

FLUID MECHANICS SERIES



Flows and Chemical Reactions in Homogeneous Mixtures

Roger Prud'homme

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List of Main Symbols

Latin characters

a	surface strain rate
a, b	partial derivatives of pressure with respect to ξ and A respectively
A	chemical affinity; chemical species; or monatomic species
A_2	diatomic species
\underline{A}	column matrix of chemical affinities in a multi-reactive medium
A, B	Arrhenius coefficients
c	speed of sound; or molecular speed
c_K	characteristic celerity in a multi-reactive mixture
$c_1, c_\mu, c_\varepsilon, c_k$	coefficients of the $k - \varepsilon$ method
C	total number of moles per unit volume; or Germano's parameter
C_f	friction coefficient
C_j	molar concentration per unit volume

C_p, C_v	specific heat at constant pressure or constant volume respectively (c_p, c_v for the unit of mass)
Cr	crispation number
d	molecular diameter; distance; or differential
D	diffusion coefficient; or diameter
$\bar{\bar{D}}$	strain rate tensor
Da	Damköhler number
D_T	thermal diffusion coefficient
D_T, D_p	partial derivatives of $\ln n$ with respect to $\ln T$ and $\ln p$ respectively
e	roughness thickness
\bar{e}_i	orthonormal basis vector
E	internal energy (e per unit mass)
$E(t_e)$	residence time distribution in a chemical reactor
$E(k)$	energy spectrum of turbulence
E_a	activation energy
$\mathcal{E}, \mathcal{E}_j$	chemical species
f	parameter; or reduced chemical production rate
f', f''	Reynolds, Favre fluctuation, respectively
\vec{f}	force acting on each unit mass
\vec{f}_j	force acting on the unitary mass of the species j

F	Helmholtz free energy (f for the unit of mass); generalized force; or any extensive value (f for the unit of mass)
\vec{F}	force
G	Gibbs free enthalpy (g for the unit of mass); or production rate of entities per unit volume of the phase space
$G(\vec{x}, t)$	filter in the physical space
$G(\vec{k}, \omega)$	filter in the Fourier space
\vec{g}	acceleration due to gravity (of modulus g)
g_j	chemical potential per unit mass of the species j in a mixture
H	enthalpy (h per unit mass)
h_0	stagnation enthalpy
$\vec{1}$	unit tensor
$I(\alpha)$	distribution of ages
j	chemical species
\vec{J}_{Dj}	diffusion flux of the species j
J_0, J_1	Bessel functions
k	Boltzmann's constant; wave number; or kinetic energy of turbulence
$k(T)$	specific reaction rate
K	kinetic energy (k per unit mass); compressibility; number of chemical reactions in a mixture; heat exchange coefficient; or wave number

K_F	turbulent exchange coefficient for the quantity F
K_C, K_p	equilibrium constants for the concentrations and the partial pressures, respectively
l	latent heat per unit mass; or mean free path
ℓ	length of transfer; or integral scale of turbulence
L	length; molar latent heat; number of chemical elements in a mixture; size of a crystal; or phenomenological coefficient of a chemical reaction
ℓ_D	diffusion thickness of a non premixed flame
ℓ_f, ℓ_δ	thickness of preheating, of reaction of a premixed flame, respectively ℓ_G, ℓ_K : length scales of Gibson, of Kolmogorov, respectively
Le	Lewis number
Lp	Prandtl mixing length
$\underline{\underline{L}}$	matrix of phenomenological coefficients of chemical reactions
\mathcal{L}	resolved strained tensor (in LES)
$\mathcal{L}(f)$	derivation operator in cylindrical coordinates
m	total mass
M	molecular mass; diluent; or Mach number
\mathcal{M}	molar mass
m_j	mass of the species j
\mathcal{M}_j	molar mass of the species j
\dot{m}	unit mass flow rate; or mass flow rate of a nozzle

n	total number of moles
n_j	number of moles of the species j
N	number of species; number of molecules per unit volume; or coordinate normal to an interface
\vec{n}, \vec{N}	unitary normal to an interface
p	thermodynamic pressure
P	probability density
$\vec{\vec{P}}$	pressure tensor
Pr	Prandtl number
q	any parameter; or heat flux
\dot{q}	volume flowrate
\vec{q}	heat flux vector
Q	partition function; or quantity of heat
\dot{Q}	heat released per unit time at the walls of a chemical reactor
$(\mathcal{Q}_f^0)_j = (H_0^0)_j$	molar enthalpy of formation of the species j ($(q_f^0)_j$ per unit mass)
r	constant of perfect gases per unit mass; radius; or caloric power received per unit volume
R	universal molar gas constant; radius; or number of independent chemical species in a mixture
$R(\xi)$	correlation coefficient
Re	Reynolds number

R_j	mass production of species j by chemical reaction
s	Arrhenius exponent
S	entropy (s per unit mass); area of the cross-section of a nozzle
s_L, s_L^0, s_t	laminar combustion velocity, standard, and turbulent, respectively
S, \mathcal{S}	surface
S	symmetrical part of the velocity gradient tensor
Sc	Schmidt number
t	time; diffusion thickness
t_e	residence time in a chemical reactor
T	absolute temperature; or Chapmann-Jouguet detonation point
T_a, T_{ad}	activation temperature, adiabatic temperature of a reaction, respectively
$\bar{\bar{T}}, T$	double-filter tensor (in LES)
$\bar{\bar{T}}, \mathcal{T}$	unresolved Reynolds tensor (in LES)
u, v, w	velocity \vec{v} components in Cartesian coordinates (v_r, v_θ, v_z in cylindrical coordinates)
U, U_∞	reference velocity
\vec{U}, \vec{v}	velocity vector; or barycentric velocity vector in a composite fluid
v, v'	speed, turbulence intensity respectively
V	speed; force; volume in the phase space; or potential

\vec{V}	vector; velocity vector; or velocity vector in the phase space $(\vec{x}, \vec{\zeta})$
\mathcal{V}	volume; or control volume
\vec{v}_j	velocity vector of the species j
\vec{V}_j	diffusion velocity of the species $\vec{v}_j - v$
\vec{w}	velocity of a surface (normal component w); or $d\vec{\zeta}/dt$ in the phase space
\vec{W}	local velocity vector of a discontinuity
\dot{W}_F	rate of production of the quantity F (\dot{W}_j for species j)
$\dot{W}_{E\alpha, \text{int}}$	rate of production of energy for the internal degrees of freedom of the species j
x, y, z	Cartesian coordinates; x along a nozzle axis
\vec{x}	position vector
X_j, Y_j	molar and mass fraction of the species j respectively
Z	fraction of mixture

Greek symbols

α	species; or age of an entity in a chemical reactor
β_j, β_T	reduced concentration, respectively reduced temperature
δ	thickness of a viscous layer; $\delta(x)$: Dirac distribution
Δ	difference; Laplacian; size of a filter (in LES); ΔH : heat of a reaction

ε	small dimensionless parameter; or turbulent dissipation rate
ε_δ	relative roughness
ϕ	velocity potential; $\phi(\bar{x}, t)$: weight function
ϕ_j	partial molar quantity associated with the quantity ϕ
γ	isentropic coefficient c_p/c_v ; damping of a wave
Γ	circulation of a vortex; second partial derivative of enthalpy
χ	scalar local dissipation rate
η	partial bulk viscosity; or reduced coordinate
κ	thermal diffusivity $\lambda/\rho c_p$; or mean curvature of a surface
λ	coefficient of thermal conductivity; eigenvalue; Taylor's micro-scale
Λ	coefficient of head-loss; or heat transfer coefficient
μ	coefficient of shear viscosity; Gibbs free energy per mole; or absorption coefficient per unit of wave length
μ_j	molar chemical potential of a species j in a mixture
ν	kinematic viscosity μ/ρ
ν_t	turbulent kinematic viscosity
ν_j	algebraic stoichiometric coefficient $\nu_j = \nu''_j - \nu'_j$
ν'_j, ν''_j	stoichiometric coefficient of the direct reaction, or its inverse respectively
$\bar{\bar{\Pi}}$	viscous pressure tensor

Π_i	dimensionless group
θ	temperature; or angular coordinate
ϑ	volume per unit mass (inverse of the density)
ρ	density (volumetric mass)
ρ_j	partial density
σ	surface tension
Σ	surface; area of a surface; $\Sigma(x)$ area of the cross-section of a nozzle
$\bar{\bar{\Sigma}}$	stress tensor
$\sigma_k, \sigma_\varepsilon$	Prandtl numbers of the $k - \varepsilon$ method
τ	characteristic time; crossing time in a chemical reactor; dimensionless energy of reaction $\tau = \Delta H / c_p T_1$
ω	speed of rotation; or pulsation of an oscillating wave; function of β_T
$\bar{\omega}$	rotation vector
Ω	speed of rotation
$\bar{\bar{\Omega}}$	rotation vector
ξ	progress variable per unit mass; reduced coordinate; or correlation length
$\underline{\xi}$	column matrix of the progress variables
ψ	stream function; or probability in the space phase
ζ	progress variable per unit volume; or reduced variable

$\dot{\zeta}$ rate of production of a chemical reaction

$\vec{\zeta}$ vector of the phase space

Subscripts, superscripts, and other symbols

a of activation; or relative to the quantities per unit area of the interface

ad adiabatic

b burned gases

c concentration; or cut-off

C critical point

chem chemical

$CO-E_{\beta v}$ coupling CO molecule - vibrational energy

d relative to small dissipative eddies

D direct; of dissociation; or diffusive

e equilibrium flow; exit of a reactor; residence; or large eddies

eff effective

EBU relating to the “Eddy break-up” model

f frozen composition; fresh gases; or flame

$_G, ^g$ gas

α, β, i, j of species

i internal; relative to imaginary part; or irreversible

int	internal degrees of freedom of a molecule
K	for the K frozen progress variables
l	liquid
L	line; liquid; or laminar
m	mixture; mass
mec	mechanical
p	at constant pressure; or solid phase
q	extinction limit of a flame
r	chemical reaction; or reference
R	reverse; or recombination
$R-K$	relative to the $R - K$ progress variables at equilibrium
s	steady state; surface; or isentropic
o	entry of a reactor
S	surface; relative to the specific or intensive interfacial quantities
st	stoichiometric; or steady
t	for translational energy mode of a molecule; turbulent
T	temperature; turbulent; or at constant temperature
T	second order tensor; or transpose of a tensor
$^{\circ}$	deviator of a tensor
th	thermal

v , or ϑ	at constant volume
v	vapor
//	parallel to a surface
\perp	normal to a surface
0	standard reference value
•	pure simple substance
'	per unit time; or for a rate of production
—	thermodynamic value per mole; average quantity; or Reynolds average
'	Reynolds disturbance in relation to an average value
"	Favre disturbance in relation to an average value
$S()$	symmetrical part of a matrix or a tensor
\sim	transposed tensor; transposed matrix; or Favre average
$\langle \rangle$	ensemble average
\wedge	pre-exponential factor; or relative to a test filter in LES
$()_T^0$	standard thermodynamic function
\times	vector product
\otimes	tensor product
\cdot	scalar product (singly-contracted tensor product)
$:$	dyadic product (doubly-contracted tensor product)
\wedge	exterior product

$*$	sonic conditions; or reference state; or virtual
$\vec{\nabla}$	nabla (gradient operator)
$[\]^{\pm}$	jump of a quantity across an interface
d/dt	material derivative equal to $\partial/\partial t + \vec{v} \cdot \vec{\nabla}$
$\partial/\partial t$	partial time derivative
$d_{\mathbf{W}}/dt$	material derivative associated with the velocity $\vec{\mathbf{W}}$ equal to $\partial/\partial t + \vec{\mathbf{W}} \cdot \vec{\nabla}$
\rightleftharpoons	for a reversible chemical reaction

Preface

This book – a follow-up to the author's previous publication, *Flows and Chemical Reactions* [PRU 12] – is devoted to the applications of such flows and reactions.

Remember that the former book on *general equations* comprised three chapters:

1. Simple fluids;
2. Reactive mixtures; and
3. Interfaces and lines.

It is unsurprising that the examples chosen for this book relate mainly to reactive homogeneous mixtures, because on the one hand, numerous examples of non-reactive fluids were discussed in Chapter 1 of the earlier work and, on the other, heterogeneous flows, notably including interfaces and lines, will be the topic of a third, forthcoming publication.

Diffusion phenomena are overlooked in Chapter 1, but the reactions are of crucial importance. Thus, the focus is on the propagation of sound and on mono-dimensional flows in nozzles. Damköhler numbers and differences from chemical equilibrium play an important part, and relate to the performances of thrusters. In this chapter, the balance equations for non-equilibrium flows are extended to non-equilibrium of the internal modes of molecule energy, which is one way of dealing with the problems of bodies' re-entry into the atmosphere.

Chapter 2, on chemical reactors, is very conventional, and the main point discussed is that of homogeneous, perfectly stirred reactors, where the analytical computations can be pursued further – particularly with regard to the stability of stationary operating points. Many different types of instability are to be found in this chapter, and we can deal with these by using control parameters linked particularly