COMPARISON OF THE SYMMETRIC HYPERBOLIC THERMODYNAMICALLY COMPATIBLE FRAMEWORK WITH HAMILTONIAN MECHANICS OF BINARY MIXTURES

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"We speak different languages, as usual," responded Woland, "but this does not change the things we speak about. Well?..."

–M. Bulgakov [1]

How to properly describe continuum thermodynamics of binary mixtures where each constituent has its own momentum? The Symmetric Hyperbolic Thermodynamically Consistent (SHTC) framework and Hamiltonian mechanics in the form of the General Equation for Non-Equilibrium Reversible-Irreversible Coupling (GENERIC) provide two answers, which are similar but not identical, and are compared in this article. They are compared both analytically and numerically on several levels of description, varying in the amount of detail. The GENERIC equations, stemming from the Liouville equation, contain terms expressing self-advection of the relative velocity by itself, which lead to a vorticity-dependent diffusion matrix after a reduction. The SHTC equations, on the other hand, do not contain such terms. We also show how to formulate a theory of mixtures with two momenta and only one temperature that is compatible with the Liouville equation and possesses the Hamiltonian structure, including Jacobi identity.

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Homogeneous mixtures (for instance the air, petrol, aqueous solutions, or plasma in fusion reactors) are ubiquitous in everyday life and industry. Although their behaviour can in most cases be well explained by means of equilibrium thermodynamics or fluid mechanics \([2, 3]\), there are processes that are difficult to describe theoretically. For instance, when a two species are mixing with high relative velocity, dynamics of the relative velocity affects the overall behaviour of the mixture (stress, heat flux, or possibly even rates of chemical reactions \([4]\)). Our goal is to derive dynamics of binary mixtures with evolving relative velocity. A particular feature of our model is that the relative velocity is advected by itself when it has non-zero vorticity. After a reduction, this leads to a diffusion equation with a vorticity-dependent diffusion matrix. Consequently, the diffusion flux does not need to be aligned with the gradient of chemical potential, in constrast with the standard theory of mixtures \([5]\).

Binary homogeneous mixtures can be described by various non-equilibrium thermodynamic models. These models can be classified based on the chosen state variables (fields that are equipped with their own time-evolution equations). In Classical Irreversible Thermodynamics (CIT), the mixture models have only one momentum density or velocity, typically the barycentric one \([5]\), or they have none, being in the mechanical equilibrium \([6]\). In Rational Thermodynamics each constituent of the mixture can be equipped with its own momentum \([7]\). In Extended Rational Thermodynamics and Extended Irreversible Thermodynamics the constituents can also have different temperatures \([8, 9, 10]\). These classical approaches take the conservation laws of mass, momentum, and energy for granted while seeking the undetermined fields like the stress tensor, heat flux, and diffusion flux via an entropic closure. There is, however, no unique way how to find such closure, which is why the theory of mixtures is still an active area of research. Alternative approaches exploit variational principles and the Lagrange→Euler transformation \([11]\), which are the directions where we also aim.

A closure found in \([4]\) leads to a mixture with several velocities and only one temperature, allowing for the diffusion to affect chemical reactions and for identification of partial pressure for non-ideal mixtures \([12]\). Especially in the non-isothermal case, however, there are many possibilities of finding the closures, and construction of the models is rather cumbersome when relying on the closures. In \([13]\) another theory was developed, leading to similar results, but facing difficulties when identifying the partial pressure of ideal gases in equilibrium. Yet another approach was developed in \([14]\), using a definition of time-reversal parity dependent on the choice of the physical units, making the Onsager-Casimir reciprocal relations dependent on the units as well. In \([15]\) a theory of mixtures is obtained from the kinetic theory of rarefied gases, similarly as in \([5]\), but equations for partial momenta of all

### 1 Introduction

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components are not provided. All these theories of mixtures are based on entropic closures and share the property that the closure can not be identified uniquely.

In this article, on the other hand, we show different ways towards theory of mixtures, relying on geometric mechanics or on the requirement of hyperbolicity. We present two approaches to binary mixtures: (i) the Symmetric Hyperbolic Thermodynamically Compatible (SHTC) equations, which is a set of first-order quasilinear hyperbolic equations \cite{16,17,18}, and (ii) the General Equation for Non-Equilibrium Reversible-Irreversible Coupling (GENERIC), which relies on geometric mechanics, in particular Hamiltonian mechanics \cite{19,20,21,22}.

The SHTC system can be seen as constructed from a Lagrangian master system of equations guaranteeing its mathematical properties \cite{23,24,25}. GENERIC, on the other hand, is constructed from four geometric building blocks: a Poisson bracket, an energy functional, a dissipation potential, and an entropy functional. Both approaches are compatible for the simple continuum \cite{17}, where the SHTC form of governing equations possesses the GENERIC structure. In the case of (binary) mixtures, the SHTC equations still possess the GENERIC structure. However, the projection from the Liouville equation (for the N-particle distribution function) within GENERIC leads to additional terms expressing self-advection of the relative velocity, which are not observed in the SHTC framework. We demonstrate the effects of those additional terms both analytically and numerically in this article.

On top of the two momenta, binary mixtures can have two entropies (or temperatures). By direct projection from the (Hamiltonian) Liouville equation, we obtain a Hamiltonian theory of mixtures where each constituent has its own density, momentum density, and entropy density (or temperature) \cite{22}. But models with only one entropy density are more difficult to obtain because it is not straightforward to fulfil the Jacobi identity, which expresses the self-consistency of Hamiltonian mechanics \cite{26}. Therefore, we introduce a Jacobi closure relation for the entropy difference, keeping only the overall entropy of the mixture, so that Jacobi identity is satisfied.

In Sec. 2, we recall the SHTC approach to binary mixtures. In Sec. 3, we first construct the GENERIC model for binary mixtures by projection from the Liouville equation and, subsequently, we compare it with the SHTC model. Moreover, a model with only one entropy is constructed via the Jacobi closure. In Sec. 4, some difference between reduced versions of the SHTC and GENERIC models are discussed and compared both analytically and numerically.

2 SHTC FRAMEWORK

The SHTC equations are a class of partial differential equations of continuum physics with two crucial properties. Firstly, they are symmetric hyperbolic in the sense that they can be written, after a possible change of variables, in the form

$$A(q) \cdot \frac{\partial q}{\partial t} + B_n(q) \cdot \frac{\partial q}{\partial x_n} + C(q) \cdot q = 0,$$  

(1)

with \(q\) being the vector of state variables and where the matrices \(A\) and \(B_n\) are symmetric and \(A\) is positive definite \cite{27,28,29}. One of the reasons to work with such restricted class of PDEs is that hyperbolic first order systems guarantee finite speed of propagation, unlike second order parabolic equations such as Navier-Stokes, and thus do not violate the concept of relativistic causality. Another reason is that symmetric hyperbolic systems are locally well posed\(^1\), since a unique and stable solution exists at least locally in time \cite{28,29}. Moreover, the SHTC equations are compatible with thermodynamics because they satisfy the first and second laws of thermodynamics.

\(^1\) Note that only hyperbolicity is not enough to establish the local in-time well-posedness of the Cauchy problem for a general quasilinear system (1) with non-symmetric matrices \cite{29}.
Due to the restriction of SHTC to first order PDEs, classical models with higher derivatives, such as Navier-Stokes equations, are not within the framework directly. However, it has been shown via an asymptotic expansion in a relaxation parameter that solutions to the Navier-Stokes-Fourier model are approximated by the solutions to the SHTC equations [30, 31].

We focus on a simplified setting close to the thermal equilibrium that can be modelled with just one entropy, see [32], and on homogeneous mixtures, (neglecting volume fractions). Therefore, we aim neither at multi-temperature mixtures, like electrons and ions in low-temperature plasma, nor at heterogeneous mixtures, like water vapour with droplets. The following section addresses binary one-temperature homogeneous mixtures within the SHTC framework.

\subsection{SHTC equations for binary mixtures}

Let us consider a homogeneous binary mixture composed of fluids of two kinds, denoted as species 1 and 2. A possible set of state variables describing the mixture are the pairs of densities, momentum densities, and entropy densities of the two species, \( \rho_1, \rho_2, \) Eulerian mass densities of the two components, (2a) \( \mathbf{u}_1, \mathbf{u}_2, \) momentum densities of the two components, (2b) \( s_1, s_2, \) Eulerian entropy densities (per volume) of the two components. (2c)

Within the SHTC framework, binary mixtures are expressed in terms of the following state variables

\begin{align*}
\rho_1 &= \rho_1, & \text{mass density of the first component,} \quad (3a) \\
\rho &= \rho_1 + \rho_2, & \text{(total) mass density,} \quad (3b) \\
\mathbf{m} &= \mathbf{u}_1 + \mathbf{u}_2, & \text{(total) momentum density,} \quad (3c) \\
\mathbf{w} &= \mathbf{u}_1 - \mathbf{u}_2, & \text{velocity difference,} \quad (3d) \\
s &= s_1 + s_2, & \text{total entropy density.} \quad (3e)
\end{align*}

Their SHTC time-evolution equations are

\begin{align*}
\frac{\partial \rho_1}{\partial t} &= - \partial_i (\rho_1 \mathbf{E}_{\mathbf{m}_i}) - \partial_i \mathbf{E}_{\mathbf{w}_i}, \quad (4a) \\
\frac{\partial \rho}{\partial t} &= - \partial_i (\rho \mathbf{E}_{\mathbf{m}_i}), \quad (4b) \\
\frac{\partial \mathbf{m}_i}{\partial t} &= - \rho \partial_i \mathbf{E}_\rho - \rho_1 \partial_i \mathbf{E}_{\rho_1} - s \partial_i \mathbf{E}_s - m_j \partial_i \mathbf{E}_{\mathbf{m}_j} - \partial_j (m_1 \mathbf{E}_{\mathbf{m}_j}) \\
&\quad + \mathbf{E}_\mathbf{w}_j \partial_i \mathbf{w}_j - \mathbf{E}_{\mathbf{w}_j} \partial_i \mathbf{w}_j, \quad (4c) \\
\frac{\partial \mathbf{w}_i}{\partial t} &= - \partial_i \mathbf{E}_\rho - \mathbf{E}_{\mathbf{m}_i} \partial_i \mathbf{w}_i - \mathbf{w}_j \partial_i \mathbf{E}_{\mathbf{m}_j} - \frac{1}{\tau} \mathbf{E}_{\mathbf{w}_i}, \quad (4d) \\
\frac{\partial s}{\partial t} &= - \partial_i (s \mathbf{E}_{\mathbf{m}_i}) + \frac{1}{\tau} \mathbf{E}_s \mathbf{E}_{\mathbf{w}_i}, \quad (4e)
\end{align*}

where \( \tau \) is a positive relaxation parameter specifying the rate of dissipation, see [18]. The dissipation is purely algebraic (involving no spatial gradients).

In order to close the system of evolution equations, we have to specify the energy and the relaxation parameter. The theory so far has been independent of the physical system under consideration and thus general. The energy can be obtained by the means of statistical physics or by geometrical arguments based on the maximisation of entropy, see [22]. The dissipation parameter can be obtained for instance by a dynamic reduction [22], by the fluctuation-dissipation theorem [21], or, of course, it can be measured experimentally [33].
For binary mixtures the energy is composed from the kinetic and the internal energy,
\[
E = \frac{u_1^2}{2\rho_1} + \frac{u_2^2}{2\rho_2} + \varepsilon_{\text{int}}(\rho_1, \rho, s) = \frac{m^2}{2\rho} + \frac{\rho_1(\rho - \rho_1)}{2\rho}w^2 + \varepsilon_{\text{int}}(\rho_1, \rho, s).
\] (5)

Therefore, the velocity is conjugate to the momentum density through \( E_m = \frac{m}{\rho} = v \). Once the internal energy is prescribed, for instance by the Sackur-Tetrode relation [34] or in any other way [30], the energy becomes an explicit function of the state variables. Both the energy and \( \tau \) will be chosen later in Sec. 4 explicitly. In the following section we discuss the particular properties of SHTC equations like hyperbolicity.

### 2.2 Properties of the SHTC Equations

Evolution equations (4) can be written as a symmetric quasilinear system (1) of first-order partial differential equations [35, 32, 17]. Therefore, one can expect local in-time well-posedness of the Cauchy problem for (4), provided that we have regular initial data [29] and convex energy \( E \). The symmetrization of (4) can be accomplished by introducing a generating potential and generating variables, as described, for example, in [36]. It should be noted that for the presented version of SHTC equations (4), it is difficult to define a physically reasonable internal energy that is convex over a wide range of state parameters. To formulate the SHTC model, in which the energy is a convex function, it is necessary to extend the system (4) by including the equation for the evolution of the volume fraction, as it is done in [36], and to define the internal energy of the mixture as the mass averaged internal energy of constituents’ internal energies. In this paper, however, we exclude the volume fraction from the set of state variables and consider simplified versions of both SHTC and GENERIC equations in order to focus on the relative velocity evolution equation, which is the main equation describing transport of the constituents.

Furthermore, the reversible part of the SHTC equations (4), obtained by disregarding the relaxation terms with the prefactor \( 1/\tau \), is a particular realization of Hamiltonian mechanics [17]. The validity of the Jacobi identity can be shown for instance using program [37].

Finally, system (4) admits the total energy conservation law, see [35, 32, 17], and therefore it is compatible with the first law of thermodynamics. Additionally, the irreversible part of (4) (the relaxation terms) can be seen as the gradient of a quadratic dissipation potential, see [17], and therefore the entropy production is guaranteed. This implies the compatibility with the second law of thermodynamics.

### 3 GENERIC FRAMEWORK

Within the GENERIC framework, summarized in monographs [21, 22], the time evolution of any state variables \( q \) is split into reversible and irreversible parts. The reversible part is generated by a Poisson bracket \( \{\cdot, \cdot\} \) with the Hamiltonian (or energy) of the system \( E \), while the irreversible part is described by a dissipation potential \( \Xi \), and entropy \( S \). The time evolution of any functional \( A \) of the state variables is given by
\[
\dot{A} = \{A, E\} + \langle A_q, \Xi_{q^*} \rangle, \tag{6}
\]
where subscripts stand for functional derivatives, angle brackets for the \( L_2 \) scalar product, and \( q^* = S_q \) are the conjugate variables. The evolution equation for a state variable \( q^i \) is obtained by plugging \( A = q^i \) into Eq. (6).
Let us now discuss the GENERIC building blocks in more detail. The Poisson bracket is a skew-symmetric bilinear operator, \( \{ F, G \} = - \{ G, F \} \), and it satisfies the Leibniz rule and the Jacobi identity,

\[
\{ F, G \} H = G \{ F, H \} + \{ F, G \} H \\
\{ F, \{ G, H \} \} + \{ G, \{ H, F \} \} + \{ H, \{ F, G \} \} = 0
\]

for any \( F(q) \) and \( G(q) \). In particular, the skew-symmetry implies conservation of energy. When the dissipation potential is convex with a minimum at zero in conjugate variables\(^2\), entropy is being produced, which guarantees compatibility with the second law of thermodynamics. An interesting feature of GENERIC is the fact that once the given requirements are met, the first and second laws of thermodynamics are automatically satisfied by construction, so every GENERIC model is thermodynamically compatible.

The dissipation potential is usually assumed to be quadratic, which makes it compatible with the concept of dissipative brackets \([39, 21]\), although it does not have to be. The Poisson bracket can be obtained by a series of projections. For instance, Hamiltonian continuum mechanics can be obtained from the N-particle Liouville Poisson bracket, as in this article, or by other geometric techniques like variational principles \([40]\), dynamics on Lie algebra duals \([41, 42, 43]\), or semidirect products \([44, 45]\). Once a set of state variables is declared, the Poisson bracket is usually derived in a unique way \([46]\). When, moreover, entropy or energy density are among the set of state variables, only one of the pair \( E \) and \( S \) is necessary, since one can be then expressed in terms of the other, similarly as in the so called one-generator framework \([47]\). The whole model for a chosen set of state variables only requires the knowledge of the energy of the system and of the dissipation potential, since these describe the particular material of the system. This is, for instance, the case when formulating SHTC within GENERIC \([17]\). In the next section, we show a GENERIC formulation of binary mixtures.

### 3.1 Hamiltonian mechanics of mixtures by projection from the Liouville equation

Let us briefly summarise the derivation of Hamiltonian mechanics for binary mixtures by projection from the Liouville equation. Any system composed of classical particles can be described by means of the N-particle distribution function, \( f_N \), evolution of which is expressed by the Liouville equation \([22]\). The Liouville equation is a particular realisation of the Lie-Poisson Hamiltonian mechanics, and is thus constructed from a Poisson bracket, called Liouville-Poisson bracket, and from an N-particle energy \([48, 46]\).

When the system is composed of particles of two kinds, the N-particle distribution function can be projected onto state variables of continuum mechanics \((2)\).

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\(^{2}\) see \([38]\) for non-convex dissipation potentials
Such projection turns the Liouville Poisson bracket for the $N$-particle distribution function to another Poisson bracket for state variables (2),

$$\{F, G\}_{\text{binary}} = \int d\rho_1 \left( \partial_i F_{\rho_1} G_{u_{1i}} - \partial_i G_{\rho_1} F_{u_{1i}} \right)$$

(9)

$$+ \int d\rho_2 \left( \partial_i F_{\rho_2} G_{u_{2i}} - \partial_i G_{\rho_2} F_{u_{2i}} \right)$$

$$+ \int (\partial_i F_{s_1} G_{u_{1i}} - \partial_i G_{s_1} F_{u_{1i}})$$

$$+ \int (\partial_i F_{s_2} G_{u_{2i}} - \partial_i G_{s_2} F_{u_{2i}})$$

see for instance [46, 22]. The resulting reversible evolution equations (before adding dissipative dynamics) are

$$\frac{\partial \rho_a}{\partial t} = \partial_i (\rho_a E_{u_{ai}})$$

(10a)

$$\frac{\partial u_{ai}}{\partial t} = -\rho_a \partial_i E_{\rho_a} - u_{aj} \partial_i E_{u_{aj}} - \partial_j (u_{ai} E_{u_{aj}})$$

(10b)

$$\frac{\partial s_a}{\partial t} = -\partial_i (s_a E_{u_{ai}})$$

(10c)

for $a = 1, 2$. The total energy of the system is denoted by $E$ and the subscripts stand for functional derivatives. If the energy is of an algebraic type, $E = \int e(\rho_1, u_1, s_1, \rho_2, u_2, s_2) d\mathbf{r}$, where the volumetric energy density $e$ is a smooth function of its arguments, the functional derivatives become identical with the partial derivatives of the energy density. State variables $\rho_1, \rho_2, u_1, u_2, s_1,$ and $s_2$ are, however, not those in which the SHTC equations are usually expressed. The purpose of the following section is to adapt the variables closer to the SHTC framework.

### 3.2 Transformation to the SHTC-like variables with two entropies

Let us now transform the state variables so that the total density, total momentum density, and total entropy density are included, [16],

$$\begin{align*}
\rho_1 &= \rho_1, & \text{(mass density of the first component)} \\
\rho &= \rho_1 + \rho_2, & \text{(total mass density)} \\
u &= u_1 + u_2, & \text{(total momentum density)} \\
w &= \frac{u_1 - u_2}{\rho_1 - \rho_2}, & \text{(velocity difference)} \\
s &= s_1 + s_2, & \text{(total entropy density)} \\
\Delta s &= \frac{s_1}{\rho_1} - \frac{s_2}{\rho_2}, & \text{(specific entropy difference)}
\end{align*}$$

(11)

If we excluded the specific entropy difference $\Delta s$, we would have the same state variables as in SHTC.
Note that the relaxation parameter $\tau$ is in general a symmetric (by the Onsager-Casimir reciprocal relations) positive semidefinite second-order twice covariant tensor even with respect to the time-reversal transformation [40].
The resulting system of evolution equations, including the terms expressing the mutual friction, reads
\[
\frac{\partial \rho_1}{\partial t} = - \partial_i (\rho_1 E_{m_i}) - \partial_i E_{w_i},
\]
\[
\frac{\partial \rho}{\partial t} = - \partial_i (\rho E_{m_i}),
\]
\[
\frac{\partial m_i}{\partial t} = - \rho \partial_i \rho - \rho_1 \partial_i E_{\rho_1} - s \partial_i E_s - m_j \partial_i E_{m_j} - \partial_j (m_i E_{m_j})
\]
\[
+ E_{w_j} \partial_i w_j - \partial_j (w_i E_{w_j}) - \Delta s \partial_i E_{\Delta s} - \left( s_1 \frac{\partial_i}{\rho_1} - s_2 \frac{\partial_1}{\rho_2} \frac{1}{\rho - \rho_1} \right) E_{\Delta s},
\]
\[
\frac{\partial w_i}{\partial t} = - \partial_i \rho_1 - \partial_i w_i E_{m_j} - w_j \partial_i E_{m_i} + \Delta s \partial_i E_s
\]
\[
\left( \left( \frac{s_1}{\rho_1^2} - \frac{s_2}{(\rho - \rho_1)^2} \right) \partial_i E_{\Delta s} - \left( \frac{s_1}{\rho_1} \frac{\partial_i}{\rho_1} - \frac{s_2}{\rho - \rho_1} \frac{\partial_1}{\rho_2} \frac{1}{\rho - \rho_1} \right) E_{\Delta s} \right)
\]
\[
+ \frac{\rho}{\rho_1 (\rho - \rho_1)} \left( \frac{\partial_i}{\rho} m_j - \frac{\partial_j}{\rho} m_i \right) E_{w_j}
\]
\[
+ \frac{1}{\rho_1} (\partial_i w_j - \partial_j w_i) E_{w_j}
\]
\[
+ \frac{\rho}{\rho_1 (\rho - \rho_1)} \left( \frac{\partial_i}{\rho} m_j - \frac{\partial_j}{\rho} m_i \right) E_{w_j} \left( \frac{\partial_i}{\rho} \frac{1}{\rho} w_j - \frac{\partial_j}{\rho} \frac{1}{\rho} w_i \right) E_{w_j} - \frac{1}{\tau} E_{w_i},
\]
\[
\frac{\partial s}{\partial t} = - \partial_i (s E_{m_i}) - \partial_i (\Delta s E_{w_i}) - \frac{1}{\tau} \frac{1}{E_{w_i}} (E_{w_i})^2,
\]
\[
\frac{\partial \Delta s}{\partial t} = - \partial_i (\Delta s E_{m_i}) + \left( s_1 \frac{\partial_i}{\rho_1} - s_2 \frac{\partial_1}{\rho_2} \frac{1}{\rho - \rho_1} \right) E_{m_i}
\]
\[
- \partial_i \left( \left( \frac{s_1}{\rho_1^2} - \frac{s_2}{(\rho - \rho_1)^2} \right) E_{w_i} + \left( \frac{s_1}{\rho_1} \frac{\partial_i}{\rho_1} - \frac{s_2}{\rho - \rho_1} \frac{\partial_1}{\rho_2} \frac{1}{\rho - \rho_1} \right) E_{w_i},
\]

where the boxed terms are not present in the SHTC framework. In particular, we have to eliminate the \( \Delta s \) variable from the equations in order to be compatible with the one-temperature SHTC system (4).

At the moment, we cannot prove the well-posedness of system (15) via its symmetrization as it can be done for the SHTC system (4). We hope to clarify this question in the future. The following section contains a reduced model with only one entropy.

3.3 Reduction to only one entropy

The SHTC equations contain only the overall entropy \( s \), not the entropy difference \( \Delta s \), which is why we shall reduce the model and eliminate \( \Delta s \). The elimination consists of two steps. First, only energy functionals independent of \( \Delta s \) are considered, and, secondly, the entropy difference is expressed in terms of the remaining state variables, \( \Delta s(\rho_1, \rho, s, m, w) \) while keeping Jacobi identity valid. The second step is called a Jacobi closure [50]. The whole bracket (12) of course satisfies the Jacobi identity because it is just a transformation of the Poisson bracket (9), and if we drop the lines with \( s \) and \( \Delta s \), it still satisfies Jacobi identity\(^4\). Such bracket with no entropies is suitable for isothermal mixtures, as shown in [51]. Here, however, we aim at non-isothermal mixtures, keeping \( s \) among the state variables.

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\(^4\) Jacobi identity can be checked using program [37].
Since $\Delta s$ is no longer a state variable, the total energy does not explicitly depend on it, so we have
\[ E_{\Delta s} = 0, \]
which means that $E_{\Delta s} = \frac{\rho_1 - \rho_2}{\rho} (E_{s_1} - E_{s_2}) = 0$ and consequently $T_1 = E_{s_1} = E_{s_2} = T_2$, which means that the temperatures of the two constituents are equal. Therefore the restriction to only the overall entropy is possible only if the two constituents of the mixture have the same temperature. This is not satisfied only in rather extreme cases of homogeneous mixtures like electrons and ions in cold plasma [52].

The last four lines of (12), which generate equation (15f), disappear, but the fifth line of (12) still contains $\Delta s$, which translates to the boxed terms in equation (15e) and in the first line of (15d). Using a program [37], we now check whether there exists an admissible formula for $\Delta s$ such that the remaining terms of (12) (without the last four lines) fulfil Jacobi identity. We first assume a general dependence $\Delta s(\rho, \rho_1, m, w, s)$ and get a necessary condition that it does not depend on $m$ to satisfy the Jacobi identity. Then we consider $\Delta s$ independent of $m$ which yields that $\Delta s$ must be independent of $w$ as well. Choosing such entropy difference, we get that $\Delta s$ must be $\delta$-homogeneous, that is $\Delta s = \Delta s(\phi, \psi)$, where $\phi = \rho/s$ and $\psi = \rho_1/s$. The next iteration of this procedure gives the condition
\[ \partial_\psi \Delta s - \Delta s (\phi \partial_\phi \Delta s + \psi \partial_\psi \Delta s) = 0, \]
particular solution of which is
\[ \Delta s = \frac{\phi_0 - \phi}{\phi_0 \psi - \phi \psi_0} \]
for arbitrary parameters $\phi_0, \psi_0$. Note, however, that this class does not contain all solutions, for instance the constant solution. Finally, using again the program [37], it becomes necessary that
\[ \psi_0 = 0 \quad \text{or} \quad \psi_0 = \phi_0 \]
in order that the Jacobi identity be fulfilled. Even though we have not studied all possible solutions of (17), we have found a family of reductions satisfying Jacobi identity. The constant solution, however, does belong to that family.\(^5\)

\(^5\) Another possibility to find $\Delta s$ unambiguously is to focus directly on Eq. (16). Using results from [22] for a binary mixture of two ideal gases with the same atomic masses, we obtain that $\Delta s$ should be equal to $\frac{\Delta F}{\Delta F} \ln \left( \frac{\rho_1}{\rho_1 - 1} \right)$, which, however, does not satisfy the Jacobi identity.
To sum up, the above choice of $\Delta s$ (condition (18a)) leads to a simplified Poisson bracket which fulfils the Jacobi identity. In terms of equations, system (15) then simplifies to

\[
\begin{align*}
\frac{\partial \rho_1}{\partial t} &= - \partial_i (\rho_1 E_{m_i}) - \partial_i E_{w_i}, \\
\frac{\partial \rho}{\partial t} &= - \partial_i (\rho E_{m_i}), \\
\frac{\partial m_i}{\partial t} &= - \rho \partial_i E_\rho - \rho_1 \partial_i E_{\rho_1} - s \partial_i E_s - m_j \partial_i E_{m_j} - \partial_i (m_j E_{m_j}) + E_{w_i} \partial_i w_j - \partial_j (w_j E_{w_j}), \\
\frac{\partial w_i}{\partial t} &= - \partial_i E_{\rho_1} - E_{m_j} \partial_j w_i - w_j \partial_i E_{m_i} - \Delta s \partial_i E_s + \frac{\rho}{\rho_1 (\rho - \rho_1)} \left( \partial_i \frac{m_i}{\rho} - \partial_j \frac{m_i}{\rho} \right) E_{w_j} + \frac{1}{\rho_1 (\rho - \rho_1)} \left( \partial_i \frac{\rho_1 w_i}{\rho} - \partial_j \frac{\rho_1 w_j}{\rho} \right) E_{w_i} - \frac{1}{\tau} E_{w_i}, \\
\frac{\partial s}{\partial t} &= - \partial_i (s E_{m_i}) - \partial_i (\Delta s E_{w_i}) + \frac{1}{\tau s} (E_w)^2,
\end{align*}
\]

where $\Delta s$ is a function of $\rho/s$ and $\rho_1/s$. This is a two-fluid model with one temperature derived from the Liouville equation only through projections and a Jacobi closure. The total mass, momentum, and the total energy are conserved by equations (15) and (19). This model is Hamiltonian and fulfils the Jacobi identity.

There is also another way to obtain a Hamiltonian model with only the overall entropy. If we first drop the second, third and fourth lines of (12), which represent the difference between the SHTC evolution and the evolution stemming from the Liouville equation, then, following the above procedure based on the program [37], we get that the Jacobi identity is satisfied as long as $\Delta s$ is constant. In other words, if we drop the three boxed terms not containing $\Delta s$, we can leave the others and reduce the model to single entropy $s$ as long as $E_{\Delta s} = 0$ and $\Delta s$ is constant. If actually $\Delta s = 0$, we obtain the SHTC equations as a special case. Thus the SHTC model is Hamiltonian, and stays Hamiltonian even after adding the boxed terms containing constant $\Delta s$. However, it is derived from the Liouville equation not just by projections, but also by the further neglectation of the boxed terms. The Liouville equation leads to the SHTC equations extended by extra terms that express self-advection of the relative velocity field $w$ and extra advection of total entropy by that field. This difference is demonstrated in the following section while noting that $\Delta s = 0$ requires identical specific partial entropies rather than equal temperatures.

4 REDUCTION AND COMPARISON OF SHTC AND GENERIC

In order to describe the difference between the SHTC and GENERIC models for binary mixtures, we further reduce the models so that the effects of the self-advection of $w$ are highlighted. Systems (4) and (19) are reduced to simpler systems of equations containing less detail. Assuming that the dynamics of the $w$ field is fast (relaxation parameter $\tau$ sufficiently small), solutions to the full systems of equations should be close to solutions to reduced systems without $w$ as a state variable. One way to carry out that reduction is asymptotic analysis [30]. Here we follow another way, called the Dynamic Maximum Entropy reduction (DynMaxEnt), which is based on the geometric character of the evolution equations.
4.1 DynMaxEnt reduction of GENERIC

DynMaxEnt is motivated by contact geometry, and it is typically compatible with asymptotic analysis [53, 22, 54]. Let us denote the energetic conjugate variables as \( \rho_1^\dagger = E_{\rho_1}, \rho_1^\ddagger = E_\rho, m_1^\dagger = E_m, w_1^\dagger = E_w, \) and \( s_1^\dagger = E_s \). The DynMaxEnt reduction of \( w_1 \) is carried out in these steps: (i) Set \( w_1 \) to its maximum entropy (MaxEnt) value [34] (here \( w_1 = 0 \)), which corresponds to the minimum of energy (5), (ii) calculate \( w_1^\dagger \) from the evolution equation of \( w_1 \), and (iii) plug the calculated \( w_1 \) and \( w_1^\dagger \) into the remaining equations.

From Eq. (19d) we get that

\[
\tau \Gamma = - (1 - \alpha \Omega) w_1^\dagger, \tag{20}
\]

where

\[
\Gamma = \nabla \rho_1^\dagger + \Delta s \nabla s_1^\dagger, \quad \Omega_{ij} = \delta_{1i} m_1^\dagger - \delta_{1j} m_1^\dagger, \quad \text{and} \quad \alpha = \frac{\tau \rho}{\rho_1 (\rho - \rho_1)}. \tag{21}
\]

Denoting \( \Theta = (1 - \alpha \Omega) \), we obtain a relation for \( w_1^\dagger \),

\[
w_1^\dagger = - \tau \Theta^{-1} \Gamma, \tag{22}
\]

that is to be substituted into the remaining equations (for \( \rho, \rho_1, \) and \( m_1 \)). By introducing quantities

\[
a = - \alpha (\delta_{11} m_1^\dagger - \delta_{12} m_1^\dagger), \quad b = - \alpha (\delta_{11} m_1^\dagger - \delta_{22} m_1^\dagger), \quad \text{and} \quad c = - \alpha (\delta_{22} m_1^\dagger - \delta_{33} m_1^\dagger), \tag{23}
\]

which are proportional to the overall vorticity, matrix \( \Theta \) can be rewritten as

\[
\Theta = \begin{pmatrix} 1 & a & b \\ -a & 1 & c \\ -b & -c & 1 \end{pmatrix}. \tag{24}
\]

Moreover,

\[
\det(\Theta) = 1 + a^2 + b^2 + c^2 > 0, \quad \Theta > 0, \quad \text{and}
\]

\[
\Theta^{-1} = \frac{1}{\det(\Theta)} \begin{pmatrix} 1 + c^2 & -a - bc & -b + ac \\ a - bc & 1 + b^2 & -c - ab \\ b + ac & c - ab & 1 + a^2 \end{pmatrix} \approx \begin{pmatrix} 1 & -a & -b \\ a & 1 & -c \\ b & c & 1 \end{pmatrix} = \Theta^{-1},
\]

which is an approximate inverse of matrix \( \Theta \) in the regime of low overall vorticity. Matrices \( \Theta, \Theta^{-1}, \Theta^{-1} \) are positive definite because their symmetric parts are positive definite although the eigenvalues of \( \Theta, \{1, 1 \pm \sqrt{-a^2 - b^2 - c^2}\}, \) are not all real (bearing in mind that the matrices are not symmetric).

System of equations (19) is then reduced to

\[
\frac{\partial \rho_1}{\partial t} = - \delta_{11} (\rho_1 m_1^\dagger) + \nabla \cdot \left( \tau \Theta^{-1} \Gamma \right), \tag{25a}
\]

\[
\frac{\partial \rho}{\partial t} = - \delta_{11} (\rho m_1^\dagger), \tag{25b}
\]

\[
\frac{\partial m_1}{\partial t} = - \rho \delta_{11} \rho_1^\dagger - \rho_1 \delta_{11} \rho_1^\ddagger - s \delta_{11} s^\dagger - m_2 \delta_{11} m_1^\dagger - \delta_{11} (m_1 m_1^\dagger), \tag{25c}
\]

\[
\frac{\partial s}{\partial t} = - \delta_{11} (sm_1^\dagger) + \nabla \cdot \left( \Delta s \tau \Theta^{-1} \Gamma \right) + \frac{1}{s^\dagger} \left( \tau \Theta^{-1} \Gamma \right)^2, \tag{25d}
\]

which no longer contains \( w_1 \) as a state variable.

Let us now discuss the properties of this reduced system of equations. Firstly, entropy is produced because the right-hand side of (25d) consists of divergence terms and positive terms. Secondly, equation (25a) can be interpreted as advection of \( \rho_1 \).
by the velocity and as diffusion of $\rho_1$ with a vorticity-dependent non-symmetric diffusion matrix. When using the approximate inverse $\Theta^{-1}$ and neglecting the entropies (the isothermal case), the flux $J$ becomes

$$J \approx -\tau \nabla \rho_1^\dagger + \tau \alpha \omega \times \nabla \rho_1^\dagger,$$

where $\omega = \nabla \times v$ is the overall vorticity. The flux then consists of two terms, one proportional to the gradient of chemical potential and the other perpendicular to that gradient and the vorticity. We shall study the effects of the latter term later in this section.

### 4.2 DynMaxEnt reduction of SHTC

Similarly as in the case of GENERIC, DynMaxEnt reduces the SHTC equations (4) to

$$\frac{\partial \rho_1}{\partial t} = -\partial_i (\rho_1 m_i^\dagger) + \nabla \cdot \left( \tau \Theta^{-1} \nabla \rho_1^\dagger \right), \quad (26a)$$

$$\frac{\partial \rho}{\partial t} = -\partial_i (\rho m_i^\dagger), \quad (26b)$$

$$\frac{\partial m_i}{\partial t} = -\rho \partial_i \rho^\dagger - \rho_1 \partial_i \rho_1^\dagger - s \partial_i s^\dagger - m_j \partial_i m_j^\dagger - \partial_j (m_i m_j^\dagger), \quad (26c)$$

$$\frac{\partial s}{\partial t} = -\partial_i (s m_i^\dagger) + \frac{\tau}{s^\dagger} \left( \nabla \rho_1^\dagger \right)^2. \quad (26d)$$

This model has similar features as model (25).

The main difference between GENERIC and SHTC for binary mixtures is the self-advection of $w$. In the following section, we confine ourselves to the isothermal case to highlight this difference.

### 4.3 The isothermal regime in two-dimensions

The reduction of both the SHTC and GENERIC models ((26), (25)) to isothermal case (dropping all terms with the entropy) leads to

$$\frac{\partial \rho_1}{\partial t} = -\partial_i (\rho_1 m_i^\dagger) + \nabla \cdot \left( \tau \Theta^{-1} \nabla \rho_1^\dagger \right), \quad (27a)$$

$$\frac{\partial \rho}{\partial t} = -\partial_i (\rho m_i^\dagger), \quad (27b)$$

$$\frac{\partial m_i}{\partial t} = -\rho \partial_i \rho^\dagger - \rho_1 \partial_i \rho_1^\dagger - m_j \partial_i m_j^\dagger - \partial_j (m_i m_j^\dagger), \quad (27c)$$

where the difference between the two models is encoded into the “diffusion matrix” $\Theta^{-1}$. Next, we linearise the “diffusion matrix” $\Theta^{-1}$ to $\Theta^{-1}$ and restrict ourselves to two dimensions, which gives

$$\Theta^{-1} \approx \begin{pmatrix} 1 & -a \\ a & 1 \end{pmatrix} \quad (28)$$

with

$$a = 0, \quad \text{for SHTC,} \quad (29)$$

$$a = -\alpha \left( \partial_1 \left( \frac{m_1}{\rho} \right) - \partial_2 \left( \frac{m_2}{\rho} \right) \right) = -\alpha \text{curl} \left( \frac{m}{\rho} \right) \quad \text{for GENERIC.} \quad (30)$$

Let us now interpret the quantities $a$ and $\alpha$. From the definition (21) it follows that $\alpha \sim \frac{\tau}{\rho}$, the units of $\alpha$ are thus seconds, and $\alpha$ represents the microscopic time scale due to the relative velocity $w$, $t_{\text{micro}}$. The units of the vorticity $\Omega$ are $s^{-1}$.
and thus the vorticity represents the macroscopic time scale related to the overall vortices, $t_{\text{macro}}$. Quantity $a$ represents the ratio of the microscopic relative velocity time scale and the macroscopic vorticity time scale, $a \sim t_{\text{micro}}/t_{\text{macro}}$.

In order to compare both approaches quantitatively, we have to provide an energy functional and a formula for the relaxation parameter. In the isothermal case the energy can be substituted with the free energy, see [22]. Therefore, we choose a simplified free energy of two ideal gases

$$E = \frac{m^2}{2p} + \frac{\kappa}{\alpha} (\rho_1 \log(\rho_1) - (\rho_1 - \rho) \log(\rho - \rho_1)),$$

where $\kappa$ and $\alpha$ are constants. Furthermore, the choice of $\alpha$ also defines the relaxation parameter $\tau$ through relation (21).

We now write (27) in a compact divergence form as

$$\frac{\partial \rho_1}{\partial t} = -\text{div} \left( \rho_1 \frac{m}{\rho} - \frac{\kappa}{\alpha} \rho \right),$$

$$\frac{\partial \rho}{\partial t} = -\text{div}(m),$$

$$\frac{\partial m_i}{\partial t} = -\text{div} \left( \frac{m_i m}{\rho} + p e_i \right), \quad i = 1, 2,$$

where the pressure $p$ stands for

$$p = -e + \rho \frac{de}{d\rho} + \rho_1 \frac{de}{d\rho_1} + m \cdot \frac{de}{dm}.$$ (33)

Even more explicitly, we obtain that

$$\frac{\partial \rho_1}{\partial t} = -\text{div} \left( \rho_1 \frac{m}{\rho} \right) + \text{div} \left( \tau \Theta^{-1} \nabla \rho_1 \right),$$

$$\frac{\partial \rho}{\partial t} = -\text{div}(m),$$

$$\frac{\partial m_i}{\partial t} = -\text{div} \left( \frac{m_i m}{\rho} + \frac{\kappa}{\alpha} \rho \right), \quad i = 1, 2.$$ (34c)

The pressure can be rewritten as $p = \frac{\kappa}{\alpha} \rho$. Evaluating gradients in the right-most term of (34a), gives

$$\text{div} \left( \tau \Theta^{-1} \nabla \left( \frac{\kappa}{\alpha} (\log(\rho_1) - \log(\rho - \rho_1)) \right) \right) = \text{div} \left( \tau \Theta^{-1} \nabla \rho_1 - \tau \Theta^{-1} \frac{\rho_1}{\rho} \nabla \rho \right)$$

$$= \text{div} \left( \kappa \Theta^{-1} \rho \nabla \left( \frac{\rho_1}{\rho} \right) \right).$$ (35)

The system of equations then simplifies to

$$\frac{\partial \rho_1}{\partial t} = -\text{div} \left( \rho_1 \frac{m}{\rho} - \kappa \Theta^{-1} \rho \nabla \left( \frac{\rho_1}{\rho} \right) \right),$$

$$\frac{\partial \rho}{\partial t} = -\text{div}(m),$$

$$\frac{\partial m_i}{\partial t} = -\text{div} \left( \frac{m_i m}{\rho} + \frac{\kappa}{\alpha} \rho \right), \quad i = 1, 2,$$

which we solve both analytically and numerically.

### 4.4 Analytical comparison

In this section, we illustrate the difference between SHTC and GENERIC formulations by analytical means, solving the simplified system (36). Equation (36a) gets within the SHTC model the following form,

$$\frac{\partial \rho_1}{\partial t} =
On the other hand, within the GENERIC model, we obtain
\[
\frac{\partial \rho_1}{\partial t} = -\text{div} \left( \rho_1 \frac{m}{\rho} \right) + \kappa \Delta \rho_1 - \kappa \rho_1 \frac{\partial}{\partial \rho} \frac{\partial \rho}{\partial \rho} \nabla \rho + \kappa \left( \frac{\partial a \rho_1}{\partial y} - \frac{\partial a \rho_1}{\partial x} \right) - \kappa \rho_1 \left( \frac{\partial a \rho_1}{\partial y} - \frac{\partial a \rho_1}{\partial x} \right)
\]
\[\Rightarrow \frac{\partial \rho_1}{\partial t} = -\text{div} \left( \rho_1 \frac{m}{\rho} \right) + \kappa \Delta \rho_1 - \kappa \rho_1 \frac{\partial}{\partial \rho} \frac{\partial \rho}{\partial \rho} \nabla \rho + \kappa \left( \frac{\partial a \rho_1}{\partial y} - \frac{\partial a \rho_1}{\partial x} \right) - \kappa \rho_1 \left( \frac{\partial a \rho_1}{\partial y} - \frac{\partial a \rho_1}{\partial x} \right)
\]  
(38)

Realising that the equations (36b) and (36c) are not coupled with (36a), we first search for stationary \( m \) and \( \rho \), solving Eqs. (36b) and (36c), and then for a non-stationary \( \rho_1 \), solving Eq. (36a). The following functions indeed represent stationary solutions,
\[
\rho = 1,
\]
\[
v = (v_1, v_2) = (10 \sin(y), 0),
\]  
(39)
\( (40) \)
where \( v \) is the velocity field defined by \( m = \rho v \). Plugging these solutions into Eqs. (37) and (38), we get
\[
\frac{\partial \rho_1}{\partial t} = -\text{div} \left( \rho_1 \frac{m}{\rho} \right) + \kappa \Delta \rho_1 \quad \text{for SHTC},
\]
\[
\frac{\partial \rho_1}{\partial t} = -\text{div} \left( \rho_1 \frac{m}{\rho} \right) + \kappa \Delta \rho_1 + \kappa \left( \frac{\partial a \rho_1}{\partial y} - \frac{\partial a \rho_1}{\partial x} \right) \quad \text{for GENERIC}.
\]  
(41)
\( (42) \)
We now recall the vorticity diffusion ratio \( a \), that for GENERIC takes the form
\[
a = -\alpha (\partial_x v_2 - \partial_y v_1) = \alpha \partial_y v_1.
\]  
(43)
As a result, \( \partial_x a = 0 \) and \( \partial_y a = \alpha \partial_y v_1 = -10 \alpha \sin(y) = -\alpha v_1 \). Plugging this into Eq. (42) yields
\[
\frac{\partial \rho_1}{\partial t} = -\text{div} \left( \rho_1 \frac{m}{\rho} \right) + \kappa \Delta \rho_1 - \kappa \alpha v_1 \frac{\partial \rho_1}{\partial x}.
\]  
(44)
Since \( v_1 \) does not depend on \( x \) and \( v_2 = 0 \), we get
\[
\frac{\partial \rho_1}{\partial t} = -(1 + \kappa \alpha) \text{div} \left( \rho_1 \frac{m}{\rho} \right) + \kappa \Delta \rho_1.
\]  
(45)
In summary, both SHTC and GENERIC models contain advection and diffusion of \( \rho_1 \). The advection in GENERIC, however, has a coefficient \( 1 + \kappa \alpha \) while in SHTC the coefficient equals 1, even though the velocity field is identical in both cases. This is an effect of the vorticity-dependent part of the diffusion matrix in the reduced GENERIC model. Let us now examine these effects in more detail numerically.

4.5 Numerical comparison

We now solve the reduced system (36) numerically in order to illustrate the differences between the reduced SHTC and GENERIC systems. The numerical implementation is realised in the software library PyPDE [55], using ADER-WENO [56, 30] method for solution to equations in the form:
\[
\frac{\partial q}{\partial t} + \nabla F(q, \nabla q) + B(q) \cdot \nabla q = S(q),
\]  
(46)
where \( q \) is the vector of state variables, \( S \) represents the vector of source terms, \( F \) are the conservative terms, and \( B \) the non-conservative terms. In particular, for system (36) we have \( B = S = 0 \).

The presented examples are solved with the scheme of third order and the Rusanov flux. For laminar flow and the Gresho vortex, periodic and transitive boundary conditions are applied, respectively. Parameters are chosen as \( \kappa = 1 \) and \( \alpha = 1 \) in Eq. (30). Computational examples run till the final time \( T_{\text{final}} = 0.5 \) in 100 time steps on a \( 100 \times 100 \) mesh. Let us now discuss the laminar channel flow.
Figure 1: Steady laminar flow of a binary mixture with periodic boundary conditions. The density of the first component is diffused and advected by the flow, for three times (from left to right $t = 0, T_{\text{final}}/2, T_{\text{final}}$) under the SHTC model (top), and the GENERIC model (middle). The bottom line shows one-dimensional density profiles of the first component along x-axis at the middle of the y-axis.

4.5.1 Laminar channel flow

The first example corresponds to the setting in Sec. 4.4. The computation domain is $\Omega = [0, 2\pi] \times [-\pi/2, 3\pi/2]$ and initial conditions are

$$\rho_1 = 0.5 + 0.25 \sin(x),$$

$\rho$ and $v$ being prescribed by formulas (39).

Figure 1 shows the numerical solution to the system (36b), (36c), (45). Similar profiles of SHTC and GENERIC solutions at times $T_{\text{final}}$ (Fig. 1 top-right) and $T_{\text{final}}/2$ (Fig. 1 middle-bottom), respectively, indicate that advection within the reduced GENERIC model is (with the chosen material parameters $\kappa$ and $\alpha$) twice faster than in the reduced SHTC model.

4.5.2 Gresho vortex

The second computational example is based on the Gresho vortex for the Euler equation, where the centrifugal force is balanced by the pressure gradient, resulting in a stable time-independent vortex [57]. In our case, the mixture density, plays the role of the pressure, as can be in from Eq. (36c).
Figure 2: Time evolution of the difference between \( \rho_1 \) in SHTC model and the GENERIC model, \( \rho_1^{\text{SHTC}} - \rho_1^{\text{GENERIC}} \) for initial data of the Gersho vortex. We present six times, in the reading order, \( t = 0, 1/5T_{\text{final}}, 2/5T_{\text{final}}, 3/5T_{\text{final}}, 4/5T_{\text{final}}, T_{\text{final}} \).  

Let the computation domain be a square \( \Omega = [0, 1] \times [0, 1] \). Initially we prescribe a Gresho body vortex outside of the origin,

\[
\rho = \begin{cases} 
5 + \frac{25}{2} r^2, & r < 0.2 \\
9 - 4 \ln(0.2) + 4 \ln(r) - 20r + \frac{25}{2} r^2, & 0.2 \leq r \leq 0.4 \\
3 + 4 \ln(2), & 0.4 < r 
\end{cases}, 
\]

\( \rho_1 = 2.5 \), \( (48) \)

\[
v = e_\phi \begin{cases} 
5r, & r < 0.2 \\
2 - 5r, & 0.2 \leq r \leq 0.4 \\
0, & 0.4 < r 
\end{cases} , 
\]

\( (50) \)

where \( r = \sqrt{(x - 0.5)^2 + (y - 0.5)^2} \) and \( e_\phi = (-y - 0.5, x - 0.5)/r \).  

Figure 2 shows the time evolution of the difference in the density of the first component \( \rho_1^{\text{SHTC}} - \rho_1^{\text{GENERIC}} \). We can see that the vorticity-dependent diffusion matrix within the reduced GENERIC model causes extra interaction between the vortex and \( \rho_1 \). Field \( \rho_1 \) now flows partly in the direction perpendicular to the (radial) gradient of chemical potential, that is also in the azimuthal direction. Those extra terms break the radial symmetry of the solution\(^6\). Comparison with experimental data is, however, out of scope of the present paper.

5 Conclusion

The main goal of this manuscript is to compare two recent frameworks of continuum thermodynamics, the SHTC equations and GENERIC, in the context of binary

\(^6\) More precisely, the symmetry is broken by the boundary conditions, but the extra terms highlight this symmetry breaking in the solution.
homogeneous mixtures. Using GENERIC, we can start from the Liouville equation and obtain equations for binary mixtures with additional terms that are not present in the SHTC framework, namely the terms containing the self-advection of the relative velocity.

These terms can be analysed on simplified versions of the SHTC and GENERIC models, letting the relative velocity \( w \) relax to a quasi-equilibrium value. Within GENERIC, we obtained a vorticity-dependent diffusion matrix. Consequently, the density of the first constituent flows not only against the gradient of the chemical potential but also in the direction perpendicular to the gradient and the vorticity pseudovector. This implies for instance, different advection rates in the two models or symmetry breaking of the solution in the presence of vorticity, see Figs. 1 and 2.

Apart from the terms with self-advection of the relative velocity, the mixture models can have two entropies, the overall entropy, or no entropy at all. The first option is observed for instance in cold plasma, where light electrons and heavy ions absorb electromagnetic energy with different efficiency. Second possibility assumes that the components have the same temperature, and the third option is isothermal. The first option (two entropies) has uniquely determined Poisson bracket, that is derived from the Liouville equation. The second option (one entropy) is, however, much more difficult in the context of Hamiltonian mechanics. But we have shown that there is a family of Hamiltonian binary mixture model with only the overall entropy that still contains the self-advection terms of the relative velocity while satisfying the Jacobi identity. The entropy difference \( \Delta s \) is given by solutions to (17), for example by formulas (18a), (18b). Finally, the isothermal case then again has a unique Poisson bracket.

The structure of the SHTC model (4), which does not contain the self-advection terms, is also Hamiltonian (considering only the reversible part) and furthermore admits constant \( \Delta s \) (without violating Jacobi identity), unlike the GENERIC model.

In future, we would like to compare the results with 2D experimental results on diffusion in the presence of vorticity. Furthermore, it remains to generalise the analysis to heterogeneous mixtures, taking volume fractions among the state variables.

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REFERENCES

[1] M. Bulgakov. The Master and Margarita. Vintage Books, 1996.

[2] L.D. Landau and E.M. Lifschitz. Statistical physics. Number pt. 1 in Course of theoretical physics. Pergamon Press, 1969.
[3] L.D. Landau and E.M. Lifshitz. *Fluid Mechanics*. Number v. 6. Elsevier Science, 2013.

[4] M. Pavelka, F. Maršík, and V. Klika. Consistent theory of mixtures on different levels of description. *International Journal of Engineering Science*, 78(0):192 – 217, 2014.

[5] S. R. de Groot and P. Mazur. *Non-equilibrium Thermodynamics*. Dover Publications, New York, 1984.

[6] S. Kjelstrup and D. Bedeaux. *Non-Equilibrium Thermodynamics of Heterogeneous Systems*. Series on Advances in Statistical Mechanics. World Scientific, 2008.

[7] R. M. Bowen. *Continuum Physics*, volume 3. Academic Press, New York, 1976.

[8] I. Müller. *Thermodynamics*. Interaction of Mechanics and Mathematics Series. Pitman, 1985.

[9] I. Müller and T. Ruggeri. *Rational extended thermodynamics*. Springer tracts in natural philosophy. Springer, 1998.

[10] D. Jou, J. Casas-Vázquez, and G. Lebon. *Extended Irreversible Thermodynamics*. Springer-Verlag, New York, 4th edition, 2010.

[11] Sergey Gavril'yuk, Henri Gouin, and Yuriy Perepechko. A variational principle for two-fluid models. *Comptes Rendus de l’Académie des Sciences - Series IIB - Mechanics-Physics-Chemistry-Astronomy*, 324(8):483 – 490, 1997.

[12] V. Samohyľ, I. Samohyľ, and Petr Voňka. Partial pressures in thermodynamics of classical fluid mixtures. *Acta Chimica Slovaca*, 5(1):29–36, 2012.

[13] O. Souček, V. Průša, J. Málek, and K. R. Rajagopal. On the natural structure of thermodynamic potentials and fluxes in the theory of chemically non-reacting binary mixtures. *Acta Mechanica*, 225(11):3157–3186, 2014.

[14] D. Bothe and W. Dreyer. Continuum thermodynamics of chemically reacting fluid mixtures. *Acta Mechanica*, 226(6):1757–1805, 2015.

[15] J.O. Hirschfelder, C.F. Curtiss, R.B. Bird, and University of Wisconsin. Theoretical Chemistry Laboratory. *Molecular theory of gases and liquids*. Structure of matter series. Wiley, 1954.

[16] E. I. Romensky. Hyperbolic systems of thermodynamically compatible conservation laws in continuum mechanics. *Mathl. Comput. Modelling*, 28(10):115–130, 1998.

[17] I. Peshkov, M. Pavelka, E. Romenski, and M. Grmela. Continuum mechanics and thermodynamics in the Hamilton and the Godunov-type formulations. *Continuum Mechanics and Thermodynamics*, 30(6):1343–1378, 2018.

[18] E. Romenski, G. Reshetova, I. Peshkov, and M. Dumbser. Modeling wavefields in saturated elastic porous media based on thermodynamically compatible system theory for two-phase solid-fluid mixtures. *Computers & Fluids*, 206:104587, 2020.

[19] M. Grmela and H. C. Öttinger. Dynamics and thermodynamics of complex fluids. I. Development of a general formalism. *Phys. Rev. E*, 56:6620–6632, Dec 1997.

[20] H. C. Öttinger and Miroslav Grmela. Dynamics and thermodynamics of complex fluids. II. Illustrations of a general formalism. *Phys. Rev. E*, 56:6633–6655, Dec 1997.
[21] H. C. Öttinger. *Beyond Equilibrium Thermodynamics*. Wiley, 2005.

[22] M. Pavelka, V. Klika, and M. Grmela. *Multiscale Thermo-Dynamics*. de Gruyter (Berlin), 2018.

[23] S. K. Godunov and E. Romensky. *Computational Fluid Dynamics Review*, chapter Thermodynamics, conservation laws and symmetric forms of differential equations in mechanics of continuous media, pages 19–31. Wiley: New York, NY, USA, 1995.

[24] S. Godunov, T. Mikhailova, and E. Romenskii. Systems of thermodynamically coordinated laws of conservation invariant under rotations. *Siberian Mathematical Journal*, 37(4):690–705, 1996.

[25] S. K. Godunov and E I Romenskii. *Elements of continuum mechanics and conservation laws*. Kluwer Academic/Plenum Publishers, 2003.

[26] M. Fecko. *Differential Geometry and Lie Groups for Physicists*. Cambridge University Press, 2006.

[27] K. O. Friedrichs. Symmetric hyperbolic linear differential equations. *Comm. Pure Appl. Math.*, 7:345–392, 1954.

[28] K. M. Dafermos. *Hyperbolic Conservation Laws in Continuum Physics*. Springer-Verlag Berlin Heidelberg, 2016.

[29] S. Benzoni-Gavage and D. Serre. *Multi-dimensional hyperbolic partial differential equations*, volume 325 of *Grundlehren der mathematischen Wissenschaften*. Oxford University Press, Berlin, Heidelberg, nov 2006.

[30] M. Dumbser, I. Peshkov, E. Romenski, and O. Zanotti. High order ader schemes for a unified first order hyperbolic formulation of continuum mechanics: Viscous heat-conducting fluids and elastic solids. *Journal of Computational Physics*, 314:824–862, 2016.

[31] I. Peshkov and E. Romenski. A hyperbolic model for viscous Newtonian flows. *Continuum Mech. Thermodyn.*, 28:85–104, 2016.

[32] E. Romenski, A. Belozerov, and I. Peshkov. Conservative formulation for compressible multiphase flows. *Quarterly of Applied Mathematics*, 74, 05 2014.

[33] E. A. Mason and A. P. Malinauskas. *Gas transport in porous media: the dusty-gas model*. Number v. 17 in Chemical engineering monographs. Elsevier, 1983.

[34] H. B. Callen. *Thermodynamics: an introduction to the physical theories of equilibrium thermostatics and irreversible thermodynamics*. Wiley, 1960.

[35] E. Romenski, A. D. Resnyansky, and E. F. Toro. Conservative hyperbolic formulation for compressible two-phase flow with different phase pressures and temperatures. *Quarterly of Applied Mathematics*, 65(2):259–279, apr 2007.

[36] E. Romenski, D. Drikakis, and E. F. Toro. Conservative models and numerical methods for compressible two-phase flow. *Journal of Scientific Computing*, 68, 2009.

[37] M. Kroeger and M. Huetter. Automated symbolic calculations in nonequilibrium thermodynamics. *Comput. Phys. Commun.*, 181:2149–2157, 2010.

[38] A. Janečka and M. Pavelka. Non-convex dissipation potentials in multiscale non-equilibrium thermodynamics. *Continuum Mechanics and Thermodynamics*, 30(4):917–941, 2018.
[39] P. J. Morrison. Bracket formulation for irreversible classical fields. *Physics Letters A*, 100(8):423–427, 1984.

[40] H. Goldstein. *Classical Mechanics*. Pearson Education, 2002.

[41] V. I. Arnold. Sur la géometrie différentielle des groupes de lie de dimension infini et ses applications dans l’hydrodynamique des fluides parfaits. *Annales de l’institut Fourier*, 16(1):319–361, 1966.

[42] O. Esen and H. Gümrul. Tulczyjew’s triplet for Lie groups I: Trivializations and reductions. *Journal of Lie Theory*, 24:1115–1160, 2014.

[43] O. Esen and H. Gümrul. Tulczyjew’s triplet for Lie groups ii: Dynamics. *ArXiv e-prints*, March 2015.

[44] J Marsden, T Ratiu, and A Weinstein. Semidirect products and reduction in mechanics. *Transactions of the american mathematical society*, 281(1):147–177, 1984.

[45] P. Vágner, M. Pavelka, and O. Esen. Multiscale thermodynamics of charged mixtures. *Continuum Mechanics and Thermodynamics*, Accepted, 2020.

[46] M. Pavelka, V. Klika, O. Esen, and M. Grmela. A hierarchy of Poisson brackets in non-equilibrium thermodynamics. *Physica D: Nonlinear phenomena*, 335:54–69, 2016.

[47] A. N. Beris and B. J. Edwards. *Thermodynamics of Flowing Systems*. Oxford Univ. Press, Oxford, UK, 1994.

[48] J. E. Marsden, P. J. Morrison, and A. Weinstein. The hamiltonian structure of the bbgky hierarchy equations. *Cont. Math. AMS.*, 28:115–124, 1984.

[49] M. Pavelka, V. Klika, and M. Grmela. Time reversal in nonequilibrium thermodynamics. *Phys. Rev. E*, 90(062131), 2014.

[50] M. Grmela, L. Hong, D. Jou, G. Lebon, and M. Pavelka. Hamiltonian and godunov structures of the grad hierarchy. *Physical Review E*, 95(033121), 2017.

[51] A. El Afif and M. Grmela. Non-fickian mass transport in polymers. *Journal of Rheology (1978-present)*, 46(3):591–628, 2002.

[52] F. F. Chen. *Introduction to plasma physics*. Plenum Press, 1974.

[53] V. I. Arnold. *Mathematical methods of classical mechanics*. Springer, New York, 1989.

[54] V. Klika, M. Pavelka, P. Vágner, and M. Grmela. Dynamic maximum entropy reduction. *Entropy*, 21(715), 2019.

[55] H. Jackson and N. Nikiforakis. A numerical scheme for non-newtonian fluids and plastic solids under the gpr model. *Journal of Computational Physics*, 387:410 – 429, 2019.

[56] E. F. Toro. *Riemann Solvers and Numerical Methods for Fluid Dynamics: A Practical Introduction*. Springer Berlin Heidelberg, 2009.

[57] P. M. Gresho and S. T. Chan. On the theory of semi-implicit projection methods for viscous incompressible flow and its implementation via a finite element method that also introduces a nearly consistent mass matrix. part 2: Implementation. *International Journal for Numerical Methods in Fluids*, 11(5):621–659, October 1990.