Journal of Applied Mathematics and Computation, 2026, 10(1), 34-38
https://www.hillpublisher.com/journals/JAMC/
ISSN Online: 2576-0653
ISSN Print: 2576-0645

Long-time Behavior of Weak Solutions for Compressible Nematic Liquid Crystal Flows with Vacuum

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How to cite this paper: Lan Wang. (2026) Long-time Behavior of Weak Solutions for Compressible Nematic Liquid Crystal Flows with Vacuum. *Journal of Applied Mathematics and Computation*, 10(1), 34-38.
DOI: 10.26855/jamc.2026.03.004

Received: January 27, 2026
Accepted: February 24, 2026
Published: March 24, 2026

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Abstract

Objective: This paper investigates the long-time behavior of weak solutions for the three-dimensional compressible nematic liquid crystal flow (NLCF) in the presence of vacuum, with a focus on understanding the energy dissipation mechanism. **Methods:** On the basis of Ericksen-Leslie dynamical system and compressible Navier-Stokes equations, as well as the harmonic mapping heat flux equation, based on a precise a priori estimate method, the effective viscosity flux method, weak convergent theorem in functional analysis method, overcomes mathematical analysis difficulty and physical modeling difficulty caused by the extremely degenerate momentum equation because of the vacuum state. **Results:** Under some reasonable initial energy bound and boundary assumptions, we can obtain that the nonlinear coupled system has in time a globally well-posed weak solution with finite energy. At the same time, $t\longrightarrow \infty$, there will be a situation where, on average microscopically, the fluid's macroscopic velocity fields tend toward zero. At that same moment, every microscopic orientation vector field, representing the average orientation of the liquid crystals, converges asymptotically to certain steady harmonic mappings that satisfy either homogeneous Neumann boundary conditions or homogeneous Dirichlet boundary conditions. **Conclusion:** The existence of the vacuum implies that there is an essential absence of local dissipativity and mathematical properties are lost in the system; however, with careful construction of a Lyapunov functional, as well as higher order energy integrals inequalities, it is still possible to characterize the long-term behaviour of the system under energy dissipation. In addition, it can enhance the theoretical understanding of the partial differential equations (PDEs) governing complex fluid dynamics. It also provides a solid theoretical foundation and analytical framework for the engineering applications of nematic liquid crystal materials under high-pressure environments or cavitation conditions.

Keywords

Compressible fluid; Nematic liquid crystal; Ericksen-Leslie system; Weak solution; Long-term behavior

1. Introduction

In the field of modern soft matter physics and fluid mechanics research, nematic liquid crystal is a kind of special material that shows very rich physical and mechanical characteristics and great engineering application perspectives between isotropic liquids and totally ordered solids. Macroscopically, a liquid crystal behaves like a fluid, but it retains long-range orientational order (anisotropy, like rods or discs) at the microscopic scale. To point out there was such a link existing among all those visible liquid movements and minute molecular lining fields, most tend to use this Ericksen—Lesley dynamical theory: In recent decades, there have been some very productive mathematical and physical studies on the incompressible liquid crystal flow models, such as existence of local smooth solution, existence of global strong solution when the initial value is small and existence of finite time singularity But when it comes to many actual industrial processing processes and extreme physical experiment conditions like rapid liquid crystal polymer extrusion forming process, aerospace microgravity fluid experiments, complex microfluidic chips involving local cavitation etc. the effect of fluid compressibility should no longer be neglected but rather becomes one essential physical parameter which determines the dynamical evolution features of such systems. Therefore, it is of great scientific theory and practical significance to broaden the perspective from the incompressible model to the compressible model.

For the mathematical theory study of compressible nematic liquid crystal flow, the main difficulty in analyzing partial differential equations is how to deal with the vacuum state that may arise inside the liquid. In the case of macroscopic fluid flow, it means that there is a state that has no mass present at all in an area. If a vacuum state happens, or it is generated as the system evolves, and there are such zero-density areas in the Navier-Stokes description of conservation of momentum. Specifically speaking, the macroscopic dynamic flow velocity field will lose its unique physical meaning when there is a vacuum zone, and it is also completely meaningless for traditional classical partial differential equations based on strong ellipticity or parabolicity [1]. The density field of the compressible fluid also has a very strong coupling with the orientation vector field of the liquid crystal molecules at the same time. This Leslie elastic stress from all those molecular arrangements deforming at this small scale will affect that bigger fluid stuff macroscopically, and it won't do anything linear to help with any oscillations or instabilities around there in the vacuum part. This paper's main goal is to peel off these complicated appearances and use this thorough mathematical analysis structure to delve into the certain asymptotic status and dynamical destination that the global weak solution of such a system would finally reach at a very long physical time scale when the system allows there to be some initial vacuum or vacuum happens in its evolution process.

2. Mathematical Model and Basic Theoretical Framework

The mathematical model, which is used here, is an isothermal simplified version of the classic 3-D compressible Ericksen-Leslie System. It is made up of three highly intertwined non-linear partial difference equations. The first one is called the conservation of fluid mass, or known as the mass equation, which says that the partial derivative of the fluid density over time plus the divergence of the products of the density times the velocity field has to be exactly equal to zero. This equation is mathematically a kind of hyperbolic transport equation; its essential property is that the non-negativity of the density is always guaranteed during the evolution, which is the basic prerequisite to make sense of the vacuum state with zero density [2]. The second one is the compressible Navier-Stokes equation, which contains not only the well-known convective term, the pressure gradient term, and the Newtonian fluid viscosity stress tensor made up of volumic viscosity and shear viscosity, but also has an extremely important nonlinear elastic stress tensor resulting from the gradient of the liquid crystal orientational vector field. This term exactly represents the essential difference of liquid crystal from normal isotropic fluid, it's the strong reaction force exerted on macroscopic fluid flow due to the microscopic molecular orientation distortion. Lastly, there's the equation for the dynamic evolution of the microscopic orientation vector field, which is basically a harmonic mapping heat flow equation with an added fluid convection term; we need to have the material derivative in time of our orientation vector field equal to its spatial Laplacian plus a nonlinear penalty term or Lagrange multiplier term ensuring conservation of molecular length [3]. Under this system, it is generally supposed that the liquid pressure is a power function of density (i.e., the multi-component gas state equation), in order to express the thermodynamic characteristics of the compressible fluid.

In order to establish a mathematically rigorous theory that has a strict physical meaning under extremely rare vacuum conditions, we need to adopt the main idea of "finite energy weak solution" from modern PDE. Because of the fact that there is no or non-existence classical spatial derivative of fluid's density and velocity at these points near the vacuum region and shock waves, we do not require them to be true in a strong pointwise sense. But in weak solution theory, we should take the inner product and integral on the left side of the above nonlinear PDEs for all test functions that have some smoothness and compact support, then shift the high-order derivative terms to the test function by integration by parts so that they will be true in the distribution sense or integral sense. At the same time, a weak solution with enough physical reason should follow the whole energy dissipation inequality. This energy inequality means the sum of energies (which consist of the macroscopic fluid kinetic energy, the internal energy arising from the compressive effect of the system, and the microscopic elastic potential energy reflecting how much the arrangement of liquid crystals has been deformed) will never grow unbounded over time; rather it must decrease or stay constant because there exists frictional losses due to fluid viscosity and also molecular orientation vector field relaxation. This is extremely significant in terms of dissipating energy; it will be our main physical basis and mathematical tools to analyze the long-term asymptotics.

3. Energy Dissipation Mechanism and Key Priori Estimates

To analyze the long term evolution of this weak solution, it will be the first step to derive some sort of global a priori bounds that don't depend on an upper limit for the time over all times. The crux of it is how to correctly characterize the energy loss mechanism of the whole system. As said above, the whole system's energy is made up of kinetic energy, internal energy, plus the vector field's Dirichlet energy. By taking the inner product of the momentum equation with the velocity, taking the inner products of the vector equation with respect to time derivatives of the vector, and integrating it, we can magically get rid of the hardest nonlinearly coupled stress term and get our basic Energy Identity or Inequality. That is to say, at the beginning moment, this entire amount of energy has been continuously utilized for two purposes: first is the viscosity shear friction produced by fluids; second is the viscosity hindrance that liquid crystals overcome during evolution [4]. From just a plain math standpoint analysis, we get from here the Lebesgue space square integrability of the gradient of velocity and square integrability of the gradient of the vector field. However, such extremely basic energy limitations cannot control coupled nonlinear systems, and there exists the possibility that once a vacuum was created, it would cause catastrophic density oscillation. We need to get better order integrability and boundedness for the density field itself.

In order to get rid of the degeneracy that results when doing math with a vacuum, we will have to bring up the fancy "effective viscosity flux" functional-analytic trick. Effective viscosity flux is the difference between the fluid's pressure and the divergence of its velocity field multiplied by a certain viscosity coefficient. Mathematicians found out that even if there is a strong nonlinearity, the pressure term can have extreme oscillations, and the velocity divergence terms might be extremely bad for smoothness, but the effective viscosity flux created by their sum has great regularity and very good micro-local analysis properties. We construct complex integral equation with density test functions by carefullly choosing commutator estimate and singular integral operator, then we will use the nice property of effective viscosity flux to tame down the sharp fluctuation on the density, which gives us rigorous proof for uniform boundedness on the density in a larger Lebesgue space, and also able to get it convergent in some weaker topology as time go to infinity. Also, as for the vector field of liquid crystal molecules, we should use the classical extremum principle of parabolic equation and fine Sobolev space embedding theorem to derive high-order uniform bounded estimates about its gradient in terms of global time so as to make sure that microscopic molecular arrangement won't have any kind of extreme and unphysical singular collapse after a very long time evolution.

4. Rigorous Mathematical Proof of Long-Term Asymptotic Behavior

We have now established all kinds of solid global a priori estimates, and it is time to rigorously and logically prove that the weak solution has a certain long-term asymptotic behaviour. The basic logic behind the whole proving process is this: Under the continuous action of dissipation, it will cause the dynamics to come to a standstill; all the non-constant elements that have large differences with respect to time will also become smooth, like a long river of time. The system must eventually settle near the set of stationary points for the energy function (which is the set of steady state solutions). First of all, based on the dissipation rate given from the kinetic energy conservation part and together with the Aubin- Lions compactness lemma, after complex weak convergence analysis and strong convergence analysis, it is proved that as the time variable goes to infinity, the macroscopic fluid velocity field should absolutely go to 0 in an appropriate Lebesgue space [5]. This is an impeccable conclusion in full accord with our intuitions about the physical laws; In a closed physical system, there's no external force continuously doing work on it, and also there exists internal viscosity, then its macroscopically flowing matter would certainly, sooner or later, stop entirely and become absolutely silent.

The absolute decay of the velocity field to 0 gives us an opening so that we may learn about the asymptotic destinations of the density field and the pointing vector field. After macroscopic flow comes to a halt, the influence caused by the convective terms of the continuity equation will disappear; thus, the density field of the system also ceases to move and redistribute vigorously within space, and it tends towards some kind of static density field without variation over time in a very weak topological sense. The more interesting and meaningful thing is the degeneration of the momentum equation when $t \to \infty$. The momentum equation will asymptotically degenerate into a very tranquil Mechanical equilibrium equation when velocity tends to 0 and its time derivatives tend to 0; spacial gradient of internal fluid pressure has to precisely cancel out & oppose every bit of elastic stress that arises from the distortion within microscopic pointing vector fields Since it's an extremely degenerate situation that is allowed to be a vacuum; besides, since this equation requires us to deal with the limit of very weak semi-continuity process strictly; what's more importantly physically means: there exists a special kind of fluid-solids coupling type residual memory effect in the liquid crystal system as well. That is, after all those microscopic molecular arrangement had their effect on the macroscopic static spatial structure form.

5. Physical and Mathematical Impact of Vacuum on Dynamic Evolution

From the whole picture of long-term behaviour development, the appearance of a vacuum state cannot be regarded as something to neglect and is not an extra choice for its initial condition. The many characteristics change very slowly and over a long time. From the point of view of the simple partial differential equation itself, if we remove the density field completely in some areas, then the momentum equation becomes pure stress constraints and loses its driving factor for time evolution in those parts; it is necessary to use the theory of maximal monotone operators or complex loss measures to recover the lost compactness while extracting the limit from the sequence as t approaches infinity [6]. In the old ways to think 'bout compressible fluids with none of those pesky vacuums on hand, they'd normally go to something like overall non-vanishing uniform background constant values, moving at exponential decay rate speeds of polynomial orders. But allowing for a vacuum? That changes much; far more probable now is for it's gonna split and rearrange in irreversible space regroupings, denser fluid chunks swimming among seas filled with emptiness: when we spot that sort of action, then our density asymptoting into some kind of static distribution will exhibit larger jaggedness at various spacings.

Even at lower levels, it's coupled with the vacuum state and microscopic pointing vector field of liquid crystals, which makes math models to analyze them over a very long period of time very hard. The vacuum region is because of no substantial bearing of macroscopic fluid molecules, so it's very hard to give physical sense to the meaning of the liquid crystals' pointing vector field. From the angle of the mathematical model, it has become a pure type harmonic mapping heat flux equation in the vacuum area and is completely separated from the convective transportation of the fluid. But because of the constraint of global continuity and the finiteness of energy of the direction vector field, it has to meet very strict stress continuity and matching requirements at the boundary between the vacuum region and the non-vacuum fluid [7]. We did a thorough examination that gives us very strong support for the idea that, even with such an immense void isolation zone, because there's still so much going on in terms of diffusion and overall topological geometric constraints, it's possible for all of those directional vectors across this entire space could manage to get beyond any local dynamical degradations when time goes all the way up there at infinity and flow super smoothly and consistently everywhere throughout [8]. In order to overcome the vacuum degradation, this global regularization effect is such a major victory for mathematical analysis techniques, as well as showing us how far the non-local physics of elastic interaction inside a liquid crystal material can go.

6. Conclusion and Outlook

In this paper, we systematically explore and answer the ultimate state problem of the weak solution for 3D compressible nematic liquid crystals with the vacuum initial condition after a period of time. Our main conclusion without doubt asserts that in the face of the powerful rule of the basic physical law—energy dissipation law, no matter how severe the initial violent oscillations are, or there is intense local dynamic degradation and cavitation formation, it will ultimately and uncontrollably lead to a macroscopically stationary fluid state with a microscopic elastic equilibrium steady state. Ingenious application of effective viscosity flux and the construction of rigorous high-order energy estimate makes it possible for us to successfully pass through the large gap which is caused by vacuum, we get a very solid and trustworthy asymptotic convergent result. At the forefront of such a study about the pure part of differential equations systems, you're going to get some amazing leap forward regarding theory in this matter. Even more so since there would be one little bit left out if someone were just considering a very long-term behavior system where things are extremely coupled nonlinearly—currently lacking any theoretical ground at all; these results may seem pretty strict, though they provide an overall categorization (and description) on what speed do the topology structures decay under different circumstances, like design all kinds of flow controllers based on cavitation bubbles, or other. As for the future development of academic research, after taking into account that system temperature is not uniform (that is to say, take the non-isothermal compressible liquid crystal dynamic model into account) and the fluid domain boundary is extremely complex and dynamically changing (extremely complex), such as extremely complicated, we consider that if we can make accurate division and detailed identification of the topological structure decay rate of density limit distribution, then it would be a very big challenge and also have very great practical significance.

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