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Regularized equations for multicomponent compressible gas mixture flows and their finite-defference approximations

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Statement of the problem. Equations describing compressible multicomponent gas mixture dynamics are of great theoretical and applied interest, since they describe flows that are widespread in nature and technology. Systems of equations describing the dynamics of multicomponent mixtures are represented in numerous monographs, including: Landau L.D., Lifshitz E.M. (1986); Nigmatulin R.I. (1987); Pilyugin N.N., Tirskiy G.A. (1989); Rajagopal K.L., Tao L. (1995); Giovangigli V. (1999); Brennen C.E. (2005); Ruggeri T., Sugiyama M. (2021).

Quasi-gasdynamic (QGD) and quasi-hydrodynamic (QHD) systems of equations are regularized systems of Euler and Navier-Stokes equations of viscous compressible heat-conducting gases and are used for computer modeling of a wide range of gas dynamics problems. For more detailas see also the monographs of Chetverushkin B.N. (2004); Elizarova T.G. (2007); Sheretov Yu.V. (2009, 2016); Elizarova T.G., Shirokov I.A. (2018), as well as numerous articles. These systems of equations are suitable for discretization and construction of simple and reasonably effective explicit numerical methods. They have been used in computer modeling of various gas dynamics problems for several decades and remain relevant today. Accordingly, the QGD system is used at any, and the simpler QHD system at moderate Mach numbers. Their important mathematical properties, similar to those discussed in this dissertation, have been proven in the following works: Zlotnik A.A., Chetverushkin B.N. (2008); Zlotnik A.A. (2008, 2010); Sheretov Yu.V. (2009).

However, despite the extensive literature on regularized systems of equations for single-component gases and binary mixtures and their applications, the mathematical theory for multicomponent mixtures is poorly developed.

Actuality of the theme. QGD and QHD systems of equations for both multi-velocity and multi-temperature, and single-velocity and single-temperature binary gas mixtures were developed, considered and applied, in particular, in the works of Elizarova T.G. (2007); Elizarova T.G., Zlotnik A.A., Chetverushkin B.N. (2014); Balashov V.A., Savenkov E.B. (2018); Kudryashova T., Karamzin Y., Podryga V., Polyakov S. (2018); Elizarova T.G., Zlotnik A.A., Shilnikov E.V. (2019); Elizarova T.G., Shilnikov E.V. (2021); Balashov V., Zlotnik A. (2021), including the derivation of the entropy balance equation with non-negative entropy production which was given for some models in: Elizarova T.G., Zlotnik A.A., Chetverushkin B.N. (2014);

Elizarova T.G., Zlotnik A.A., Shilnikov E.V. (2019). The fulfillment of the entropy balance equation is an important physical property of the model and a mathematical property of the corresponding system of differential equations.

Construction of entropy-correct discretizations of systems of gas dynamics equations for which the entropy balance equation with non-negative entropy production is satisfied at a discrete level is also of great interest, see, for example: Amosov A.A., Zlotnik A.A. (1987); Tadmor E. (2003); Prokopov G.P. (2007); Tadmor E. (2016); Carpenter M.H. et al. (2016).

Level of progress in the theme. In the one-component case, QGD and simpler QHD systems of equations as regularized systems of Euler and Navier-Stokes equations of a viscous compressible heat-conducting gas are quite thoroughly studied in monographs of Chetverushkin B.N. (2004); Elizarova T.G. (2007); Sheretov Yu.V. (2009); Elizarova T.G., Shirokov I.A. (2017). Entropy balance equations with non-negative entropy production, in particular, were derived for them. Such important mathematical properties of these systems as Petrovsky's uniform parabolicity and dissipativity of solutions of linearized systems were proven in A.A. Zlotnik, B.N. Chetverushkin. (2008), Zlotnik A.A. (2008, 2010).

Generalizations of QGD and QHD systems on the case of binary mixtures of gases with different densities, velocities and temperatures in the absence of diffusion fluxes and chemical reactions were given in: Elizarova T.G. (2007); Elizarova T.G., Zlotnik A.A., Chetverushkin B.N. (2014); for the case of multicomponent mixtures, see: Podryga V.O. (2017). Recently, corresponding generalizations have been derived for the practically important case of homogeneous gas mixtures with a common velocity and temperature, as well as with common or several regularizing velocities, including the case of taking into account the interphase interaction of the components of the mixture, see: Balashov V.A., Savenkov E.B. (2018); Elizarova T.G., Zlotnik A.A., Shilnikov E.V. (2019), Zlotnik A., Lomonosov T. (2023). At the same time, the properties of equations for multicomponent mixtures have not been studied to such an extent, and some properties have not been studied at all. For example, the above models do not take into account diffusion fluxes between the components of the mixture, which are significant in numerous tasks. The use of numerical methods based on QGD and QHD systems of equations for binary mixtures with a common regularizing velocity has proven its efficiency in a number of computer modeling problems, see: Balashov V., Zlotnik A., Savenkov E. (2017);

Elizarova T.G., Zlotnik A.A., Shilnikov E.V. (2019); Balashov V., Zlotnik A. (2020), Balashov V., Zlotnik A. (2021); Elizarova T.G., Shilnikov E.V. (2021).

Regularized QGD and QHD systems of equations in the barotropic case were also previously considered in the literature. The one-component barotropic case was considered in Zlotnik A.A., Chetverushkin B.N. (2008); Zlotnik A.A. (2008, 2012) , and the case of barotropic binary two-velocity mixtures — in Elizarova T.G., Zlotnik A.A., Chetverushkin B.N. (2014). Various numerical methods for computer modelling of such mixtures have been proposed in recent years, in the works of Li Z., Oger G., Le Touzé D. (2020), Sondermann C.N. et al. (2021).

Numerical methods constructed on the basis of regularized equations of a one-component gas are presented in detail, for example, in the monographs of Chetverushkin B.N. (2004); Elizarova T.G. (2007); Sheretov Yu.V. (2009) and many subsequent articles. It should be noted that a large number of different numerical methods have been developed for solving systems of equations of one-component gas dynamics, including the monographs: LeVeque R.J. (2004); Kulikovsky A.G., Pogorelov N.V., Semenov A.Yu. (2012); Abgrall R., Shu C.W., eds. (2016, 2017). Discretizations for QGD and QHD systems of equations for binary mixtures in the absence of chemical reactions, including mixtures with a common velocity and temperature of the components, were constructed and successfully tested in numerical simulations, including in: Elizarova T.G. (2007); Balashov V., Zlotnik A., Savenkov E. (2017); Podryga V.O. (2017); Kudryashova T., Karamzin Y., Podryga V., Polyakov S. (2018); Elizarova T.G., Zlotnik A.A., Shilnikov E.V. (2019); Balashov V., Zlotnik A. (2021); Elizarova T.G., Shilnikov E.V. (2021), Podryga, V. O., Churbanov A. G., Tarasov N. I., Polyakov S. V., Trapeznikova M. A., Churbanova N. G. (2022). At the same time, due to the great complexity of systems of differential equations that arise while describing the dynamics of mixture flows, there are relatively few rigorous mathematical results about their properties, as well as about the properties of their discretizations. Note also that usually QGD and QHD regularizations were studied separately.

Entropy-correct discretizations of systems of gas dynamics equations were proposed, in particular, in: Amosov A.A., Zlotnik A.A. (1987); Tadmor E. (2003, 2016); Prokopov G.P. (2007); Carpenter M.H. et al. (2016). In the article: Zlotnik A.A. (2012) a symmetric three-point discretization of this type was constructed for the one-dimensional QGD gas dynamics equations for a perfect polytropic one-component gas, conservative in mass, momentum and total energy. Subsequently, similar discretizations were developed for the case of general gas state equationse, as considered in: Gavrilin V.A., Zlotnik A.A. (2015), as well as for the multidimensional case: Zlotnik A.A. (2017). These discretizations were successfully tested in numerical simulations.

It should be metioned that alternative regularized systems of equations in the one-component case have been studied and applied, for example, in: Feireisl E., Vasseur A. (2010); Guermond J.L., Popov B. (2014); Svärd M. (2018); Feireisl E. et al. (2020); Dolejší V., Svärd M. (2021). However, until now their practical testing has been quite limited, in contrast to QGD and QHD systems of equations.

The aim of this dissertation is the analysis of the properties of QGD and QHD systems of equations for multicomponent gas mixtures and construction of entropy-correct spatial discretizations for them. To achieve this goal, the following **objectives** have been set.

1. To derive an entropy balance equation with non-negative entropy production and study the L^2-dissipativity properties of the linearized system for an aggregated QHD system of equations for a homogeneous multicomponent gas mixture with common regularizing velocity in the presence of diffusion fluxes.
2. To derive an entropy balance equations with non-negative entropy production for aggregated QGD and QHD systems of equations for a homogeneous multicomponent gas mixture in the presence of diffusion fluxes; to construct linearized systems of equations and prove the existence, uniqueness and L^2-dissipativity of weak solutions of the initial boundary value problem; to analize the original system of equations and derive strong parabolicity and local time classical unique solvability of the Cauchy problem.
3. To study the properties of QGD and QHD systems of equations for single-velocity multicomponent gas mixtures in the barotropic case.
4. To construct entropy-correct discretizations of one-dimensional QGD and QHD systems of equations for the dynamics of both multi-velocity and multi-temperature, and single-velocity and single-temperature (in the presence of diffusion fluxes) multicomponent gas mixtures.

Scientific significance. In the present work QGD and QHD systems of equations (binary or single-component) known in the literature are generalized on the multicomponent case.

Firstly, a generalization of the aggregated QHD system of equations for a homogeneous gas mixture with a general regularizing velocity is carried out from the binary case to the multicomponent one, taking into account diffusion fluxes. An entropy balance equation with non-negative entropy production is derived for it. In the linearized formulation, the property of L^2-dissipativity is proven.

Secondly, a generalization on the multicomponent case of QGD and QHD systems of equations for a homogeneous gas mixture is constructed. Moreover, the additional diffusion fluxes are considered. These systems of equations are studied both in the case where the components of the mixture are perfect polytropic gases, and in the barotropic case. Entropy balance equations with non-negative entropy production are derived. Linearized systems of equations are constructed and the existence, uniqueness and L^2-dissipativity of weak solutions of the initial boundary value problem are analized. Such properties as strong parabolicity and local time classical unique solvability of the Cauchy problem for the original system are proven. The QGD and QHD systems of equations are studied not separately, but uniformly.

Thirdly, by generalizing the discretization for a single-component gas, an original entropy-correct discretizations of one-dimensional QGD and QHD systems of equations for multi-velocity and multi-temperature systems, as well as single-velocity and single-temperature in the presence of diffusion fluxes for a multicomponent gas mixture, is obtained. It should be noted that the discretization for the second systems is obtained by aggregating the discretizations for the first systems.

Theoretical and practical significance lies in the derivation of the important mathematical properties of the considered systems of equations of gas mixtures, as well as in the construction of entropy-correct discretizations in the one-dimensional case. These properties include the fulfillment of the entropy balance equation with non-negative entropy production, the existence, uniqueness and L^2-dissipativity of solutions for the linearized systems of equations and Petrovsky parabolicity and the classical unique solvability of the Cauchy problem for the original systems of equations. These properties confirm the physical correctness of the systems of equations under consideration, and also justify their mathematical regularizing properties. The developed discretizations can be used for numerical simulation of mixture flows.

Research methodology and methods. In the dissertation matrix analysis, methods of mathematical and functional analysis, including elements of the theory of Lebesgue and Sobolev spaces are used. The theory of systems of partial differential equations for both weak solutions and classical solutions is also used. Methods for constructing discretization of such equations are applied.

Basic results presented to be defended.

1. Entropy balance equation with non-negative entropy production is derived for the aggregated QHD system of equations for a homogeneous multicomponent gas mixture with a common regularizing velocity in the presence of diffusion fluxes between the components of the mixture, and the L^2-dissipativity of the linearized system of equations is proven.
2. Entropy balance equations with non-negative entropy production are constructed for aggregated QGD and QHD systems of equations for a homogeneous multicomponent gas mixture in the presence of diffusion fluxes. A linearization of the system of equations on a constant solution is constructed and the existence, uniqueness and L^2-dissipativity of weak solutions of the initial-boundary value problem for it are derived. Strong parabolicity and local in time classical unique solvability of the Cauchy problem for the original system are proven.
3. The properties of QGD and QHD systems of equations for single-velocity multicomponent gas mixtures in the barotropic case are studied.
4. An entropy correct discretization of one-dimensional QGD and QHD systems of equations for the dynamics of both multi-velocity and single-velocity (in the presence of diffusion fluxes) multicomponent gas mixtures are constructed.

Reliability of the theoretical results of the work is confirmed by rigorous mathematical proofs of the corresponding theorems. The constructed discretizations were successfully tested in numerical simulations (by other authors).

Probation of the work The results of the work were reported on the following conferences:

— Annual interuniversity scientific-technical conference of students, PhD students and young specialists in the name of E.V. Armensky (Moscow, MIEM NRU HSE, 2020, 2021, 2023)

— All-Russian scientific conference “Theoretical foundations of designing numerical algorithms and solving problems of mathematical physics”, dedicated to the memory of K.I. Babenko (Pushchino, Keldysh institute of applied mathematics, 2022)

— International conference One-Parameter Semigroups of Operators (OPSO) (Online, NRU HSE, Nizhny Novgorod, 2023)

At conferences named after E.V. Armensky in 2021 and 2023 the presented reports were awarded diplomas for the best work of a PhD student. References to the published abstracts of reports are given in the dissertation text.

Author's personal contribution. Theoretical results on the analysis of QGD and QGidD systems of equations for the dynamics of multicomponent gas mixtures, as well as on the construction of entropy-correct discretizations, were obtained jointly with A.A. Zlotnik. The corresponding results in the barotropic case were obtained by the applicant independently.

Size and structure of the work. The dissertation consists of Introduction, three chapters, Conclusion and Appendix. The full volume of the dissertation is 109 pages. The work includes one table/ The bibliography contains 72 titles.

Main inferences of the research. In chapter 1 the properties of the aggregated QHD system of equations for a homogeneous gas mixture with common regularizing velocity are analyzed. In Section 1.1, the corresponding system of equations is introduced and its consequences are constructed. Section 1.2 is devoted to the derivation of the entropy balance equation for this system of equations in the presence of diffusion fluxes. Theorem 1.2.1 presents an entropy balance equation with non-negative entropy production.

In section 1.3, the expansion of the QHD system of equations is carried out with respect to the gradient of the sought functions (component densities, velocity and temperature). Further in Section 1.4, using this expansion, the system of equations is linearized on a constant solution. Then it is symmetrized. An integral identity is obtained for the symmetrized system of equations. In Theorem 1.4.1, the properties of L^2-dissipativity and uniqueness are established for its weak solutions, and an energy estimate is also derived. Further in Section 1.5, similar results are obtained for a simplified linearized QGD system of equations.

In conclusion, in Section 1.6 the type of the initial QHD system of equations for a homogeneous gas mixture is analyzed. The Fourier transform of space is applied to the original system of equations with the lower elements dropped and the coefficients frozen, which leads to a system of ordinary differential equations. It is established that in the absence of diffusion fluxes, the system of equations introduced in Section 1.1 is of a composite type, just like the system of Navier-Stokes equations for a compressible single-component gas.

In Chapter 2 the analysis of QGD and QHD systems of equations for a multicomponent gas mixture in the presence of diffusion fluxes is implemented. Both aggregated systems of equations are considered simultaneously by introducing a parameter which equals 0 for QHD system of equations and equals 1 in case of QGD system of equations. In section 2.1, the corresponding systems of equations and additional balance equations are derived. In Section 2.2, Theorem 2.2.1 regularized entropy balance equation with non-negative entropy production is presented.

Next, in Section 2.3, the expansion of the QGD and QHD systems of equations with respect to the gradient of the sought functions is performed. Then in Section 2.4 they are linearized on a constant solution and symmetrized. Lemmas 2.4.1 and 2.4.2 are related to the study of bilinear forms involved in determining the weak solution of the resulting symmetrized system of equations. Theorem 2.4.1 is devoted to the existence and uniqueness of a weak solution of the initial boundary value problem in the introduced space of vector functions, as well as its L^2 dissipativity. Corollary 2.4.1 gives a strengthened form of the L^2-dissipativity property.

Then, in Section 2.5, the parabolicity of the QGD and QHD systems of equations and the local in time classical solvability of the Cauchy problem for them are proven.

In sections 2.6 - 2.9, similar properties of barotropic QGD and QHD systems of equations are studied.

In Chapter 3, an approximation in space of one-dimensional QGD and QHD systems of equations for a multicomponent gas mixture is constructed. In Section 3.1 a one-dimensional regularized system of equations for the dynamics of a multi-velocity and multi-temperature multicomponent gas mixture is introduced. In Lemma 3.1.1 the balance equations for the kinetic and internal energies of the mixture, as well as the entropy balance equation with non-negative entropy production are derived. Next, in Section 3.2, equations are considered in the case of a single-velocity and single-temperature multicomponent gas mixture in the presence of diffusion fluxes. An entropy balance equation with non-negative entropy production is also derived.

In Section 3.3, a spatial discretization of a one-dimensional regularized system of equations for a multi-velocity and multi-temperature gas mixture is constructed. This discretization is distinguished by non-standard averaging, which further guarantees the non-negativity of entropy production in the discrete entropy balance equation. In Lemma 3.3.1, semi-discrete equations for the balance of the kinetic and internal energies of the mixture components are derived. In Theorem 3.3.1 the entropy balance equation for the spatially discrete method constructed above is derived.

The final section 3.4 examines the spatial discretization of one-dimensional QGD and QHD systems of equations for the dynamics of a single-velocity and single-temperature gas mixture in the presence of diffusion fluxes. In this case, discretization is carried out not directly, but by aggregating the semi-discrete equations for the dynamics of multi-velocity mixtures constructed in the previous section. It is this non-standard approach that ultimately ensures the fulfillment of the semi-discrete entropy balance equation with non-negative entropy production, which is the subject of Theorem 3.4.1.

All listed lemmas, statements and theorems are followed by proofs.

List of publications on the topic of the dissertation. The main results on the topic of dissertation are presented in [1–6].

The results of Chapter 1 were obtained with the financial support of the Russian Foundation for Basic Research, project No. 19-01-00262, the results of Chapter 2 were obtained with the financial support of the Russian Science Foundation, grant No. 19-11-00169.

1. *Zlotnik A. A., Fedchenko A. S.* Properties of an aggregated quasi-gasdynamic system of equations for a homogeneous gas mixture // *Dokl. Math.* – 2021. –Vol.104, no.3. Pp. 340-346.

2. *Zlotnik A. A., Fedchenko A. S.* Properties of the aggregated quasi-hydrodynamic system of equations for a homogeneous gas mixture with a common regularizing velocity // *Preprints of the Keldysh Institute of Applied Mathematics.* –2021. –Vol.77. –Pp.1-25.

3. *Zlotnik A. A., Fedchenko A. S.* On the properties of a quasihydrodynamic system of equations for a homogeneous gas mixture with a common regularizing velocity // *Diff. Equations.* – 2022. — Vol. 58., no.3. — Pp. 341-356.

4. *Zlotnik A.A., Fedchenko A.S.* On properties of aggregated regularized systems of equations for a homogeneous multicomponent gas mixture// *Math. Models in the Appl. Sci.* – 2022. – Vol. 45, no. 15. – Pp. 8906-8927.

5. *Zlotnik A.A., Fedchenko A.S., Lomonosov T.A.* Entropy correct spatial discretizations for 1D regularized systems of equations for gas mixture dynamics// *Symmetry.* – 2022. – Vol. 14, no. 10. Article 2171.

6. *Fedchenko A.S.* Properties of regularized equations for barotropic gas mixtures // *J. Math. Sci.* – 2023. – Vol. 270, no. 6. – Pp. 1-12.