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THICK FLUID INTERFACE MODELING

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ABSTRACT

Basic concepts of interface and interfacial layer are first introduced. Orthogonal curvilinear coordinate analysis, used to study interfacial zones depending of time, is presented. Classical 3D and 2D thermodynamical relations are reminded and second gradient formulation is introduced. Then general balance laws are written and examples are given to illustrate the purpose.

INTRODUCTION

Interfaces are often compared with geometrical surfaces. But these surfaces have internal physical properties and must be considered as material surfaces. They are the seat of multiple exchanges with their surrounding, i.e. the bulks in contact with them. Thermodynamical properties and balance laws of interfaces are not always simple to obtain. It is often necessary to work with several scales of analysis. At microscopic scale, 2D interfaces become 3D interfacial layers, where thermodynamical relations and balance equations must be written. A review is presented in our book [1].

Many authors were interested by interfacial modeling. Interfacial fluid layers endowed with internal capillarity were studied in particular by Casal [2,3], Germain [4], Gouin [5], Seppecher [6] and Gatignol [7]. Concept of interface extended to stretched flames were considered by Klimov [8], Sivashinski [9], Clavin and Joulin [10], Prud'homme [11]. For the concept of an "interface" with internal energy per unit area, one can cite Delhayé [12], Scriven [13], Slatery [14]. Rocard [15] gave a statistical approach and Casal, Gouin, Germain, Seppecher a macroscopic approach. Discussion about interfacial velocities were driven by Landau and Lifschitz [16], Bedeaux, Albano and Mazur [17], Napolitano [18], Prosperetti [19] and, for interfaces with surface mass, by Ghez [20,21], Prud'homme [22]. In relation with the concept of an "interfacial layer", Ishii [23], Gogosov [24], Sanfeld and Steinchen [25] utilize true quantities, and on the contrary, Landau and Lifschitz, Meinhold and Heerlein [26] excess quantities. The concept of dividing surface was utilized by Gibbs [27], Slatery [28], Defay et al. [29]. Many authors have established interfacial balance equations, but not always with the desirable strictness. One try here to point out some crucial problems and suggest solutions.

INTERFACE AND INTERFACIAL LAYER

The concept of an interface is relative. Some material surface seems very thin at a given scale and appear to be thick at a smaller one (Fig. 1).

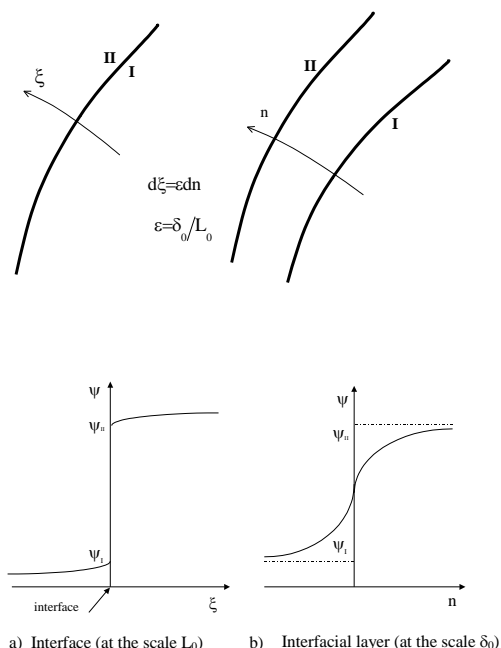


Fig. 1

As examples of interface, one can mention various systems as capillary surfaces, miscible interfaces, some flames, and so on, all systems whose properties verify the same type of balance equations at a convenient scale.

One consider here only fluid interfaces, i.e., themselves fluid, without rigidity, and located between bulk fluids.

Modeling of such interfaces means establishing equations of material surfaces (2D balance equations) and closing the obtained system by constitutive relations.

2D interfacial properties can be deduced from 3D analysis, by integration across the interfacial layer. Then, interfacial quantities ψ_a and ψ_s are deduced from local 3D properties by integration between the boundaries of the interfacial layer. It gets

$$\psi_a = \rho_a \psi_s = \int_{\xi_I}^{\xi_{II}} \rho \psi d\xi \quad (1)$$

with the surface density

$$\rho_a = \int_{\xi_I}^{\xi_{II}} \rho d\xi \quad (2)$$

Applying (1) to the fluid velocity \vec{V} , it gets

$$\rho_a \vec{V}_S = \int_{\xi_I}^{\xi_{II}} \rho \vec{V} d\xi \quad (3)$$

To calculate the integrals of the right hand member it is sometimes necessary to apply an asymptotic expansion method and to use a new coordinate n at smaller scale than ξ with $d\xi = \varepsilon dn$

$$\psi_a = \int_{\xi_I}^{\xi_{II}} \rho \psi d\xi = \varepsilon \int_{-\infty}^{+\infty} \rho \psi dn \quad (4)$$

ORTHOGONAL CURVILINEAR COORDINATES

It is generally convenient to consider the interfacial layer as a stratified structure. On each surface of this structure we suppose that the value of a characteristic parameter q (local density, temperature or concentration) is constant. Use of a system of orthogonal curvilinear coordinates can be made, and each surface of the stratified structure, on which the characteristic parameter q remains constant, can be seen as a coordinate surface $S_3(x_3, t)$ or S_3 - obtained for a given value of x_3 at time t .

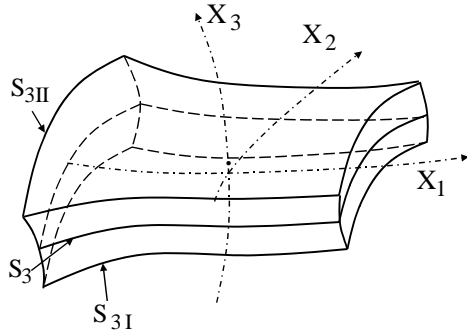


Fig. 2. Curvilinear orthogonal coordinates; coordinate surfaces.

Let us consider the following moving curvilinear system

$$\begin{aligned} x &= x(x_1, x_2, x_3, t) \\ y &= y(x_1, x_2, x_3, t), \text{ or: } \vec{x} = \vec{x}(x_1, x_2, x_3, t) \\ z &= z(x_1, x_2, x_3, t) \end{aligned} \quad (5)$$

x , y and z being the Cartesian coordinates in an orthonormal basis $(\vec{i}, \vec{j}, \vec{k})$, x_1 , x_2 and x_3 the curvilinear coordinates and t the time.

We call \vec{h}_i , the vector of components $(x_{,i}, y_{,i}, z_{,i})$. For the *orthogonal curvilinear* system of coordinates, the vectors \vec{h}_i , \vec{h}_j ($i \neq j$) are orthogonal at any point. Dividing by the norm $|\vec{h}_i| = h_i$, we obtain the normalized vector $\vec{e}_i = \vec{h}_i / h_i$ and we define the curvilinear abscissa by $dX_i = h_i dx_i$ (Fig. 2). The mean curvature of surface S_3 is then

$$\frac{1}{\delta S_3} \frac{d(\delta S_3)}{dX_3} = \vec{\nabla} \cdot \vec{e}_3 = \frac{1}{h_3} \left(\frac{h_{1,3}}{h_1} + \frac{h_{2,3}}{h_2} \right) \quad (6)$$

Projection operators can be defined [1] (for instance one define $\vec{I}_\perp = \vec{e}_3 \vec{e}_3$, and $\vec{I}_\parallel = \vec{I} - \vec{e}_3 \vec{e}_3$), and a local

velocity \vec{W} inside the interfacial layer is introduced (Fig. 3) by the formula

$$\vec{W} = \vec{V}_\parallel + w \vec{e}_3, \quad (7)$$

$$\text{with: } \vec{V}_\parallel = \vec{I}_\parallel \cdot \vec{V}, \quad \vec{w} = \frac{\partial \vec{x}}{\partial t} \cdot \vec{e}_3 \equiv \vec{h}_t \cdot \vec{e}_3, \quad w = \vec{e}_3 \cdot \vec{h}_t = \vec{I}_\perp \cdot \vec{h}_t.$$

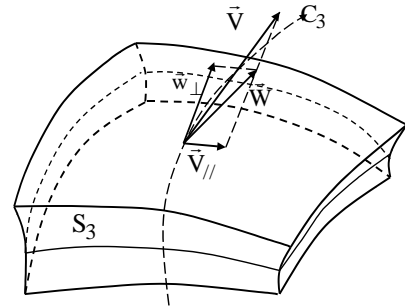


Fig. 3. Velocities inside the interface layer

The stretch of a surface S_3 moving locally at velocity \vec{W} is then

$$\frac{1}{\delta S_3} \frac{d}{dt} (\delta S_3) = \vec{\nabla} \cdot \vec{W} - \vec{\nabla}_\perp \cdot \vec{W} = \vec{\nabla}_\parallel \cdot \vec{W} \quad (8)$$

$$\text{with } \vec{\nabla}_\perp = \vec{I}_\perp \cdot \vec{\nabla}, \quad \vec{\nabla}_\parallel = \vec{I}_\parallel \cdot \vec{\nabla}.$$

Quantities defined by (6), (7) and (8) are very important for the interface description because they have physical meaning.

THERMODYNAMICAL RELATIONS

For the bulk and the interfacial layer in the case of a classical fluid mixture, the internal energy E of a given volume of fluid is an order one homogeneous

function of its entropy S , its volume \mathcal{V} and the masses of species m_j , which are extensive quantities. This gives, for the unit mass, the Euler, Gibbs and Gibbs-Duhem well known relations:

$$e = Ts - pv + \sum_{j=1}^N g^j Y^j, \quad de = Tds - p dv + \sum_{j=1}^N g^j dY^j, \quad (9)$$

$$0 = s dT - v dp + \sum_{j=1}^N Y^j dg^j$$

For the 2D interface, usual thermodynamical relations read

$$e_S = T_S s_S + \sigma / \rho_a + \sum_{j=1}^N g_S^j Y_S^j, \quad de_S = T_S ds_S + \sigma d(1/\rho_a) + \sum_{j=1}^N g_S^j dY_S^j, \quad (10)$$

$$0 = s_S dT_S + (1/\rho_a) d\sigma + \sum_{j=1}^N Y_S^j dg_S^j$$

In the case of 3D interfacial fluid layers with internal capillarity, and taking a one component fluid for simplicity, internal energy E of the stratified layer - a volume with a small thickness $\Delta \xi$ around a coordinate surface - is an order one homogeneous function of quantities S , \mathcal{V} , the mass m , and of a complementary extensive variable \mathcal{S} , which is homogeneous to an area, but is not equal to the area of the part of S_3 contained in the considered volume.

One has $\mathcal{S} = \int_{\mathcal{V}} \left| \frac{d\mathcal{V}}{d\xi} \right| d\mathcal{V}$, and the internal energy per

unit mass becomes $e = e\left(s, v, \left| \frac{d\mathcal{V}}{d\xi} \right| \right)$.

One can write

$$e = Ts - pv + \Lambda \left| \frac{d\mathcal{V}}{d\xi} \right| + g, \quad de = Tds - p dv + \Lambda d \left| \frac{d\mathcal{V}}{d\xi} \right|, \quad (11)$$

$$0 = s dT - v dp + \left| \frac{d\mathcal{V}}{d\xi} \right| d\Lambda + dg$$

More usually, one write [1, 6]

$$e = e\left(s, \rho, |\vec{\nabla} \rho|^2\right), \quad de = Tds - p d\left(\frac{1}{\rho}\right) + \lambda \vec{\nabla} \rho \cdot d(\vec{\nabla} \rho) \quad (12)$$

GENERAL BALANCE LAW

The local form of the balance equation for any property, whose volumetric value is denoted by $\rho \psi$, is

$$\frac{d_{\vec{W}}(\rho \psi)}{dt} + \rho \psi \vec{\nabla} \cdot \vec{W} + \vec{\nabla} \cdot [\vec{J} + \rho \psi (\vec{V} - \vec{W})] = \rho \phi \quad (13)$$

where velocity \vec{W} is defined by (7) and where $d_{\vec{W}}/dt$ stands for the convective derivative

associated to \vec{W} . An integration of the two sides of (13) across the interfacial layer leads to the balance law for the 2D interface

$$\frac{d_{\vec{W}_S}(\rho_a \psi_S)}{dt} + \rho_a \psi_S \vec{\nabla}_S \cdot \vec{W}_S + [(\vec{J} + \rho \psi (\vec{V} - \vec{W}_S)) \cdot \vec{\xi}] + \vec{\nabla}_S \cdot \vec{J}_{a//} = \rho_a \phi_S \quad (14)$$

with definitions (1) to (3) for the interfacial variables, \vec{W}_S being defined by (3) with \vec{W} in place of \vec{V} , and with the flux $\vec{J}_{a//} = \int_{\xi_1}^{\xi_2} [\vec{J} + \rho \psi (\vec{V} - \vec{W}_S)] d\xi$. The average velocities are shown on Fig. 4.

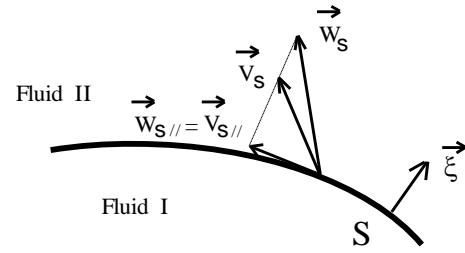


Fig. 4. The different velocities on the 2D interface S .

General surface balance law (14) can be applied to masses of species and to total mass. An alternative form of (14) may then be deduced

$$\rho_a \frac{d_S \psi_S}{dt} + [J_{\perp} + \dot{m}(\psi - \psi_S)] + \vec{\nabla}_S \cdot \vec{J}_{a//} = \rho_a \phi_S \quad (15)$$

and may be applied to momentum, total energy, internal energy and entropy. An interfacial Clausius-Duhem inequality is then written which first member is a sum of products of terms of zero, one and two tensorial order terms.

INTERFACIAL CONSTITUTIVE RELATIONS

2D closure relations

Then, the two-dimensional surface entropy production Δ_a is such that the surface dissipation

$T_S \Delta_a$ has the symbolic form:

$$T_S \Delta_a = \sum_{\alpha=1}^m \mathcal{A}_S^\alpha \mathcal{J}_S^\alpha \geq 0 \quad (16)$$

Each product corresponds to an irreversible phenomena, and \mathcal{A}_S^α and \mathcal{J}_S^α represent the generalized forces and fluxes.

This result suggests applying the general principles of Irreversible Thermodynamics [30] and writing linear closure relations between generalized forces and fluxes of same tensorial order

$$\mathcal{J}_S^\alpha = \sum_{\beta=1}^m L_S^{\alpha\beta} \mathcal{A}_S^\beta \quad (17)$$

This method is usually applied to classical problems related to capillarity at equilibrium (where $p_{II} - p_I = -\sigma \vec{\nabla} \cdot \vec{\xi}$), or out of equilibrium (where $-\llbracket \vec{T} \rrbracket \cdot \vec{\xi} + \llbracket p \rrbracket \vec{\xi} - \vec{\nabla}_S \sigma + \sigma (\vec{\nabla} \cdot \vec{\xi}) \vec{\xi} = 0$), and it is possible to introduce surface viscosities [28]. Marangoni effect, Bénard-Marangoni instability [31], surface heat transfer, evaporation-condensation, near-equilibrium surface chemical reactions, may be studied with this method. There are important simplifications for interfaces without mass [1]. Coefficients $L_S^{\alpha\beta}$ are generally deduced from molecular theory and experimental measurements. The previous method is no more valid for material surfaces far from equilibrium, but constitutive relations can be found in the literature in specific cases, as for vapor recoil [32, 33, 34], adsorption-desorption, and surface chemical reaction with non-linear kinetics.

3D closure relations

Some situations can not be directly studied using surface equations, and a preliminary study of the interfacial layer behavior is necessary.

This is the case for some wetting problems [35] where fluid layers with capillarity must be considered as 3D interfacial layers, and the second gradient method utilized [1, 2, 6]. For such a fluid inside the interfacial layer and assuming that it is without dissipation

$$\vec{\Sigma} = -p_* \vec{I} - \lambda \vec{\nabla} \rho \vec{\nabla} \rho \quad (18)$$

(In simple cases it is possible to connect surface tension σ to capillarity coefficient λ , writing [6]

$$\sigma = \int_{\xi_1}^{\xi_2} -p_*(\xi) d\xi = \int_{\xi_1}^{\xi_2} \lambda |\vec{\nabla} \rho|^2 d\xi).$$

For some generalized interfaces, as premixed flames with high activation energy [8-11], shock waves and relaxation zones behind shock waves [36, 37], interfacial layer instability between two miscible fluids

[38], interfacial layer instability in a pure heated supercritical fluid [39], some shear layers [40], it is possible to deduce surface properties. But this results from a detailed study of the interfacial layer, which obeys generally to linearized (heat and species diffusion, viscosity) or non-linear (chemical kinetics) classical constitutive relations. For premixed flames with high activation energy, the obtained combustion velocity is a linear function [10] of surface stretch $\vec{\nabla}_S \cdot \vec{W}_S$ as defined by (8), but in strongly turbulent flows the stretch dependence becomes non-linear. In the case of interfacial layer between two miscible fluids, or in the shear layers, the stability analysis shows an influence of the interfacial layer on the growing curve (ω_i in function of k) similar to the one of surface tension on Rayleigh and Kelvin-Helmholtz instability growing curve (Fig. 5). This suggests inserting of an effective surface tension.

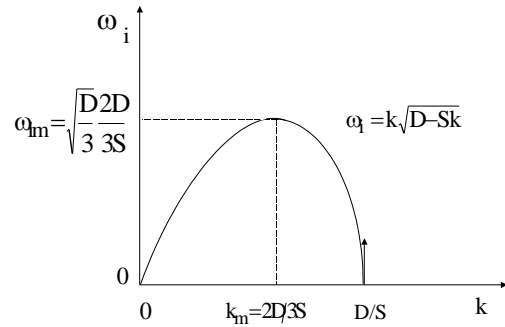


Fig. 5. Amplification factor for two semi infinite superposed fluids, without gravity in inviscid fluids with surface tension: ,

$$S = \frac{\sigma}{\rho_1 + \rho_2} \quad D = \frac{\rho_1 \rho_2 (U_1 - U_2)^2}{(\rho_1 + \rho_2)^2}$$

OTHER RELEVANT QUESTIONS

Interfacial zone appeared as a stratified region. This is a relatively comfortable situation, where the balance equation for area can be directly deduced from interfacial kinematics written in curvilinear coordinates. Indeed, the material derivative of Σ , the density of area per unit volume of the structured layer (see (8)) reads

$$\begin{aligned} \frac{1}{\Sigma} \frac{d \Sigma}{dt} &= \frac{1}{\Sigma} \frac{d \delta S_3}{dt} - \frac{1}{\delta \mathcal{V}} \frac{d \delta \mathcal{V}}{dt} \\ &= \vec{\nabla}_{//} \cdot \vec{W} - \vec{\nabla} \cdot \vec{W} = -\vec{\nabla}_{\perp} \cdot \vec{W} \end{aligned} \quad (19)$$

This equation (in an other form) is utilized by Candel & Poinot [41] for flames. In turbulent burning flows, average quantities are introduced and source terms appear on right-hand side of (19).

An other case is the one of two-phase mixtures. Lhuillier, Morel & Delhay [42] introduce a distribution function δ_I for the interfacial area Σ per unit volume of the mixture. Writing a balance equation for δ_I , a source term γ appears, which vanishes if applied to our simple stratified interfacial layer.

In this paper, interfacial modeling of fluid was presented in such a manner that 2D description result generally from 3D analysis. The 2D description often leads to discontinuities, and it is difficult to solve numerically this type of problem. Then, some authors try to obtain continuous equations even in discontinuous situations. Phase field models have been described for solidification of alloys. The interface is considered as a transition region where averaged local quantities weighted by the liquid and solid volume fractions are introduced. At macroscopic scale, we find an enthalpy method [43] whereas at smaller case, balance equations are deduced by minimization of free energy in functional analysis [44]. Jamet et al. [45] use a second gradient method with an artificially thickened interface, and Jamet and Petitjeans [46] apply phase field models to interfaces of diffusion.

NOMENCLATURE

\mathcal{A}_S^α	interfacial generalized force
\mathcal{J}_S^α	interfacial generalized flux
k	wave number
L_0	hydrodynamic scale
$L_S^{\alpha\beta}$	interfacial phenomenological coefficient
n	normal coordinate at small scale
p_*	interfacial pressure
q	physical parameter
S_3	coordinate surface
t	time
$\bar{\mathbf{T}}$	bulk viscous stress tensor
\mathbf{U}	velocity
$\vec{\mathbf{V}}$	local fluid velocity
$\vec{\mathbf{w}}$	velocity of the surface S_3
x, y, z	Cartesian coordinates
x_1, x_2, x_3	curvilinear coordinates
$\bar{\mathbf{x}}$	position of a point
δ_0	interfacial thickness
ε	small parameter $\varepsilon = \delta_0 / L_0 \ll 1$
ψ	any property per unit mass
ξ	normal coordinate at any scale
$\bar{\xi}$	unit normal to the interface
ρ	fluid density

σ surface tension

$\bar{\Sigma}$ bulk stress tensor

ω_i amplification factor

$[[\varphi]]$ jump $\varphi_{II} - \varphi_I$

Subscripts

1, 2 both sides for superposed fluids

I, II lower and upper limits of an interfacial layer

$,i$ space derivative $\partial/\partial x_i$

//, S parallel to the interface

\perp normal to the interface

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