Heat and Mass Transfer Made Visible

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Abstract. Heat and mass transfer in fluid flows traditionally is examined in terms of temperature and concentration fields and heat/mass-transfer coefficients at fluid-solid interfaces. However, heat/mass transfer may alternatively be considered as the transport of a passive scalar by the total advective-diffusive flux in a way analogous to the transport of fluid by the flow field. This Lagrangian approach facilitates heat/mass-transfer visualisation in a similar manner as flow visualisation and has great potential for transport problems in which insight into (interaction between) the scalar fluxes throughout the entire configuration is essential. This ansatz furthermore admits investigation of heat and mass transfer by well-established geometrical methods from laminar-mixing studies, which offers promising new research capabilities. The Lagrangian approach is introduced and demonstrated by way of representative examples.

Introduction

Laminar heat and mass transfer is key to a wide variety of industrial processes of size extending from microns to metres. Examples range from the traditional mixing and thermal processing of viscous fluids [1] via compact processing equipment for process intensification [2] down to emerging micro-fluidics applications [3]. Such systems traditionally are examined in terms of temperature and concentration fields and heat/mass-transfer coefficients at fluid-solid interfaces. However, heat/mass transfer may alternatively be considered as the transport of a passive scalar by the total advective-diffusive heat/mass flux in a way analogous to the transport of fluid by the flow field. The paths followed by this total scalar flux are the natural counterpart to fluid trajectories and facilitate heat/mass-transfer visualisation in a similar manner as flow visualisation.

To date the Lagrangian concept has been restricted to 2D steady flows [4–6]. Recent studies proposed its generalisation to generic unsteady flows by considering heat/mass transfer as the unsteady “motion” of a “fluid” subject to continuity [7–9]. This ansatz is particularly suited for laminar flows and low to moderate Péclet numbers $P_e$ (typically $P_e \lesssim O(100)$), characteristic of small-scale systems in process intensification and micro-fluidics, and has great potential for cases in which insight into (interaction between) scalar fluxes throughout the entire configuration is essential. It furthermore admits investigation of scalar transport by well-established geometrical methods from laminar-mixing studies, which offers promising new research capabilities [8, 9].

The Lagrangian heat/mass-transfer analysis is demonstrated by way of a simple model problem representative of compact processes. Two cases of practical relevance are considered: heat transfer in the presence of chaotic mixing and simultaneous heat and mass transfer.
Model Problem

Considered is the heat and mass transfer in a (chaotic) time-periodic flow (period time $\tau = 1$) set up by a horizontally-oscillating vortex pair inside a non-dimensional periodic channel (width $W = 1$; height $H = 1/2$). The velocity field is given by the analytical expressions $u(x, t) = \bar{u}(x_+, t) + \bar{u}(x_-, t) = \bar{u}(x, t+1)$, with $x_+ = (1/4 - \Delta x(t), 1/4)$ and $x_- = (3/4 - \Delta x(t), 1/4)$ the positions of left and right vortices, respectively, and $\Delta x(t) = \epsilon \sin(2\pi t)$ their time-periodic horizontal oscillation at amplitude $\epsilon$. The basic solenoidal velocity components read $\bar{u}_x(x, y) = \sin (2\pi x) \cos (2\pi y)$ and $\bar{u}_y(x, y) = -\cos (2\pi x) \sin (2\pi y)$.

Heat and mass transfer are described by the non-dimensional advection-diffusion equation

$$\frac{\partial \phi}{\partial t} + u \cdot \nabla \phi = Pe^{-1} \nabla^2 \phi,$$

for the scalar quantity $\phi$, which may represent both temperature $T$ and mass concentration $C$ [4]. System parameter $Pe$ is the well-known Péclet number $Pe = UL/\kappa$, with $U$ and $L$ characteristic velocity and length scale, respectively, and $\kappa$ the diffusion coefficient for $\phi$. Heat and mass fluxes are set up through permeable top (constant $\phi_{top}$) and bottom (constant $\phi_{bottom} < \phi_{top}$) walls. Scalar transport, unless stated otherwise, is investigated in terms of temperature $T$ hereafter, which can be done without loss of generality. Numerical methods are detailed in [9].

Lagrangian Transport Analysis

Key to the Lagrangian concept by [7–9] is that heat transfer occurs along paths (“thermal trajectories”) delineated by the total heat flux, in non-dimensional form reading

$$q = q_c + q_d, \quad q_c = uT, \quad q_d = -\frac{1}{Pe} \nabla T,$$

with $q_c$ and $q_d$ representing thermal transport by advection (or “convection”) and diffusion (or “conduction”), respectively. These thermal trajectories $x_T$ are described by

$$\frac{dx_T}{dt} = v, \quad \frac{\partial T}{\partial t} + \nabla \cdot (T v) = 0, \quad v = u - \frac{1}{Pe} \nabla (\ln T),$$

and are the thermal analogy to the Lagrangian fluid trajectories, governed by

$$\frac{dx}{dt} = u, \quad \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0,$$

by which fluid transport takes place (here $\rho = 1$). This exposes $T$, $v$ and $x_T$ as the thermal analogies to the fluid density $\rho$, fluid velocity $u$ and fluid trajectories $x$ and thus enables representation of heat transfer entirely in terms of the “motion” of a “fluid” subject to continuity.

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1Some terminology: advection is transport by fluid motion; diffusion is transport by molecular motion. In heat-transfer problems, advection and diffusion are usually denoted “convection” and “conduction,” respectively. Generic laminar transport involves both transport mechanisms; mixing is only by advection.
Important to note is that the convective flux $q_c$ in (2) in fact identifies with the enthalpy flux and thus, inherently, is defined only relative to a preset reference state. The minimum temperature inside the domain of interest is the commonly-used definition in literature (consult e.g. [4–6]) and therefore also adopted here. However, a recent study contends this definition, albeit without solid physical justification, and proposes the mean temperature as alternative, which significantly alters the thermal trajectories [10]. The present study nonetheless adheres to the minimum temperature yet with the annotation that a general consensus on the reference state remains outstanding. It must be stressed that the choice of reference state has no conceptual consequences; it affects the appearance – and physical interpretation – of thermal trajectories yet not the Lagrangian framework per se.

The Lagrangian formulation (3) admits heat-transfer analyses by well-established Lagrangian methods from laminar-mixing studies. These methods lean on the property that continuity “organises” fluid trajectories $x$ into sets of coherent structures (“flow topology”) that geometrically determine the fluid transport [11–13]. The thermal trajectories $x_T$, by virtue of the fluid-motion analogy, form a thermal topology of essentially equivalent composition that demarcates the transport routes of heat. Topological analysis of this thermal topology offers promising new thermal-analysis capabilities. This is demonstrated below by way of the above model problem.

### Mixing Characteristics

The steady flow topology ($\epsilon = 0$) coincides with the streamline portrait shown in Fig. 1(a) and consists entirely of closed streamlines defining recirculation zones (“islands”), signifying absence of any mixing. The time-periodic flow topology can be visualised by Poincaré-sections of passive tracers (subsequent tracer positions at time levels $t \in [0, \tau, 2\tau, \ldots]$ as if illuminated by a stroboscope) released at “strategic” locations in the flow [11]. Fig. 1(b) shows the Poincaré-section (black dots) of passive tracers released on the line $y = 1/4$ for $\epsilon = 0.1$, disclosing two kinds of coherent structures: (i) chaotic sea; (ii) islands embedded in the chaotic sea. The chaotic sea is an essentially unsteady phenomenon that ensues from disintegration of (parts of) islands; the remaining islands are remnants of their (partially-disintegrated) steady-state counterparts [11]. The black and gray curves within the sea (termed “manifolds”) delineate the principal transport directions upon progression and regression in time, respectively. These manifolds effectuate chaotic advection and are key to the accomplishment of “efficient mixing” [11–13]. The flow topology thus directly exposes the poor and good mixing zones.

### Heat Transfer under Steady Conditions

Fig. 2 visualises the thermal topology by way of the thermal streamline portrait and the corresponding temperature fields for “low” and “high” $Pe$ in case of steady flow. The thermal topology comprises two distinct coherent structures: (i) the thermal path, facilitating heat transfer from bottom to top wall (ii) thermal islands, entrapping and clock-wise recirculating thermal energy. The thermal path always exists in the presence of non-adiabatic walls [7, 8]; thermal islands emerge only in case of sufficient advective heat transfer. The thermal topologies thus
demonstrate the progression from a diffusion-dominated state (near vertical thermal streamlines) to an advection-dominated state (emergence of thermal islands and confinement of the thermal path) with increasing $Pe$. The effect of advection may in the advection-dominated state (Fig. 2(b)) nonetheless exhibit appreciably spatial variation. The strong correlation between isotherms (bright curves) and thermal streamlines in the thermal path signifies locally diffusion-dominated heat transfer. The poor correlation in the thermal islands, on the other hand, indicates that advection has the upper hand in these regions.

**Heat transfer in the Presence of Chaotic Mixing**

The present Lagrangian approach, contrary to conventional Eulerian methods, enables direct investigation of the connection between chaotic mixing and heat transfer. This is a topic of great practical relevance that nonetheless remains ill-understood to date (see e.g. [1]). Fig. 3 demonstrates the transformation of the steady-state thermal topology for $Pe = 10$, shown in Fig. 2(b), upon introduction of chaotic advection ($\epsilon = 0.1$). Panel (a) visualises the time-periodic thermal topology by combination of thermal manifolds (chaotic zone) and instantaneous thermal streamlines at time levels $t \in [0, \tau, 2\tau, \ldots]$ (thermal path); panel (b) visualises the thermal topology
Simultaneous Heat and Mass Transfer

Thermofluid processing and reactive flows in general involve simultaneous heat and mass transfer, which are characterised by the respective Péclet numbers $Pe_\alpha = U L / \alpha$ and $Pe_D = U L / D$, with $\alpha$ the thermal diffusivity and $D$ the mass-diffusion coefficient. This introduces an additional system parameter: the Lewis number $Le = \alpha / D = Pe_D / Pe_\alpha$ [14]. Typically $\alpha \sim O(10^{-7} \text{m}^2/\text{s})$ and $D \sim O(10^{-9} \text{m}^2/\text{s})$, yielding $Le \sim O(100)$ and implying a significant difference in the relative role of (chaotic) advection in both transport processes. Fig. 4 gives the transport topologies for heat and mass transfer for $Pe_D = 1000$ and $Le$ as indicated. The mass-transfer topology (bottom) consists entirely of manifolds, save the narrow instantaneous path centred on $x \approx 0.5$, signifying almost fully chaotic mass transfer. The thermal topology (top), in contrast, typically contains a thermal path – with essentially non-chaotic heat transfer – that covers a sizeable region (Fig. 4(a)) if not the full domain (Fig. 4(b)). The visualisation thus reveals that for typical $Le$ chaotic mass transfer coexists with directional heat transfer through a thermal path. This gener-
ally is the sought-after situation for thermofluids processing and reactive flows, to which rapid dispersion of additives and continuous throughflow of heat usually is essential. Transport visualisation by the present Lagrangian approach facilitates methodical optimisation of such systems.

\[ a) \text{Le} = 100 \]
\[ b) \text{Le} = 500 \]

Figure 4: Transport topologies for heat (top) and mass (bottom) transfer in terms of manifolds and instantaneous path connecting top and bottom walls at \( t \in [0, \tau, 2\tau, \ldots] \) for \( Pe_D = 1000 \).

Conclusions

The present study introduces a Lagrangian formulation of heat and mass transfer that hinges on its representation as the “motion” of a “fluid” subject to continuity. Its key advantage over conventional Eulerian methods is that it facilitates heat/mass-transfer visualisation in a similar manner as flow visualisation, which has great potential for the analysis of a wide range of systems in particular in the areas of process intensification and micro-fluidics.

The Lagrangian approach is demonstrated by way of a representative model problem. Two cases of practical relevance are considered: heat transfer in the presence of chaotic mixing and simultaneous heat and mass transfer. This reveals that chaotic mixing accomplishes (local) chaotic heat transfer. However, in general a thermal path effectuating directional – and thus non-chaotic – heat transfer between non-adiabatic walls remains, the extent of which depends primarily on the degree of advection (determined by the Péclet number \( Pe \)) yet only marginally on its nature. The analysis furthermore reveals that simultaneous heat and mass transfer usually is characterised by chaotic mass transfer in coexistence with directional heat transfer via a thermal path. This generally is the sought-after situation for thermofluids processing and reactive flows; the present Lagrangian approach facilitates methodical optimisation of such systems.

The Lagrangian representation of heat and mass transfer, though demonstrated here for 2D systems, admits generalisation to 3D unsteady systems [8, 9]. Furthermore, this approach can in principle be extended to the transport of a wide range of scalar quantities in e.g. double-diffusive, reactive or two-phase systems [4, 15]. However, a number of conceptual and technical challenges remain that must be tackled in order for the Lagrangian analysis of (un)steady heat transfer to fully come of age [9]. Efforts to address these challenges are underway.
References