Boundary-layer formation for viscosity approximations in transonic flow

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The boundary-layer formation for viscosity approximations in one-dimensional transonic flow models in a bounded interval with a source or a force-collision term is considered. The energy equation is replaced by a pressure–density relationship. The values of the density are imposed at the ends of the interval. The models are used in steady-state hydrodynamic modeling of semiconductor devices where the force term is a force-collision integral operator of the density. Also, the model represents the steady-state nozzle flow, where the source term accounts by geometrical effects. It is shown that the viscosity approximation converges to a solution of the equation arising from these models. As expected, a limiting solution can develop shocks that only occur from supersonic to subsonic regions satisfying the jump condition (i.e., equal flux) and the classical entropy condition (i.e., pressure and density increase across a shock in the direction of the particle path). More interesting is the boundary behavior of the limiting solution. The boundary layer has a condition that determines the possible range of discontinuities for the density. Values of the density at the upstream boundary in the limit $\epsilon \to 0$, must remain subsonic if the prescribed value is subsonic. Values of the density at the upstream boundary in the limit $\epsilon \to 0$, if different from the prescribed subsonic or sonic one, must become supersonic with bigger flux than the flux of the prescribed one. This can be thought of as trying to impose boundary values inside the range of a forming shock.

I. INTRODUCTION

We report here on the construction of solutions of one-dimensional transonic flow models for semiconductor devices (or gas-dynamic equations) via the viscosity method in a bounded interval.

We prove that the viscosity solutions of the regularized problem converge to a weak solution of the limiting equations satisfying the entropy condition given by the second law of thermodynamics for normal fluids, namely, the entropy, pressure, and density increase across a shock wave in the direction of the flow.

It is worthwhile noticing that the flux function is continuous and therefore discontinuities in the density can occur only from supersonic to subsonic conjugate values (i.e., of equal flux).

It is also interesting to note that the range of possible discontinuities at the boundary is restricted: values of the density at the upstream boundary in the limit $\epsilon \to 0$, even when different from the prescribed value, must remain subsonic. On the other hand, values of the density at the downstream boundary in the limit $\epsilon \to 0$, if different from the prescribed one, must not only become supersonic, but further be of bigger flux than the flux of the prescribed one.

This can be thought of as trying to impose boundary values inside the range of a forming shock.

Numerical simulations related to this problem in the modeling of semiconductor devices can be found in Ascher *et al.*,[1] Fatemi and co-workers,[2,3] Gardner,[4] and Gardner *et al.*[5]

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We consider the following system of steady-state conservation laws in one space dimension:

$$(\rho u)_x = 0, \tag{1a}$$

$$F(\rho,\rho u)_x + S(\rho,\rho u,x) = 0, \tag{1b}$$

in the interval $I = (0,1)$. Here F is a strictly convex function of ρ (Fig. 1) and S is locally bounded. Examples of the system above are

$$F(\rho,\rho u) = [(\rho u)^2/\rho] + p(\rho), \tag{2a}$$

where $p(\rho)$ is the pressure function, which represents the steady-state Euler equations for gas dynamics, where conservation of energy is replaced by a pressure–density relationship, namely

$$p(\rho) = \rho^\gamma, \quad \gamma > 1. \tag{2b}$$

This represents a classical model of transonic flow with a source term (e.g., those accounting for geometric effects). For example, when $S(\rho,\rho u,\phi_x) = c(x)h(u)$, this system represents the steady-state model of transonic gas flow in a duct of variable cross section $c(x)$ where both $h(u)$ and $h'(u)$ are nonzero and never change sign. For references regarding work done on this model see Courant and Friedrichs[6] (Chap. 5), Glaz and Liu,[7] Glimm *et al.*,[8] Hsu and Liu,[9] and Liu.[10]

Also, this system is found in the modeling of semiconductors. There,

$$S(\rho,\rho u,\phi_x) = -\rho\phi_x + \frac{\rho u}{\tau(\rho,\rho u)}, \quad \text{with } \phi_{xx} = \rho - C(x). \tag{3}$$

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That is, in this case, S involves an integral operator of ρ. Thus, (1)–(3) describe the steady state of a hydrodynamic model (or Euler–Poisson model) for semiconductors. The model has the form of the Euler equations for a gas of charged particles [with a force term proportional to the electric field, given by the first term in (3)] modified by momentum relaxation terms. This term, the second one in (3), originates from the moments of the collision operator which, in contrast to gas dynamics, do not vanish in the semiconductor case and, usually, is modeled by a relaxation time approximation (see Blotekjaer[11] and Markowich *et al.*[12]).

Thus in (1)–(3) $u(x)$, $\rho(x)$, and $\phi(x)$ denote the electron density, velocity, and electrostatic potential, respectively, and the function $\tau(\rho,\rho u)$ is the momentum relaxation time which we assume

$$0<\tau_0<\tau(\rho,\rho u)\leqslant\tau_M, \quad \forall(\rho,\rho u)\in(0,\infty)\times\mathbb{R}. \tag{4}$$

The function $C(x)$ in (3) is called the doping profile and is usually assumed to be a step function.

We are interested in the behavior of a solution ρ of (1b) at the ends of I if we try to impose Dirichlet data at both ends of the interval I.

II. EXISTENCE OF SOLUTIONS

Introducing the current density $j=\rho u$, the steady-state system becomes

$$j(x)=\text{const}, \tag{5a}$$

$$F(\rho,j)_x+S(\rho,j,x)=0, \tag{5b}$$

for $x\in I$, with prescribed values

$$\rho(0)=\rho_0, \ , \rho(1)=\rho_1.$$

Since F is not monotone, simple examples show that it is necessary to impose some sort of an entropy condition to select the physical solution. In accordance with the second law of thermodynamics for fluids with normal thermodynamic properties, this entropy condition says that the entropy, density, and pressure increases across the shock in the direction of the particle path (see Courant and Friedrichs,[6] Raizer and Zel'dovich,[13] and Menikoff and Plohr[14]).

One classical way of doing that is by adding an artificial term $\epsilon\rho_{xx}$ to (5b). This term might be called, more properly, a diffusivity term since it is a modification of second order in the density variable. Notice that it carries the opposite sign to the usual artificial viscosity as $\rho_{xx}=-(ju_x/u)_x$. That is, we add a "viscous" term of the form $\epsilon(ju_x/u)_x$.

Under suitable growth conditions on F and S (which are satisfied in the examples above), one can show (see Gamba[15]) the existence of solutions of the viscosity approximations,

$$j(x)=\text{const}>0, \tag{6a}$$

$$F(\rho^\epsilon,j)_x+S(\rho^\epsilon,j,x)+\epsilon\rho^\epsilon_{xx}=0, \tag{6b}$$

with boundary data

$$\rho^\epsilon(0)=\rho_0, \quad \rho^\epsilon(1)=\rho_1. \tag{6c}$$

More precisely, in Ref. 15, we have shown that there exists a solution ρ^ϵ in I with second bounded derivatives of the ϵ-viscosity boundary-value problem (6a)–(6c), which is bounded above and below by strictly positive constants independent of ϵ, depending only on the boundary data ρ_0, ρ_1, the constant j from (5a), the exponent γ (larger than 1), from (2b), and on condition (4) for the momentum relaxation time function $\tau(\rho,j)$. In particular, ρ^ϵ is uniformly bounded away from cavitation. Also, $\epsilon\rho^\epsilon_x$ is bounded uniformly in $\overline{I}$, independently of ϵ. For the semiconductor device equations, the interesting case becomes as $\gamma=1$, for which the result remains valid under the additional assumption that the vector field $-\phi_x$ remains strictly negative in the interval I.

By taking the limit as ϵ goes to zero, we find a weak solution of the problem (5a) and (5b) in the sense of the integral identity,

$$\int_I[-F(\rho)\varphi_x+S(\rho,j,x)\varphi]dx=0, \tag{7}$$

which is valid for any smooth φ defined in I such that φ and its derivatives are zero at the boundary of I.

We now discuss the physical properties of the approximating sequences of the limiting solution. Let us recall that the sonic value ρ_{sonic} is the value of ρ where F attains its minimum, changing the equation's type (in the two-dimensional problem this model would mean the equation changes from elliptic to hyperbolic type),

$$F(\rho_{\text{sonic}})=\min_{\rho\in(0,\infty)}F(\rho). \tag{8}$$

An important role is played by the function $\mathscr{H}(\rho)$ defined as

$$\mathscr{H}(\rho)=[F(\rho)-F(\rho_{\text{sonic}})]\operatorname{sgn}(\rho-\rho_{\text{sonic}}). \tag{9}$$

This function is now strictly monotone in ρ.

We prove (the entropy condition)

$$\mathscr{H}(\rho(x))+Cx \text{ is monotone increasing,} \tag{10}$$

where $C=\sup_I S(\rho^\epsilon,j,x)$. That is, $\mathscr{H}(\rho)_x$ is a measure bounded below by $-C$.

The sign of the "added viscosity" is crucial in demonstrating (10) and depends on the sign of the constant j. Actually, $j=\rho u$, with u the velocity, represents a constant current flow, going to the right, and the viscosity must retard the flow in the direction in which the flow moves.

We point out that (10) represents the classical "entropy condition" for the transonic case in the sense of Oleĭnik,[16] Vol'pert,[17] and Kružkov.[18] Note that if the problem is transonic we do not expect ρ but $\mathscr{H}(\rho)$ to have a derivative almost everywhere. Furthermore, (10) implies that a weak solution ρ of (7), given by the vanishing viscosity method, can be written as a sum of a monotone increasing function plus a term that is only Hölder continuous with exponent 1/2. This means the discontinuities of ρ can only be jumps from smaller to bigger values of ρ in the direction of the flow (classical entropy condition).

Moreover, the function $F(\rho(x))$ is a continuous function defined on I with bounded derivatives. That means the quantity $F(\rho(x))$ conserved across the discontinuity points of $\rho(x)$ for every x, so we can say that $\rho(x)$ can only develop admissible shocks, from supersonic to subsonic conjugate values ρ and ρ^* satisfying the jump condition

$F(\rho) = F(\rho^*)$.

In order to obtain this convergence result, we showed that

$$\int_I |\mathscr{H}(\rho^\epsilon)_x|dx$$

is bounded independently of ϵ (see Sec. 3 in Ref. 6).

Once we know the family $\{\mathscr{H}(\rho^\epsilon)\} = \{\mathscr{H}_\epsilon\}$ is uniformly of bounded variation, which means the above integral is uniformly bounded independently of ϵ, classical completeness and compactness theorems [Helly's theorem in one dimension, Kolmogorov's compactness condition in one (or eventually more) dimensions; see Ref. 19] assure us that we can extract a sequence $\{\mathscr{H}_{\epsilon_n}\}$, $\epsilon_n \to 0$ as $n \to \infty$, that converges pointwise in I and in every $L^p(I), 1 \leqslant p < \infty$, to a bounded variation function $\mathscr{H}_0(x)$ [that is, $\mathscr{H}_0(x)$ has a derivative almost everywhere].

Further, $\{\mathscr{H}(\rho^{\epsilon_n})\}$ being uniformly bounded, $\phi(\mathscr{H}(\rho^{\epsilon_n}))$ converges to $\phi(\mathscr{H}_0(x))$ in $L^1(I)$ and pointwise for any continuous function ϕ. Thus, as $\mathscr{H}(x)$ is continuous and increasing, $\mathscr{H}^{-1}(x)$ is a well-defined continuous function.

Taking $\mathscr{H}^{-1}$ as the ϕ above, we can recover the physical density ρ as

$$\rho(x) = \lim_{n \to \infty} \mathscr{H}^{-1}(\mathscr{H}_{\epsilon_n}(x)) = \mathscr{H}^{-1}(\mathscr{H}_0)(x). \quad (11)$$

satisfies what is an admissible solution of (7), (9), (10), and $F(\rho(x))$ is a Lipschitz function on I.

III. DISCUSSION OF THE BEHAVIOR AT THE BOUNDARY OF THE LIMITING SOLUTION ρ

Finally, we investigate what the boundary layer looks like near the ends for the viscous boundary-value problem:

$$(F(\rho^\epsilon))_x + S(\rho^\epsilon, j, x) = -\epsilon\rho^\epsilon_{xx}, \quad x \text{ in } I = (0,1),$$
$$\rho^\epsilon(0) = \rho_0 \text{ and } \rho^\epsilon(1) = \rho_1 \text{ for every } \epsilon. \quad (12)$$

A boundary layer may develop at both ends of the boundary, and explicit examples can be constructed for $S \equiv 0$ by rescaling in ϵ and solving the global ordinary differential equation (ODE) $(F(\rho) + \rho_x)_x = 0$. Indeed, this equation becomes $F(\rho) + \rho_x = M$. If the constant M is smaller than $F(\rho_{\text{sonic}})$ then the solutions are not admissible (these solutions, when rescaled, give a vertical line).

If M is larger than $F(\rho_{\text{sonic}})$, there are two types of solutions. The first type are bounded increasing ones where the limit at minus infinity is the (supersonic) conjugate value of the (subsonic) limit at infinity by the function F. These limits at plus and minus infinity depend on M. The other type are unbounded decreasing ones.

The bounded increasing ones, when rescaled, either give examples of internal shocks or give the condition at the downstream boundary by choosing the interval of definition appropriately. More precisely, rescaling the interval $(-\epsilon^{-1}, \epsilon^{-1})$ to $(0,1)$, and letting ϵ go to zero, an exact discontinuity (i.e., of equal flux) develops in the limiting nonviscous solution as the limit of a forming internal shock. Analogously, the interval $[-\epsilon^{-1}, \alpha(\epsilon)]$, with $\epsilon\alpha(\epsilon)$ going to zero, as ϵ goes to zero, is rescaled to $(0,1)$ for the condition at the downstream boundary, where the data is $\rho_\epsilon(1) = \rho_\epsilon(\alpha(\epsilon)) = \rho_1$. With this rescaling of the interval of definition, the viscous solution forms a shock at distance $\epsilon\alpha(\epsilon)$ from the downstream boundary point $x = 1$. Thus, letting ϵ go to zero, a discontinuity will form in the limiting nonviscous solution at the boundary, where the value from the left of $x = 1$ approaches the limit at minus infinity of the viscous solutions, and the value at $x = 1$ is ρ_1.

Note that with the above rescaling a discontinuity does not necessarily form at a distance ϵ from the boundary, making it undetectable with standard boundary-layer analysis.

An unbounded decreasing solution reduces to an upstream boundary layer when rescaling $(0, \epsilon^{-1})$ to $(0,1)$.

Therefore, further analysis of the boundary layer is needed for the general problem, and is given in Ref. 15, Sec. 4, where it has been shown that the limiting nonviscous solution of the problem (6a)–(6c) satisfies the properties described below in detail.

In general, if $\rho(x) = \mathscr{H}^{-1}(\mathscr{H}_0)(x) = \lim_{\epsilon \to 0} \rho^\epsilon(x)$ for every x in I, where this convergence is not uniform in ϵ, it means the respective lateral limits of $\rho(x)$ for x approaching the boundary points from inside I may not coincide with the prescribed values ρ_0 and ρ_1 at the boundary points $x = 0$ and $x = 1$. [These lateral limits exist since $\mathscr{H}(\rho)$ has a derivative almost everywhere.] Thus the boundary layer cannot have oscillations with wavelength going to zero as ϵ goes to zero.

Actually, we shall see that if the prescribed values ρ_0 and ρ_1 are subsonic, that is, $\rho_0, \rho_1 > \rho_{\text{sonic}}$ with $F(\rho_{\text{sonic}}) = \min_{\rho \in (0,\infty)} F(\rho)$, a "subsonic" boundary layer may be formed in the "upstream" boundary, which in our particular problem is at $x = 0$, and a "shock-boundary layer" may be formed in the "downstream" boundary $x = 1$. That is, the upstream boundary limiting value

$$\rho_0^+ = \lim_{\substack{x \to 0 \\ x > 0}} \rho(x)$$

must stay subsonic, i.e.,

$$\rho_0^+ \geqslant \rho_{\text{sonic}}. \quad (13)$$

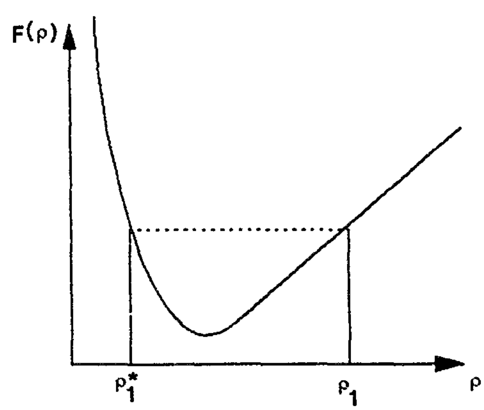

FIG. 1. Typical $F(\rho)$.

On the other hand, the downstream boundary limiting value

$$\rho_1^- = \lim_{\substack{x\to 1\\ x<1}} \rho(x),$$

if different from ρ_1, not only must become supersonic, but further, stay below to the conjugate value of ρ_1, i.e.,

$$\rho_1^- = \rho_1, \tag{14a}$$

or

$$\rho_1^- < \rho_1^* < \rho_{\text{sonic}} \text{ with } F(\rho_1^*) = F(\rho_1). \tag{14b}$$

This can be interpreted as follows: At the upstream boundary, a layer may form, but it must stay subsonic, i.e., close to the prescribed value. Downstream a discontinuity forms only if one attempts to prescribe values at a point where a shock is formed by jumping from a supersonic value ρ_1^- to its subsonic conjugate $(\rho_1^-)^*$ larger than ρ_1 (Fig. 2).

This result is obtained by studying the behavior of $F(\rho^\epsilon(x))$ as a boundary layer is forming. We exploit the following formula, obtained by integrating the ϵ equation (12),

$$F(\rho^\epsilon(b^\epsilon)) - F(\rho^\epsilon(a^\epsilon)) = -\int_a^b S(\rho^\epsilon, j, x)\,dx - \epsilon\rho_x^\epsilon(b^\epsilon) + \epsilon\rho_x^\epsilon(a^\epsilon), \tag{15}$$

for points b^ϵ and a^ϵ at "both sides" of the forming layer. The factor $\int_a^b S(\rho^\epsilon, j, x)\,dx$ is not essential since S is uniformly bounded so that the difference $F(\rho_1^-) - F(\rho_1)$ is of order $F(\rho^\epsilon(b^\epsilon)) - F(\rho^\epsilon(a^\epsilon))$, whose sign can be controlled by choosing a^ϵ and b^ϵ carefully, depending on the difference $\rho_1^- - \rho_1$ (resp. $\rho_0^+ - \rho_0$), so that we can make the sign of the right-hand side of

$$F(\rho_1^-) - F(\rho_1) = -\int_a^b S(\rho^\epsilon, j, x)\,dx - \epsilon\rho_x^\epsilon(b^\epsilon) + \epsilon\rho_x^\epsilon(a^\epsilon) + [F(\rho_1^-) - F(\rho^\epsilon(b^\epsilon))] + [F(\rho^\epsilon(a^\epsilon)) - F(\rho_1)] \tag{16}$$

either positive or negative.

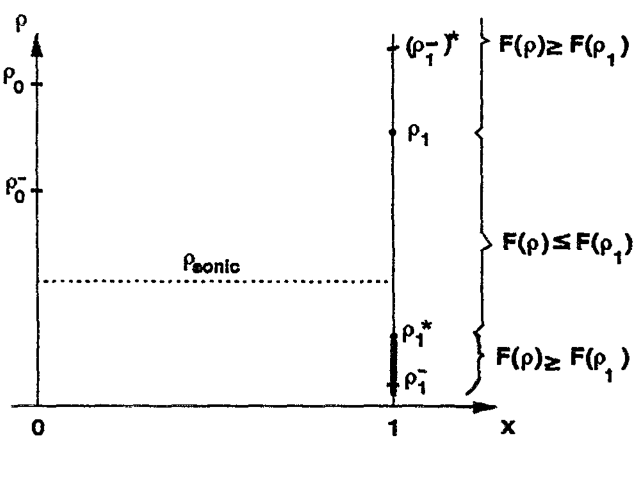

FIG. 2. Diagram of possible boundary discontinuities.

IV. CONCLUSIONS

These results show that in an ideal limit (no viscosity) the shock wave is an exact discontinuity in density, velocity, and pressure. That is, mass and momentum are conserved, or equivalently, the discontinuities occur from supersonic to subsonic values with equal flux. This allows us to conclude immediately that, for a strictly convex momentum flux with one critical value achieved at the sonic value, supersonic flow will be smooth and produce no shock waves. The transition from subsonic flow to supersonic flow is also smooth. The transition from supersonic flow to subsonic flow might develop a shock wave, that is, a wave over which density and velocity and pressure change very rapidly. These conclusions are in agreement with conclusions obtained by Gardner using numerical experiments.[4]

The boundary-layer conditions (13), (14a), and (14b) were proposed and shown in Ref. 15. The same boundary-layer conditions are proposed by Hsu and Liu.[9] They might provide a test to check when shocks appear to develop in numerical computations of transonic one-dimensional flow.

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