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Internal mass and heat transfer between a single deformable droplet and simple extensional creeping flow

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ABSTRACT

This work studied numerically the internal mass/heat transfer of a deformable droplet immersed in a simple extensional flow. The droplet would deform gradually from prolate spheroid to 'peanut' in uniaxial extensional flow, or from oblate spheriod to 'red-blood-cell' in biaxial extensional flow. Based on the analytical solution of Stokes flow over a deformable droplet, the convection-diffusion transport equation was numerically solved by the finite difference method. The results show that the heat/mass transfer behaviors of a deformable droplet were different when compared with that of a spherical one. The effects of Pe ($1 \leq Pe \leq 10000$), capillary number Ca ($0 \leq Ca \leq 0.5$), viscosity ratio λ ($0.01 \leq \lambda \leq 100$) and the extensional flow direction on the Sh and mean concentration were numerically investigated. It shows that the internal mass/heat transfer rate was always enhanced with the increased degree of drop deformation in the diffusion-dominated case in both uniaxial/biaxial extensional flows. However, in the convection-dominated case, the flow direction has opposite influence on transport rates of mass/heat transfer with different deformation rates. The stabilized mass transfer rate decreased for droplets with different deformation in the order: 'red-blood-cell' shaped droplet, oblate droplet, prolate droplet and 'peanut' shaped droplet. At last, we proposed the empirical correlations to predict the internal mass/heat transfer rate of a deformable droplet (by adding the parameter Ca to represent the deformation of a droplet) in simple extensional flow.

1. Introduction

As a basic form of fluid flow, the extensional flow field and multiphase dispersed flow are not only frequently encountered in traditional industrial operations and applications (such as extrusion, coating, spinning of fiber [1]), but also are ubiquitous in newly developed industries and processes (such as microfluidics technology [2] and DNA dynamics [3]). For example, hydrodynamic trapping is a new non-contact technique to observe particles in a stagnation point. The non-contact properties can be used as a high-precision experimental method to study DNA molecules [4,5], extensional rheometry [6], and dissolution of liquid microdroplets [2]. The fundamental researches of a simplified single particle system can provide a theoretical guide for the actual industrial process and lay a solid foundation for more realistic models.

Experimental investigations, theoretical studies and numerical simulations about fluid mechanics, heat and mass transfer of a droplet in ambient fluid have been widely reported [7–17]. While for creeping extensional flow, the related researches were commonly reported with theoretical analysis. Taylor [18,19] gave the analytical solutions of flow field for a single spherical particle in simple shear flow and the experimental observation of deformation of emulsion droplets in four-roller apparatus. Afterwards, Acrivos et al. [20–23], Tatsuo and Buskue [24], Torza et al. [25], Chin and Han [26,27], Powell [28] and Kaloni [29], reported the flow fields, deformation, and breakup of a single drop/bubble in detouring flow, shear flow or extensional flow at low Reynolds numbers. Furthermore, Stone and Leal [30] studied the effect of surfactants on droplet behaviors and the surfactant-induced Marangoni effect. Then, Stone and Leal [31] used the boundary element method to simulate the concentric double emulsion droplets in extensional flow.

Those researches on hydrodynamic characteristics served as a good basis to study the interphase mass/heat mass transfer mechanism. Most of the literature were focused on the mass/heat

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Notation

a	sphere radius, m
c	concentration, kg/m^3
C	concentration (dimensionless)
$\overline{C}$	mean concentration of droplet (dimensionless)
Ca	$=\mu_1 Ea/\sigma$, Capillary number (dimensionless)
D_i	diffusivity, m^2/s
e	strength of the extension rate, s^{-1}
$\mathbf{E}$	rate of strain tensor
Fo	$=\tau/Pe$, Fourier number
L	shortest semi-axes, m
Pe	$=\lvert e\rvert a^2/D$, Peclet number
Pe'	$= Pe/(1+\lambda)$, modified Pe number
r	radial coordinate (dimensionless)
S	longest semi-axes, m
Sh	Sherwood number, defined in Eq. (15)
t	time, s
u	velocity (dimensionless)
$\mathbf{U}$	velocity vector, m
$\mathbf{X}$	position vector, m

Greek Symbols

θ	spherical polar angle, rad
λ	interior-to-exterior viscosity ratio
μ	viscosity, Pa·s
ξ	deformation ratio
ρ	density, kg /m^3
σ	surface tension, N/m
τ	$=\lvert e\rvert t$, dimensionless time
φ	spherical azimuthal angle, rad
ψ	stream function, m^3 /s
ω	cylindrical azimuthal angle, rad

Subscripts

0	initial time
1	outside the droplet
2	inside the droplet
start	first measurement location
end	second measurement location
r	spherical radial component
x	cylindrical component
z	cylindrical component
θ	spherical polar component
φ	spherical azimuthal component
∞	far from the droplet or finite large time

Superscript

s	droplet interface

transfer for a single rigid spherical droplet. For example, Freidlander [32], Acrivos et al. [33–35], Ruckenstein [36], Cox [37], and Abramzon and Borde [38] modeled theoretically the heat/mass transfer of a single spherical particle in creeping flow fields (detouring flow, shear flow or extensional flow) and proposed the correlations of Sherwood/Nusselt number. Oliver [39] studied the internal mass transfer of a spherical droplet suspended in an uniform electric field. With the development of computer technology, Juncu [40] used the numerical method to simulate the internal unsteady heat/mass transfer from a fluid particle in creeping flow, whereas did not give the correlation of Sh number. Zhang et al. [13,14] studied in detail the steady internal/external/conjugate mass and heat transfer of a single sphere in simple extensional creeping flow, and presented the corresponding correlation formula. The Zhang-Yang-Mao model [14] has been reported to successfully predict the droplet dissolution in extensional flow [2]. Subsequently, Li et al. [12] studied the steady conjugate mass/ heat transfer of a single sphere in shear flow. For readers' convenience, a short summary about the mass/heat transfer correlations has been listed in Table 1.

The drop would experience deformation, rather than keep the fixed shape (mostly assumed spherical), in viscous flow, which in turn affects the flow structure and the heat/mass transfer process. Although the numerical method has been developed greatly in this

Table 1
Summary of transfer correlations of a single particle in infinite stokes flow.

Case	Correlation and limitation
Rigid sphere in detouring flow[a] [32]	$Nu_1 = 0.991 Pe_1^{1/3}$, $100 < Nu < 100,000$
Rigid sphere in detouring flow[a] [35]	$Nu_1 = 2 + 0.5Pe_1 + 0.25Pe_1^2 \ln(Pe_1) + 0.03404Pe_1^2 + O(Pe_1^3)$, $0 \leqslant Nu < 1$
Rigid sphere in shear flow[a] [34]	$Nu_1 = 2 + \frac{0.9104}{(2\pi)^{0.5}} Pe_1^{0.5} + \ldots, Nu \leqslant 1$
Spherical droplet in any flow[c] [38]	$\frac{1}{Nu} = \lambda \frac{1}{Nu_1} + \frac{1}{Nu_2}$, $0 \leqslant Nu < 1000$
Spherical droplet in potential flow[c] [36]	$Sh_1 = 4/\sqrt{(3\pi)} Pe_1^{1/2}$, $Pe_1 >> 1$
Rigid sphere in extensional flow[a] [41]	$Sh = 0.5 + (0.125 + 0.745Pe_1)^{1/3}$, $0 \leqslant Pe_1 < 100,000$
Spherical droplet in extensional flow[a] [14]	$Sh_1 = \frac{1}{\lambda+1}[0.6 + (0.16 + 0.48Pe_1)^{1/2}] + \frac{\lambda}{\lambda+1}[0.5 + (0.125 + 0.745Pe_1)^{1/3}] + f_1 + f_2 \exp(-Pe^{1/6}/f_3)$
	$f_1 = -19.844 + 17.846 \frac{1}{\lambda+1} + 19.491 \exp\left(\frac{-2.174}{\lambda+1}\right)$
	$f_2 = -1.781 + 2.746 \exp\left[-\left(\frac{1.336}{\lambda+1} - 0.664\right)^2\right]$
	$f_3 = -1.478 - 0.371 \exp(-0.274\lambda) - 0.251 \exp(-0.072\lambda)$, $0 \leqslant Pe_1 < 100,000$
Spherical droplet in extensional flow[b] [14]	$Sh_2 = 14.09 - \frac{10.87}{1+\left(\frac{Pe_2}{45.81(1+\lambda)}\right)^{1.830}}$, $0 \leqslant Pe_2 < 100,000$
Spherical droplet in shear flow[a] [12]	$Sh_1 = \frac{-40.3+9.15\ln Pe_1 - 0.3(\ln Pe_1)^2 + 29\lambda}{1-0.079\ln Pe_1 + 6.3\lambda}$, $1000 \leqslant Pe_1 < 100,000$
Spherical droplet in shear flow[b] [12]	$Sh_2 = \frac{2.885-2.065\ln Pe_2 + 0.470(\ln Pe2)^2 + 38.515\lambda}{1-0.634\ln Pe2 + 0.124(\ln Pe2)^2 + 11.703\lambda}$, $10 \leqslant Pe_2 < 50,000$
Deformation droplet in extensional flow[a] [42,43]	$Sh_1 = \sqrt{\frac{3}{2\pi(1+\lambda)}}\left[1 \pm \frac{4(4+31\lambda)Y}{315(1+\lambda)} Ca\right] Pe_1^{0.5}$, $1 << Pe_1$

[a] External mass/heat transfer.
[b] Internal mass/heat transfer.
[c] Conjugate mass/heat transfer.