

Transport equations on curved interfaces with finite thickness

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1988 J. Phys. A: Math. Gen. 21 2273

(<http://iopscience.iop.org/0305-4470/21/9/040>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 129.252.86.83

The article was downloaded on 01/06/2010 at 06:41

Please note that [terms and conditions apply](#).

COMMENT

Transport equations on curved interfaces with finite thickness

A Grauel

Theoretische Physik, Universität Paderborn, Postfach 1621, 4790 Paderborn, Federal Republic of Germany and Abteilung Theoretische Physik, Naturwissenschaftliches und Medizinisches Institut an der Universität Tübingen in Reutlingen, Postfach 2362, 7410 Reutlingen, Federal Republic of Germany

Received 4 January 1988, in final form 5 February 1988

Abstract. In this comment we discuss transport equations on a curved interface which is semipermeable. The moving interface has finite thickness and separates two media with different physical properties. We introduce a thermodynamical field theory with the material properties of such an inhomogeneous system.

There exist in the literature many studies of the description of shells as a material body. Here we give two extensions: first, that the surface geometry is time dependent; and second that the thin region is semipermeable and therefore in material and heat exchange with the surrounding media. Furthermore, the temperature as an additional field is taken into account.

We consider a moving three-dimensional region embedded in and interacting with a three-dimensional continuum where one dimension of the moving region is much smaller than the other two (interface with finite thickness). The balance equations together with the constituent equations represent field equations for the thermodynamical fields. Mathematically speaking, the equations form a closed set of boundary conditions for moving boundaries.

We consider a body $\mathcal{L}(t)$ with the volume $\mathcal{V}(t)$. We assume that this volume is divided into the volumes $\mathcal{V}^+(t)$ and $\mathcal{V}^-(t)$ by a thin region of parallel surfaces with body $b(t)$ and volume $V(t)$. The volume $\mathcal{V}(t) = \mathcal{V}^+(t) \cup \mathcal{V}^-(t) \cup V(t)$ is bounded by

$$\partial\mathcal{V}(t) = \partial\mathcal{V}^+(t) \cup \partial\mathcal{V}^-(t) \cup \Omega(t).$$

Let Ψ be an additive property of $V(t)$ and Ψ_v the amount of Ψ in a partial volume v of $V(t)$. Ψ_v is given by

$$\Psi_v = \int_v \psi(x^i, t) \, d\tau \tag{1}$$

where $\psi(x^i, t)$ is the density of Ψ_v . Let us assume that (1) holds for every partial volume of $V(t)$, moreover we assume additivity of (1) to obtain the total amount of Ψ of $V(t)$. $V(t)$ is bounded by the curved surface $\Sigma^{(\xi_1)}(t)$, $\Sigma^{(\xi_2)}(t)$ and the lateral surface Ω .

We consider a smooth surface $\Sigma(t)$ in the Euclidean space E^3 with orthonormal base vectors b_i , $i = 1, 2, 3$, where the position vector r of any point $P(u^1, u^2, t)$ on the moving surface is given by $\Sigma^{(0)}(t)$:

$$r = b_i x^i \quad \text{where } x^i = \chi^i(u^A, t) \text{ and } A = 1, 2. \tag{2}$$

The u^A are curvilinear coordinates on $\Sigma^{(0)}(t)$ called surface coordinates and t represents time. Throughout we use covariant notation and summation convention. The quantity dr on $P(u^1, u^2, t)$ directed tangentially to the u^B coordinate curve is

$$dr = \frac{\partial r}{\partial u^B} du^B \tag{3}$$

or in components

$$dx^i = x^i_{;B} du^B \tag{4}$$

where the quantities $x^i_{;B}$ are components in space directed tangentially to the surface coordinates u^1, u^2 . The square of length of arc on $\Sigma(t)$ is given by $(ds)^2 = g_{ij} dx^i \otimes dx^j$ and with (4) it follows that

$$(ds)^2 = g_{AB} du^A \otimes du^B \tag{5}$$

where $g_{AB} = g_{ij} x^i_{;A} \otimes x^j_{;B}$ is the metric tensor on $\Sigma(t)$ and $g_{ij} = \delta_{ij}$ in space E^3 where \otimes means tensor product. The normal vector perpendicular to $\Sigma(t)$ has the representation

$$e_i = \frac{1}{2} \varepsilon^{AB} \varepsilon_{ijk} x^j_{;A} \otimes x^k_{;B} \tag{6}$$

where $e^i e_i = 1$ and $e_i x^i_{;A} = 0$ at all times t . The curvature tensor b_{AB} is given by definition

$$b_{AB} = -x^i_{;A} \otimes e_{i,B} = e_i \otimes x^i_{;AB} \tag{7}$$

Let us denote by $\Sigma^{(\xi)}(t)$ the surface, smooth by hypothesis, obtained by laying off equal distances ξ along the normal e^i to $\Sigma^{(0)}(t)$ and $\Sigma^{(\xi)}(t)$ is laid to be parallel to the surface $\Sigma^{(0)}(t)$. $\Sigma^{(\xi)}(t)$ is determined by

$$\Sigma^{(\xi)}(t): R = r + \xi b_i e^i \tag{8}$$

where R is the position of any point on the surface $\Sigma^{(\xi)}(t)$ and r is defined by (2). Written in components we have

$$\kappa^i = \chi^i(u^A, t) + \xi e^i(u^A, t) \tag{9}$$

Formally $\xi \in [\xi_1, \xi_2]$, where ξ_1 and ξ_2 are finite distances from the middle surface at $\xi = 0$. With foregoing conventions we have

$$\kappa^i_{;A} = x^i_{;A} + \xi e^i_{;A} = (\delta^B_A - \xi b_{AB}) x^i_{;A} \tag{10}$$

and the metric and curvature tensor at any parallel surface is given by

$$G_{AB} = (1 - \xi^2 k_G) g_{AB} - 2\xi(1 - \xi k_M) b_{AB} \tag{11}$$

and

$$B_{AC} = \xi k_G g_{AC} + (1 + \xi k_M) b_{AC} \tag{12}$$

where k_M and k_G are the mean and the Gaussian curvature of b_{AB} . The determinant of the expression in front of $x^i_{;A}$ in (10) can be written in terms of k_M and k_G as

$$F(\xi) = 1 - 2\xi k_M + \xi^2 k_G \tag{13}$$

The rate of change of Ψ in $V(t)$ is given by

$$\frac{d\Psi}{dt} = -\Phi(\Psi) + P(\Psi) + S(\Psi) \tag{14}$$

where $\Phi(\Psi)$ is the flux through the surface $\partial V = \Sigma^{(\xi_1)} \cup \Sigma^{(\xi_2)} \cup \Omega$. $P(\Psi)$ is a production term

$$P(\Psi) = \int_V P \, d\tau \tag{15}$$

and represents the production of Ψ in V , for example the mass production in V via chemical reactions, and

$$S(\Psi) = \int_V S \, d\tau \tag{16}$$

is the supply of Ψ , for example by radiation, in the volume V from outside of the volume V . P and S are densities, namely the production density and the density of supply. The flux $\Phi(\Psi)$ consists of two parts, namely a convection flux $\hat{\Phi}(\Psi)$ and a non-convective part

$$\int_{\partial V} \Phi^j \eta_j \, dA \tag{17}$$

where Φ^j is the density of the non-convective flux through ∂V , dA is a surface element of ∂V and η_j are the covariant components of a surface vector perpendicular to ∂V .

In the following formulae v^j is the velocity in the volume $V(t)$, σ^j the velocity of the surface $\partial V(t)$, w_n the velocity parallel to e^i and \dot{u}^A are the components of a velocity in the lateral surface $\Omega(t)$. Now we obtain from (14) the generalised transport equation

$$\partial_t \psi_s + (\dot{g}/2g) \psi_s + w_{n,A} \psi_s^A + (\psi_s \dot{u}^A + \Phi^A + \hat{\Phi}^A)_{;A} + [F(\xi) \{ \psi (v^j - \sigma^j) e_j + \Phi^j e_j \}] = p + s \tag{18}$$

which is valid for all points of the interfacial region. The quantity $\xi = \xi_2 - \xi_1$ is the thickness of the interfacial region and the other quantities are defined as follows.

The mean value of the density field in $V(t)$:

$$\Psi_s = \int_{\xi_1}^{\xi_2} F(\xi) \psi \, d\xi. \tag{19}$$

The vector-valued surface quantity:

$$\Psi_s^A = - \int_{\xi_1}^{\xi_2} (E^{AB}(\xi) \psi_{;B} + D^{AB}(\xi)_{;B} \psi) \xi \, d\xi. \tag{20}$$

The non-convective flux through the lateral surface $\Omega(t)$:

$$\Phi^A = x_{j,B} \int_{\xi_1}^{\xi_2} \Phi^j D^{BA}(\xi) \, d\xi. \tag{21}$$

The convective flux through $\Omega(t)$:

$$\hat{\Phi}^A = \int_{\xi_1}^{\xi_2} \psi \{ D^{AB}(\xi) (v_j x^j_{;B} + \xi w_{n;B}) - F(\xi) \dot{u}^A \psi \} \, d\xi. \tag{22}$$

The production density in $V(t)$:

$$p = \int_{\xi_1}^{\xi_2} F(\xi) P \, d\xi. \tag{23}$$

The density of supply from the region outside of $V(t)$ into $V(t)$:

$$s = \int_{\xi_1}^{\xi_2} F(\xi) S \, d\xi. \tag{24}$$

Also

$$g = \det(g_{AB}) \tag{25}$$

$$D^{AB}(\xi) = F(\xi) g^{AB} - E^{AB}(\xi) \tag{26}$$

$$E^{AB}(\xi) = -\xi^2 k_G g^{AB} + \xi b^{AB}. \tag{27}$$

The notation $[\cdot]$ is introduced as the jump of a physical quantity ψ on any thin region and is defined by

$$[F(\xi)\psi] = F(\xi_2)\psi|_{\xi_2} - F(\xi_1)\psi|_{\xi_1} \tag{28}$$

where $\psi|_{\xi_2}$ is the value of the field quantity $\psi(u^A, \xi, t)$ for $\xi = \xi_2$. $F(\xi_1)$ and $F(\xi_2)$ are limit values of $F(\xi)$ on $\Sigma^{(\xi_1)}(t)$ and $\Sigma^{(\xi_2)}(t)$. Equation (18) represents the generalised transport equation which is valid for interfacial regions of finite thickness $\xi = \xi_2 - \xi_1$. We obtain equations of balance if we identify the quantities in (18) with the fields in the interfacial region (Grauel 1982a, b, 1987).

Now let us study the limiting behaviour of (19)-(27). To that end we consider a thin region between two of the surfaces $\Sigma^{(\xi_1)}(t)$ and $\Sigma^{(\xi_2)}(t)$ of constant thickness ε and we set $\xi_1 = -\frac{1}{2}\varepsilon$ and $\xi_2 = \frac{1}{2}\varepsilon$. We assume the following.

(i) The surface field $\psi^+(u^A, t)$ is given by definition

$$\psi^+(u^A, t) =: \lim_{\substack{x^i \in \mathcal{V}^+(t) \\ x^i \rightarrow \mathcal{X}^i \in \Sigma^{(\xi_2)}(t)}} \psi(x^i, t) \tag{29}$$

and $\psi^-(u^A, t)$ by an analogous definition.

(ii) The limits of integrals over fields exist and are non-vanishing smooth functions of the coordinates u^A and time t . Let $G(u^A, \xi, t)$ be a scalar-valued function. Then

$$g(u^A, t) = \lim_{\varepsilon \rightarrow 0} \int_{-\varepsilon/2}^{\varepsilon/2} G(u^A, \xi, t) \, d\xi \tag{30}$$

is the scalar-valued field on the surface or interface. Similarly we introduce vector-valued functions on surfaces and interfaces by

$$f^j(u^A, t) = \lim_{\varepsilon \rightarrow 0} \int_{-\varepsilon/2}^{\varepsilon/2} F^j(u^A, \xi, t) \, d\xi. \tag{31}$$

The limiting values of the surface quantities (17), (26) and (27) are $F(0) = 1$, $D^{AB}(0) = g^{AB}$, $E^{AB}(0) = 0$ and

$$\lim_{\varepsilon \rightarrow 0} \int_{-\varepsilon/2}^{\varepsilon/2} \xi^p h(u^A, \xi, t) \, d\xi = 0$$

where $p > 0$.

Therefore $\psi_s^A = 0$ and (22) takes on the form

$$\hat{\Phi}^A = \lim_{\varepsilon \rightarrow 0} \int_{-\varepsilon/2}^{\varepsilon/2} F(\xi) \psi(u^A, \xi, t) (v^A - \dot{u}^A) \, d\xi. \tag{32}$$

By definition the velocity field u^A is introduced into the theory independently of certain motion of particles on the surface $\Sigma^{(0)}$ and therefore Φ^A represents a diffusion of particles on the surface if we identify $\psi(u^A, \xi, t)$ with the density of mass. If the diffusion flux $\hat{\Phi}^A$ on the surface is zero we obtain an expression of the velocity field

$$\psi_s \dot{u}^A = \lim_{\varepsilon \rightarrow 0} \int_{-\varepsilon/2}^{\varepsilon/2} F(\xi) \psi(u^A, \xi, t) v^A d\xi \tag{33}$$

where

$$\psi_s(u^A, t) = \lim_{\varepsilon \rightarrow 0} \int_{-\varepsilon/2}^{\varepsilon/2} F(\xi) \psi(u^A, \xi, t) d\xi.$$

Equation (18) in the limit $\varepsilon \rightarrow 0$ has the following form:

$$\partial_t \psi_s + \frac{\dot{g}}{2g} \psi_s + (\psi_s w^A + \Phi^A)_{;A} + [\psi(v^j - w^j) e_j + \Psi^j e_j] = \pi + \sigma \tag{34}$$

where

$$\begin{aligned} \Phi^A(u^A, t) &=: x_{p,B} g^{AB} \lim_{\varepsilon \rightarrow 0} \int_{-\varepsilon/2}^{\varepsilon/2} F(\xi) \Phi^p(u^A, \xi, t) d\xi \\ \pi(u^A, t) &=: \lim_{\varepsilon \rightarrow 0} \int_{-\varepsilon/2}^{\varepsilon/2} F(\xi) P(u^A, \xi, t) d\xi \\ \sigma(u^A, t) &=: \lim_{\varepsilon \rightarrow 0} \int_{-\varepsilon/2}^{\varepsilon/2} F(\xi) S(u^A, \xi, t) d\xi. \end{aligned} \tag{35}$$

Equation (34) takes on the same form which we have given in previous papers (Grauel 1980, 1982a, b). With the definitions in those papers for a mixture of $\delta = 1, \dots, \lambda$ chemically reacting fluids we obtain the equations of balance of mass, momentum and internal energy in the following form:

$$\begin{aligned} \partial_t \gamma_\delta + \frac{\dot{g}}{2g} \gamma_\delta + (\gamma_\delta w_\delta^A)_{;A} + [\rho_\sigma (v_\sigma^j - w_\lambda^j) e_j] &= \pi_\delta & \pi_\delta &= \sum_{r=1}^n \zeta_\delta^r m_\delta z_r \\ \partial_t (\gamma_\delta w_\delta^k) + \frac{\dot{g}}{2g} \gamma_\delta w_\delta^k + (\gamma_\delta w_\delta^k \otimes w_\delta^A - T_\delta^{kA})_{;A} &+ [\rho_\sigma v_\sigma^k \otimes (v^j - w^j) - t_\sigma^{kj}] e_j &= m_\delta^k + \gamma_\delta F_\delta^k \\ \partial_t (\gamma E_s) + \frac{\dot{g}}{2g} \gamma E_s + (\gamma E_s w^A + Q^A)_{;A} - T^{kA} w_{k;A} &+ [\rho (\varepsilon + \frac{1}{2} (v^k - w^k)^2) (v^j - w_\lambda^j) e_j + q^j e_j - t^{kj} (v_k - w_k) e_j] \\ &= \sum_{\delta=1}^\lambda \gamma_\delta (F_\delta^k U_k^\delta + r_{s\delta}) \end{aligned} \tag{36}$$

where $[\cdot]$ represents the jump of a physical quantity on the surface or interface and σ runs over different values for the bulk media outside the interface. $U_\delta^k = w_\delta^k - w^k$ is the diffusive velocity in the mixture.

For the entropy we assume the following.

(i) On the interface exists an additive quantity called the interface entropy η which is balanced according to (34) by

$$\partial_t (\gamma \eta_s) + (\dot{g}/2g) \gamma \eta_s + (\gamma \eta_s w^A + \Phi^A)_{;A} + [\rho \eta (v^j - w_\lambda^j) + \Phi^j] e_j - \gamma \sigma_{\eta_s} = \pi_{\eta_s} \tag{37}$$

where π_{η_s} is the production of entropy.

(ii) For each thermodynamic process on the interface the production of entropy π_{η_s} shall not be negative; therefore we have

$$\pi_{\eta_s} \geq 0 \quad (38)$$

or

$$\partial_t(\gamma\eta_s) + \frac{\dot{g}}{2g}\gamma\eta_s + (\gamma\eta_s w^A + \Phi^A)_{;A} + [\rho\eta(v^j - w_\lambda^j) + \Phi^j] e_j - (a_k F^k + br_s)\gamma \geq 0 \quad (39)$$

where the specific supply of entropy $\gamma\sigma_{\eta_s}$ on the interface is given by the supplies of momentum and internal energy.

The balance equations together with the entropy balance (39) describe the interaction of the embedded surface in the bulk phases correctly. If we supplement constituent equations for the constituent quantities z_r , T_δ^{kA} , m_δ^k , E_s and Q^A to the equations (36) then (37) is restrictive for the theory (Grauel 1982a, b).

The transport equation together with the quantities (19)–(24) can be applied to fluid films, interfacial fluid membranes, boundary layers, etc with the possibility of momentum, heat and material exchange with the surrounding media. Equation (19) shows that we can take into account density distributions and chemically active materials. By a limiting process $\varepsilon \rightarrow 0$ we obtain a closed set of boundary conditions for a moving boundary. This boundary can be semipermeable and chemical reactions can occur in the interfacial fluids. Moreover equations (36) can be applied to phase boundary problems and stability considerations of fluid interfaces.

References

- Grauel A 1980 *Physica* **103A** 468
 — 1982a *J. Math. Modelling* **3** 17
 — 1982b *Habilitationsschrift* University of Paderborn
 — 1987 *Chin. Phys. Lett.* **5**