kinetic theory these parameters are fixed due to the given viscosity, temperature and molecule type. That is, the RET theory is restricted to a particular particle model and interaction. The thermal conductivities are the same. In the framework of non-equilibrium thermodynamics these parameters are free, only the positivity must be satisfied due to the positive entropy production. In the kinetic model the number of unknown material parameters could be the two relaxation times for a given gas if one knows the classical parameters \( \lambda, \nu, \rho, c_v, a \). This could be a disadvantage of the non-equilibrium thermodynamics from this point of view.

**Remark:** The applied entropy density and entropy current is the same as in case of ballistic-conductive model. Let us recall that we are modeling the same: propagation in
a rarefied gas, only the type of the gas is different. The ballistic conduction in rarefied
gases in the continuum model represented in the same way as in kinetic theory, there is
no interaction between the molecules, and they scatter on the boundary.

Nevertheless, one must pay attention to the closure problem of kinetic theory. The system (2.78) can cover phenomena beyond the classical Navier-Stokes-Fourier behavior but its validity is restricted to rarefied gases, the parameters are fixed with the detailed properties. This property will be demonstrated on the low temperature experiments in the next chapter. The more general modeling involves higher number of fitted parameters. There are also experiments that could be used to test these models. Sluijter et al. [105, 106] measured the sound absorption at low temperatures (77K and 90K) and at room temperature also, with different types of molecules. Similar measurements are made by Rhodes [107], Greenspan [108] and Sette et al. [109]. From the kinetic theory point of view, these experimental results were elaborated in detail by Arima et al. [87–89,104]. The non-equilibrium thermodynamic theory (2.89) should be analyzed further in the respect of experiments but it is not the goal of this thesis.

2.3 Environment of the solution method

2.3.1 Dimensionless formulation

The ballistic-conductive model has a dimensionless form where all of the parameters are
dimensionless [2,3]. It is useful to decrease the number of parameters and to remove the
irrelevant, not physical part of the model, e.g. units. In the further parts of this thesis
only the heat pulse type experiments are analyzed in 1+1 dimension.

Boundary conditions [2,3]: the heat pulse itself is applied at the front side:

\[ q_0(t) = q_{x=0,t} = \begin{cases} 
q_{\text{max}} \left(1 - \cos \left(2\pi \cdot \frac{t}{t_p}\right)\right) & \text{if } 0 < t \leq t_p, \\
0 & \text{if } t > t_p.
\]

On the rear side, there is an adiabatic or cooling boundary condition depending on the
particular measurement. The adiabatic boundary condition is defined as \( q(x = L, t) = 0 \),
where \( L \) is the length of the sample. The cooling boundary condition is defined as \( q(x = L, t) = h(T - T_0) \) where \( h \) is the heat transfer coefficient (HTC) and \( T_0 \) is the constant
environmental temperature.

Initial conditions [2,3]: the temperature \( T_0 \) is used as a homogeneous initial condi-
tion which induces zero fluxes at the initial time instant.

For such experimental boundary conditions the preferred choice to reduce the parameters is to introduce the dimensionless variables \( \hat{t}, \hat{x}, \hat{T}, \hat{q}, \hat{Q}, \hat{h} \) for time, space, temperature, heat flux, internal variable and heat transfer coefficient, respectively,

\[ \hat{t} = \frac{\alpha t}{L^2}, \quad \hat{x} = \frac{x}{L}, \quad \hat{T} = \frac{T - T_0}{T_{\text{end}} - T_0}, \quad \hat{q} = \frac{q}{q_0}, \quad \hat{Q} = \sqrt{\frac{\kappa_{12}}{\kappa_{21}}} q_0 Q, \quad \hat{h} = h \frac{t_p}{\rho c L}, \]

(2.91)
where $\alpha$ is the thermal diffusivity, $t_p$ is the length of the heat pulse, $T_{\text{end}}$ is the maximum or equilibrium temperature value in the adiabatic case, $\bar{q}$ is the mean value of the heat pulse [2, 3]. Furthermore, the following dimensionless parameters are also introduced, correspondingly

$$\hat{\tau}_\Delta = \frac{\alpha t_p}{L^2}; \quad \hat{\tau}_q = \frac{\alpha \tau_q}{L^2}; \quad \hat{\tau}_Q = \frac{\alpha \tau_Q}{L^2}; \quad \hat{\kappa} = \sqrt{-\frac{\kappa_{12} \kappa_{21}}{L}},$$ (2.92)

where $\hat{\tau}_\Delta$ is the dimensionless pulse length, $\hat{\tau}_q$ and $\hat{\tau}_Q$ are the dimensionless relaxation times and $\hat{\kappa}$ is the dimensionless square root of the dissipation parameter [2, 3]. The dimensionless heat pulse boundary condition is:

$$q_{x=0} = \begin{cases} 
1 - \cos(2\pi \cdot \frac{\hat{t}}{\hat{\tau}_\Delta}) & \text{if } 0 < \hat{t} \leq \hat{\tau}_\Delta, \\
0 & \text{if } \hat{t} > \hat{\tau}_\Delta.
\end{cases}$$

Finally, we obtain the ballistic-conductive equation in a non-dimensional form [2, 3]:

$$\hat{\tau}_\Delta \partial_t \hat{T} + \partial_x \hat{q} = 0,$$
$$\hat{\tau}_q \partial_t \hat{q} + \hat{q} + \hat{\tau}_\Delta \partial_x \hat{T} + \hat{\kappa} \partial_x \hat{Q} = 0,$$
$$\hat{\tau}_Q \partial_t \hat{Q} + \hat{Q} + \hat{\kappa} \partial_x \hat{q} = 0.$$ (2.93)

From now on only dimensionless quantities are used. In the following we do not use the hats.

### 2.3.2 Numerical method

At this point all of the equations are known, now they must be solved with the given initial and boundary conditions. In case of Fourier equation, there are well-known boundary conditions, such as Dirichlet, Neumann and 3\textsuperscript{rd} type boundaries where the temperature, the temperature gradient and the heat transfer is defined, respectively. However, in case of non-Fourier heat conduction these boundary conditions do not have the same physical meaning. The temperature gradient does not correspond to the heat flux, therefore it is inconvenient to work only with the temperature field. The heat flux is not proportional to the temperature gradient.

For $q$-driven boundary conditions we introduce a special method, called shifted fields. Instead of the usual one sided derivation for the temperature field we assume that the fields of temperature and $Q$ are a consequence by the given heat flux at the boundary. This is a natural physical point of view. We know that the physical quantities are not independent at the boundaries. The concept is demonstrated on Fig. 2.5.

**Remark:** There are schemes such as two-step Lax-Wendroff, leapfrog or Finite-Difference-Time-Domain (FDTD) method which applies values at half time or half space step to update a grid point at the next time instant [110]. In the multigrid method the goal is to increase the accuracy by applying finer and finer meshes [110]. Here this is not the case. These methods do not avoid the application of temperature related boundary conditions. Feynman in [111] also presents a technique for time integration of the dynamics of a mass point where a similar shifting is used in time by a half step. Yee discuss the problem of electromagnetic wave propagation and apply the FDTD method to solve the Maxwell equations, and also discuss the possible boundary conditions for such wave propagation problem [112]. However, none of these examples use shifted fields to eliminate boundary conditions, as we do.
In the discretization the finite difference method is used. It has some advantages and disadvantages.

- The discretization is simple, the accuracy can be well-estimated and it can be used independently from the boundary conditions. It can be programmed easily.

- There is the possibility of artificial numerical phenomena such as dispersion and phase error. It is difficult to handle suddenly changing solutions like shock waves.

My goal was to write an explicit scheme which can be used for similar equation structures and can be easily extended. The presented heat conduction equations have a very similar structure thus the application of the discretization method for different constitutive equations is straightforward. The scheme is explicit then it is conditionally stable. The calculation of the stability conditions is inevitable and presented after the discretized forms. Moreover, according to Lax-Richtmyer theorem [113], the consistency of a scheme should be proved to ensure the convergence.

In our discretization scheme (Fig. 2.5), one of the fields, it is \( q \), goes from zero to the end of the space domain. The other fields are shifted by \( \frac{\Delta x}{2} \). By this kind of discretization one can distinguish surface-like and volume-like quantities. The one that covers the whole domain is a surface-like quantity, its values are given on the cell’s boundary. On the other hand the points of shifted fields are in the middle of the cells, these are called volume-like quantities [2,3].

The discretized form of the balance equation of internal energy:

\[
T_j^{n+1} = T_j^n - \frac{\Delta t}{\tau \Delta x} (q_{j+1}^n - q_j^n),
\]

(2.94)

where \( n \) stands for the time steps and \( j \) denotes space steps. Let us continue with the constitutive equations.

- Fourier equation:

\[
q_j^{n+1} = -\frac{\tau \Delta}{\Delta x} (T_j^n - T_{j-1}^n).
\]

(2.95)

- Guyer–Krumhansl equation:

\[
q_j^{n+1} = q_j^n - \frac{\Delta t}{\tau_q} q_j^n - \frac{\tau \Delta \Delta t}{\tau_q \Delta x} (T_j^n - T_{j-1}^n) + \frac{\kappa^2 \Delta t}{\tau_q \Delta x^2} (q_{j+1}^n - 2q_j^n + q_{j-1}^n).
\]

(2.96)

It can be reduced for the MCV equation via the substitution \( \kappa = 0 \).
Ballistic-conductive equation:

\[ q_j^{n+1} = q_j^n - \frac{\Delta t}{\tau_q} q_j^n - \frac{\tau_\Delta \Delta t}{\tau_q \Delta x} (T_j^n - T_{j-1}^n) - \frac{\kappa \Delta t}{\tau Q} \Delta x (q_j^n - q_{j-1}^n), \]  

(2.97)

\[ Q_j^{n+1} = Q_j^n - \frac{\Delta t}{\tau Q} Q_j^n - \frac{\kappa \Delta t}{\tau Q \Delta x} (q_j^{n+1} - q_j^n). \]  

(2.98)

In the ballistic-conductive model, not only the temperature is represented as a shifted field but the internal variable \( Q \) as well.

Unfortunately, this kind of forward in time discretization has only first order accuracy. Naturally, there are several possibilities to improve accuracy, e.g. by applying spectral methods [114]. However, our goal was to obtain a numerical method where the stability conditions can be calculated and applicable in the scheme, using more points to improve accuracy was not a problem.

Stability

A numerical scheme is stable if the error of the approximation is bounded. The method of Neumann with Jury conditions will be used in this section. First, let us see the detailed steps of the Neumann method. Assume the solutions of the difference equations in the form

\[ \phi_j^n = \xi^n e^{ikj\Delta x}, \]  

(2.99)

where \( i \) is the imaginary unit, \( k \) is the wavenumber, \( j \Delta x \) denotes the discretized position and \( n \) is the index of the time step. The scheme will be stable if \( |\xi| \leq 1 \) stands for the growth factor \( \xi \). If \( |\xi| = 1 \) then the scheme is conservative. Equation (2.99) must be substituted into various discretized equations: (2.94) + (2.95), (2.94) + (2.96), (2.94) + (2.97) + (2.98), respectively. For (2.94) and (2.95) it yields

\[ \xi q_0 + \frac{\tau_\Delta}{\Delta x} \left( 1 - e^{-ik\Delta x} \right) T_0 = 0, \]

\[ (\xi - 1) T_0 + \frac{\Delta t}{\tau_\Delta \Delta x} \left( e^{ik\Delta x} - 1 \right) q_0 = 0. \]  

(2.100)

Then the system of linear algebraic equations is obtained in the form

\[ \begin{pmatrix} \xi - 1 & \frac{\Delta x}{\tau_\Delta \Delta x} \left( e^{ik\Delta x} - 1 \right) \\ \frac{\tau_\Delta}{\Delta x} \left( 1 - e^{-ik\Delta x} \right) & \xi \end{pmatrix} \begin{pmatrix} T_0 \\ q_0 \end{pmatrix} = 0. \]

If the determinant of the coefficient matrix is zero, the system has a nontrivial solution. The characteristic polynomial \( F(\xi) \) of the coefficient matrix is

\[ F(\xi) = \xi^2 - \xi - \frac{\Delta t}{\Delta x^2} (2 \cos(k\Delta x) - 2). \]  

(2.101)

According to Jury conditions [115], the coefficient of the highest order term must be positive. If not, then the polynomial must be rearranged accordingly. It is easy to see in the simple case with second order polynomial. The ballistic-conductive model leads to a third order polynomial, thus one must pay attention to the coefficient of the highest order term. When the order of the characteristic polynomial is odd, one of the Jury condition changes. If the Jury conditions are fulfilled, the roots of the characteristic polynomial are
inside the unit circle on the complex plane and the solution of the difference equation is asymptotically stable.

A $n^{th}$ order polynomial $F(\xi) = a_n \xi^n + a_{n-1} \xi^{n-1} + \ldots + a_1 \xi + a_0$ requires $n+1$ conditions. According to Jury criteria [115], the stability of a third order polynomial requires:

1. $F(\xi = 1) \geq 0$,
2. $F(\xi = -1) \geq 0$ if $n$ is even and $F(\xi = -1) \leq 0$ if $n$ is odd,
3. $|a_0| \leq a_n$, if the coefficient of the highest order term is 1, it will ensure that the zeroth order term will not be higher than 1 in the case of a trivial solution,
4. $b_0 > |b_2|$, where $b_0 = \begin{vmatrix} a_0 & a_3 \\ a_3 & a_0 \end{vmatrix}$ and $b_2 = \begin{vmatrix} a_0 & a_1 \\ a_3 & a_2 \end{vmatrix}$.

If these conditions are fulfilled then the scheme is stable and for the growth factor $|\xi| \leq 1$ will be valid. Hereinafter only the coefficients of characteristic polynomial are written and the number of the criterion is referred.

- **Fourier equation**: here (2.101) is the characteristic polynomial. The cos term is considered with its extrema: $-1$ in every case. The corresponding Jury conditions are:

  1. $\frac{4 \Delta t}{\Delta x^2} > 0$; it is fulfilled in every case.
  2. $1 + \frac{2 \Delta t}{\Delta x^2} > 0$; it is valid for every parameter.
  3. $\Delta t < \frac{\Delta x^2}{2}$; this third criterion gives a condition for the time step.

It must be emphasized that this condition is not the same as the well-known Courant condition due to the different discretization.

- **Guyer–Krumhansl equation**: here the coefficients of characteristic polynomial of (2.94) and (2.96) are

  $$
  a_2 = 1, \\
  a_1 = \frac{\Delta t}{\tau_q} - 2 - \frac{k^2 \Delta t}{\tau_q \Delta x^2} (2 \cos(k \Delta x) - 2), \\
  a_0 = 1 - \frac{\Delta t}{\tau_q} + \frac{k^2 \Delta t}{\tau_q \Delta x^2} (2 \cos(k \Delta x) - 2) - \frac{\Delta t^2}{\tau_q \Delta x^2} (2 \cos(k \Delta x) - 2).
  $$

Then one obtains the conditions as:

1. $\frac{4 \Delta t}{\tau_q \Delta x^2} > 0$;
2. $\frac{\Delta x^2}{4} \left(\frac{2 \tau q}{\Delta t} - 1\right) + \frac{\Delta t}{2} > \kappa^2$.
3. The third inequality has two solutions because of the absolute value. The first one is $\Delta t - \frac{\Delta x^2}{4} < \kappa^2$. The other one is $\frac{\Delta x^2}{4} \left(\frac{2 \tau q}{\Delta t} - 1\right) + \Delta t > \kappa^2$. This is weaker than the previous from the second Jury criterion, because $\frac{\Delta t}{2} < \Delta t$.

These conditions can be simplified to the MCV case if $\kappa = 0$. 
Ballistic-conductive equation: the system (2.94), (2.97) and (2.98) consists of three equations, therefore the characteristic polynomial is a third order one. The coefficients are

\[ a_3 = 1, \]
\[ a_2 = \frac{\Delta t}{\tau_q} + \frac{\Delta t}{\tau_Q} - 3, \]
\[ a_1 = \frac{\Delta t^2}{\tau_q} + 3 - \frac{2\Delta t}{\tau_q} - \frac{2\Delta t}{\tau_Q} - \left( \frac{\kappa^2 \Delta t^2}{\tau_{qQ} \Delta x^2} + \frac{\Delta t^2}{\tau_q \Delta x^2} \right) (2 \cos(k\Delta x) - 2), \]
\[ a_0 = \frac{\Delta t}{\tau_q} + \frac{\Delta t}{\tau_Q} - \frac{3\Delta t^2}{\tau_Q \tau_q} - 1 + \left( \frac{\kappa^2 \Delta t^2}{\tau_{qQ} \Delta x^2} - \frac{\Delta t^2}{\tau_q \Delta x^2} \left( \frac{\Delta t}{\tau_Q} - 1 \right) \right) (2 \cos(k\Delta x) - 2). \]

As conditions become more and more complicated a numerical evaluation is recommended. We do not give an explicit solution of the inequalities here. The formulas in principle can be derived analytically as well, but it is not necessary.

Consistency

The stability is ensured by the given conditions. The proof of consistency is required to show the convergence of the scheme by Lax-Richtmyer theorem. There are two levels of consistency, the weak and the strong one. In case of weak consistency one does not expect that some properties of the original partial differential equation, like conservation of particular quantities, are preserved by the discretization [116,117]. In this case, only the weak-consistency of our scheme is proved which is enough for convergence.

If a numerical solution of a partial differential equation tend to the original solution while space and time steps \( \Delta x, \Delta t \) tend to zero, then a numerical scheme is weakly consistent. In order to prove this property it is necessary to expand the appropriate terms in Taylor series and substitute back the expression into the scheme. It yields the numerical (‘discrete’) operators for each field. The last step is to calculate the limit when the step sizes go to zero and subtract from the original, continuous operators. If the result is zero then the scheme is weakly consistent.

First of all, let us see the balance equation of internal energy, it is rewritten as:

\[ \tau \Delta \partial_t T + \partial_x q = \hat{P}_1 T + \hat{P}_2 q = 0, \]
\[ \hat{P}_1 = \tau \frac{\partial}{\partial t}; \quad \hat{P}_2 = \frac{\partial}{\partial x}, \]

where \( \hat{P}_1 \) and \( \hat{P}_2 \) are the given differential operators. Let us recall (2.94):

\[ \tau \Delta \frac{T^{n+1}_j - T^n_j}{\Delta t} + \frac{q^m_{j+1} - q^m_j}{\Delta x} = 0. \]

The discrete time and space differences can be expressed in a form of Taylor series,

\[ T^{n+1}_j = T^n_j + \Delta t \partial_t T + \frac{\Delta t^2}{2} \partial_{tt} T + O(\Delta t^3), \]
\[ q^n_{j+1} = q^n_j + \Delta x \partial_x q + \frac{\Delta x^2}{2} \partial_{xx} q + O(\Delta x^3), \]

and substituting into the equation (2.103) yields

\[ \tau \Delta \left( \partial_t T + \frac{1}{2} \Delta t \partial_{tt} T + O(\Delta t^2) \right) + \left( \partial_x q + \frac{1}{2} \Delta x \partial_{xx} q + O(\Delta x^2) \right) = \hat{P}_{1\Delta t, \Delta x} T + \hat{P}_{2\Delta t, \Delta x} q, \]

31
where $\hat{P}_{1,\Delta t,\Delta x}$ and $\hat{P}_{2,\Delta t,\Delta x}$ are the discrete operators. If $\Delta t$ and $\Delta x$ tend to zero in the expression above, then we obtain (2.102). Therefore the discrete scheme of the energy equation is weakly consistent.

Let us present the proof only for the GK equation because the structure of the equations and the steps are the same. The discrete terms to be expanded into Taylor series in (2.96), therefore we need

\[
T^n_{j-1} = T^n_j - \Delta x \partial_x T + \frac{1}{2} \Delta x^2 \partial_{xx} T - O(\Delta x^3),
\]

\[
q^n_{j-1} = q^n_j - \Delta x \partial_x q + \frac{\Delta x^2}{2} \partial_{xx} q - \frac{\Delta x^3}{6} \partial^3_x q + \frac{\Delta x^4}{24} \partial^4_x q - O(\Delta x^5),
\]

\[
q^n_{j+1} = q^n_j + \Delta x \partial_x q + \frac{\Delta x^2}{2} \partial_{xx} q + \frac{\Delta x^3}{6} \partial^3_x q + \frac{\Delta x^4}{24} \partial^4_x q + O(\Delta x^5),
\]

\[
q^n_{j+1} = q^n_j + \Delta t \partial_t q + \frac{1}{2} \Delta t^2 \partial_{tt} q + O(\Delta t^3).
\]

The two terms of the heat flux with a spatial deviation are expanded up to the 4th term because of the second order derivative in the scheme. Substituting back into the equation (2.96), one obtains:

\[
\tau_q \left( \partial_t q + \frac{1}{2} \Delta t \partial_{tt} q + O(\Delta t^2) \right) + q^n_j + \tau_{\Delta} \left( \partial_x T - \frac{1}{2} \Delta x \partial_{xx} T - O(\Delta x^2) \right) + \\
- \kappa^2 \left( \partial_{xx} q + \frac{1}{12} \Delta x^2 \partial^4_x q + O(\Delta x^4) \right) = \hat{P}_{1,\Delta t,\Delta x} T + \hat{P}_{2,\Delta t,\Delta x} q.
\]

One can see that the discretized second order spatial derivative has second order accuracy due to the first term in Taylor series, but the lowest order of the scheme is the relevant one, hence it remains first order. It follows that the scheme is convergent in first order [118].

Let us summarize the consequences. We have proved that the finite difference schemes for equations (2.94, 2.95, 2.96, 2.97, 2.98) are conditionally stable and weakly consistent. Therefore, if the initial value problem of our system of partial differential equations is well-posed then the schemes are convergent. The initial value problem is well-posed if

1. the solution is existing and unique,

2. the solution depends continuously on the initial and boundary conditions,

where the existence and uniqueness requires the checking the initial and boundary conditions as well. One can easily define well-posed problems for symmetric hyperbolic systems [19] such as the ballistic-conductive equation. Further and more detailed mathematical discussion can be found in [119]. The analysis of the existence and uniqueness for the ballistic-conductive system is still an open problem.
Chapter 3

Heat conduction at low temperature

So far we have seen the theoretical background. In this chapter I present solutions of ballistic-conductive model and I compare them to the results of Dreyer and Struchtrup [101] and Y. Ma [120, 121]. I have put emphasis on the modeling of ballistic heat conduction. In my related paper [122], I investigated the corresponding informations from literature regarding NaF experiments. Furthermore, in this paper I demonstrated a reproduction of one measurement, the section 'Analysis of NaF experiments' presents the main conclusions based on [122]. The complete reproduction of NaF experiments is my latest result and is under publication.

3.1 Brief historical background

Low temperature physics was fascinating for the researchers since the beginning of XX. century. The story of non-Fourier heat conduction has been started by predicting the phenomenon of second sound, a dissipative, wave-like propagation of temperature by Tisza and Landau [123, 124]. Then it was first measured by Peshkov in liquid He II in 1944 [125]. The heat conduction properties of He II are remarkable. At atmospheric pressure and under around 2 K, He I goes through the \( \lambda \) - point and He II is formed. Under 25 atm. it is a superfluid. Its viscosity is practically zero, as London remarks it, He II has 'super-properties' [126]. It is also interesting that He I is contracting when cooled but He II is expanding [126]. Donnelly emphasizes the viscosity properties of He II as a paradox: “The oscillations of a torsion pendulum in helium II will gradually decay with an apparent viscosity about one-tenth that of air, but if liquid helium is made to flow through a very fine tube, it will do so with no observable pressure drop – the apparent viscosity is not only small, it is zero!” [127].

For experimental discovery, a new technique, the application of heat pulses was also crucially important. Figure 3.1 (left side) indicates the arrangement of Peshkov’s measurement. It is not the scheme of the original measurements, it is a simpler version. Here, \( T \) denotes the thermometer, \( H \) is the heater, \( G \) stands for the glass tube, \( A \) and \( B \) are tubes with adjustable positions. That was necessary for better observation of the reflecting waves. A small electric current at \( H \) generates a small temperature signal which can be detected by the thermometer.

On the right hand side of Fig. 3.1 a picture can be seen from the video\(^1\) of Alfred Leitner. The arrangement of the experiment is the same as it is shown at the left hand

\(^1\)Available online at 31/10/2016: https://www.youtube.com/watch?v=sKOIfR5OcB4
side, furthermore the measured signal of wave propagation can be seen on the oscilloscope, in the middle.

The crucial point of the modeling of second sound is the signal propagation speed. Figure 3.2 presents its temperature dependence by Lane et al. [128]. The solid line with circles represents their measured results and the broken line presents the theoretical prediction of Tisza. It is also in good agreement with Landau’s theory.

Ward and Wilks derived the same result as Landau but in different way with different theoretical basis [129]. Let us note that on Fig. 3.2 the curves start around 1.1 K. Less than 1 K, the wave speed increases considerably as it is indicated on Fig. 3.3, based on the measurements of Atkinson and Osborn [130]. This temperature sensibility of the wave speed represents well that the detection and modeling of a related phenomenon can be difficult.

Chester made a quantitative estimation for the relaxation time based on the kinetic theory to describe the wave propagation speed [131]. Later, Guyer and Krumhansl obtained the so-called window condition [132], which was helpful to detect second sound in solids as well and plays an important role in recent studies [20,133–136]. This condition was used by Ackerman et al. to further analyze the wave propagation speed in solids [137]. An overview about the history of this topic is given by Joseph and Preziosi, Ván, Cimmelli and coworkers [138–146].

3.2 Analysis of NaF experiments

Later on, the ballistic-type propagation was detected by Jackson, Walker and McNelly, this is the so-called ‘NaF experiment’ [147–149]. This propagation mode is more complicated, more difficult to observe and to detect the presence of such effect; it is very sensitive to boundary conditions. Various theories have been developed to provide explanation and modeling [101,120,150–156]. Interestingly, none of the mentioned models can describe the ballistic propagation quantitatively. This chapter is about the modeling of the NaF experiment with the help of the ballistic-conductive model (2.22).
Figure 3.2: The temperature dependence of the propagation speed of second sound in He II [128].

Figure 3.3: The temperature dependence of the propagation speed of second sound in He II based on [130].
Figure 3.4 shows the arrangement of the NaF experiments [149]. The sample is cube-like, excited at the front side and the temperature is measured at the rear side. The results can be seen on Fig. 3.5. Here, L and T denote the longitudinal and transversal ballistic signal. It is followed by the peak of second sound. The NaF crystals were prepared particularly for these experiments. Due to the high purity of the crystals the thermal conductivity is about hundred times higher than in the best conductor at room temperature, it is about $10000 \, \text{W/mK}$. There were at least six different samples prepared with different sizes and purities, five of them are mentioned in [148] and one in [157]. Based on the papers of Jackson et al. [147, 148], the crystals can be identified only by their length and by impurity classes such as 'very pure', 'less pure', etc. This twofold identification is crucial when we are seeking for the proper parameters of the respective measurement data. The thermal conductivity depends on the temperature and on the crystal impurity, see Fig. 3.6. Walker presents the thermal conductivity curves for several crystals, the relevant ones being NaF #1 and #2 [158]. These crystals are not related to the measured results presented on Fig. 3.5. The maximum thermal conductivity of #1 (around $50000 \, \text{W/mK}$) is approximately the double of the peak value of the second one. Interestingly, this sample has not been used in measurements in spite of the seemingly better properties.

Thermal conductivity is not the only relevant material parameter, one requires density and specific heat as well. The temperature dependency of thermal conductivity is well-discussed in the literature but the density is not. Bargmann and Steinmann [159] give the value of density and specific heat according to the Gmelin Handbook [160]. Hardy and Jaswal have calculated the temperature dependency of specific heat, which changes significantly between 9 K and 17 K [161]. This property is analyzed by Coleman and Newmann [162], too. However, one cannot find information regarding the crystal impurity dependency of the specific heat.
Figure 3.5: Original results of NaF experiments: the right one was published in [147] and the left one in [148]. L and T denote the longitudinal and transversal peaks of ballistic propagation, respectively.

Figure 3.6: Temperature and purity dependence of the NaF crystals, Fig 3 of [148]. The purity is decreasing from A to E.

The relaxation times are determined from the measurements via fitting to the model equations; therefore, different models can lead to different relaxation times. In the ballistic-conductive model, the ballistic speed is not an independent further parameter:
As it is mentioned, the presence of the ballistic signal significantly depends on the boundary conditions. There are two important questions about the boundary conditions. How long is the input pulse? Can the rear end be adiabatic? According to McNelly et al. [157] the pulse length is between 0.1 µs and 1 µs. The theoretical analyses use various values within this interval. Dreyer and Struchtrup apply the lower limit, 0.1 µs [101]. Yanbao Ma used two different values, 0.24 µs and 0.36 µs, for the evaluation of the same experiment [121]. As Kovács and Ván state [122]: “Regarding the other question, Jackson et al. [148] do not provide any direct information about the rear boundaries. The flattening of the measured curves on the left side of Fig. 3.5 indicates that the sample cools back non-negligibly during the time scale of the measurement. Theoretical modeling did not use this observation up to now.

The presence of shear and longitudinal ballistic propagation indicates that the experiment cannot be completely modeled in one spatial dimension. Moreover, according to the experimental arrangement in [149], the specimen is cube-like and the heat excitation affects only the middle part of the front face. Therefore only two dimensional modeling could provide reliable quantitative agreement with experimental results. However, model calculations are mostly one dimensional [2, 3, 101], except for [121]. Moreover, except [121], the transversal, rather than the longitudinal, ballistic peak is reproduced in these one dimensional models [2, 3, 101]. In principle, only the longitudinal ballistic propagation that can be connected to one-dimensional models, in the form of volumetric thermoelastic effects [84], while the transversal one cannot be interpreted within such framework. However, the signal speed can be calibrated by the proper material parameters in both cases. Hence, in this work we choose the simultaneous reproduction of the peak of the transversal ballistic propagation and of the second sound in order to keep our results comparable to results of other theories.”

### 3.2.1 Theory versus experiments

The reproduction of NaF measurements is presented and compared to the 9-field approximation of the kinetic theory by Dreyer and Struchtrup [101], and the complex viscosity calculations of Yanbao Ma [120]. First, let us consider the measurement from Fig. 3.5 at 13 K. Here, the propagation modes can be clearly distinguished from each other and it is used as a test for the ballistic-conductive model. It must be mentioned that there is no vertical scale on the original figure (Fig. 3.5) hence an extra constraint must be introduced. The relative amplitude of the signals is considered as a fitting parameter.

**Results of Dreyer and Struchtrup**

The evolution equations of RET are derived from kinetic theory by particular phonon-phonon interactions [19, 101, 153, 163] as it is already discussed in the previous chapter. The 9-field approximation results in a set of equations that is similar to ours. The parameters are the specific heat, thermal conductivity and the two relaxation times. These parameters are fitted to the NaF measurements. However, the goal of Dreyer and Struchtrup was only a qualitative reproduction. The ballistic propagation speed cannot match because of theoretical reasons, only 3 momentum equations are used. Although the ballistic-conductive equation (2.93) is very similar, it contains one more parameter, \( \kappa \), which
allows us to adjust the proper ballistic propagation speed. Its value is calculated directly from the characteristic propagation speed (2.25).

Let us analyze Fig. 5.1/b from [101] (Fig. 3.7). One needs to consider the material parameters of the pure crystal at 13 K to reproduce this simulation. Let the thermal conductivity be \( k = 13500 \frac{W}{mK} \) based on Figure 3/curve B of [148] (here Fig. 3.6), which corresponds to the 'less pure' case. The mass density is \( \rho = 2866 \frac{kg}{m^3} \) and specific heat is \( c_v = 1.8 \frac{J}{kgK} \) [159], where the temperature dependency is accounted according to [161]. Then the thermal diffusivity can be calculated: \( \alpha = \frac{k}{\rho c_v} = 2.617 \frac{m^2}{s} \). In [101], there is no explicit data about the length of the specimen, however, there is a correlation on the top of the figures: \( \frac{x}{c \Delta t} = 23 \), where \( x \) is the sample length, \( c \) denotes the Debye speed and \( \Delta t \) is the pulse length. Here, \( \Delta t = 10^{-7} s \) is given, regarding the Debye speed \( c = \sqrt{\frac{3\alpha}{\tau R}} \) one can find \( c = 2747.5 \frac{m}{s} \), because \( \tau_R = 10.4\Delta t \) is also given. Then one obtains that the length of the sample is \( x = 6.3\,mm \). The second relaxation time is also given as \( \tau = 2.1\Delta t \). Hence all parameters are reproduced to calculate the dimensionless coefficients of our model:

\[
\tau_q = 0.0686; \quad \tau_Q = 0.0138; \quad \tau_\Delta = 0.0066; \quad \kappa = 0.102.
\]

Applying adiabatic boundary condition at the rear side of the sample, the temperature history at rear side according to the ballistic-conductive model (2.93) can be seen on Fig. 3.8.

Let us note that the length of the crystal is not the same as it is given in [148], where \( L = 7.9 \) mm. Moreover, the pulse length, which is not given exactly in the experimental papers, is different from the one used by Y. Ma [121]. In their calculations, Dreyer and Struchtrup used Laplace transformations, with environmental temperature at the infinity [101]. This assumption is a particular realization of cooling at the rear side of the finite sample. In case of adiabatic conditions, the final temperature depends on the energy content of the pulse and corresponds to \( T = 1 \) according to (2.91). Therefore, as a summary, one can say that the difference in the material parameters of the two models (the extra \( \kappa \) coefficient in our case) does not play a role in the qualitative reproduction of their calculation.
Results of Yanbao Ma

Y. Ma applied a hydrodynamic theory [120,121,164], where relaxation effects are modeled by complex viscosity [93,150]. He obtained a good quantitative matching with the experimental results with both ballistic speed values [121]. In his case, the duration of the input heat pulse is 0.24 µs, and the length of the sample is \( L = 7.9 \text{mm} \). He does not provide any information about the rear side boundary condition. The published relaxation times are \( \tau_R = 0.937 \mu s \); \( \tau = 0.248 \mu s \) and the speed of sound is also given, \( c = 3186 \frac{m}{s} \), which is determined from the original measurement data. In these papers there is no information about the other material parameters, thus we use the same values as in the previous case, \( \alpha = 2.617 \frac{m^2}{s} \). Therefore the dimensionless parameters are

\[
\tau_q = 0.0393; \quad \tau_Q = 0.0091; \quad \tau_\Delta = 0.01; \quad \kappa = 0.123.
\]

Then the temperature history at the rear side according to the ballistic-conductive model (2.93) can be seen on Fig. 3.9.
Apparently, these parameters do not reproduce the measurement data, the difference is significant. The structure of the equations is not the same and the uncertainty in the boundary conditions also seems to be an important factor.

**Results of non-equilibrium thermodynamics**

According to the inherently two-dimensional arrangement of the measurements with a point-like heat pulse at the front end [149], it is reasonable to assume that the internal energy is not conserved. Moreover, even if we assume that the thermal insulation at the rear end is not perfect, one cannot obtain sufficient heat loss to explain the diffusive tail of the measurement in [148]. Therefore, a source term, a heat exchange between the bulk crystal and the pulse channel is introduced in the balance equation (2.1):

\[
\frac{\partial e}{\partial t} + \frac{\partial x}{\partial q} = -a(T - T_0),
\]  

(3.1)

where \(a\) is the heat exchange parameter and \(T_0 = 13\) K is the environmental temperature. This is an emulation of the real three-dimensional effect in a one-dimensional framework. The dimensionless form of the equation is

\[
\tau_\Delta \frac{\partial T}{\partial t} + \frac{\partial x}{\partial q} + \hat{a} T = 0,
\]  

(3.2)

with

\[
\hat{a} = \frac{t_p}{\rho c} a.
\]  

(3.3)

Comparing the information from [148] and [149], the heat conduction values seem to be contradictory. The crystal in the experiment according to [148] is the one labeled as "B" on Fig. 3 of [148] (here, Fig. 3.6) which has the peak thermal conductivity around 15000 \(\frac{W}{mK}\). However, McNelly points out regarding Fig. 32 in [149] (here, Fig. 3.10), that this crystal is a different one (namely #7204205W [149]), with peak thermal conductivity value around 12000 \(\frac{W}{mK}\). Thus \(\lambda = 10200 \frac{W}{mK}\) is applied instead of the value 13500 \(\frac{W}{mK}\) based on the Appendix of thermal conductivity data in [149]. The relaxation times were determined from the transversal ballistic propagation speed and by the proper fit to the second sound peak, and they are \(\tau_q = 0.355\) \(\mu s\) and \(\tau_Q = 0.21\) \(\mu s\). The additional parameter \(\kappa = 0.523\) mm is calculated with the help of the characteristic propagation speed (2.25) and relaxation times to obtain the appropriate ballistic propagation speed. The heat exchange coefficient is the third fitted parameter, it is \(a = 3.2 \frac{W}{mm^3K}\).

Therefore, the dimensionless parameters of the ballistic-conductive theory are:

\[
\tau_q = 0.0113; \quad \tau_Q = 0.0067; \quad \tau_\Delta = 0.0076; \quad \kappa = 0.0663; \quad \hat{a} = 0.149.
\]

The corresponding solution of the ballistic-conductive equation is shown on Fig. 3.11, and also shown together with the originally measured curve (Fig. 3.12). Due to the two additional parameters, the slope of the diffusive tail and the ratio of the amplitudes are properly given, too. This result is published in [122].
Figure 3.10: Measurement results on four different NaF samples. This figure is the page 103 in [149]. The peak thermal conductivities are indicated in the caption. The path length corresponds to the length of the crystal in the direction of heat pulse. Figure B is the relevant one.

Figure 3.11: NaF experiment: reproduction of the NaF experiment at 13K in [148]. The ratio of amplitudes is calculated without considering the longitudinal wave.
3.2.2 A complete reproduction of NaF experiments

Only one curve is reproduced so far but one can reproduce the other curves as well in the same way. Furthermore, one more constraint is introduced, namely the ratio of relaxation times $\tau_q/\tau_Q$ is considered as a monotonic function which cannot be different by orders of magnitude between two measurements for the same crystal. This fitting procedure cannot be considered as a conventional one. The exact reproduction or fitting is impossible because of the lack of some details of experimental data. However, there is no better measurement in the literature up to now which could be a test of ballistic heat conduction theories. Tables 3.1 and 3.2 sums up the known material parameters without the relaxation times for both crystals [149,159,161]. The remaining parameters are determined by the particular curves and they are considered as temperature dependent.

<table>
<thead>
<tr>
<th>Temperature</th>
<th>Thermal conductivity $[\frac{W}{m\cdot K}]$</th>
<th>Specific heat $[\frac{J}{g\cdot K}]$</th>
<th>Mass density $[\frac{kg}{m^3}]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>@11 K</td>
<td>8573</td>
<td>1.118</td>
<td>2866</td>
</tr>
<tr>
<td>@13 K</td>
<td>10200</td>
<td>1.8</td>
<td>2866</td>
</tr>
<tr>
<td>@14.5 K</td>
<td>10950</td>
<td>2.543</td>
<td>2866</td>
</tr>
</tbody>
</table>

Table 3.1: Classical material parameters for crystal #607167J
Table 3.2: Classical material parameters for crystal #7204205W

<table>
<thead>
<tr>
<th>Temperature</th>
<th>Thermal conductivity [W/mK]</th>
<th>Specific heat [J/kgK]</th>
<th>Mass density [kg/m³]</th>
</tr>
</thead>
<tbody>
<tr>
<td>@9.6 K</td>
<td>8500</td>
<td>0.7123</td>
<td>2866</td>
</tr>
<tr>
<td>@12.5 K</td>
<td>17300</td>
<td>1.62</td>
<td>2866</td>
</tr>
<tr>
<td>@15 K</td>
<td>21750</td>
<td>2.735</td>
<td>2866</td>
</tr>
<tr>
<td>@17.3 K</td>
<td>22880</td>
<td>4.45</td>
<td>2866</td>
</tr>
</tbody>
</table>

Let us see now the whole series of curves for both crystals, started with the sample #607167J (Fig. 3.13) and then the results of sample #7204205W (Fig. 3.14) is discussed. Fig. 3.16 shows two side effects that are not covered by the ballistic-conductive model. In case of the sample #607167J, there is a widening effect between the ballistic signal and the peak of second sound along the increasing temperature. In case of the other one, #7204205W, at the end the temperature decreases below the initial temperature. The fitted parameters are summarized in Tables 3.3 and 3.4.

It is interesting to compare the series of parameters to each other. The tendency of temperature dependence of the fitted parameters are precisely opposite in the two cases, see Fig. 3.15. Furthermore, the higher internal heat transfer coefficient seems to be natural in the purer sample. It is interesting to compare our results to other approaches. The available results [19] from phonon hydrodynamics are presented (Fig. 3.17) where only 3 momentum equations (2.61) are used. The purer sample (#7204205W) is more conclusive, the different approaches show great variations.
Figure 3.13: The result of the simulations of rear side temperature history for sample #607167J at different temperatures
Figure 3.14: The result of the simulations of rear side temperature history for sample #7204205W at different temperatures
Figure 3.15: The temperature dependence of the fitted parameters for different crystals
<table>
<thead>
<tr>
<th></th>
<th>Relax. time I. ($\tau_q$) [µs]</th>
<th>Relax. time II. ($\tau_Q$) [µs]</th>
<th>Heat transfer coeff. ($a$) $[\frac{W}{mm^2K}]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>@11 K</td>
<td>0.471</td>
<td>0.18</td>
<td>3.34</td>
</tr>
<tr>
<td>@13 K</td>
<td>0.586</td>
<td>0.22</td>
<td>2.8</td>
</tr>
<tr>
<td>@14.5 K</td>
<td>0.65</td>
<td>0.24</td>
<td>2.31</td>
</tr>
</tbody>
</table>

Table 3.3: The fitted parameters for crystal #607167J

<table>
<thead>
<tr>
<th></th>
<th>Relax. time I. ($\tau_q$) [µs]</th>
<th>Relax. time II. ($\tau_Q$) [µs]</th>
<th>Heat transfer coeff. ($a$) $[\frac{W}{mm^2K}]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>@9.6 K</td>
<td>1.17</td>
<td>0.25</td>
<td>6.8</td>
</tr>
<tr>
<td>@12.5 K</td>
<td>0.961</td>
<td>0.1</td>
<td>12.63</td>
</tr>
<tr>
<td>@15 K</td>
<td>0.833</td>
<td>0.085</td>
<td>17.6</td>
</tr>
<tr>
<td>@17.3 K</td>
<td>0.707</td>
<td>0.07</td>
<td>15.94</td>
</tr>
</tbody>
</table>

Table 3.4: The fitted parameters for crystal #7204205W

Figure 3.16: Summarized result of the simulations and experiments, the red curves correspond to the calculations. The appearance of two mentioned side-effects can be seen clearly.
3.2.3 Comparison with the RET model

As we have discussed in the previous chapter, the ballistic propagation speed cannot be reproduced precisely with three momentum equations. Really, in the calculations of Dreyer and Struchtrup [101] this physical parameter is different from the measured value. However, in phonon hydrodynamics only two relaxation time parameters are to be fitted, while in ballistic-conductive model, three parameters are to be fitted. In our model one of the parameters is related to the cooling of the sample, an effect not considered by the RET model. The result of the original calculations can be seen on Fig. 3.17.

It is interesting to compare the tendency of temperature dependency of relaxation times. For simplicity, the relaxation time parameters from RET are summarized in the Tables 3.5 and 3.6 below based on [19]. Let us recall the correspondence between the parameters of these different models:

\[ \tau_q = \tau_R, \quad \tau_Q = \tau. \]

<table>
<thead>
<tr>
<th>Relax. time I. ((\tau_q)) [(\mu s)]</th>
<th>Relax. time II. ((\tau_Q)) [(\mu s)]</th>
</tr>
</thead>
<tbody>
<tr>
<td>@11 K</td>
<td>1.56</td>
</tr>
<tr>
<td>@13K</td>
<td>1.04</td>
</tr>
<tr>
<td>@14.5K</td>
<td>0.74</td>
</tr>
</tbody>
</table>

Table 3.5: The fitted parameters for crystal #607167J

<table>
<thead>
<tr>
<th>Relax. time I. ((\tau_q)) [(\mu s)]</th>
<th>Relax. time II. ((\tau_Q)) [(\mu s)]</th>
</tr>
</thead>
<tbody>
<tr>
<td>@9.6 K</td>
<td>3</td>
</tr>
<tr>
<td>@12.5 K</td>
<td>3</td>
</tr>
<tr>
<td>@15 K</td>
<td>3</td>
</tr>
<tr>
<td>@17.3 K</td>
<td>3</td>
</tr>
</tbody>
</table>

Table 3.6: The fitted parameters for crystal #7204205W

The tendency shows decreasing relaxation time with increasing temperature for both crystals which is in partial agreement with the presented results from ballistic-conductive model. It is remarkable to note that the \(\tau_q\) time is constant in this case for the purer crystal. Beside the inappropriate value of thermal conductivity, the relative amplitudes seem to be also inaccurate. Moreover, a clear ballistic signal at 12.5 K is predicted by the theory but it does not exists in the experiment.

As a final conclusion, one can see that the results of phonon hydrodynamics are rather a qualitative model test than a reproduction of the experiments. The ballistic-conductive model consists of three equations with three parameters to fit along with the emulation of cooling effect as well on a real spatial domain. In the phonon hydrodynamic model one must solve 30 momentum equations with increasing tensorial order to obtain realistic ballistic propagation speed. In order to obtain the cooling effect they solved the equations on a semi-infinite domain. It is also remarkable that the values of material parameters in the calculations are not clear.
Figure 3.17: Summarized result of the simulations from phonon hydrodynamic model with three momentum equations [19]
3.2.4 Comparison with the hybrid phonon gas model

The difference between the theory and the experiment is stronger in case of Y. Ma’s hybrid phonon gas model [120,121]. Fig. 3.18 compare the theoretical results to the experiments. Tables 3.7 and 3.8 summarize the fitted relaxation time parameters. In [121], the values of $\tau_R (= \tau_q)$ and $\tau_N$ are given hence $\tau (= \tau_Q)$ must be calculated according to the kinetic theory:

$$\frac{1}{\tau} = \frac{1}{\tau_R} + \frac{1}{\tau_N}. \tag{3.4}$$

In case of crystal #7204205W @9.6 K, there is no clear sign of the second sound thus Ma adjusted $\tau_N$ as infinite, i.e. $\tau_R = \tau$. Moreover, a clear analogy can be observed with the results of Dreyer and Struchtrup [101]. The parameter $\tau_R$ is constant as a function of temperature. In the other cases, the relaxation times become smaller by increasing temperature. Furthermore, as Ma states, the signal of second sound is significantly broadened for the crystal #7204205W probably because of the constant $\tau_R$ [121]. This theory also predicts ballistic signal where one cannot identify it at the experiments (Fig. 3.18/b). It is remarkable also that in these publications the boundary conditions are missing and Y. Ma uses wrong heat conduction coefficients, like Dreyer and Struchtrup.

![Figure 3.18: Summarized result of the simulations from hybrid phonon gas model [121]](image)

<table>
<thead>
<tr>
<th>@11 K</th>
<th>1.056</th>
<th>0.281</th>
</tr>
</thead>
<tbody>
<tr>
<td>@13K</td>
<td>0.937</td>
<td>0.248</td>
</tr>
<tr>
<td>@14.5K</td>
<td>0.723</td>
<td>0.208</td>
</tr>
</tbody>
</table>

Table 3.7: The fitted parameters for crystal #607167J

<table>
<thead>
<tr>
<th>@9.6 K</th>
<th>1.56</th>
<th>1.56</th>
</tr>
</thead>
<tbody>
<tr>
<td>@12.5 K</td>
<td>1.56</td>
<td>0.294</td>
</tr>
<tr>
<td>@15 K</td>
<td>1.56</td>
<td>0.245</td>
</tr>
<tr>
<td>@17.3 K</td>
<td>1.56</td>
<td>0.17</td>
</tr>
</tbody>
</table>

Table 3.8: The fitted parameters for crystal #7204205W
3.3 Dispersion relations

The goal of this section is to demonstrate how the theory can support the experiments. The results presented here are not yet published and based only on my own research.

Dispersion relations are important characteristics of plane wave propagation in various field theories. A dispersion relation is a functional relationship between the frequency and the wavenumber of a plane wave, it is a characteristics of the linearized field equations. Let us assume the solution in a form of a plane wave, i.e.

\[ \chi = Ae^{i(\omega(k)t-kx)}, \quad (3.5) \]

where \( A \) is the wave amplitude, \( k \) is the wavenumber and \( \omega(k) \) is the frequency of the wave which depends on the wavenumber. The phase velocity is the velocity of a single plane wave \( v_p = \frac{\omega}{k} \) and the group velocity is the velocity of a wave pocket and given by the relation \( v_g = \frac{d\omega}{dk} \) [165]. If \( w(k) \) is not linear, the phase velocity differs from the group velocity: they are equal only in case of the wave equation \( \partial_{tt}\phi = v^2 \partial_{xx}\phi \). The difference between the two velocities indicates the presence of dispersion: wave pockets are broadening when propagating. Gerasik and Stastna analyzes the physical role of these velocities from energy aspects [166]. It needs to be noted that the calculation of the dispersion relation is a useful utility to stability analysis. The dispersion relation can give a complex function for \( w(k) \). Then the imaginary part characterizes the damping, the real part is related to dispersion properties of the continua if the linearization is around the local thermodynamic equilibrium. If the imaginary part of \( w(k) \) is negative, then the amplitude of the wave is increasing, the equilibrium state of the linearized continuum is not stable. One expects positive imaginary part for real physical theories.

The present analysis is intended to show the role of the dispersion relations in the detection of second sound and demonstrate the difference between the parabolic and hyperbolic equations.

The wavenumber is complex and the frequency is real, i.e. \( k := \frac{2\pi}{\lambda}; k \in \mathbb{C}_0, \omega \in \mathbb{R}_0^+ \), where \( \lambda \) is the wavelength. In dimensionless formalism, the wavenumber and frequency can be written as \( \hat{k} = kL, \hat{\omega} = \omegaL^2/\alpha \). In the following, these hats are also neglected and all quantities are dimensionless.

Remark

There is an important aspect of dispersion relations which is not yet investigated in detail in the literature. The role of boundary conditions is essential and influence that the wavenumber and frequency are complex or real numbers. For example in [102], one can see different ways of looking at dispersion relation in stability analysis.

In most of the cases one assumes infinite media and then the dispersion relation is characteristics of the field equation. One of the counterexample is [167]. Here Banach analyzes the hyperbolic system of equations of phonon hydrodynamics [167]. In this paper, the initial and boundary conditions of the momentum system are considered and it is recognized that beyond three momentums initial and boundary conditions for further momentums are missing. Here the wavenumber is declared to be complex and the frequency is real. Further examples are demonstrated in the papers by Banach et al. [168] and Muracchini et al. [169]. In our analysis the role of boundary conditions is not investigated.
3.3.1 Window condition

As it is mentioned, the so-called window condition provided by Guyer and Krumhansl was helpful to detect the second sound in solids [132]. A simple analysis is presented in [101], where the phonon hydrodynamic model (9-field theory) is compared to the results of Guyer and Krumhansl. The theoretical requirement of undamped second sound in phonon hydrodynamics requires vanishing resistive collisions among phonons and only normal interactions are allowed. However, it is only an ideal case, cannot be valid for a real process. Then the goal is to minimize the dissipative terms, i.e. the imaginary part of the phase velocity. In phonon hydrodynamics, it leads to the following condition:

$$\frac{1}{\tau_R} \ll \omega \ll \frac{1}{\tau_N}. \quad (3.6)$$

This formula implies $\tau_N \ll \tau_R$, i.e. large purity and low temperature are needed, however “the temperature must not be too low, because that would prevent enough normal processes to satisfy $\tau_N \ll \tau_R$” [101]. The formula (3.6) is valid only in a small temperature range. Moreover, the condition constraints the pulse length in heat pulse experiments, i.e. the heat pulse must satisfy the given condition. The question naturally arises: what is the value of these relaxation times? The presented heat pulse experiment is one of the possible methods to measure it. Various theories may predict and explain the presence of second sound but the parameters and their values depend in different ways on the particular details of the detection. E.g. the evaluation of NaF experiments leads to different relaxation times in different theories.

The presence of wave phenomena is sensitive to the purity, excitation, boundary conditions, etc. Moreover, this window condition is valid only for second sound and it does not provide any information about the ballistic signal. Let us see now the dispersion relation of the ballistic-conductive system (2.93). We look for solution in the form of (3.5). After substitution, one obtains a coefficient matrix, let us denote it by $M$. The condition of a nontrivial propagating plane wave solution results the dispersion relation:

$$\text{det}(M) = 0, \quad (3.7)$$

where

$$M = \begin{pmatrix} i\tau_\Delta \omega & -ik & 0 \\ -ik\tau_\Delta & 1 + i\tau_q \omega & -ik\kappa \\ 0 & -ik\kappa & 1 + i\tau_Q \omega \end{pmatrix}, \quad (3.8)$$

and it yields a polynomial of $k$. In case of ballistic-conductive equation one obtains

$$k = \pm \sqrt{\frac{\omega(1 + i\tau_q \omega)(\tau_Q \omega - i)}{1 + ik^2\omega + i\tau_Q \omega}}. \quad (3.9)$$

The dispersion relation of GK equation comes with the condition $\tau_Q = 0$. The $\pm$ sign corresponds to the direction of wave propagation. To calculate the phase speed $v_p = \frac{\omega}{k}$, let us divide equation (3.9) by $\omega$ and take its reciprocal. The analytical derivation is omitted, Wolfram Mathematica is used to evaluate the phase speed. Its imaginary part characterizes dissipation. To demonstrate the difference between hyperbolic and parabolic theories, the MCV, and GK models are investigated.
Maxwell-Cattaneo-Vernotte equation

The phase speed for MCV equation reads as

\[ v_p = \sqrt{\frac{\omega}{\tau_q \omega - i}}, \quad (3.10) \]

and the imaginary part of its square can be expressed simply by

\[ \Im(v_p^2) = \frac{\omega}{(\tau_q \omega)^2 + 1}. \quad (3.11) \]

Let us note that the infinite frequency limit is

\[ \lim_{\omega \to \infty} \Im(v_p) = 0. \quad (3.12) \]

For a given \( \tau_q \), it has a maximum at \( 1/\tau_q \) and plotted on Fig. 3.19. The MCV model predicts low dissipation for high frequencies. This is a characteristic property of a hyperbolic system.

![Figure 3.19: Imaginary part of the phase speed for MCV equation at \( \tau_q = 1 \).](image)

Guyer-Krumhansl equation

The case of GK equation is more interesting, the phase speed is

\[ v_p = \sqrt{\frac{\omega(1 + i\kappa^2 \omega)}{\tau_q \omega - i}}, \quad (3.13) \]

The imaginary part of its square is expressed:

\[ \Im(v_p^2) = \frac{\omega - \kappa^2 \omega^2 + \tau_q \kappa^2 \omega^3}{(\tau_q \omega)^2 + 1}. \quad (3.14) \]

For high frequencies if \( \tau_q > 0 \) and \( \kappa > 0 \),

\[ \lim_{\omega \to \infty} \Im(v_p) = \infty, \quad (3.15) \]
this is a characteristic property of a parabolic partial differential equation.

Remark: let us note that the requirement of positive entropy production leads directly to the conditions $\tau_q > 0$ and $\kappa > 0$.

When $\tau_q > \kappa^2$ then one can demonstrate the window condition in the following way.

On Fig. 3.20 one can see a minimum point of the imaginary part of (3.13). Let it be explained. The frequency is inversely proportional with the excitation, hence if one applies a short heat pulse (for example based on MCV model) the GK model predicts high dissipation and the short pulse is possibly not satisfying. However, one can calculate the optimal frequency as:

$$\frac{d\text{Im}(v_p)}{d\omega} = 0,$$

for solving to $\omega$, then the pulse length can be determined which leads to the less dissipated signal.

Moreover, when $\kappa \ll 1$, it approximates the MCV equation (Fig. 3.21) and in the limit, $\kappa = 0$, the dispersion relation of the GK equation is reduced to MCV equation.

Figure 3.20: Imaginary part of the phase speed for GK equation at $\tau_q = 0.08, \kappa = 0.05$.

Figure 3.21: Imaginary part of the phase speed for GK equation at $\tau_q = 0.1, \kappa = 0.0001$. 

55
The interpretation of dispersion relation for ballistic-conductive model is more difficult.

Conclusion

The analysis of low temperature heat pulse experiments validated the ballistic-conductive non-equilibrium thermodynamic theory. Our model with two internal variables with generalized entropy current proved to be compatible with RET hierarchy and comparable in quantitative reproduction of the celebrated NaF experiment. It is shown that a simpler system is also can be effective or more effective than the corresponding other theories with more complexity. It is interesting to see: what could be changed by the underlying theory, how it influences the coefficients in the equations. Moreover, the main difference between the parabolic and hyperbolic equations is demonstrated. There is an important general question regarding this property of models:

Is the world hyperbolic or parabolic?

The first answer is straightforward: hyperbolic - naturally - due to the finite speed of propagation. However, the common experience shows that the parabolic models are in good agreement with the heat pulse experiments and the seemingly contradictory physical content does not matter for practical applications in engineering. The second law of thermodynamics always proposes a parabolic model, a hyperbolic one is derived by a simplification. This statement holds for the ballistic-conductive equation, it is only a simplified version of a parabolic system. Seemingly, our world seems to be parabolic, therefore the description is more universal, they covers the hyperbolic models as special cases and incorporates the effects of non-Fourier heat conduction. Moreover, it advertises the most common and general aspect: the world is imperfect and dissipative.
Chapter 4

Deviation from Fourier heat conduction at room temperature

At low temperature heat conduction the deviation from Fourier’s law was due to the presence of non-negligible higher order terms in the momentum hierarchy. This is usually attributed to the rarity of the gas (large mean free path and Knudsen number) or, in case of phonon hydrodynamics, to different channels of phonon propagation (see the two relaxation times in the Callaway collision integral). In solids at room temperature these mechanisms cannot play a role, moreover, the phonons are self-scattering, the quasiparticle approach is not applicable, the Boltzmann equation itself is not valid.

The classical law of heat conduction is valid for homogeneous materials which practically do not exist in reality. This chapter is intended to present a series of experiments, the way of finding non-Fourier heat conduction at room temperature in inorganic materials. These experiments have been performed at the Department of Energy Engineering, BME. First, the development of the experiments is presented to introduce the physical interpretation behind the deviations and then a discussion of the theoretical background follows.

The case of organic materials with its experimental background is discussed in the next chapter, it belongs to biological heat conduction despite of the applied temperature range.

4.1 Motivation

In recent years several experiments were performed to demonstrate non-Fourier heat conduction in biological systems, too [170]. Mitra et al. [171] showed the wave-nature of heat conduction in processed meat, see Fig. 4.1. It was a similar experiment as the 'Book experiment' presented in the next section. Processed meat is situated suddenly onto a preheated plate and the temperature is measured by thermocouples inside the meat. However, later the experiment could not be repeated. Other, follow up measurements led to contradictory results, see Scott et al. [172], Herwig and Beckert [173,174].

The general approach is still looking for the MCV equation as the first feasible extension of Fourier’s law. Luikov [175,176] also proposed the MCV equation to model heat propagation in porous structures at room temperature on the basis of theoretical considerations. As it is shown in the chapter of biological heat conduction, most of the researchers use the MCV or the DPL-type extensions of Fourier’s law with more or less success.
Regarding to heat conduction in rocks, an effective model can be helpful in the measurement of thermal diffusivity and in transient processes where the thermo-mechanical effects play a role. An example of such effects is shown on Fig. 4.2. There one can see the role of temperature fluctuations on the strain of rock, measured by extensometers [177].

Another famous example to detect non-Fourier effects is the Kaminski experiment [178]. The arrangement of experiment can be seen on Fig. 4.3. The examined materials were sand and glass ballotini among others. These are grained materials and the different time scales may exist due to the voids among the particles. As a conclusion of this experiment, it is found that there is a significant time lag between the excitation and signal observation. As Kaminski states, if the Fourier’s law would be valid, the signal should be arrived after 5 to 10 s. However, the signal was observed much later, between 100 to 200 s,
see Fig. 4.4. Unfortunately, these results could not be reproduced, too [173,174,179].

4.2 Experimental background

A simple inhomogeneous structure consists of parallel layers with different material parameters. It can be realized by a book and while the most important material in these experiments was layered paper, this first stage is called ’book experiment’.
4.2.1 Book experiment

This experiment was performed by Gróf et al. [180] and the setup can be seen on Fig. 4.5. Two measurements were published, in the first one, five thermocouples were used while the first thermocouple built in the surface of the thermostat. In the other one, eight thermocouples were utilized; moreover all thermocouples are situated inside the book. Hence the main difference is how to measure and model the boundary conditions. The result of the second experiment and the fitting of nonlinear Fourier equation and Guyer-Krumhansl equation can be seen on Fig. 4.6.

**Remark:** I joined to the research group at this point. My first paper is connected to book experiment [181].

In these experiments the non-Fourier effects were not significant and therefore the results were not convincing and not decisive. Let us notice that in these experiments the material is transversally isotropic: the periodic layered structure is perpendicular to the direction of the heat flux.

![Figure 4.5: The schematic arrangement of book experiment, taken from [180].](image)

![Figure 4.6: The results of the first experiment, taken from [180]. Left side: results of the fitting of nonlinear Fourier equation. Right side: results of the fitting of Guyer-Krumhansl equation.](image)
4.2.2 EGR-capacitor experiment

Our first successful measurement of a significant deviation from Fourier’s law in heterogeneous media was published in [182]. This is due to a collaboration of our department research group and it is based on a heat flash experimental equipment developed here by Gy. Gróf and Á. Gyenis, therefore we call that EGR experiment. S. Both prepared the capacitor samples and performed the experiments with P. Ván. My role was to help in the sample preparation and to evaluate the experimental data. Á. Lovas joined to the research at this point under my supervision and his role was to prepare the samples and perform the experiments.

The schematic arrangement is presented on Fig. 4.7, which is valid for a heat pulse experiment in general. The sample contains a periodic layer structure and the layers and the direction of heat flux are parallel. A flash light is the source of the heat pulse at the front end of the sample and temperature is measured by a pin-thermocouple (K-type) at the rear end. The thermocouple and the detector are insulated from the heat pulse and from the electromagnetic noises. The heat pulse is measured directly at the front end by a photovoltaic cell, providing the triggering signal for the data acquisition.

Figure 4.7: The schematic arrangement of EGR-capacitor experiment, taken from [182].

Figure 4.8: Photo of the sample holder with the inserted specimen. The photovoltaic detector is on the right-hand side [182].
This photovoltaic detector is also used to measure the shape of the heat pulse (Fig. 4.9). However, in numerical simulations this particular shape is not used because the length of the pulse is shorter than the characteristic time of the measured signal, therefore the measured data is not sensitive to that [47].

Figure 4.9: The form of the heat pulse, measured by a photovoltaic cell [182].

The studied specimen in the experiment has a disk shape with \( L = 3.9 \text{ mm} \) thickness and \( d = 19 \text{ mm} \) diameter. The specimen is composed of aluminum (5 \( \mu \text{m} \)) and polystyrene (15 \( \mu \text{m} \)) layers, arranged parallel to the heat pulse. The front side is painted black to ensure uniform boundary conditions as well as to eliminate the transparency of the sample. At the rear side, a silver painting is applied for better electric coupling of the thermocouple and to measure an effective temperature of the heterogeneous material. The experimental device was calibrated using several samples with known thermal diffusivity. The measurement was performed at 21°C room temperature. The measured time dependent dimensionless temperature data with the corresponding fitting of Fourier and GK equations can be seen on Fig. 4.10 and 4.11.

Figure 4.10: The thin noisy line is the experimentally measured data of the rear side temperature as the function of time. The dashed line is the best fit solution of the Fourier equation with thermal diffusivity \( \alpha = 2.144 \cdot 10^{-6} \text{ m}^2/\text{s} \) [182].
4.2.3 Physical interpretation

What is the particular reason applying the GK equation? First of all, there is no such wave front in the signal which could correspond to the MCV equation. Moreover, the experience shows the GK equation seems to be the next appropriate extension of Fourier’s law to explain non-Fourier heat conduction at room temperature. Beyond the experience there is a further explanation for this phenomenon which allows us to characterize the deviation precisely. Let us substitute the GK equation into the energy balance to obtain the differential equation for the temperature, the heat conduction equation:

\[
\tau_q \partial_t T + \partial_t T = \alpha \partial_{xx} T + \kappa^2 \partial_{txx} T, \quad (4.1)
\]

where the terms can be divided into two parts: it contains the original Fourier equation and its time derivative as well with different coefficients as a hierarchy of Fourier equations [60]. There are two different time scales in the equation. The first one comes from the classical theory, \( t_1 = L^2/\alpha \). It is a natural time scale for the diffusion, predicted by the Fourier’s law. Here \( L \) is the characteristic length scale of the sample. The next one is the ratio of the extra material parameters, \( t_2 = \tau_q L^2/\kappa^2 \). When these different time scales are equal to each other, i.e. \( \alpha = \kappa^2/\tau_q \), there is no deviation from Fourier’s law and it is called Fourier resonance condition [182]. The role of the boundary condition appears here, the length of the heat pulse determines the second time scale. Furthermore, when \( \kappa^2/\tau_q > \alpha \) holds, it represents an over-diffusive solution. When \( \kappa^2/\tau_q < \alpha \) holds, then the wave-like behavior of MCV equation appears [60]. The equation (4.1) is rearranged in the following form in order to obtain a single parameter to characterize this deviation better,

\[
\tau_q \partial_t (\partial_t T - b\alpha \partial_{xx} T) + \partial_t T - \alpha \partial_{xx} T = 0, \quad (4.2)
\]

where the parameter \( b \) is:

\[
b = \frac{\kappa^2}{\tau_q \alpha}. \quad (4.3)
\]
In this form, \(b > 1\) indicates the over-diffusive domain and \(b < 1\) stands for the wave-like regime.

**Remark:** This kind of hierarchy repeating the Fourier equation is not exceptional in the framework of non-equilibrium thermodynamics \([60,183]\).

The thermodynamic theory predicts the same governing equations for the same measured temperatures, for various macroscopic mechanisms. We will see that the layered structure of the sample of the EGR-capacitor experiment is not the only possible heterogeneity which leads to deviation from Fourier’s law. In the following sections, finite element simulations and experiments on rock and metal foam samples are presented.

### 4.2.4 Finite element modeling of the EGR-capacitor experiment

With the help of a well understood microscopic mechanism we were able to simulate the low temperature NaF experiments. The layered sample of the EGR-capacitor experiment may be a way to look for a more detailed explanation. In this section we elaborate possible temperature profiles from this point of view.

As it is mentioned in the previous section, two materials with different thermal diffusivity are connected to each other parallel with the heat flux. One may expect that only two layers may be able to produce such deviation. It seems too simple and unnecessary at first glance. At second glance, it could be a checkpoint to understand the phenomenon in a totally controlled environment. During the modeling, every parameter can be adjusted and are under full control.

**Remark:** Ádám Lovas in his work for scientific student association \([184]\) created the basis of these finite element models under my supervision. The results based on these models demonstrate the physical interpretation of the previous section. However, the phenomenon in reality is more complex and more general.

The strategy was to build a geometry similar to the one of the EGR-capacitor experiment, starting from the simple two-layer model then applying progressively more and more layers, that is 5, 20 and 50 layers in the same overall volume. The boundary condition at front end is the same as in the numerical simulations, a smooth half-cosine function is applied. Adiabatic boundary condition is used at the rear end. To ensure the similarity with the capacitor experiment, a silver layer is situated at the rear end in every case where the probes record the temperature history.

![Figure 4.12: The sketch of model with indicating the direction of heat flux, the size of the geometry ([in mm]) and the place of the probes](image-url)

(a) Sketch of the geometry  
(b) The place of the probes at the rear end
Fig. 4.12 presents the sketch of the model and the place of the probes. The temperature history is recorded at four different points. It was necessary to check the correspondence with the experiments because the pins of thermocouples are connected at different points of the silver layer. It was concluded that there is no significant difference between the temperature histories at these points. The simulations were made by ANSYS\textsuperscript{1}.

The thermal conductivity of the better conductor was a parameter and adjusted in the interval from 10 to 250 $\frac{W}{mK}$. Its density, 8933 $\frac{kg}{m^3}$, and specific heat, 385 $\frac{J}{kgK}$, are constant. The other layer is a bad thermal conductor with lower thermal conductivity, mass density and specific heat as 4.5 $\frac{W}{mK}$, 4900 $\frac{kg}{m^3}$ and 800 $\frac{J}{kgK}$, respectively. The properties of the silver layer for thermal conductivity, mass density and specific heat are 429 $\frac{W}{mK}$, 10500 $\frac{kg}{m^3}$ and 235 $\frac{J}{kgK}$, respectively.

Two-layer model

The finite element model with the applied mesh is presented on Fig. 4.13. The number of nodes is 25344. During the simulation, the minimum time step was 0.001s, the maximum was 0.01s.

![Mesh of the global model](image1)

![Mesh of the silver layer](image2)

**Figure 4.13: The mesh of the finite element model**

It is important whether the outer or the inner layer is the better conductor thus two different series of results are presented according to the position of the better conducting layer. Let us begin with the case when the inner layer is the better conductor (Fig. 4.16). It is clear that for certain pairs of thermal conductivities one can observe a strong deviation from the Fourier case, it becomes similar to wave propagation. On Fig. 4.16 a Fourier fit is also presented to demonstrate the deviation and to calculate the corresponding effective thermal conductivity of the composite medium. The first, the third and the fourth simulation are presented here. On Fig. 4.16(b), the rear side temperature can be reproduced almost perfectly with the Fourier equation. The further results on Figs. 4.16(c) and 4.16(d) present clearly a non-Fourier effect. The deviation on Fig. 4.16(c) is similar to the measured one from previous section but weaker, see Fig. 4.10.

Regarding the other case when the outer layer is the better conductor (Fig. 4.17), already the first thermal conductivity pair (Fig. 4.17(b)) lead to more significant deviation from Fourier’s law. The type of deviations in this case differ from the previous one, it seems that these curves are in the under-diffusive region, i.e. in the MCV domain. Indeed, the result represents a solution for MCV domain, as it is demonstrated for the case of Fig.

\textsuperscript{1}Version: 17.2; with student license; applied module: transient thermal with classical Fourier equation.
4.17(d) (see Fig. 4.14), i.e. $\kappa^2/\tau_q < \alpha$. However, no wave propagation is experienced. Furthermore, the deviation from Fourier’s law is not apparent at first glance.

Figure 4.14: The solid line is the simulated data of the rear side temperature by finite element method (Fig. 4.17(d)). The dashed line is the solution of the GK equation with thermal diffusivity $\alpha = 4.23 \cdot 10^{-6} \text{ m}^2/\text{s}$, $\tau_q = 0.101 \text{ s}$, $\kappa^2 = 2.475 \cdot 10^{-7} \text{ m}^2$.

Let us note that the maximum applied thermal conductivity is $250 \frac{W}{mK}$ in the examples. The application of copper as inner layer with thermal conductivity of $398 \frac{W}{mK}$ leads to interesting result, see Fig. 4.15. The effect is similar as on Fig. 4.16(d) but stronger and there is an example to this characteristic in the section of rock samples without layers, namely in the case of Kantavár limestone, see Fig. 4.20.

Figure 4.15: The solid line is the simulated data of the rear side temperature by finite element method. The dashed line stands for the Fourier fit with thermal diffusivity $\alpha = 5 \cdot 10^{-6} \text{ m}^2/\text{s}$.
Figure 4.16: The solid lines are the results of simulations when the inner layer is the better conductor. Figures b), c) and d) present the Fourier fit by dashed line to demonstrate the deviation. The value of thermal conductivity corresponds to better conductor; the effective thermal diffusivity is obtained by Fourier fit.

(a) Summarized results of the simulations

(b) The applied parameters are: $\lambda = 10 \frac{W}{mK}$, $\alpha = 1.2 \cdot 10^{-6} \frac{m^2}{s}$

(c) The applied parameters are: $\lambda = 50 \frac{W}{mK}$, $\alpha = 2.4 \cdot 10^{-6} \frac{m^2}{s}$

(d) The applied parameters are: $\lambda = 150 \frac{W}{mK}$, $\alpha = 3 \cdot 10^{-6} \frac{m^2}{s}$
(a) Summarized results of the simulations

(b) The applied parameters are: \( \lambda = 10 \, \text{W m}^{-1} \text{K}^{-1} \), \( \alpha = 1.5 \cdot 10^{-6} \, \text{m}^2 \text{s}^{-1} \)

(c) The applied parameters are: \( \lambda = 50 \, \text{W m}^{-1} \text{K}^{-1} \), \( \alpha = 3 \cdot 10^{-6} \, \text{m}^2 \text{s}^{-1} \)

(d) The applied parameters are: \( \lambda = 150 \, \text{W m}^{-1} \text{K}^{-1} \), \( \alpha = 4 \cdot 10^{-6} \, \text{m}^2 \text{s}^{-1} \)

Figure 4.17: The solid lines are the results of simulations when the outer layer is the better conductor. Figures b), c) and d) present the Fourier fit by dashed line to demonstrate the deviation. The value of thermal conductivity corresponds to better conductor; the effective thermal diffusivity is obtained by Fourier fit.
5-20-layer models

In these models, the number of layers is greater, the sample is more and more similar to the one from EGR-capacitor experiment. According to the simulations, the order, that is which material is at the center, does not play a role. The overall number of nodes in these models is around 30000. The models are also tested for mesh dependency with satisfactory results. The time steps are also the same as in the two-layer model. The summarized results of these models can be seen on Fig. 4.18. The 5-layer model results in similar characteristics to the case 2-layer model when the better conductor is the outer layer (Fig. 4.17). It is shown that the effective parameters are in the MCV domain again, see Fig. 4.18(c).

Conclusion

The presented finite element simulations support the theoretical prediction that in heterogeneous samples there is a deviation from Fourier’s law. Although, so far only the over-diffusive domain is detected in the experiments. According to these simulations, it could be possible to reach the MCV domain, too. The derivation of the effective model, namely the GK equation, in the framework of non-equilibrium thermodynamics cannot give an explanation of the mechanism neither the dependency of effective parameters from the classical material properties such as thermal conductivity, specific heat and mass density of the components.
(a) Summerized results for 5-layer model

(b) Summerized results for 20-layer model

(c) The applied parameters are: $\lambda = 150 \frac{W}{mK}$, $\alpha = 4.03 \cdot 10^{-6} \frac{m^2}{s}$, $\tau_q = 0.132s$, $\kappa^2 = 3.15 \cdot 10^{-7}m^2$

Figure 4.18: The solid lines are the results of simulations for 5-20-layer models. Fig. 4.18(c) presents the fit of the GK equation for 5-layer model with parameters in the MCV domain.
4.3 Rock samples

Measurements of five rock samples are shown in this section, namely

- Crystalline limestone from Villány,
- Leucocratic rock,
- Boda red aleurolite,
- Kantavár limestone,
- Reddish partially porphyric monzogranite.

Remark: My related publication is [185]. In this paper the preliminary measurements of rock samples are presented.

The size of the samples is approximately the same, Fig. 4.19 shows for instance the crystalline limestone from Villány. The thickness of the samples can be found in Table 4.1.

![Figure 4.19: Crystalline limestone from Villány.](image)

The scheme and the evaluation of the measurement is the same as in the EGR-capacitor experiment. The experiments are repeated several times to validate and check the data, see Table 4.1 which contains the corresponding fitted parameters. In case of Kantavár limestone, the Fourier’s law describes precisely the beginning of the temperature history but the asymptotic part is unexpected (Fig. 4.20). It is similar to the one from finite element analysis, see Fig. 4.15. However, here there was no visible heterogeneity in the sample.

The strongest effect is produced by the limestone sample from Villány (Fig. 4.21 and 4.22). Similar results are shown by Fig. 4.23 for Boda red aleurolite and Leucocratic rock. As it is seen, the deviation occurs in the same way as for the layered sample and it holds in every other case, too. A detailed finite element modeling of such inhomogeneous structure can be facilitated by implementing the effective material parameters which are measured and evaluated by the extended theory. It represents clearly the general point of view behind the extension, such inhomogeneity is more general and untraceable than a layered structure, it shows greater variety in the nature and the effective theory can be useful to deal with such materials.
Some of the measurements show a decreasing, cooling tail for the temperature, hence in the evaluation two extra fitting parameters are introduced. One of them describes the rear end boundary condition, let us recall eq. (2.91):

\[ \hat{h} = h \frac{t_p}{\rho c L} \]  

where \( h \) is the heat transfer coefficient (HTC) at the rear side and \( \hat{h} \) is its dimensionless version. The real heat transfer coefficient cannot be calculated because the density and specific heat of the sample are unknown. Nevertheless, it can be estimated according to the dimensionless parameter due to the known heat pulse length, thickness and approximation of heat capacity. It yields the order of magnitude around 0.1 and 1 \( \frac{W}{m^2 K} \). The other parameter introduces the temperature scale, it is the ratio between the asymptotic temperature and maximum point of the measured temperature curve. This is the asymptotic temperature ratio. It is necessary because an unknown amount of energy goes to the environment during the measurement. When there is a ‘ - ’ sign in Table 4.1, then it was not necessary to use this parameter.

Figure 4.20: Measurement results (solid noisy line) and Fourier fitting (dashed line) of Kantavár limestone sample (22/02/2016, second experiment).

Figure 4.21: Measurement results (solid noisy line) and Fourier fitting (dashed line) of crystalline limestone sample from Villány (22/02/2016, second experiment).
Conclusion

Several rock samples were identified that show deviation from Fourier’s law. In principle, precise constituent analysis of the structure could be helpful to understand the origin of observed deviations. Practically, it is far more complicated than the effective modeling. Differences can be observed between the measurements made on different occasions. It could be caused by changed environmental conditions such as humidity, room temperature and so on. In order to obtain more consistent data, stricter measurement protocol is applied in the series of experiments in autumn 2016. It means enough time for the samples to relax between each experiment. It is clear that an effective model can be helpful in the measurement of thermal diffusivity and in transient processes where the thermo-mechanical effects play a role. The case of Kantavár limestone is remarkable due to the corresponding model of finite element analysis.
Figure 4.23: Summarized fitting results for Boda red aleurolite (/III.) and Leucocratic rock (/I.) samples. The experimental results are given by a solid noisy line, the fitting results are denoted with dashed line. The deviation is apparent. Measurement data: 22/02/2016.
<table>
<thead>
<tr>
<th>Sample</th>
<th>Length [mm]</th>
<th>Fourier Thermal diffusivity [mm²/s]</th>
<th>Thermal diffusivity [mm²/s]</th>
<th>Relaxation time [s]</th>
<th>Dissipation parameter [mm²/s]</th>
<th>HTC (h)</th>
<th>Asymptotic temperature ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>CLfV 12/02/II.</td>
<td>1.4</td>
<td>0.456</td>
<td>0.216</td>
<td>1.1591</td>
<td>0.7680</td>
<td>2·10⁻⁵</td>
<td>0.962</td>
</tr>
<tr>
<td>CLfV 12/02/II.</td>
<td>1.4</td>
<td>0.486</td>
<td>0.263</td>
<td>1.3720</td>
<td>0.8980</td>
<td>1.78·10⁻⁴</td>
<td>0.86</td>
</tr>
<tr>
<td>CLfV 22/02/I.</td>
<td>1.4</td>
<td>0.26</td>
<td>0.26</td>
<td>1.055</td>
<td>0.6664</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>CLfV 22/02/II.</td>
<td>1.4</td>
<td>0.26</td>
<td>0.26</td>
<td>1.055</td>
<td>0.6664</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>CLfV 26/09/1. - V.</td>
<td>1.4</td>
<td>0.3</td>
<td>0.20</td>
<td>1.176</td>
<td>0.5096</td>
<td>7·10⁻⁵</td>
<td>0.915</td>
</tr>
<tr>
<td>RPPM 12/02/I.</td>
<td>1.4</td>
<td>0.58</td>
<td>0.321</td>
<td>1.2226</td>
<td>0.9424</td>
<td>4.3·10⁻⁵</td>
<td>0.958</td>
</tr>
<tr>
<td>RPPM 12/02/II.</td>
<td>1.4</td>
<td>0.773</td>
<td>0.262</td>
<td>1.3881</td>
<td>0.8196</td>
<td>1.8·10⁻⁴</td>
<td>0.848</td>
</tr>
<tr>
<td>RPPM 22/02/I.</td>
<td>1.4</td>
<td>0.5</td>
<td>0.5</td>
<td>0.6272</td>
<td>0.49</td>
<td>-</td>
<td>-</td>
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<tr>
<td>RPPM 22/02/II.</td>
<td>1.4</td>
<td>0.3</td>
<td>0.3</td>
<td>0.6533</td>
<td>0.49</td>
<td>1.1·10⁻⁴</td>
<td>0.9</td>
</tr>
<tr>
<td>RPPM 22/02/III.</td>
<td>1.4</td>
<td>0.45</td>
<td>0.45</td>
<td>0.6968</td>
<td>0.49</td>
<td>4·10⁻⁵</td>
<td>0.98</td>
</tr>
<tr>
<td>Leucocratic rock 12/02/I.</td>
<td>1.75</td>
<td>0.46</td>
<td>0.46</td>
<td>1.1318</td>
<td>0.98</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Leucocratic rock 12/02/II.</td>
<td>1.75</td>
<td>0.57</td>
<td>0.57</td>
<td>0.9133</td>
<td>0.92</td>
<td>5.5·10⁻⁵</td>
<td>0.95</td>
</tr>
<tr>
<td>Leucocratic rock 22/02/I.</td>
<td>1.75</td>
<td>0.5</td>
<td>0.5</td>
<td>1.0412</td>
<td>0.9187</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Leucocratic rock 22/02/II.</td>
<td>1.75</td>
<td>0.52</td>
<td>0.52</td>
<td>1.0012</td>
<td>0.8575</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Kantavár limestone 12/02/I.</td>
<td>1</td>
<td>0.59</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Kantavár limestone 12/02/II.</td>
<td>1</td>
<td>0.64</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Kantavár limestone 22/02/I.</td>
<td>1</td>
<td>0.6</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Kantavár limestone 22/02/II.</td>
<td>1</td>
<td>0.63</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Boda red aleurolite 12/02/I.</td>
<td>1.45</td>
<td>0.075</td>
<td>0.075</td>
<td>0.4765</td>
<td>0.1219</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Boda red aleurolite 12/02/II.</td>
<td>1.45</td>
<td>0.078</td>
<td>0.078</td>
<td>0.4582</td>
<td>0.1135</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Boda red aleurolite 12/02/III.</td>
<td>1.45</td>
<td>0.08</td>
<td>0.08</td>
<td>0.4467</td>
<td>0.1135</td>
<td>4·10⁻⁵</td>
<td>0.95</td>
</tr>
<tr>
<td>Boda red aleurolite 22/02/I.</td>
<td>1.45</td>
<td>0.085</td>
<td>0.085</td>
<td>0.4947</td>
<td>0.1156</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Boda red aleurolite 22/02/II.</td>
<td>1.45</td>
<td>0.1</td>
<td>0.1</td>
<td>0.4205</td>
<td>0.1051</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Boda red aleurolite 22/02/III.</td>
<td>1.45</td>
<td>0.075</td>
<td>0.075</td>
<td>0.5046</td>
<td>0.1051</td>
<td>5·10⁻⁵</td>
<td>0.91</td>
</tr>
</tbody>
</table>

Table 4.1: Heat conduction parameters for rock samples. Abbreviations: CLfV = Crystalline limestone sample from Villány; RPPM = Reddish partially porphyric monzogranite sample. Date of the experiment is indicated after the name of sample (format: dd/mm); all of them is made in 2016.
4.4 Metal foam samples

Foams belong to the most pioneering material structures [186–189]. Inclusions are artificially situated inside the material during a special regulated gasifying process. The aim is to preserve good mechanical properties along with a lightened structure. The role of metal foams in aerospace, automotive industry, moreover in the field of heat exchangers is growing [188]. In our experiments, two different aluminum based foams are used. In the first one (type-1, Fig. 4.24(a)) the size of inclusions is around $1 \text{ mm}$. In the second one (type-2, Fig. 4.24(b)) the inclusions are bigger, around $2 - 3 \text{ mm}$. The type-2 structure shows the strongest deviation from Fourier heat conduction among all investigated samples.

(a) Metal foam, type-1  
(b) Metal foam, type-2

Figure 4.24: Metal foam samples used in the experiments

Figure 4.25 presents two typical measurement results. Fig. 4.25(a) corresponds to type-1 metal foam, it shows weaker effect compared with the type-2 metal foam (Fig. 4.25(c)). The GK equation is adequate to model these deviations (Fig. 4.25(b) and 4.25(d)). As the experiment shows, for short transient processes there is a significant difference between the prediction of the Fourier theory and the observed temperature history. The solutions are in the over-diffusive domain again. Table 4.2 presents the parameters from fitting of the Fourier and the GK equations.

The deviation from Fourier’s law at room temperature is demonstrated with different samples with different types of inhomogeneity. In the next chapter the scope is placed to organic materials in the framework of biological heat conduction.
Figure 4.25: Summarized fitting results for type-1 (\(I\)) and type-2 (\(II\)) metal foam. The noisy line corresponds to the measured data, the dashed presents the fitting. Measurement date: 12/02/2016.
<table>
<thead>
<tr>
<th>Sample</th>
<th>Length [mm]</th>
<th>Fourier</th>
<th>Guyer-Krumhansl</th>
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</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Thermal diffusivity [mm$^2$/s]</td>
<td>Thermal diffusivity [mm$^2$/s]</td>
</tr>
<tr>
<td>Metal foam, type-1 12/02/I.</td>
<td>5.2</td>
<td>5.7</td>
<td>5.17</td>
</tr>
<tr>
<td>Metal foam, type-1 12/02/II.</td>
<td>5.2</td>
<td>5.75</td>
<td>5.215</td>
</tr>
<tr>
<td>Metal foam, type-1 14/10/I. – IV.</td>
<td>5.2</td>
<td>9</td>
<td>7.7</td>
</tr>
<tr>
<td>Metal foam, type-2 12/02/I.</td>
<td>5.1</td>
<td>2.5</td>
<td>2.712</td>
</tr>
<tr>
<td>Metal foam, type-2 12/02/II.</td>
<td>5.1</td>
<td>2.5</td>
<td>2.65</td>
</tr>
<tr>
<td>Metal foam, type-2 22/02/I.</td>
<td>5.1</td>
<td>3.5</td>
<td>3.5</td>
</tr>
<tr>
<td>Metal foam, type-2 22/02/II.</td>
<td>5.1</td>
<td>2.35</td>
<td>2.35</td>
</tr>
<tr>
<td>Metal foam, type-2 22/02/III.</td>
<td>5.1</td>
<td>2.35</td>
<td>2.35</td>
</tr>
</tbody>
</table>

Table 4.2: Fitted parameters for metal foam samples. Date of the experiment is indicated after the name of sample (format: dd/mm); all of them is made in 2016. The roman numbers indicates the number of repetition.
Chapter 5

Biological heat conduction

In the previous chapters the existence of non-Fourier effects are demonstrated in case of inorganic materials. Although, these are the most important type of material for practical engineering applications, the role of theoretical predictions of heat conduction in organic materials is increasing by biological applications.

Remark: I have extended my research to biology. My goal here is to demonstrate the effectiveness of ballistic-conductive model and extend its limit of applications. I criticize the existing biological heat conduction models and I evaluated a heat pulse experiment from literature. These are my latest results and are under publication.

The experiment of Mitra et al. [171] and its shortcomings are already presented and motivates the investigation of this chapter. Banerjee et al. [190] made a series of laser flash experiments with 3 different materials, namely processed meat, tissue phantoms and fiber composites, with macroscopic length scale. The authors successfully used the MCV equation to explain their results; nevertheless, there is no wave phenomenon in this experiment. The experimental setup with their result is presented on Fig. 5.1. It must be noted that the thickness $z$ of the sample is 8 mm, but the authors did not mention which thickness corresponds to the curves on Fig. 5.1(b), i.e. what is the distance from the front end.

Jaunich et al. made a very similar series of experiments on multi-layered tissue phantoms, see Fig. 5.3 for details [191]. The MCV equation is also considered in modeling of temperature history along the radial and axial axis but the results can be explained neither with the Fourier’s law nor with the MCV equation (Fig. 5.3(c)). The series of experiments by Dhar et al. on translucent tissue should be mentioned here, too [192]. The scheme of the experimental arrangement is practically the same as on Fig. 5.3(b). Fig. 5.2 shows the temperature history versus the subsurface depth. It is evaluated by analytically solving Pennes’ model with moderate success. Among the numerous experiments, the one performed by Tang et al. is mentioned here [193]. These results will be reproduced in the framework of non-equilibrium thermodynamics and will be discussed later in the corresponding section.

The field of biological heat conduction seems to lack of suitable models for reproducing experiments. The applied models sometimes ad-hoc or devoid the strong thermodynamic basis. The next section presents the most frequently used models, moreover, analyze them from the point of non-Fourier heat conduction.

\footnote{The next section is devoted to present the heat conduction models in biology.}
5.1 Heat conduction in biological materials

We have demonstrated in the previous chapter that material heterogeneity may result in non-Fourier heat conduction. In biological systems such heterogeneity can be the porous structure (in analogy with foams and colloids), the blood vessels within several layers of skin, and so on. From the practical point of view, e.g. precision surgical application of lasers in medical sciences requires the prediction of temperature distribution in operations. A little difference in temperature distribution above the admissible level can cause irreversible damage in cellular level [194,195].
Figure 5.3: The original figures about the experimental setup and results of Jaunich et al. [191]
5.1.1 Pennes’ model

Pennes analyzed the steady-state temperature distribution of tissues and arterial blood in human forearm [196]. Pennes managed to obtain sink and source terms to extend the balance equation of internal energy. Pennes’ equation reads as

\[ \rho_c c_t \partial_t T = k_t \partial_{xx} T + \rho_b c_b \omega_b (T - T_a) + q_{met}, \]  

where \( \rho_t, c_t, k_t \) are the mass density, the specific heat and the thermal conductivity corresponding to the tissue, respectively. \( \omega_b \) is the blood perfusion rate and \( \rho_b, c_b \) are the mass density and the specific heat corresponding to the blood, \( T_a \) is the arterial blood temperature and \( q_{met} \) corresponds to the metabolic heat generation. One can see, that this model obeys the Fourier’s constitutive equation. From the anatomical point of view, Pennes applied the following simplifying assumptions [197]:

- the directional dependence of blood flow is neglected,
- the blood is at the temperature of the body core and instantaneously equilibrates with the tissue temperature,
- the local vascular geometry is not considered in this model.

According to Zolfaghari and Maerefat [198], the metabolic heat generation and the blood perfusion effects are simplified and considered as homogeneous and isotropic in the tissue. Moreover, Zolfaghari and Maerefat also noted the main shortcomings of this model, namely the oversimplified vascular geometry, the directionality of the blood perfusion is not accounted and the blood temperature is not equal to the body core temperature contrary to the Pennes’ model [197,198].

5.1.2 Chen-Holmes (CH) model

In 1980, Chen and Holmes proposed [199] a model which is the most detailed one from a physiological point of view. Chen and Holmes modeled separately the tissue and the blood by separating their volumes. Its brief derivation is presented below with the original notations.

Let us choose a differential control volume \( \delta V \) which can be divided into \( \delta V = \delta V_s + \delta V_b \), where \( \delta V_s \) represents the volume of the solid tissue and \( \delta V_b \) stands for the vascular space. It is assumed that \( \phi \equiv \frac{\delta V_b}{\delta V} \ll 1 \). Then a local mean temperature is defined by volume averaging:

\[
T_s = \frac{1}{\delta V_s} \int_{\delta V_s} TdV, \]

\[
T_b = \frac{1}{\delta V_b} \int_{\delta V_b} TdV. \]  

(5.2)

There are two different balance equations for the energy. The first one corresponds to the solid tissue and it is expressed as

\[
\delta V_s \rho_s c_s \partial_t T_s = \delta Q_{ks} + \delta Q_{b-s} + \delta Q_m, \]  

(5.3)
where \( \rho_s \) and \( c_s \) are the tissue density and the specific heat, \( \delta Q_{ks} \) is the conductive heat gain, \( \delta Q_{bs} \) stands for the heat gain from the blood and \( \delta Q_m \) represent the metabolic term. The second balance corresponds to the blood and reads as

\[
\delta V_b \rho_b c_b \partial_t T_b = \delta Q_{kb} + \delta Q_{b-s} \int_S \rho_b c_b T u dS,
\]

(5.4)

where \( \rho_b \) and \( c_b \) are the blood density and specific heat, \( \delta Q_{kb} \) is the conductive contribution, the integral over the surface \( S \) is the convective energy transport due to the blood and \( u \) represents the velocity vector of the flow field. This term represents the main difference between the Chen-Holmes model and the Pennes’ model. Moreover, it makes CH model harder to implement. It requires detailed description of the anatomy, the exact knowledge about the blood flow field, moreover, the accurate modeling of the vascular system [200]. Adding equations (5.3) and (5.4), then dividing by \( \delta V \), it results:

\[
\rho c \partial_t T_t = q'_k + q'_m + q'_p,
\]

(5.5)

where \( \rho = (1 - \phi) \rho_s + \phi \rho_b, \ c = 1/\rho ((1 - \phi) \rho_s c_s + \phi \rho_b c_b) \) and \( T_t \) is the local mean tissue temperature which can be expressed as

\[
T_t = \frac{1}{p c} ((1 - \phi) \rho_s c_s T_s + \phi \rho_b c_b),
\]

(5.6)

and approximately equal to \( T_s \) in case of \( \phi \ll 1 \) [199]. Here \( q'_k \) and \( q'_m \) corresponds to the heat flux from Fourier’s law and metabolic heat generation, respectively. Furthermore,

\[
q'_p = \frac{1}{\delta V} \int_S \rho_b c_b T u dS.
\]

(5.7)

The Chen-Holmes model reads as

\[
\rho c \partial_t T_t = (k + k_p) \partial_{xx} T_t + \rho_b c_b u \cdot \nabla T_t + W c_b (T_t - T_{art}) + q_m,
\]

(5.8)

where \( k \) is the thermal conductivity of the tissue and \( k_p \) is called the perfusion conductivity. It accounts the enhanced conduction by blood perfusion. The blood perfusion term differs from the Pennes’ model, here \( W \) is the perfusion rate and \( T_{art} \) represent the upstream blood temperature in the arteriole instead of the body core temperature. Zolfaghari and Maerefat mention that this description does not deal with the effect of the counter-current artery-vein pairs [198]. This kind of shortcoming is corrected in the model of Weinbaum, Jiji and Lemons. The CH model also apply the Fourier’s law, but Gou and Cai refers to this model as non-Fourier equation and present the equation (5.8) with an extra, second time derivative term [201].

### 5.1.3 Weinbaum-Jiji-Lemons (WJL) and Weinbaum-Jiji (WJ) models

The counter-current like behavior of the vascular system have been implemented in these models. The WJL model is also called as three temperature model due to the identification of three different vascular layers of the skin, namely the deep, intermediate and cutaneous layers [197]. Khanafer and Vafai pointed out that the WJL model is mainly valid within the intermediate layer ( [194], p23).
Let us start the discussion with the WJL model [202]. One can define the heat gain by conduction per unit length through the wall of the artery and veins:

\[
\rho b c b \pi r^2 \mathbf{u} \frac{dT_{art}}{ds} = -q_{art},
\]

\[
\rho b c b \pi r^2 \mathbf{u} \frac{dT_v}{ds} = -q_v,
\]

where \( \rho \) and \( c \) are the mass density and the specific heat, \( r \) is the vessel radius, \( \mathbf{u} \) stands for the mean velocity in either the artery or vein, thus the WJL model apply the same velocity for inlet and outlet blood flow. \( T_{art} \) and \( T_v \) are the bulk mean temperatures inside the blood vessel and \( s \) stands for the unit normal vector of the blood vessel surface. It results in the following equation for the tissue temperature in one spatial dimension:

\[
\rho_t c_t \partial_t T_t = k_t \partial_{xx} T_t + n g \rho_b c_b (T_{art} - T_v) - \rho_b c_b n \pi r^2 \mathbf{u} \frac{d(T_{art} - T_v)}{ds} + q_{met},
\]

(5.10)

where \( g \) is the perfusion bleed-off velocity per unit vessel surface area and \( n \) is the number of arteries or veins. This approach considers the artery and vein diameters to be equal, neglects the lymphatic fluid loss to obtain the same mass flow rate in the vein as in the artery, also assumes the bleed-off perfusion as spatially uniform and the axial conduction through vessels [203] is neglected. It is difficult to implement into practical tasks, the \( T_{art} \) and \( T_v \) are unknown parameters [198], thus in 1985, Weinbaum and Jiji have simplified this model [204].

In order to avoid the difficulties with three different temperatures, the tissue temperature \( T_t \) is approximated with the average of the artery and vein temperatures, moreover, \( q_{art} \approx q_v \approx \sigma k_b(T_{art} - T_v) \), where \( \sigma \) is the geometrical shape factor to characterize the resistance between two parallel vessels embedded in an infinite medium [198]. It means that the heat from the artery goes almost completely to the vein.

Weinbaum and Jiji [204] introduced an effective thermal conductivity to model the enhancement in the tissue conductivity due to the blood flow and in one dimension reads as

\[
k_{eff} = k \left( 1 + \frac{\pi^2}{4 \sigma k^2} n^2 h_b^2 P e^2 \right),
\]

(5.11)

where \( P e \) is the Peclet number and \( k \) belongs to the isotropic tissue thermal conductivity. This kind of modeling theoretically can result in around 3.5 times higher effective thermal conductivity for the tissue [204]. As it can be seen, the WJ model requires lot of anatomical informations, just like the CH model. The simplifying assumptions can be easily violated and according to [198], it is not an accurate model to predict the temperature field. It must be emphasized that the vascular anatomy is different from the superficial tissues [200], for example this happens in tumors.

5.1.4 Wulff model

Wulff in [205] directly criticized Pennes’ model in the sense of incorrect formulation of thermal transport by blood and proposed a modified constitutive equation:

\[
\mathbf{q} = -k_t \nabla T_t + \rho_b h_b \mathbf{U}_h,
\]

(5.12)

where the index ‘\( t \)’ and ‘\( b \)’ refers to the tissue and blood properties; \( h_b \) is the specific enthalpy of the blood and \( \mathbf{U}_h \) denotes the local mean blood velocity. It is clear that
the temperature of a given point of the tissue depends on the blood flow. However, this expression means that the material behavior of the tissue – the constitutive equation – depends on the blood flow which is physically questionable from the point of view of objectivity. Blood transport influences the heat transfer but it does not modify the tissue as a material. Wulff’s model totally differs from the CH and Pennes model in this respect.

The second term on the right hand side in equation (5.12) is introduced in order to extend the heat flux between tissue and blood with the enthalpy flux. The specific enthalpy is expressed as follows:

\[
h_b = \int_{T_0}^{T_b} c_b(T) dT + \frac{P}{\rho_b} + \Delta H_f (1 - \epsilon),
\]

where \(P\) is the blood pressure, \(\Delta H_f\) is the enthalpy correspond to metabolic reaction and \(\epsilon\) is the degree of reaction. The integration of the velocity field over the entire solid angle \(\Omega (=4\pi)\) results in

\[
U_h = \frac{1}{4\pi} \int_{\Omega} u d\omega.
\]

This leads to the following expression by applying the balance equation for internal energy,

\[
\rho c_t \partial_t T_t = -\nabla \cdot \left[ -k_t \nabla T_t + \rho_b U_h \left( \int_{T_0}^{T_b} c_b(T_b^*) dT_b^* + \frac{P}{\rho_b} + \Delta H_f (1 - \epsilon) \right) \right],
\]

where the operation \(\nabla \cdot\) stands for the divergence. It must be mentioned that the term \(\nabla \cdot P\) introduces the acceleration of the blood by Cauchy’s equation of motion from continuum mechanics. Furthermore, in this framework a relative motion is introduced into the constitutive equation which is not allowed by objectivity [206–208] which is one of the central problems of continuum mechanics.

Wulff introduced the following simplifications:

- the mechanical part \(\frac{P}{\rho_b}\) is neglected,
- the divergence of the term \(\rho_b U_h\) is considered as zero,
- the temperature of the blood is equal to the temperature of the tissue,
- material parameters are constant and independent on the direction, i.e. isotropic.

These assumptions lead to a more simplified equation for tissue temperature:

\[
\rho c_t \partial_t T_t = k_t \nabla^2 T_t - \rho_b c_b U_h \nabla T_t + q_m,
\]

where the internal metabolic production term is expressed as \(q_m = \rho_b U_h \Delta H_f \nabla \epsilon\). Let us note the following. The terms

\[
\rho c_t \partial_t T_t + \rho_b c_b U_h \nabla T_t
\]

almost forms a material time derivative except the different material parameters. It highlights the questions about the physical background of this model.

One of the main conclusions of Wulff’s paper that the blood flow affects only slightly the temperature distribution in the tissue. Then it would be straightforward to model effectively such effect without introducing the flow field into the equations. It would be easier to solve, too.
5.1.5 Klinger model

Klinger divided the heat flux in the tissue into two parts [209]. The first one corresponds to the Fourier’s law and the second one represents the heat convection in the perfused tissue. The material parameters are considered as constant. Klinger found an analytical solution for infinite medium with constant convection field in space and time. Klinger used this general solution to analyze the temperature distribution in perfused tissues [210]. This framework is very similar to Wulff’s model, however, there are slight differences. Klinger’s model reads as

\[ \rho c (\partial_t T + v(x, t) \cdot \nabla T) = k \nabla^2 T + q_V(x, t), \]  

(5.18)

where all of the material parameters correspond to the tissue and the internal heat generation \( q_V(x, t) \) is considered as time and space dependent. Here \( v(x, t) \) represents the velocity field. The incompressibility of the blood is also used. On the left-hand side one can see a real material time derivative, contrary to Wulff’s model. This treatment of the convection field makes the description more general but in parallel, more difficult to solve.

5.1.6 Small artery model (SAM)

The SAM model is developed by Anderson and Valvano [211] to describe the connection between the self-heated thermal thermistor measurements and perfusion. Moreover, its goal is to improve the Pennes and KEFF [212, 213] models. This model specifically developed for the anatomy of kidney vascular system due to its highest perfusion rate among the organs. In this sense, the modeling approach is similar to WJ model, it is highly based on the anatomy as it follows from the definition of the heat flux,

\[ q_a = n F a \text{avg} [1 + \lambda - 2\lambda \xi] \rho_b c_b T_b - T_t - \Delta z, \]

where \( n \) is the vessel density, \( \rho_b \) and \( c_b \) are the usual blood density and specific heat. The last fractional term means the temperature difference between the sides of the control volume and it is considered only in direction \( z \) which is parallel to the artery. The term \( F a \text{avg} \) means the ‘average flow of a typical interlobular artery’, \( \lambda \) is the bleed-off term, \( \xi \) is the dimensionless distance and these quantities completely depend on the current anatomy [211]. The definition reads the same as for veins. Kreith et al. call attention to its discrete formalization because it does not allow to apply it in inverse problems, only in the case where the exact vessel density is known [203].

5.1.7 Simplified thermo-regulatory bioheat model (STB)

Zolfaghari and Maerefat [214] investigate the thermo-regulatory control mechanisms such as regulatory sweating, shivering and so on. The authors emphasize that these mechanisms are able to change the body core temperature which is considered constant in Pennes’ model. This approach combines Pennes’ model with Gagge’s thermal comfort model [215]. Hensen emphasizes the significance of the comfort models and environmental conditions due to their considerable impact to the body core temperature [216].

The governing equation of STB model is very similar to the one from Pennes’ model:

\[ \rho_t c_t \partial_t T_t = k_t \partial_{xx} T_t + \rho_b c_b W_b (T_b - T_t) + q_{net}, \]  

(5.19)

where the indices \( t \) and \( b \) refer to the tissue and blood properties, \( W_b \) is the perfusion rate of the blood, \( T_b \) corresponds to the blood temperature and \( q_{net} \) stands for the metabolic
heat generation. It modifies the perfusion term by a minus sign regarding the Pennes’
model and applies time dependent boundary conditions to consider the environmental
conditions. Based on the paper of Lv and Liu [217], the boundary condition for skin
surface is
\[-k_t \partial_x T_t = h(T_t - T_a) + \sigma \varepsilon ((T_t + 273)^4 - (T_a + 273)^4) + (3.054 + 16.7h\omega_{skin})(0.256T_t - 3.37 - P_a), \tag{5.20}\]
where \(T_a\) denotes the air temperature, \(P_a\) is the water vapor pressure in the air, \(h\) is the
convective heat transfer coefficient, \(\varepsilon\) is the skin emissivity and \(\sigma\) stands for the Stefan-
Boltzmann constant, \(\omega_{skin}\) is the skin wettedness. In [217], the body core temperature
is considered as constant, however, in this model it varies in time according to the following
condition:
\[(1 - \alpha) \rho_b c_b \frac{dT_{cr}}{dt} = r_m q_m - \frac{(K_{eff} + c_b\dot{m}_b)(T_{cr} - T_{sk})}{l_b}, \tag{5.21}\]
where \(\alpha\) is the fraction of total body mass concentrated in the skin compartment, \(T_{cr}\) is
the body core temperature, \(T_{sk}\) is the skin temperature, \(K_{eff}\) is the effective conductance
between core and skin compartments and \(r_m\) is called as remaining metabolic coefficient
and it is defined as
\[r_m = 1 - \eta - 0.0014(34 - T_a) - 0.0173(5.87 - P_a), \tag{5.22}\]
where \(\eta\) is the external mechanical efficiency which is insignificant in many applications
[214]. The characteristic length of the body \(l_b\) is needed and defined as
\[l_b = \frac{V_b}{A_D}, \tag{5.23}\]
where \(A_D\) is the nude body surface and \(V_b\) is the body volume. Equations (5.20) and
(5.21) are coupled to each other by \(T_{sk} = T_t\) on the skin surface.

As it is presented, the STB model contains several empirical factors that depend on
many parameters of environment and anatomy. There is no further information provided
how the \(K_{eff}\) is determined. Furthermore, such system of partial differential equations
with time dependent radiative nonlinear boundary conditions is hard to solve, even with
modern numerical methods. Despite of these properties, the STB model is validated
through experiments and shows good agreement. It must be noted that the characteristic
time of such thermo-regulatory processes is several minutes or hours. It means that such
model cannot be used for fast processes such as laser operations where the characteristic
time can be less than seconds.

The models so far obeyed the Fourier’s law and devoted to consider the source or sink
terms in the body more accurately. It is not an easy task due to the great number of varia-
tions in properties among the organs and skin structure. Based on the experiments, these
models are not applicable for problems where the time scale is relevant and heterogeneity
induces non-Fourier heat conduction.

### 5.1.8 DPL model revisited

The physical basis of DPL equation is already discussed. However, in the field of biological
heat conduction it is a popular model and many authors applied this type of extension.
Zhou et al. used this approach to predict the thermal damage in irradiated tissues [218].
Zhang proposed the so-called generalized DPL (GDPL) model [219] where the DPL equation (2.39) is extended by the corresponding heat transfer terms. It is straightforward that in case of zero relaxation times the model reduces to Pennes’ model.

Zhang proposed explicit formulas to calculate the relaxation times analytically [219], based on the work of Minkowycz et al. [220],

\[
\tau_q = \frac{\varepsilon(1-\varepsilon)}{C_{tb}} \rho_b c_b G, \\
\tau_T = \frac{\varepsilon(1-\varepsilon)}{K_{tb}} \rho_b c_b G ,
\]

(5.24)

where \( C_{tb} = \rho_t c_t / (\rho_b c_b) \) is the ratio of heat capacities and \( K_{tb} = k_t / k_b \) is the ratio of the thermal conductivities, the index \( t \) and \( b \) corresponds for the tissue and blood and \( \varepsilon \) represents the porosity of the tissue. \( G \) is the so-called lumped convection-perfusion parameter, it depends on the vascular diameter, heat transfer coefficient and the perfusion rate of the blood. Zhang evaluated the relaxation times for several cases. It has an important consequence during the interpretation of these results. It clearly shows when the relaxation times \( \tau_q \) and \( \tau_T \) are equal then Fourier-type solution is experienced. It is related to the Fourier-resonance condition proposed in the previous chapter. Let us note two cases in this respect. When the porosity is zero then it results in Fourier-type solution due to the zero relaxation times, the structure reduced to a homogeneous one. In the other case when the ratio of heat capacities is equal to the ratio of thermal conductivities, it leads to the equality of the relaxation times, the structure is homogeneous again. Zhang used [219] these formulas (5.24) in a test problem proposed by Yuan [221]. The estimated relaxation times obey the condition proposed by Fabrizio discussed in the chapter of nonequilibrium thermodynamics. Nevertheless, it should be observed that the dimensional parameters in equation (5.24) correspond only to blood instead of the tissue.

Hooshmand et al. present the analytical solutions for DPL and GDPL equations for adiabatic boundary conditions [222]. The solutions are tested by laser irradiation experiments made by Museux et al. [223] and compared to each other, see Fig. 5.4. It is found that the anatomy based extensions lower the temperature distribution below the predicted values by the DPL equation (Fig. 5.4(a)). Unfortunately, these calculations are found to be far from the experiment which presented by Fig. 5.4(b).

According to Afrin et al. [224], the solutions of the GDPL model can be really different from the DPL or the Fourier model which statement is in good agreement with Hooshmand et al. [222]. Afrin et al. analyzed the impact of the used model to the thermal damage and concluded that in most of the cases, the Fourier’s law overestimates the temperature.

A demonstrative analysis is made by Liu and Chen [225]. The DPL model is used for predicting the temperature distribution during a tumor treatment, furthermore, the solutions are compared to the experiments from Andrä et al. [226] and the results are in good agreement, see Fig. 5.5.

Sahoo et al. investigated the temperature history in a wet tissue and applied the DPL and type-3 DPL equations to model the laser irradiation [63]. Fig. 5.6 presents the result of the experiment and fitting of the equations. It must be noted as a conclusion that further Taylor series expansion is seemingly not helpful in the modeling. Moreover, the type-3 equation is more complicated, harder to solve and it does not improve the solution. Instead of the improvement, it introduces extra propagation effects that are not proved experimentally.
(a) Temperature distribution along skin tissue depth at different time instants

(b) Temperature history in the experiment and calculations

Figure 5.4: The original figure about the calculations and experimental results of Hooshmand et al. [222]

Figure 5.5: The original figure about the experimental results and calculations from Liu and Chen [225]
5.2 Experiment revisited

In this section the already mentioned experiment of Tang et al. is discussed in detail [193]. It is also a heat pulse experiment but the sample is a processed meat similar to the one from the paper of Mitra et al. [171]. The diameter of the samples is 10 mm, their shape is cylindrical. The experiment is repeated with three different sample lengths, i.e. $L = 2$, 3 and 4 mm. The pulse time is 1 s, which is considerably higher than the one from capacitor experiment (0.01 s). The front end of each specimen is blackened by using graphite spray. At the rear end, Cu film is applied with thickness of 0.01 mm. The results can be seen on Fig. 5.7, [193].
At first sight, the non-Fourier behavior seems to be clear from the deviation between the fitting and measured data (Fig. 5.7). The cooling of the specimen is relevant in the case where the length $L$ is 2 and 3 mm. The evaluation of such measured result is the same as it was presented in the last chapter for our own experiments. However, in these cases the dimensionless temperature cannot reach one, not even theoretically, due to cooling. Thus in the second and third cases the fitting should be reconsidered.

The fitting is reproduced in the framework of non-equilibrium thermodynamics, see Fig. 5.9. It is clear that in the first case the deviation from Fourier’s law is real. However, when cooling is present, the Fourier fitting of Tang et al. [193] is not appropriate and there is no such deviation in the experimental data, the Fourier’s law is applicable in these cases, see Figs. 5.9(c) and 5.9(d). Moreover, as it can be seen on Fig. 5.8, the deviation is considered as a wave propagation which produces an overshoot instead of cooling tail [193] and it leads to equilibrium below the dimensionless temperature one.

![Figure 5.8: The original figure about the experimental results and comparisons from Tang et al. [193]](image)

**Conclusion**

The heat conduction models with biologically inspired extensions are presented. We have seen that only the MCV and the DPL equations are used to model non-Fourier effects. The other, biologically inspired theories are not appropriate to model fast transient phenomena or non-Fourier effects in heat conduction.

The next aspect is to model a complex medium. Among the great variety of anatomical structures such as organs, muscles and differences between human beings, the heat transfer processes are more complex due to the small size and unknown or at least hardly measurable quantities. The need for an effective and universal model with strong physical basis is required in the field of biological heat conduction.
(a) Fourier fit for the first case; $\alpha = 1.1 \cdot 10^{-7} m^2/s$

(b) GK fit for the first case $\alpha = 9.4 \cdot 10^{-8} m^2/s$, $\tau_q = 3.574 s$, $\kappa^2 = 5.44 \cdot 10^{-7} m^2$

(c) Fourier fit for the second case; $\alpha = 7.7 \cdot 10^{-8} m^2/s$

(d) Fourier fit for the third case; $\alpha = 7 \cdot 10^{-8} m^2/s$

Figure 5.9: Solid line denotes the measured data from Tang et al. [193], the dashed line presents the fitting
Summary and Theses

The Fourier’s law can be derived easily from non-equilibrium thermodynamics in local equilibrium [13,51]. In this work, non-equilibrium thermodynamics with internal variables and Nyíri-multipliers was applied to extend the classical theory out of local equilibrium. The comparison with other theories and experimental discovery of the prediction is the subject of this Ph.D. dissertation. In classical irreversible thermodynamics the coupling is forbidden between a vectorial and a tensorial thermodynamical interaction. With the help of internal variables and Nyíri-multipliers one can overcome this difficulty. This is the key aspect of our theory of heat conduction out of local equilibrium.

1. Thesis

I have applied one vectorial and one second-order tensorial internal variable along with generalized entropy current by Nyíri-multipliers in the framework of non-equilibrium thermodynamics to derive the ballistic-conductive model of heat conduction. I have compared this theory of non-equilibrium thermodynamics to the kinetic theory based Rational Extended Thermodynamics in case of heat conduction in solids and rarefied gases in 1+1 dimensions. I have derived the conditions of equivalence of these two theories.

Related publications: [2,3]

The ballistic-conductive model is solved numerically with the particular initial and boundary conditions of heat pulse experiments. Shifted field discretization method is applied in order to use only physical boundary conditions for the heat flux. The finite difference scheme is explicit therefore stability conditions are required. To obtain a complete framework for numerical solution, the convergence of the scheme is proved.

2/A. Thesis

I have developed an explicit finite difference scheme based on the discretization of shifted fields to solve the ballistic-conductive model of the 1. Thesis.

2/B. Thesis

I have derived the stability criteria of the developed numerical scheme with the help of Neumann method and Jury conditions. I have proved the weak consistency of the developed numerical scheme. The convergence of the scheme follows.

Related publications: [2,3]
The 1. and 2. Theses are the basis to test the performance of our non-equilibrium thermodynamical framework on heat pulse experiments. First, the ballistic-conductive model is tested on NaF experiments of Jackson et al. [147–149]. The goal was to model the wave forms of heat conduction, namely the phenomena of second sound and ballistic propagation. The numerical modeling shows that our theory is competitive with the Rational Extended Thermodynamical one. Moreover, the temperature dependency of relaxation times is also shown.

3. Thesis

I have applied the ballistic-conductive system of equations to model the ballistic heat propagation in NaF crystals observed by Jackson et al. [147–149]. I have calculated the material parameters along with the temperature dependency of thermal relaxation times.

Related publications: [3,122]

The low temperature experiments are a demonstrative and comprehensive test of the ballistic-conductive model. However, the practical problems in engineering sciences require experiments under not so extraordinary conditions. Hence, heat pulse experiments at room temperature, at the Department of Energy Engineering, BME were performed. In this dissertation, the theoretical framework is universal, in the sense that it is independent from a particular micro- or mesomechanism. Therefore, the deviation from Fourier’s law is not related to the existence of phonons. The non-equilibrium thermodynamic theory does not exclude non-Fourier heat conduction under different, more common conditions, e.g. because of material inhomogeneity at room temperature. Our prediction was confirmed by experiments. The simplified ballistic-conductive model, namely the Guyer-Krumhansl equation is used to evaluate the measured deviation. Here, the hierarchy of Fourier equation was helpful to introduce a parametrization of the deviation from Fourier’s law. The investigation of room temperature experiments covers the organic and inorganic materials as well.

4. Thesis

I have realized the hierarchy of Fourier equation in the Guyer-Krumhansl equation. I have introduced the parametric characterization of deviation from Fourier’s law at room temperature based on the experiments performed at the Department of Energy Engineering, BME and the experiments of Tang et al. [193].

Related publications: [3,60,182,185]
Összefoglalás és tézisek

A technológiai fejlődés napjainkban megköveteli a fizika klasszikus törvényeinek érvényességi körén túlmutató jelenségek hasznosítását. Így például alacsony hőmérsékleten (< 10 K) vagy nanométeres léptéken lezajló jelenségeket kell modelleznünk. Ahhoz, hogy leírhatóak legyenek az itt előforduló, a klasszikustól eltérő transzport jelenségek, szükségessé válik a konstitutív egyenletek kiterjesztése. Ez az említett fizikai körülmények alatti anyagi viselkedés megértését jelenti.

Ebben a munkában a belső változókkal és a Nyíri-szorzókkal általánosított nemegyen-súlyú termodinamikai elméletet használtuk a klasszikus lokális egyensúlytól való eltérés leírására. A termodinamika második főtélétele fizikai alapelvekért az egyetlen kényszerként szolgál a konstitutív és fejlődési egyenletek levezetésében. A vizsgálatainkban szilárd testek és ritka gázok hővezetési jelenségeinek leírására foglalkozunk.

A klasszikus Navier-Stokes-Fourier rendszer is könnyen levezethető a nemegyen-súlyú termodinamikai keretein belül a klasszikus egyensúlyi hipotézis segítségével. Itt a termikus disszipációt vektori, a mechanikát másodrendű tenzori változók írják le. A vonatkozó konstitutív egyenletek izotróp anyagokban közvetlenül nem csatoltak, csak a mérlege-gyenleteken keresztül. A klasszikus irreverzibilis termodinamika a Curie-elven keresztül tiltja a különböző tenzori rendő mennyiségek konstitutív egyenleteken belüli csatolását. Azonban a lokális egyensúlytól túl a belső változók és Nyíri-szorzók alkalmazása feloldja ezt a korlátozást. Ez egy különszintességű pontja a hővezetés lokális egyensúlyon kívüli leírásának.


A célunk egy egyesítő kontinuum elmélet levezetése a nemegyen-súlyú termodinamikai keretein belül. A belső változók és a Nyíri-szorzók alkalmazása lehetővé teszi számunkra, hogy a második főtéltelel kompatibilis módon hozzunk létre kapcsolatot a termikus és mechanikai mezők, illetve különböző tenzori rendő mennyiségek között a konstitutív egyenletekben.

Ez a Ph.D. értekezés két részre bontva tárgyalja a kísérleteket. Az első rész Jackson és társai alacsony hőmérsékletű kísérleteirel foglalkozik és a hő hullámtermészetét vizsgálja. A másik rész a BME Energetikai Gépek és Rendszerek Tanszéken a kutatócsoportunk által végzett, úgynevezett szoba-hőmérsékletű EGR-kísérleteket mutatja be. Itt a cél az anyagi inhomogenitások hővezetésre gyakorolt hatásának a kimutatása volt. A felállított nem-
Egyensúlyi termodinamikai elmélet megjósolja a nem-Fourier viselkedést szobahőmérsékleten is, ezen a nyomon elindulva sikerült közönséges körülmények között is kimutatni a nem klasszikus viselkedést, például fémhabokban és több különböző közettípusnál.

Az értekezés célja az eredményeink összehasonlítása más vonatkozó elméletekkel és az elméleti predikció kísérleti felfedezésének a bemutatása.

Elméleti szempontból nézve, a ballisztikus-konduktív modellhez vezető általánosítást már bemutattuk. A levezetett általánosított egyenlet megoldásához egy egyedileg kidolgozott numerikus módszert használtunk fel, mely az eltolt mezőkön alapul. A gyakorlati szempontokat is szem előtt tartva, hőimpulzus kísérletek segítségével sikerült kimutatni a megjósolt jelenséget. A hőimpulzus kísérletek szolgáltatták az értekezés gyakorlati alapját. Ez a mérési módszer az anyagok hőfokvezetési tényezőjének a meghatározására szolgáló alapvető eljárás a mérnöki gyakorlatban. A klasszikustól eltérő esetekben a Fourier-törvény nem használható, azonban ugyanaz a mérési módszer használható a kiterjesztett elméletben megjelenő új paraméterek meghatározására. Ugyanez az elrendezés érvényes az alacsony hőmérsékletű kísérletekre is, így ugyanaz az állapotot értékelhető ki ezek a különböző kísérletek. A mérés kiértékeléséhez a hőmérséklet változásokban és a lehűlést jellemző hőátadási paraméterek bevezetésére is szükség volt.

Tézisek és eredmények

Az elméleti háttér egy erős alapot szolgáltat a nem-Fourier hővezetés modellezésére függetlenül az anyagi inhomogenitás jellegétől vagy az anyag állapotától. A Nyíriszorzókkal és a belső változók bevezetése egy olyan kontinuum modellhez vezet, amely képes egyesíteni a nem-Fourier hővezetés ismert aspektusait. Az 1. tézis ezt az eredményt fogalmazza meg.

1. Tézis

Egy vektori és egy másodrendű tenzori belső változót alkalmaztam a Nyíriszorzókkal általánosított entrópiaárammal együtt a nemegyensúlyi termodinamikai elméletben a hővezetés ballisztikus-konduktív egyenletének levezetéséhez. Ezt az elméletet összehasonlítottam a kinetikus elméleti alapú Racionális Kiterjesztett Termodinamika szilárd testek és ritka gázok hővezetésére vonatkozó elméleteivel 1+1 dimenzióban. Megadtam a két elmélet ekvivalenciájához szükséges feltételeket.

Vonatkozó publikációk: [2,3]

A levezetett ballisztikus-konduktív modell megoldását numerikusan állítottam elő egy explicit véges differencia séma segítségével. Az 1. és a 2. Tézispontok fektetik le az alapot a nem-Fourier hővezetés megértéséhez. Továbbá, ezek elengedhetetlenek a kísérletek kiértékeléséhez.

2/A. Tézis

Kidolgoztam egy eltolt mezőkön alapuló explicit véges differencia sémát az 1. Tézisben megfogalmazott ballisztikus-konduktív modell megoldásához.
2/B. Tézis

Levezettem a kidolgozott numerikus séma stabilitási feltételeit a Neumann és Jury módszerek segítségével. Bebizonyítottam a séma gyenge konzisztenciáját. Ezek együtt biztosítják a séma konvergenciáját.

Vonatkozó publikációk: [2, 3]

A ballisztikus-konduktív modellt először Jackson és társai NaF kísérletein teszteltük [147–149]. A cél a hővezetés egyes hullámtöltött formáinak, azaz a második hangnak és a ballisztikus terjedésnek a modellzése volt. A numerikus modellezés megmutatta, hogy az elméletünk versenyképes a Racionális Kiterjesztett Termodinamika vonatkozó elméletével. Továbbá kimutattuk a termikus relaxációs idő hőmérsékletfüggését.

3. Tézis


Vonatkozó publikációk: [3, 122]

A nemegyensúlyi termodinamikai elmélet nem feltételez fononokat, ezért nem zárja ki, hogy a sokkal közönségesebb és a mérnöki gyakorlatban gyakrabban előforduló körülmények között is létrejöjjön nem-Fourier hővezetés. Szobahőmérsékleten az anyagi inhomogenitások megléte vezet el idáig. Az elméletünk jóslatát kísérletileg bizonyítottuk. Az egyszerűsített ballisztikus-konduktív egyenletet (\(\tau_Q = 0\)), azaz a Guyer-Krumhansl-e格林letet használtuk az EGR-kísérletek kiértékeléséhez. Itt megjelenik a Fourier-e格林let hierarchiájának a szerepe, mely segítségünkre volt a Fourier-törvénytől eltérő viselkedés parametrikus jellemzésében. A szobahőmérsékletű kísérletekben használt anyagok között előfordult szerves és szervetlen minta is.

4. Tézis


Vonatkozó publikációk: [3, 60, 182, 185]
Bibliography


[45] P. M. Mariano. Finite speed heat propagation as a consequence of microstructural events.


