Correspondenc - "On a Unified Approach to the Study of Transfer Processes"

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On a Unified Approach to the Study of Transfer Processes

In a recent survey of the transport equations, Fulford and Pei (*3*) have presented a general differential equation and listed the special forms that it takes for mass, momentum, and energy transport. The linear constitutive equations are incorporated into the governing equations, and the macroscopic balances are given. The starting point for the presentation by Fulford and Pei may be taken as their governing differential equation for the conservation of some property P in a flowing medium.

$$\underset{(1)}{\frac{\partial P}{\partial t}} = \underset{(2)}{-\left[\frac{\partial}{\partial x}(v_x P) + \frac{\partial}{\partial y}(v_y P) + \frac{\partial}{\partial z}(V_z P)\right]} - \underset{(3)}{\left[\frac{\partial \Pi_x}{\partial x} + \frac{\partial \Pi_y}{\partial y} + \frac{\partial \Pi_z}{\partial z}\right]} - \underset{(4)}{\left[\frac{\partial F}{\partial x} + \frac{\partial F}{\partial y} + \frac{\partial F}{\partial z}\right]} + \underset{(5)}{G} \quad (1)$$

The terms in Equation 1, reading from left to right, were described by Fulford and Pei as follows:

1. Rate of accumulation of P per unit volume
2. Net addition of P per unit volume by convection (bulk flow)
3. Net rate of addition of P per unit volume due to molecular fluxes
4. Rate of generation of P per unit volume *at surfaces*
5. Rate of generation of P per unit volume in the bulk of the system

As a preliminary step to forming the macroscopic balances, Fulford and Pei expressed Equation 1 (their equation 2) in vector form to obtain

$$\frac{\partial P}{\partial t} = -\nabla\cdot(\boldsymbol{v}P) - \nabla\cdot\boldsymbol{\Pi} - \nabla F + G \quad (2)$$

This form was then integrated to yield a macroscopic balance (equation 9 of Fulford and Pei).

In the physical interpretation of the terms in Equation 1 we see a surface source term never before encountered in the development of the transport equations (*1*, pp 74, 76, and 311), and while one is free to assign whatever names one wishes to the various terms in a balance equation, the use of a surface source has led to some conceptual and mathematical difficulties. This is seen quite clearly in Equation 2 where each term, with the exception of ∇F, is a scalar, while the errant surface source term is a vector. Since we require all of our physical laws to be invariant under coordinate rotations, Equation 2 cannot properly describe any real physical phenomena. The error has resulted from treating the surface source term as being independent of the outwardly directed unit normal, while in actual fact one can prove (*6*) that all surface flux or surface source terms for *nonsingular* surfaces are linear vector functions of the outwardly directed unit normal to the surface. Equation 1 also contains the error of not being invariant to coordinate rotations, and in addition has the disturbing feature that it is not equal to Equation 2, for the term ∇F is the gradient of a scalar and is given by (*5*, p 301)

$$\nabla F = \boldsymbol{i}\frac{\partial F}{\partial x} + \boldsymbol{j}\frac{\partial F}{\partial y} + \boldsymbol{k}\frac{\partial F}{\partial z} \quad (3)$$

Here we have found that the very starting point of the survey by Fulford and Pei is in error, and has led to confusion and the publication of an erroneous extension of the incorrect Equation 1. In an effort to interpret the surface sources in terms of interfacial transport rates, Chen (*2*) compounded the error in Equation 1 and suggested that it should be written in the form

$$\frac{\partial P}{\partial t} = \left[\frac{\partial}{\partial x}(v_x P) + \frac{\partial}{\partial y}(v_y P) + \frac{\partial}{\partial z}(v_z P)\right] - \left[\frac{\partial \Pi_x}{\partial x} + \frac{\partial \Pi_y}{\partial y} + \frac{\partial \Pi_z}{\partial z}\right] - \left[\frac{\partial F}{\partial x} + \frac{\partial F}{\partial y} + \frac{\partial F}{\partial z}\right] + G - [\Omega_x + \Omega_y + \Omega_z] \quad (4)$$

where Ω_x was interpreted as

$$\Omega_x = h_x b(T - T^*) \quad (5)$$

for the case of heat transfer. Here h_x is the heat-transfer coefficient in the x-direction, b is the interfacial area per unit volume, and T^* is some characteristic temperature (*1*, Sec. 13.1). The term suggested by Chen represents the sum of the scalar components of a vector and is not invariant under a coordinate rotation. For this reason it cannot adequately represent any real physical phenomena. The appearance of interphase transport terms in a differential equation results from integration of the equation, although this need not be done in a manner which leads to the traditional macroscopic balance.

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The work of Smoot (*4*), referred to by both Chen and Fulford and Pei, represents an intuitive construction of the volume-averaged form of the transport equations for multiphase systems. Derivation of this form of the transport equations is presented elsewhere (*6*), where it is shown that the general transport equation

$$\frac{\partial \psi}{\partial t} + \nabla \cdot (v\psi) = \nabla \cdot \Omega + \sigma \qquad (6)$$

takes the form

$$\epsilon_\alpha(t)\left(\frac{\partial \langle \psi_\alpha \rangle^\alpha}{\partial t}\right) + \langle \psi_\alpha \rangle^\alpha \left(\frac{\partial \epsilon_\alpha}{\partial t}\right) + \nabla \cdot (\epsilon_\alpha \langle v_\alpha \rangle \langle \psi_\alpha \rangle^\alpha) + \nabla \cdot \langle \xi_\alpha \rangle + \frac{1}{V}\int_{A_{\alpha\beta}(t)} \psi_\alpha (v_\alpha - w_\alpha) \cdot n_\alpha dA = \nabla \cdot \langle \Omega_\alpha \rangle + \frac{1}{V}\int_{A_{\alpha\beta}(t)} \Omega_\alpha \cdot n_\alpha dA + \epsilon_\alpha(t) \langle \sigma_\alpha \rangle^\alpha \qquad (7)$$

in a two phase system. In Equation 6, Ω is a tensor of order one greater than ψ and σ, which are both tensors of the same order. A detailed description of the form that Equation 7 takes for linear momentum, angular momentum, total mass, species mass, mechanical energy, and thermal energy is presented elsewhere (*6*).

Nomenclature

$A_{\alpha\beta}(t)$ = interfacial area in the averaging volume for the α and β phases (cm^2)
n = unit outwardly directed normal vector
t = time (sec)
v = mass average velocity vector (cm/sec)
w = velocity of the surface, $A_{\alpha\beta}(t)$ (cm/sec)
x, y, z = rectangular Cartesian coordinates (cm)

Greek Letters

σ = an arbitrary tensor valued function indicating a volume source term (quantity/cm^3-sec)
ϵ = volume fraction
ψ = an arbitrary tensor valued function (quantity/cm^3)
Ω = an arbitrary tensor valued function representing a surface flux (quantity/cm^2-sec)
$\langle \xi \rangle$ = dispersion vector (quantity/cm^2-sec)

Subscripts

α, β = α or β phase

Superscripts

α, β = phase averages in the α or β phases

Other Symbols

$\langle\ \rangle$ = volume average

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Stephen Whitaker

Reply to Comments of Whitaker

As pointed out in Professor Whitaker's very interesting comments on our review, the rate of generation of conserved property at the surfaces of an element, which we have denoted by F, is a difficult term to deal with. In spite of the mathematical problems involved, it has been our experience that the use of such a concept aids in providing a clear physical picture of the transfer processes in general.

In our brief review it was impossible to cover all of the mathematical situations that might arise, and in the derivation of the general conservation equation we treated F as though it were a scalar quantity, since the most frequently encountered form of F is the pressure in the equation of motion; in this way we arrived at the term ∇F in Equation 2 above, and in our equation 13, etc.

In interpreting his equation 2 (our equation 9), Professor Whitaker has considered only the case when P is a scalar quantity. In this case, F is a vector quantity, as is made clear in our Table II for the case of energy transfer, and not a scalar quantity, as assumed above. In this case, the corresponding term in the general equation should strictly be $\nabla \cdot F$—*i.e.*, we are indeed guilty of having omitted the dot in this situation. All the terms in the general equation are then clearly scalars, and should be suitably invariant, etc., and in fact the equation *will* describe real physical phenomena (see, for instance, our equation 3d, which is merely a special form of the general equation).

When P is a vector quantity (momentum transfer), F should be strictly a tensor of order two, in line with the comment after Professor Whitaker's equation 7, and again the term should appear as $\nabla \cdot F$ to give a vector quantity now. However, in the case of momentum transfer, it is only the normal components of the total pressure tensor Π that can be physically comprehended in the term F, which therefore appears to become $F = p$, with p as a scalar quantity. In this case, $\nabla \cdot F$ becomes simply ∇p, the gradient of a scalar quantity. It is still, however, a vector quantity to match the other terms in the generalized Navier-Stokes equation, which we feel sure Professor Whitaker will agree does describe many interesting real phenomena.

To sum up, we feel that the problem is merely one of nomenclature: what was needed was some general way to indicate the operation of ∇ on a quantity which, in different special cases, may be a tensor of order zero, one, or two.

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