Int. J. Heat Mass Transfer. Vol. 36, No. 18, pp. 4317–4325, 1993
Printed in Great Britain

0017-9310/93 $6.00+0.00

Thermal Taylor dispersion in an insulated circular cylinder—I. Theory

R. P. BATYCKY, D. A. EDWARDS and H. BRENNER†

Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139, U.S.A.

(*Received* 5 *January* 1993 *and in final form* 16 *June* 1993)

Abstract—Taylor–Aris dispersion techniques are used in this paper to address a broad class of convective and diffusive internal energy transport phenomena in an externally insulated circular cylinder. Expressions are derived for the mean axial thermal propagation velocity $\bar{U}^*$ and thermal dispersivity $\bar{\alpha}^*$. In general, these quantities may differ respectively from the average fluid velocity $\bar{V}$ and the fluid thermal diffusivity α_f. These generic results apply equally to laminar and turbulent flow systems.

1. INTRODUCTION

CONSIDER fully-developed flow in an insulated circular cylindrical tube of radius R_0, with the fluid manifesting varying thermophysical properties in the cross-section (R, ϕ) of the tube (Fig. 1). It will be assumed that the density $\rho(R, \phi)$, specific heat capacity $c(R, \phi)$ and thermal conductivity $k(R, \phi)$, as well as the axial velocity profile $U(R, \phi)$ are functions, at most, of only R and ϕ; specifically, each is assumed to be independent of the axial coordinate z (and of the time t). Moreover, at each cross-sectional point it will be supposed that the thermal properties are non-negative definite:

$$\{\rho, c, k\} > \{0, 0, 0\} \quad \forall (R, \phi). \tag{1}$$

Piecewise continuity of the phenomenological functions ρ, c, k and U suffices to assure continuity of the temperature and heat flux at all points; we will suppose in the subsequent analysis that the phenomenological data fulfill this piecewise continuity criterion.

Initially, the contents of the tube are at a uniform temperature T_0. At time $t = 0$ an amount of heat Q is instantaneously added to the tube over some portion of the infinite domain,

$$(0 \leqslant R < R_0, 0 \leqslant \phi < 2\pi, -\infty < z < \infty). \tag{2}$$

Subsequent convection and diffusion of this heat is governed by the energy equation,

$$\rho c\left(\frac{\partial T}{\partial t} + U\frac{\partial T}{\partial z}\right) = \frac{1}{R}\frac{\partial}{\partial R}\left(kR\frac{\partial T}{\partial R}\right) + \frac{1}{R^2}\frac{\partial}{\partial \phi}\left(k\frac{\partial T}{\partial \phi}\right) + k\frac{\partial^2 T}{\partial z^2}, \tag{3}$$

governing the temperature distribution $T(R, \phi, z, t)$ in the domain (2). Boundary conditions imposed upon T require that, for all times, it: (i) approach the initial uniform temperature at large axial positions,

$$T \to T_0 \quad \text{as} \quad z \to \pm\infty; \tag{4}$$

(ii) satisfy the condition of adiabaticity at the outer tube wall,

$$\frac{\partial T}{\partial R} = 0 \quad \text{at} \quad R = R_0, \tag{5}$$

corresponding to the tube wall being insulated on its external surface. Additionally, it is required that T be single valued and continuous in the ϕ direction, namely

$$T(\phi + 2\pi) = T(\phi) \quad \forall (R, z, t). \tag{6}$$

Introduction of heat of the amount Q into the system at time $t = 0$ is quantified by specifying an initial temperature distribution, $T(R, \phi, z, 0)$, such that

$$T = T(R, \phi, z, 0) \quad \text{at} \quad t = 0, \tag{7}$$

in which

$$Q \stackrel{\text{def}}{=} \int_{-\infty}^{\infty}\int_0^{2\pi}\int_0^{R_0} \rho(R, \phi)c(R, \phi) \times [T(R, \phi, z, 0) - T_0]R\,\mathrm{d}R\,\mathrm{d}\phi\,\mathrm{d}z, \tag{8}$$

provided that $T(R, \phi, z, 0)$ also satisfies (4).

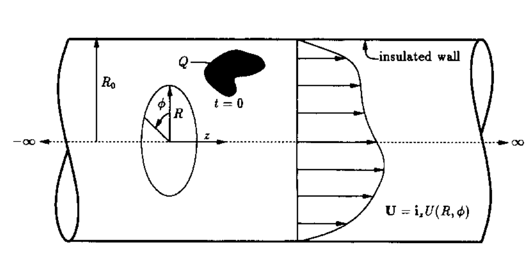

FIG. 1. Fully-developed velocity field **U** in a tube into which are introduced Q units of heat at time $t = 0$ within the indicated domain. Here, (R, ϕ, z) denote a system of circular cylindrical coordinates originating along the tube axis, with $\mathbf{i}_z$ a unit vector in the axial direction.

† Address for correspondence: H. Brenner, MIT, Room 66-562, Cambridge, MA 02139, U.S.A.

NOMENCLATURE

A_0	cross-sectional area of tube, πR_0^2
B	field defined by equations (64)–(66)
$\bar{B}$	average of the B-field
c	specific heat capacity
D	molecular diffusivity
$\bar{D}^*$	dispersivity
exp	denotes terms of exponentially small order in time as $t \to \infty$
$\mathbf{i}_z$	unit vector in the axial direction
J	flux
k	thermal conductivity
$\bar{k}$	mean thermal conductivity
$\bar{k}^*$	macroscale thermal conductivity
M_m	mth total moment of P
$\bar{M}_m$	mth total moment of $\bar{P}$
P	Green's function
P_m	mth local moment of P
Q	amount of heat introduced into the cylinder at time $t = 0$
R	radial coordinate in circular cylindrical coordinate system
R_0	outer radius of the cylinder
t	time
T	temperature
T_0	initial and far-field uniform temperature
$\bar{T}$	average temperature
u	internal energy density
U	velocity in axial direction with which heat convects
$\mathbf{U}$	velocity vector with which heat convects
$\bar{U}$	mean velocity defined in (59)
$\bar{U}^*$	mean thermal propagation velocity
$\bar{V}$	mean fluid velocity
z	axial coordinate in circular cylindrical coordinate system.

Greek symbols

α	molecular thermal diffusivity, $k/\rho c$
$\bar{\alpha}$	mean thermal diffusivity defined in (69)–(76)
$\bar{\alpha}^*$	thermal dispersivity
δ	Dirac delta function
δ_{ij}	Kronecker delta
ϕ	angular coordinate in circular cylindrical coordinate system
ρ	density
$\overline{\rho c}$	mean volumetric specific heat capacity
$\overline{\rho c}^*$	macroscale volumetric specific heat capacity.

Subscript

m	index for local and total moments.

Superscripts

$'$	initial position of impulse
∞	asymptotic form
C	convective contribution
M	molecular contribution.

Integration of (3) over the entire domain (2), together with the use of the boundary and initial conditions (4)–(8) (and the pre-initial condition that $T(R, \phi, z, t) = T_0$ for all $t < 0$) shows that the following integral is a conserved quantity for all time:

$$\int_{-\infty}^{\infty}\int_0^{2\pi}\int_0^{R_0} \rho(R,\phi)c(R,\phi) \times [T(R,\phi,z,t) - T_0]R\,\mathrm{d}R\,\mathrm{d}\phi\,\mathrm{d}z = \begin{cases} 0 & (t < 0), \\ Q & (t \geqslant 0). \end{cases} \quad \text{(9a,b)}$$

Here, the constant Q denotes the quantity defined in (8) in terms of the *initial* temperature distribution at $t = 0$; that is, owing to the adiabaticity, the amount of heat (internal energy) Q originally introduced into the system at $t = 0$ is present in the system for all subsequent times $t \geqslant 0$.

Subject to a posteriori verification via macrotransport theory [1], we speculate that after a sufficiently long time, namely

$$t \gg R_0^2/\|\alpha\| \quad (10)$$

(with $\|\alpha\|$ some norm of the thermal diffusivity, $\alpha = k/\rho c$), that a coarse-grained version of the thermal transport process will obey the macrotransport energy equation,

$$\overline{\rho c}^*\left(\frac{\partial \bar{T}}{\partial t} + \bar{U}^*\frac{\partial \bar{T}}{\partial z}\right) = \bar{k}^*\frac{\partial^2 \bar{T}}{\partial z^2}, \quad (11)$$

where $\bar{U}^*$, $\bar{k}^*$ and $\overline{\rho c}^*$ are time- and position-independent constants, respectively representing appropriate coarse-grained versions of the comparable microtransport quantities U, k and ρc. In the above, $\bar{T}(z, t)$ $(-\infty < z < \infty)$ represents some cross-sectionally-averaged temperature (whose explicit functional dependence on the microtransport temperature field $T(R, \phi, z, t)$ remains to be established; cf. equation (108)). This field is to satisfy the boundary condition,

$$\bar{T} \to T_0 \quad \text{as} \quad z \to \pm\infty \quad (12)$$

(where T_0 is the constant appearing in (4), representing the uniform initial temperature prevailing for $t < 0$), together with the initial condition

$$\overline{\rho c}^*\int_{-\infty}^{\infty} [\bar{T}(z,0) - T_0]\,\mathrm{d}z = Q, \quad (13)$$

where Q is the constant defined in (8) in terms of the initial microtransport temperature field $T(R, \phi, z, 0)$.

The system of equations (11)–(13) combine to show that heat is conserved at the macroscale in the sense that

$$\overline{\rho c}^* \int_{-\infty}^{\infty} [\bar{T}(z,t) - T_0]\, dz = \begin{cases} 0 & (t < 0), \\ Q & (t \geq 0), \end{cases} \qquad (14a,b)$$

analogous to the comparable microscale condition (9a,b).

2. GREEN'S FUNCTION FORMULATION

Analogous to the case of species dispersion [1], it will prove useful to reformulate the microscale problem (3)–(7) in terms of a Green's function [2, §8]. Define a quantity P (whose argument is as indicated below) as the kernel appearing in the following integrand:

$$T(R,\phi,z,t) - T_0 = \int_{-\infty}^{\infty}\int_0^{2\pi}\int_0^{R_0} \rho(R',\phi')c(R',\phi') \times P(R,\phi,z,t\,|\,R',\phi',z')[T(R',\phi',z',0) - T_0] \times R'\,dR'\,d\phi'\,dz'. \qquad (15)$$

By analogy to the comparable Green's function superposition case for the material transport of a Brownian tracer particle (a '*Brownion*'), the quantity $\rho'c'$ $P(R,\phi,z,t\,|\,R',\phi',z')$ appearing in the above integrand may be regarded as representing the 'conditional probability density' of finding a thermal tracer (a '*thermion*') at position (R,ϕ,z) at time t given that the thermion was originally introduced into the system at position (R',ϕ',z') at time $t = 0$. Observe upon setting $t = 0$ in (15) that P is required to satisfy the initial impulsive heat-input condition,

$$\rho(R,\phi)c(R,\phi)P(R,\phi,z,0\,|\,R',\phi',z') = \frac{1}{R}\delta(R-R')\delta(\phi-\phi')\delta(z-z'), \qquad (16)$$

where δ denotes a Dirac delta function of the indicated argument. This corresponds to a *unit* heat input (cf. (30a,b)).

The microtransport equation (3) may be regarded as being of the operational form

$$\mathscr{L}T = 0, \qquad (17)$$

where $\mathscr{L}$ is the linear operator

$$\mathscr{L} \overset{\text{def}}{=} \rho c\left(\frac{\partial}{\partial t} + U\frac{\partial}{\partial z}\right) - \left[\frac{1}{R}\frac{\partial}{\partial R}\left(kR\frac{\partial}{\partial R}\right) + \frac{1}{R^2}\frac{\partial}{\partial \phi}\left(k\frac{\partial}{\partial \phi}\right) + k\frac{\partial^2}{\partial z^2}\right]. \qquad (18)$$

Apply this operator to (15), and recognize that this (R, ϕ, z)-space operator commutes with integration over the primed variables (R', ϕ', z'). Thus, upon incorporating the initial condition (16) explicitly into the formulation, we obtain the following differential equation governing P:

$$\mathscr{L}P = \frac{1}{R}\delta(R-R')\delta(\phi-\phi')\delta(z-z')\delta(t). \qquad (19)$$

The metrical nature of this equation is such that P—rather then depending upon (z, z') and (ϕ, ϕ') separately—necessarily depends only upon the linear combination of variables $z - z'$ and $\phi - \phi'$, respectively. Thus, we may write

$$P \equiv P(R,\phi,z,t\,|\,R',\phi',z') \qquad (20)$$

$$\equiv P(R,\phi-\phi',z-z',t\,|\,R'). \qquad (21)$$

As the respective choice of origins (namely $\phi = 0$ and $z = 0$) from which ϕ and z are to be measured is arbitrary, no loss of generality arises from arbitrarily choosing

$$\phi' = 0, \qquad (22)$$

$$z' = 0. \qquad (23)$$

This choice corresponds to the initial introduction of a unit heat impulse at the point whose circular cylindrical coordinates are $(R', 0, 0)$.

In place of (19) one may thus write, explicitly,

$$\rho c\left(\frac{\partial P}{\partial t} + U\frac{\partial P}{\partial z}\right) = \frac{1}{R}\frac{\partial}{\partial R}\left(kR\frac{\partial P}{\partial R}\right) + \frac{1}{R^2}\frac{\partial}{\partial \phi}\left(k\frac{\partial P}{\partial \phi}\right) + k\frac{\partial^2 P}{\partial z^2} + \frac{1}{R}\delta(R-R')\delta(\phi)\delta(z)\delta(t), \qquad (24)$$

with $P \equiv P(R, \phi, z, t\,|\,R')$. Conditions (4)–(7) require that,

$$|z|^m\left\{P, \frac{\partial P}{\partial z}\right\} \to \{0, 0\} \quad \text{as} \quad z \to \pm\infty \quad (m = 0, 1, 2, \ldots), \qquad (25a,b)$$

$$\frac{\partial P}{\partial R} = 0 \quad \text{at} \quad R = R_0, \qquad (26)$$

$$P(\phi + 2\pi) = P(\phi) \quad \forall\,(R, z, t) \qquad (27)$$

and

$$P = 0 \quad \forall\,(t < 0). \qquad (28)$$

Conditions (25a,b) are stricter than their temperature counterparts (4). They require that P tend to zero at infinity faster than geometrically (i.e. exponentially rapidly), in order that subsequent moments of P converge (cf. (31)).

Physically, the system of equations (24)–(28) is such that $P(R, \phi, z, t\,|\,R')$ represents the temperature at the point (R, ϕ, z) at time t arising from the introduction of a unit amount of heat (cf. (30a,b)) at the point $(R', 0, 0)$ at time $t = 0$ into the insulated system which is initially at zero temperature everywhere.

Integration of (24) over the entire domain (2), together with use of the boundary conditions yields

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{-\infty}^{\infty}\int_0^{2\pi}\int_0^{R_0}\rho c P R\,\mathrm{d}R\,\mathrm{d}\phi\,\mathrm{d}z = \delta(t). \tag{29}$$

In turn, since the Dirac delta function is the derivative of the Heavyside unit step function [2, §8.3.4], integration of the latter yields

$$\int_{-\infty}^{\infty}\int_0^{2\pi}\int_0^{R_0}\rho c P R\,\mathrm{d}R\,\mathrm{d}\phi\,\mathrm{d}z = \begin{cases} 0 & (t<0), \\ 1 & (t \geqslant 0). \end{cases} \tag{30a,b}$$

Thus, the quantity (whose volumetric density is) $\rho c P$ is conserved for all time. Coupled with the (implicitly assumed) nonnegative nature of P in conjunction with the unitary value of the integral in (30a,b), this shows that the quantity $\rho c P$ may be thought of as being the probability density† for the thermion.

3. MOMENTS OF THE PROBABILITY DENSITY

3.1. *Local moments*

Define the local moments of P as

$$P_m(R,\phi,t\,|\,R') \stackrel{\text{def}}{=} \int_{-\infty}^{\infty} z^m P(R,\phi,z,t\,|\,R')\,\mathrm{d}z \qquad (m = 0,1,2,\ldots). \tag{31}$$

Differentiation with respect to t gives

$$\frac{\partial P_m}{\partial t} = \int_{-\infty}^{\infty} z^m \frac{\partial P}{\partial t}\,\mathrm{d}z. \tag{32}$$

Direct substitution of (24) into the integrand of the above gives the intermediate result

$$\begin{aligned}\rho c\frac{\partial P_m}{\partial t} &= \frac{1}{R}\frac{\partial}{\partial R}\left(kR\frac{\partial}{\partial R}\int_{-\infty}^{\infty} z^m P\,\mathrm{d}z\right) \\ &+ \frac{1}{R^2}\frac{\partial}{\partial\phi}\left(k\frac{\partial}{\partial\phi}\int_{-\infty}^{\infty} z^m P\,\mathrm{d}z\right) \\ &- \rho c U\int_{-\infty}^{\infty} z^m\frac{\partial P}{\partial z}\,\mathrm{d}z + k\int_{-\infty}^{\infty} z^m \frac{\partial^2 P}{\partial z^2}\,\mathrm{d}z \\ &+ \frac{1}{R}\delta_{m0}\delta(R-R')\delta(\phi)\delta(t),\end{aligned} \tag{33}$$

with δ_{m0} the Kronecker delta. This can be simplified by using the definition (31) while noting that integration by parts yields

$$\int_{-\infty}^{\infty} z^m\frac{\partial P}{\partial z}\,\mathrm{d}z = [z^m P]_{-\infty}^{\infty} - m\int_{-\infty}^{\infty} z^{m-1}P\,\mathrm{d}z = -mP_{m-1} \tag{34}$$

as well as

$$\begin{aligned}\int_{-\infty}^{\infty} z^m\frac{\partial^2 P}{\partial z^2}\,\mathrm{d}z &= \left[z^m\frac{\partial P}{\partial z}\right]_{-\infty}^{\infty} - m[z^{m-1}P]_{-\infty}^{\infty} \\ &+ m(m-1)\int_{-\infty}^{\infty} z^{m-2}P\,\mathrm{d}z = m(m-1)P_{m-2}.\end{aligned} \tag{35}$$

Hence, $P_m(R,\phi,t\,|\,R')$ satisfies the partial differential-recurrence equation

$$\begin{aligned}\rho c\frac{\partial P_m}{\partial t} &= \frac{1}{R}\frac{\partial}{\partial R}\left(kR\frac{\partial P_m}{\partial R}\right) + \frac{1}{R^2}\frac{\partial}{\partial\phi}\left(k\frac{\partial P_m}{\partial\phi}\right) \\ &+ \rho c U m P_{m-1} + km(m-1)P_{m-2} \\ &+ \frac{1}{R}\delta_{m0}\delta(R-R')\delta(\phi)\delta(t)\end{aligned} \tag{36}$$

in the cross-sectional domain (R,ϕ), together with the pre-initial condition

$$P_m = 0 \quad \forall\,(t<0). \tag{37}$$

Additionally, P_m satisfies the respective boundary and continuity conditions,

$$\frac{\partial P_m}{\partial R} = 0 \quad \text{at} \quad R = R_0 \tag{38}$$

and

$$P_m(\phi+2\pi) = P_m(\phi) \quad \forall\,(R,t). \tag{39}$$

3.2. *Total moments*

Define the total moments M_m of P as the following *weighted* average of the local moments P_m:

$$M_m(t\,|\,R') \stackrel{\text{def}}{=} \int_0^{2\pi}\int_0^{R_0}\rho c P_m(R,\phi,t\,|\,R')R\,\mathrm{d}R\,\mathrm{d}\phi \qquad (m = 0,1,2,\ldots). \tag{40}$$

Differentiation with respect to t gives

$$\frac{\mathrm{d}M_m}{\mathrm{d}t} = \int_0^{2\pi}\int_0^{R_0}\rho c\frac{\partial P_m}{\partial t}R\,\mathrm{d}R\,\mathrm{d}\phi. \tag{41}$$

In conjunction with (36)–(39) this yields

$$\begin{aligned}\frac{\mathrm{d}M_m}{\mathrm{d}t} &= m\int_0^{2\pi}\int_0^{R_0}\rho c U P_{m-1}R\,\mathrm{d}R\,\mathrm{d}\phi \\ &+ m(m-1)\int_0^{2\pi}\int_0^{R_0} kP_{m-2}R\,\mathrm{d}R\,\mathrm{d}\phi + \delta_{m0}\delta(t).\end{aligned} \tag{42}$$

Observe that this formulation for M_m is expressed entirely in terms of lower-order local moments P_{m-1} and P_{m-2}, rather than in terms of P_m itself, as originally in (40). Hence, information about the temporal behavior of M_m can be established without comparable knowledge of P_m itself.

† Namely the conditional probability density for finding the thermion at time t somewhere within the infinite domain (2) defining the system, given its initial introduction into the system at $(R', 0, 0)$ at time $t = 0$.

$m = 0$

Upon setting $m = 0$ in (42) we obtain

$$\frac{dM_0}{dt} = \delta(t). \tag{43}$$

Consequently,

$$M_0 = \begin{cases} 0 & (t < 0), \\ 1 & (t \geqslant 0). \end{cases} \tag{44a,b}$$

Set $m = 0$ in (36)–(39) to obtain the following system of equations governing the zero-order local moment P_0:

$$\rho c \frac{\partial P_0}{\partial t} = \frac{1}{R}\frac{\partial}{\partial R}\left(kR\frac{\partial P_0}{\partial R}\right) + \frac{1}{R^2}\frac{\partial}{\partial \phi}\left(k\frac{\partial P_0}{\partial \phi}\right) + \frac{1}{R}\delta(R-R')\delta(\phi)\delta(t), \tag{45}$$

$$P_0 = 0 \quad \forall\,(t < 0), \tag{46}$$

$$\frac{\partial P_0}{\partial R} = 0 \quad \text{at} \quad R = R_0, \tag{47}$$

$$P_0(\phi+2\pi) = P_0(\phi) \quad \forall\,(R). \tag{48}$$

These equations possess no convective contribution.

It can be shown [3, 4] that for sufficiently long times defined by (10), $P_0(R, \phi, t|R')$ possesses the steady-state solution $P_0^\infty \equiv P_0^\infty(R, \phi)$, such that, asymptotically,

$$P_0(R, \phi, t|R') \simeq P_0^\infty(R, \phi) + \exp, \tag{49}$$

where 'exp' denotes terms in R, ϕ, R' and t that are exponentially attenuated in time. The *steady-state* solution P_0^∞ is independent of R', as indicated by its argument. Upon substituting (49) into the preceding set of equations governing P_0, it is found that P_0^∞ constitutes the solution of the following boundary-value problem:

$$\frac{1}{R}\frac{\partial}{\partial R}\left(kR\frac{\partial P_0^\infty}{\partial R}\right) + \frac{1}{R^2}\frac{\partial}{\partial \phi}\left(k\frac{\partial P_0^\infty}{\partial \phi}\right) = 0, \tag{50}$$

$$\frac{\partial P_0^\infty}{\partial R} = 0 \quad \text{at} \quad R = R_0, \tag{51}$$

$$P_0^\infty(\phi+2\pi) = P_0^\infty(\phi) \quad \forall\,(R). \tag{52}$$

These possess the uniform solution

$$P_0^\infty = \text{const.}, \tag{53}$$

independent of R and ϕ. The numerical value of this constant can be obtained from the definition (40) of M_0 together with (44a,b) and (49), which combine to show that

$$\int_0^{2\pi}\int_0^{R_0} \rho c P_0^\infty R\, dR\, d\phi = 1. \tag{54}$$

Consequently,

$$P_0^\infty = \frac{1}{A_0\overline{\rho c}}, \tag{55}$$

where we have defined the constant

$$\overline{\rho c} \stackrel{\text{def}}{=} \frac{1}{A_0}\int_0^{2\pi}\int_0^{R_0} \rho c R\, dR\, d\phi, \tag{56}$$

in which

$$A_0 \equiv \pi R_0^2 \tag{57}$$

is the cross-sectional area of the tube.

$m = 1$

Set $m = 1$ in (42) and introduce the asymptotic expression (49) and (55) so as to obtain

$$\frac{dM_1}{dt} \simeq \bar{U} + \exp, \tag{58}$$

wherein $\bar{U}$ is the constant

$$\bar{U} \stackrel{\text{def}}{=} \frac{1}{A_0\overline{\rho c}}\int_0^{2\pi}\int_0^{R_0} \rho c U R\, dR\, d\phi. \tag{59}$$

Integration of (58) yields

$$M_1 \simeq \bar{U}t + \bar{B} + \exp, \tag{60}$$

where $\bar{B}$ is a constant of integration.

From (40) we have by definition that

$$M_1 = \int_0^{2\pi}\int_0^{R_0} \rho c P_1 R\, dR\, d\phi. \tag{61}$$

As a result of the temporal behavior displayed by (60), the latter suggests (subject to a posteriori verification) the following asymptotic trial solution for P_1:

$$P_1(R, \phi, t|R') \simeq P_0^\infty[\bar{U}t + B(r, \phi)] + \exp, \tag{62}$$

with P_0^∞ given by (55). Introduction of the latter into (61), together with use of the normalization condition (54), shows upon comparison of the result with (60) and use of (55) that the constant $\bar{B}$ is given by the expression

$$\bar{B} = \frac{1}{A_0\overline{\rho c}}\int_0^{2\pi}\int_0^{R_0} \rho c B R\, dR\, d\phi. \tag{63}$$

To derive the equations governing the B-field, set $m = 1$ in (36)–(39) and use (62) to obtain

$$-\frac{1}{R}\frac{\partial}{\partial R}\left(kR\frac{\partial B}{\partial R}\right) - \frac{1}{R^2}\frac{\partial}{\partial \phi}\left(k\frac{\partial B}{\partial \phi}\right) = \rho c(U - \bar{U}), \tag{64}$$

$$\frac{\partial B}{\partial R} = 0 \quad \text{at} \quad R = R_0, \tag{65}$$

$$B(\phi+2\pi) = B(\phi) \quad \forall\,(R), \tag{66}$$

with $B(R, \phi)$ uniquely determined only to within an arbitrary additive constant. As in the comparable material transport case [1], this lack of uniqueness is without physical consequence.

$m = 2$

Put $m = 2$ in (42) and use the asymptotic expansions (49) and (62) to obtain

$$\frac{dM_2}{dt} \simeq 2\bar{U}tP_0^\infty \int_0^{2\pi}\int_0^{R_0} \rho c U R\,dR\,d\phi$$

$$+2\bar{U}P_0^\infty \int_0^{2\pi}\int_0^{R_0} \rho c B R\,dR\,d\phi$$

$$+2P_0^\infty \int_0^{2\pi}\int_0^{R_0} kR\,dR\,d\phi$$

$$+2P_0^\infty \int_0^{2\pi}\int_0^{R_0} \rho c(U-\bar{U})BR\,dR\,d\phi + \text{exp.} \quad (67)$$

With use of (55) together with (59) and (63), respectively, the first integral is $\bar{U}/P_0^\infty$, whereas the second is $\bar{B}/P_0^\infty$. Hence, we obtain,

$$\frac{dM_2}{dt} \simeq 2\bar{U}^2 t + 2\bar{U}\bar{B} + 2\bar{\alpha} + \text{exp}, \quad (68)$$

where we have defined the constant

$$\bar{\alpha} \stackrel{\text{def}}{=} \bar{\alpha}^M + \bar{\alpha}^C, \quad (69)$$

in which

$$\bar{\alpha}^M \stackrel{\text{def}}{=} \frac{\bar{k}^M}{\overline{\rho c}}, \quad (70)$$

$$\bar{\alpha}^C \stackrel{\text{def}}{=} \frac{\bar{k}^C}{\overline{\rho c}}, \quad (71)$$

wherein $\bar{k}^M$ and $\bar{k}^C$ are the respective constants

$$\bar{k}^M \stackrel{\text{def}}{=} \frac{1}{A_0} \int_0^{2\pi}\int_0^{R_0} kR\,dR\,d\phi \quad (72)$$

and

$$\bar{k}^C \stackrel{\text{def}}{=} \frac{1}{A_0} \int_0^{2\pi}\int_0^{R_0} \rho c(U-\bar{U})BR\,dR\,d\phi. \quad (73)$$

An alternative expression for $\bar{k}^C$ may be derived as follows. Multiply (64) by B to obtain

$$-\frac{B}{R}\frac{\partial}{\partial R}\left(kR\frac{\partial B}{\partial R}\right) - \frac{B}{R^2}\frac{\partial}{\partial \phi}\left(k\frac{\partial B}{\partial \phi}\right) = \rho c(U-\bar{U})B, \quad (74)$$

the right-hand side of the latter identity being exactly the term appearing in the integrand of (73). By identity,

$$\frac{B}{R}\frac{\partial}{\partial R}\left(kR\frac{\partial B}{\partial R}\right) = \frac{1}{R}\frac{\partial}{\partial R}\left(BkR\frac{\partial B}{\partial R}\right) + k\left(\frac{\partial B}{\partial R}\right)^2$$

and

$$\frac{B}{R^2}\frac{\partial}{\partial \phi}\left(k\frac{\partial B}{\partial \phi}\right) = \frac{1}{R^2}\frac{\partial}{\partial \phi}\left(Bk\frac{\partial B}{\partial \phi}\right) + \frac{k}{R^2}\left(\frac{\partial B}{\partial \phi}\right)^2,$$

whence the following expression for $\bar{k}^C$ derives from (73):

$$A_0\bar{k}^C = \int_0^{2\pi}\int_0^{R_0} k\left[\left(\frac{\partial B}{\partial R}\right)^2 + \frac{1}{R^2}\left(\frac{\partial B}{\partial \phi}\right)^2\right] R\,dR\,d\phi$$
$$-\int_0^{2\pi} d\phi \left[BkR\frac{\partial B}{\partial R}\right]_0^{R_0} - \int_0^{R_0} R\,dR\frac{1}{R^2}\left[Bk\frac{\partial B}{\partial \phi}\right]_0^{2\pi}. \quad (75)$$

The last two terms are identically zero as a consequence of (65) and (66); thus,

$$\bar{k}^C \equiv \frac{1}{A_0}\int_0^{2\pi}\int_0^{R_0} k\left[\left(\frac{\partial B}{\partial R}\right)^2 + \frac{1}{R^2}\left(\frac{\partial B}{\partial \phi}\right)^2\right] R\,dR\,d\phi, \quad (76)$$

in which form the velocity field U does not appear explicitly, in contrast with the alternative formulation (73).

Observe that since, by assumption, $k > 0$ (cf. (1)), equations (72) and (76) show $\bar{k}^M$ and $\bar{k}^C$ to be non-negative, whence

$$\bar{k}^M > 0, \quad (77)$$

$$\bar{k}^C \geqslant 0. \quad (78)$$

From (76), the equality sign in the latter applies if and only if $B =$ constant for all (R, ϕ). As may be seen from the resulting *homogeneous* system of equations (64)–(66) defining the B-field this, in turn, occurs if and only if the velocity field U is spatially constant (i.e. identically zero) at all points (R, ϕ) in the cross-sectional domain. Use of (1) thereby shows that

$$\bar{\alpha}^M > 0, \quad (79)$$

$$\bar{\alpha}^C \geqslant 0, \quad (80)$$

where equality holds in the latter only when $U = 0$ everywhere in (R, ϕ). Hence, in (69),

$$\bar{\alpha} > 0. \quad (81)$$

4. MACROSCOPIC FORMULATION

Our ultimate goal is to demonstrate the applicability of the macrotransport description embodied in equations (11)–(14a,b) of the cross-sectionally averaged thermal transport process, as well as to obtain explicit expressions for the three macroscale thermophysical properties $\bar{U}^*$, $\overline{\rho c}^*$ and $\bar{k}^*$ appearing in (11) in terms of the prescribed microscale data $\rho(R,\phi)$, $c(R,\phi)$, $k(R,\phi)$, $U(R,\phi)$ and the system geometry, e.g. the radius R_0. Moreover, we wish to operationally relate the macroscale temperature field $\bar{T}$ to the microscale temperature field T. To this end, define a macroscale Green's function $\bar{P}$ as

$$\bar{P}(z,t|R') \stackrel{\text{def}}{=} \frac{1}{\overline{\rho c}^*}\int_0^{2\pi}\int_0^{R_0} \rho(R,\phi)c(R,\phi) \times P(R,\phi,z,t|R')R\,dR\,d\phi, \quad (82)$$

where the constant $\overline{\rho c}^*$ remains to be determined. Differentiate the above equation with respect to time, substitute from (24), and use the boundary conditions (25a,b) to (27). This yields

$$\overline{\rho c}^* \frac{\partial \bar{P}}{\partial t} + \frac{\partial \bar{J}}{\partial z} = \delta(z)\delta(t), \tag{83}$$

$$\bar{J} \overset{\text{def}}{=} \int_0^{2\pi} \int_0^{R_0} \left(\rho c U P - k \frac{\partial P}{\partial z} \right) R \, \mathrm{d}R \, \mathrm{d}\phi, \tag{84}$$

$$|z|^m \left\{ \bar{P}, \frac{\partial \bar{P}}{\partial z} \right\} \to \{0, 0\} \quad \text{as} \quad z \to \pm\infty \qquad (m = 0, 1, 2, \ldots). \tag{85}$$

As a consequence of its definition (82), $\bar{P}$ appearing in (83) depends upon the initial lateral position R' at which the thermion was originally introduced; however, for sufficiently long times, given by (10) (whereby the thermion has had a chance to sample all points in the tube cross section many times over), $\bar{P}$ will asymptotically become independent of R', and hence be of the asymptotic form

$$\bar{P} \approx \bar{P}(z, t), \tag{86}$$

independent of R'.†

Subject to a posteriori verification via a moment-matching scheme [1], we assume—albeit asymptotically for

$$\bar{\alpha} t / R_0^2 \gg 1 \tag{87}$$

—that $\bar{J}$ can be expressed in the macroscale convective–diffusive constitutive form

$$\bar{J} \approx \overline{\rho c}^* \bar{U}^* \bar{P} - \bar{k}^* \frac{\partial \bar{P}}{\partial z}, \tag{88}$$

where $\overline{\rho c}^*$, $\bar{U}^*$ and $\bar{k}^*$ are constants to be determined.‡ Together with (83) this yields the so-called *model* thermal macrotransport equation

$$\overline{\rho c}^* \left(\frac{\partial \bar{P}}{\partial t} + \bar{U}^* \frac{\partial \bar{P}}{\partial z} \right) = \bar{k}^* \frac{\partial^2 \bar{P}}{\partial z^2} + \delta(z)\delta(t) \quad (t \geqslant 0) \tag{89}$$

and, from (82) and (28),

$$\bar{P} = 0 \quad (t < 0). \tag{90}$$

Define the total moments $\bar{M}_m$ of the solution $\bar{P}$ of the above model equation as

$$\bar{M}_m(t) \overset{\text{def}}{=} \overline{\rho c}^* \int_{-\infty}^{\infty} z^m \bar{P}(z, t) \, \mathrm{d}z \quad (m = 0, 1, 2, \ldots). \tag{91}$$

The goal is to asymptotically match these total moments of $\bar{P}$ with the corresponding total moments M_m (40) of P:

$$\bar{M}_m(t) \simeq M_m(t) + \exp \quad \text{as} \quad t \to \infty. \tag{92}$$

That this matching proves possible to dominant terms in t, ultimately furnishes a posteriori verification of the constitutive equation (88) and, concomitantly, the macrotransport equation (89), as well as also furnishing formulas explicitly expressing $\bar{U}^*$, $\overline{\rho c}^*$ and $\bar{k}^*$ in terms of the comparable inhomogeneous microscale data, namely U, ρc and k.

Differentiate (91) with respect to time, use the model equation (89) for $\partial \bar{P}/\partial t$, and make use of boundary conditions (85) to obtain the following recurrence equation for the macroscale moments:

$$\frac{\mathrm{d}\bar{M}_m}{\mathrm{d}t} = m\bar{U}^* \bar{M}_{m-1} + \frac{\bar{k}^*}{\overline{\rho c}^*} m(m-1) \bar{M}_{m-2} + \delta_{m0}\delta(t). \tag{93}$$

$m = 0$

Setting $m = 0$ in (93) gives

$$\frac{\mathrm{d}\bar{M}_0}{\mathrm{d}t} = \delta(t). \tag{94}$$

Hence, upon integration,

$$\bar{M}_0 = \begin{cases} 0 & (t < 0), \\ 1 & (t \geqslant 0). \end{cases} \tag{95a,b}$$

Comparison with (44a,b) gives,

$$\bar{M}_0 = M_0 \quad \forall\, t, \tag{96}$$

exactly!

$m = 1$

Set $m = 1$ in (93) to obtain

$$\frac{\mathrm{d}\bar{M}_1}{\mathrm{d}t} = \bar{U}^* \bar{M}_0 \equiv \bar{U}^*. \tag{97}$$

Integration yields

$$\bar{M}_1 = \bar{U}^* t + C, \tag{98}$$

where C is a constant of integration. Comparison with (60) in the light of the requisite matching condition (92) thereby yields

$$\bar{U}^* = \bar{U} \tag{99}$$

and

$$C = \bar{B}. \tag{100}$$

Hence, from (59),

† In terms of primed variables this asymptotic behavior can be explicitly expressed as

$$\bar{P}(z, t \mid R', \phi', z') \simeq \bar{P}(z, t \mid z') \quad \text{as} \quad t \to \infty.$$

‡ Here, we are anticipating that the constant $\overline{\rho c}^*$ appearing here will be the same as that appearing in (82).

$$\bar{U}^* = \frac{1}{A_0 \overline{\rho c}} \int_0^{2\pi} \int_0^{R_0} \rho c U R \, \mathrm{d}R \, \mathrm{d}\phi. \quad (101)$$

$m = 2$

Set $m = 2$ in (93) to obtain

$$\frac{\mathrm{d}\bar{M}_2}{\mathrm{d}t} = 2\bar{U}^* \bar{M}_1 + \frac{\bar{k}^*}{\overline{\rho c}^*} 2\bar{M}_0$$

$$= 2\bar{U}^{*2} t + 2\bar{U}^* C + 2\frac{\bar{k}^*}{\overline{\rho c}^*}. \quad (102)$$

Comparison with (68) in the limit $t \to \infty$, together with use of (99) and (100), thereby yields

$$\frac{\bar{k}^*}{\overline{\rho c}^*} = \bar{\alpha}, \quad (103)$$

where $\bar{\alpha}$ is defined in (69) *et seq.*

4.1. *Relationship between $\bar{T}$ and T*

We wish to establish a relationship between an appropriately defined, transversely coarse-grained macroscale temperature field $\bar{T}(z, t)$ and its microscale precursor $T(R, \phi, z, t)$. For reasons that will subsequently become clear, it is convenient to define a quantity $\bar{T}$ by the expression (cf. (15) and (82))

$$\bar{T}(z,t) - T_0 = \frac{1}{A_0} \int_{-\infty}^{\infty} \int_0^{2\pi} \int_0^{R_0} \rho(R', \phi') c(R', \phi')$$

$$\times \bar{P}(z, t \,|\, R', \phi', z')[T(R', \phi', z', 0)$$

$$- T_0] R' \, \mathrm{d}R' \, \mathrm{d}\phi' \, \mathrm{d}z', \quad (104)$$

where the explicit dependence of $\bar{P}$ upon ϕ' and z' has been restored. Now, multiply (89) by the integrand of (104) sans the $\bar{P}$ term, integrate the resulting equation over (R', ϕ', z'), and note that the latter integration commutes with the requisite differentiations over z space. Equation (104) thereby yields

$$\overline{\rho c}^* \left(\frac{\partial \bar{T}}{\partial t} + \bar{U}^* \frac{\partial \bar{T}}{\partial z} \right) = \bar{k}^* \frac{\partial^2 \bar{T}}{\partial z^2}, \quad (105)$$

subject to the requirement that $\bar{T}$ appearing therein satisfies the initial condition

$$\bar{T}(z,0) - T_0 = \frac{1}{A_0 \overline{\rho c}^*} \int_0^{2\pi} \int_0^{R_0} \rho(R', \phi') c(R', \phi')$$

$$\times [T(R', \phi', z, 0) - T_0] R' \, \mathrm{d}R' \, \mathrm{d}\phi'. \quad (106)$$

As $\bar{P}$ satisfies (85a), we find from (104) that

$$\bar{T} \to T_0 \quad \text{as} \quad |z| \to \infty. \quad (107)$$

Furthermore, it follows directly from (15), (82) and (104) that the macroscale quantity $\bar{T}$ may be explicitly expressed in terms of its microscale precursor T as

$$\bar{T}(z,t) - T_0 = \frac{1}{A_0 \overline{\rho c}^*} \int_0^{2\pi} \int_0^{R_0} \rho(R, \phi) c(R, \phi)$$

$$\times [T(R, \phi, z, t) - T_0] R \, \mathrm{d}R \, \mathrm{d}\phi. \quad (108)$$

Finally, since we wish $\bar{T}$ appearing in the macrotransport equation (105) to represent the mean temperature based upon internal energy considerations, we choose

$$\overline{\rho c}^* = \overline{\rho c}; \quad (109)$$

moreover, upon using (69)–(71) together with (103), we have in equation (105) that

$$\bar{k}^* = \bar{k}^{\mathrm{M}} + \bar{k}^{\mathrm{C}}, \quad (110)$$

where $\bar{k}^{\mathrm{M}}$ and $\bar{k}^{\mathrm{C}}$ are defined in terms of the microscale data by (72) and either (73) or (76).

4.2. *Discussion*

Perhaps the only surprising feature of the preceding analysis is that, according to (103) (upon suppressing the asterisk superscripts), $\bar{\alpha} = \bar{k}/\overline{\rho c}$ rather than $\overline{k/\rho c}$; that is, the Taylor dispersion analysis clearly identifies the ratio of the averages rather than the average of the ratio as being the important thermophysical parameter characterizing the macroscale system. The origin of this fact can ultimately be traced to the circumstance that the conserved entity being transported is actually the internal energy u rather than the temperature T, these being related at the micro- and macroscales by the respective relations $\mathrm{d}u = \rho c \, \mathrm{d}T$ and $\mathrm{d}\bar{u} = \overline{\rho c} \, \mathrm{d}\bar{T}$. Thus, given the defining macroscale constitutive equations for the respective internal energy and thermal fluxes $\Delta \bar{J}$ relative to $\bar{U}^*$, namely $\Delta \bar{J} = -\bar{\alpha} \partial \bar{u}/\partial z$ and $\Delta \bar{J} = -\bar{k} \partial \bar{T}/\partial z$ serving to respectively define the macroscale thermophysical parameters $\bar{\alpha}$ and $\bar{k}$, it naturally arises that $\bar{\alpha} = \bar{k}/\overline{\rho c}$ rather than $\overline{k/\rho c}$.

5. SUMMARY

For any prescribed initial temperature distribution $\bar{T}(z, 0)$ (satisfying (112) below), the adiabatic mean axial dispersion of internal energy within a circular cylindrical tube of radius R_0 through which a fluid flows may be modeled by the thermal macrotransport equation,

$$\frac{\partial \bar{T}}{\partial t} + \bar{U}^* \frac{\partial \bar{T}}{\partial z} = \bar{\alpha}^* \frac{\partial^2 \bar{T}}{\partial z^2}, \quad (111)$$

$$\bar{T}(z, t) \to T_0 = \text{const.} \quad \text{as} \quad z \to \pm\infty \quad \forall t. \quad (112)$$

In these equations, the constant macrotransport parameters $\bar{U}^*$ and $\bar{\alpha}^*$ are related to the comparable microscale velocity and thermal data U, ρ, c and k—each generally functions of (R, ϕ)—by the expressions

$$\bar{U}^* = \frac{1}{\pi R_0^2 \overline{\rho c}^*} \int_0^{2\pi} \int_0^{R_0} \rho c U R \, \mathrm{d}R \, \mathrm{d}\phi, \quad (113)$$

$$\bar{\alpha}^* = \frac{\bar{k}^*}{\overline{\rho c}^*}, \quad (114)$$

in which

$$\overline{\rho c}^* = \frac{1}{\pi R_0^2} \int_0^{2\pi} \int_0^{R_0} \rho c R \, \mathrm{d}R \, \mathrm{d}\phi \quad (115)$$

and

$$\bar{k}^* = \bar{k}^{\mathrm{M}} + \bar{k}^{\mathrm{C}}, \tag{116}$$

wherein

$$\bar{k}^{\mathrm{M}} = \frac{1}{\pi R_0^2} \int_0^{2\pi} \int_0^{R_0} k R \, \mathrm{d}R \, \mathrm{d}\phi \tag{117}$$

and

$$\bar{k}^{\mathrm{C}} = \frac{1}{\pi R_0^2} \int_0^{2\pi} \int_0^{R_0} k \left[\left(\frac{\partial B}{\partial R} \right)^2 + \frac{1}{R^2} \left(\frac{\partial B}{\partial \phi} \right)^2 \right] R \, \mathrm{d}R \, \mathrm{d}\phi \tag{118}$$

or, alternatively,

$$\bar{k}^{\mathrm{C}} = \frac{1}{\pi R_0^2} \int_0^{2\pi} \int_0^{R_0} \rho c (U - \bar{U}^*) B R \, \mathrm{d}R \, \mathrm{d}\phi, \tag{119}$$

with the B-field defined by (64)–(66). The effective conductivities $\bar{k}^{\mathrm{M}}$ and $\bar{k}^{\mathrm{C}}$ represent the respective molecular ('diffusive') and convective contributions.

Acknowledgements—This research was supported in part by the Office of Basic Energy Sciences of the Department of Energy.

REFERENCES

1. H. Brenner, A general theory of Taylor dispersion phenomena, *PhysicoChem. Hydrodyn.* **1,** 91–123 (1980).
2. R. Haberman, *Elementary Applied Partial Differential Equations*. Prentice-Hall, Englewood Cliffs, New Jersey (1987).
3. I. Frankel and H. Brenner, On the foundations of generalized Taylor dispersion theory, *J. Fluid Mech.* **204,** 97–119 (1989).
4. M. Shapiro and H. Brenner, Chemically reactive generalized Taylor dispersion phenomena, *A.I.Ch.E. Jl* **33,** 1155–1167 (1987).