AGARDograph No. 41

Fundamental Data Obtained from Shock-Tube Experiments

Edited by A. FERRI

FUNDAMENTAL DATA OBTAINED FROM SHOCK-TUBE EXPERIMENTS

Editor

A. FERRI

Published for and on behalf of
ADVISORY GROUP FOR
AERONAUTICAL RESEARCH AND DEVELOPMENT
NORTH ATLANTIC TREATY ORGANIZATION

by

PERGAMON PRESS

Oxford · London · New York · Paris

1961

PERGAMON PRESS LTD.
Headington Hill Hall, Oxford
4 & 5 Fitzroy Square, London, W.1

PERGAMON PRESS INC.
122 East 55th Street, New York 22, N.Y.
1404 New York Avenue N.W., Washington 5 D.C.
Statler Center 640, 900 Wilshire Boulevard
Los Angeles 17, California

PERGAMON PRESS S.A.R.L.
24 Rue des Écoles, Paris Ve

PERGAMON PRESS G.m.b.H.
Kaiserstrasse 75, Frankfurt am Main

Library of Congress Card No. 60–14576

Set in Baskerville 10 *on* 11 *pt. and printed in Great Britain by*
Adlard & Son, Dorking, Surrey, England

PREFACE

This volume presents a collection of monographs in the fields of chemical, physical and thermodynamic problems investigated or investigable experimentally by shock-tube techniques. In the first part of the volume, including Chapters I, II and III, introductory information on unsteady flow motion and shock-tube techniques are presented.

Chapter IV and the following chapters are examples of applications, describing specific investigations in the fields of chemical physics and thermodynamics where shock-tube techniques have been used.

Antonio Ferri

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CHAPTER I

FLUID DYNAMICS OF NONSTEADY FLOW

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A. INTRODUCTION

IN THIS chapter, the basic concepts underlying the theoretical treatment of unsteady, continuous one-dimensional (and quasi-one-dimensional) motion are reviewed.

The subject matter covers a rather large variety of physically-occurring and practically-interesting flows. In spite of the simplifications introduced by the assumption of one-dimensionality, theoretical approaches are not yet capable of describing them in close form, except for a few simple cases.

In view of the complexity of the subject and in an attempt to organize logically the content, this work is divided into three main sections. The first two sections deal with the so-called ideal fluid while the third section considers deviations from this ideal fluid. Throughout the work, the "continuum", homogeneity and isotropy assumptions are made and body forces are considered negligible.

In Section B the fluid is considered to have constant composition and to be thermally and calorically perfect. The basic equations are first given under the above-mentioned body of assumptions (Section B.1) and subsequently specialized to the one- and quasi-one-dimensional motion of a non-viscous, non-conducting fluid (B.2, B.3).

Characteristic equations are derived for the general case of non-isentropic motion and pertinent finite differences, and approximate methods of solution are briefly discussed (B.4). Then specific simple cases of isentropic motions and simple wave motions are analysed (B.5). Finally, the initial value problems are investigated (B.6).

In the Section C, the fluid is considered to have variable composition as a result of chemical reactions occurring during the flow. The basic equations of a reacting mixture are given under much the same body of assumptions as in Section C.1. The motion of a non-viscous, non-conducting, non-diffusing (negligible molecular transports) fluid is presented in detail for one- and quasi-one-dimensional unsteady flow and pertinent iterative step-by-step methods of solution outlined (C.2).

In Section D, the deviations from ideal-fluid theory are considered relative to the motion of fluids of constant composition. Viscosity and heat-conduction effects (D.1) and real-gas effects (D.2) are considered separately.

A short outline of the mathematical theory of characteristics of a system of quasi-linear first order partial differential equations is given in Appendix A. Therein the properties of the characteristic curves and their bearing on the initial value problems are presented.

Thermodynamic properties of air in equilibrium at high temperature are reported in Appendix B.

B. FLUID WITH CONSTANT COMPOSITION

B.1. *Basic equations*

In this section, the fundamental equations of fluid dynamics will be given under the following assumptions:

(1) The fluid is continuous, homogeneous and isotropic.

(2) The fluid is perfect. By this it is meant that: (a) Intermolecular forces and molecular size are negligible; (b) The internal energy of the fluid is a function of temperature only; (c) Specific heat capacities are independent of temperature.

(3) The fluid is in thermodynamic equilibrium, that is, its state is uniquely determined by local conditions and can be described by any two independent parameters, usually chosen among the following: pressure, p, density, ρ, temperature, T, internal specific energy, U, specific entropy, S.

(4) Body forces are negligible.

The basic unknowns of the problems are the velocity and any three of the state parameters. The latter are usually taken to be either pressure, temperature and density; or, pressure, density and entropy.

The four necessary equations are given by the equation of state and by the three equations expressing the fundamental principles of mass, momentum and energy conservation. These equations are intrinsically necessary and sufficient for obtaining a solution if the motion is everywhere continuous. Discontinuities might arise in the flow; then this system of equations is to be integrated by the entropy equation (second law of thermodynamics) which assesses the unidirectionality of some types of transformations (Chapter II).

The basic equations are expressed as follows.[1–8*]

state equation:

$$p = \rho R T \quad \text{or} \quad p = p_0 \left(\frac{\rho}{\rho_0}\right)^{\gamma} \exp\left(\frac{S - S_0}{C_v}\right) \tag{1.1}$$

continuity equation (conservation of mass):

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} + \rho \nabla \cdot v = 0 \tag{1.2}$$

* All symbols are defined in Appendix C, p. 43.

equation of motion (conservation of momentum):

$$\rho \frac{\mathrm{d}v}{\mathrm{d}t} + \nabla p + \nabla \cdot \tau = 0 \tag{1.3}$$

energy equation (conservation of energy):

$$\frac{\mathrm{d}U}{\mathrm{d}t} + p\frac{\mathrm{d}(1/\rho)}{\mathrm{d}t} + \frac{1}{\rho}\tau : \nabla v = -\nabla \cdot J_q \tag{1.4}$$

entropy equation (Gibbs' law):

$$T\frac{\mathrm{d}S}{\mathrm{d}t} = \frac{\mathrm{d}U}{\mathrm{d}t} + p\frac{\mathrm{d}(1/\rho)}{\mathrm{d}t} \tag{1.5}$$

The time derivatives $\mathrm{d}/\mathrm{d}t$ are substantial derivatives with respect to the motion of the center of gravity, hence:

$$\frac{\mathrm{d}}{\mathrm{d}t} = \frac{\partial}{\partial t} + v \cdot \nabla \tag{1.6}$$

Two equivalent forms of the state equation are given according to whether the quantities, v, p, ρ, T, or, v, p, ρ, S, are taken as the basic unknowns.

The subscript zero indicates reference conditions.

The quantity τ is the viscous stress tensor whose components τ_{ij} are given, in Cartesian co-ordinates, by:

$$\tau_{ij} = -\mu\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right) + \frac{2}{3}\mu(\nabla \cdot v)\,\delta_{ij} \tag{1.7}$$

wherein δ_{ij} is the Kronecher delta.* It has been assumed that no viscous stresses arise for a deformation consisting of a uniform compression or expansion only. The second coefficient of viscosity, or bulk viscosity coefficient, has been accordingly taken to be equal to $-\frac{2}{3}\mu$.

The first two terms on the left-hand side of equation (1.4) represent the time rate of change of specific internal energy and the time rate at which reversible work is done, per unit mass, on the particle ($\mathrm{d}(1/\rho)/\mathrm{d}t < 0$) or by the particle ($\mathrm{d}(1/\rho)/\mathrm{d}t > 0$). Time rates are those measured by an observer fixed with respect to the motion of the center of gravity of the elementary particle (so-called local observer). The third term, often referred to as dissipation function, is the time rate at which irreversible work (per unit mass) is done on the particle. J_q is the heat flow (per unit area and unit time) given by

$$J_q = -\lambda \nabla T \tag{1.8}$$

If then one uses the expression:[9]

$$\rho \frac{\mathrm{d}Q}{\mathrm{d}t} = -\nabla \cdot J_q = \nabla \cdot (\lambda \nabla T) \tag{1.9}$$

where $\mathrm{d}Q/\mathrm{d}t$ is the time rate at which heat is added (per unit mass) to the

---

* The Kronecher delta is defined as follows:

$$\delta_{ij} = 1 \text{ for } i = j$$
$$\delta_{ij} = 0 \text{ for } i \neq j$$

particle, Eq. (1.4) expresses the first law of thermodynamics as formulated by a local observer fixed with respect to the motion of the center of gravity of the particle.

By combining Eqs. (1.4), (1.5) and (1.8), there is obtained:

$$\frac{dS}{dt} = [\nabla \cdot (\lambda \nabla T) - \frac{1}{\rho} \tau : \nabla v] \frac{1}{T} \tag{1.5a}$$

which can also be written as:

$$\frac{dS}{dt} + \nabla \cdot \left(\frac{J_q}{T}\right) = - \frac{1}{T}\left\{\frac{1}{\rho} \tau : \nabla v + \left(\frac{J_q}{T}\right) \cdot \nabla T\right\} \tag{1.5b}$$

The second term on the left-hand side of Eq. (1.5b) is the divergence of the conductive entropy current. This term obviously depends upon the previously-defined heat flux J_q. The right-hand side of Eq. (1.5b) can be interpreted as a time rate of "production" of entropy (per unit mass). Hence, for continuous motion, the only causes of entropy production are viscosity and conductivity. Each one of these factors will "produce" entropy at the rates

$$- \frac{1}{\rho T} \tau : \nabla v \quad \text{and} \quad - \frac{J_q}{T^2} \cdot \nabla T$$

respectively. In accordance with the second law of thermodynamics both rates are positive.

The applicability of the entropy equation in the form exhibited by Eq. (1.5) or Eq. (1.5a), to a system wherein gradients of velocity, pressure and temperature are different from zero can be justified provided the system itself is not too far from equilibrium conditions.[9] These conditions exist if the variations of flow properties, along distances of the same order of magnitude as the mean free path, are small. The same limitations hold true for the motion and energy equations. When the system is far away from equilibrium additional terms should be added in both equations.[7, 8]

The fundamental set of equations is largely simplified when molecular transports are considered negligible as compared to the macroscopic bulk motion. Then viscosity and conductivity can be neglected and the fluid can be considered non-viscous and non-conducting in all the field with the exception of localized regions where these effects are taken into account by introducing physical discontinuities (see Chapter II).

For the motion of a non-viscous, non-conducting fluid the basic equations reduce to:

$$p = \rho R T; \; p = \rho_0 (\rho/\rho_0)^{\gamma} \exp\{(S - S_0)/C_v\} \tag{1.10}$$

$$\frac{d\rho}{dt} + \rho \nabla \cdot v = 0 \tag{1.11}$$

$$\rho \frac{dv}{dt} + \nabla p = 0 \tag{1.12}$$

$$\frac{dU}{dt} + p \frac{d(1/\rho)}{dt} = 0 \tag{1.13}$$

$$\frac{dS}{dt} = 0 \tag{1.14}$$

The entropy production in the continuous region is zero since all the causes of irreversible processes (i.e. viscosity and heat conduction) have been assumed zero.

The system of Eqs. (1.10) through (1.14) is applicable as long as the motion of the ideal fluid is continuous. In the region of discontinuities the basic conservation principles can no longer be stated in differential form and one must resort to a different procedure. The subject will be taken up in Chapter 2 where the possible occurrence of discontinuity surfaces will be considered.

It will be noted, finally, that for continuous motion of an ideal non-viscous, non-conducting fluid the entropy equation is not an independent statement but follows directly from the energy equation. Hence, the entropy equation in the form given by Eq. (1.14) is often used as the fourth necessary equation in place of the energy equation.

An alternate form of the energy Eq. (1.13) is often useful. If

$$h = U + p/\rho \tag{1.15}$$

is the enthalpy for unit mass (specific enthalpy), combining Eq. (1.13) and Eq. (1.12) multiplied scalarly by v yields:

$$\rho \frac{\mathrm{d}}{\mathrm{d}t}\left(h + \frac{v^2}{2}\right) - \frac{\partial p}{\partial t} = 0 \tag{1.16}$$

B.2. *One-dimensional unsteady continuous motion of an ideal fluid*

In one-dimensional unsteady continuous motion all the flow properties are a function of a single space variable and time. The space variable can measure either the distance from a plane along an axis, normal to the plane; the distance from an axis; or the distance from a point. One then speaks of plane flow, cylindrically-symmetrical flow and spherically-symmetrical flow, respectively.

Rigorously speaking, plane one-dimensional flow can be termed only the flow of an ideal fluid in ducts with constant cross-sectional area. In practice, however, when the cross-sectional area varies slowly and continuously (that is, without any discontinuity in the first- or higher-order derivatives) the flow properties can be still considered as constant in any plane normal to the axis, and function only as a single space variable. This type of motion is usually referred to as quasi-one-dimensional and will be discussed in B.3.

In the subject class of flows, it is convenient to assume p, ρ, S and u, as the four basic unknowns. The pertinent set of equations is given by the state, continuity, motion and entropy equations wherein all the dependent variables are to be considered functions of one space variable and time.

The fundamental system thus reads:

$$p = p_0(\rho/\rho_0)^\gamma \exp\{(S - S_0)/C_v)\} \tag{1.17a}$$

$$\frac{1}{\rho}\frac{\partial \rho}{\partial t} + \frac{u}{\rho}\frac{\partial \rho}{\partial x} + \frac{\partial u}{\partial x} + \frac{\epsilon u}{x} = 0 \tag{1.17b}$$

$$\rho \frac{\partial u}{\partial t} + \rho u \frac{\partial u}{\partial x} + \frac{\partial p}{\partial x} = 0 \qquad (1.17c)$$

$$\frac{\partial S}{\partial t} + u \frac{\partial S}{\partial x} = 0 \qquad (1.17d)$$

Herein ϵ equals 0, 1, 2 for plane flow, cylindrically-symmetrical flow and spherically-symmetrical flow, respectively. The space variable x measures the distance along the axis in plane flow, the distance from the axis of symmetry in flows with cylindrical symmetry and the radial distance in spherically symmetrical flows.

Eqs. (1.17) form a system of quasi-linear partial-differential equations of hyperbolic type. The role played for these systems by the characteristic curves and their importance in relation to initial value problems, approximate methods of solutions and existence of simple wave flows are briefly examined in Appendix A.

Exact solutions of the subject system of equations are available in the literature[10–16] for special cases. Their usefulness is, however, limited in view of their restricted range of applicability. In the most general case, one must resort to approximate methods of solution which are based on the notion of characteristic curves.

In this section, the characteristic equations will be derived by seeking linear combinations of the subject differential equations which contain derivatives of all the unknown functions in one direction only. Such directions are called, by definition, characteristic directions (see Appendix A).

If density derivates are eliminated from Eq. (1.17b) through the state equation and Eq. (1.17d), the following system of three differential equations is obtained:

$$\left.\begin{aligned} \frac{\partial p}{\partial t} + u \frac{\partial p}{\partial x} + \rho a^2 \frac{\partial u}{\partial x} &= -\rho \frac{ua^2}{x} \epsilon \\ \frac{\partial p}{\partial x} + \rho u \frac{\partial u}{\partial x} + \rho \frac{\partial u}{\partial t} &= 0 \\ \frac{\partial S}{\partial t} + u \frac{\partial S}{\partial x} &= 0 \end{aligned}\right\} \qquad (1.18)$$

wherein the speed of sound a is defined by $a^2 = (\partial p/\partial \rho)_{S=\text{const.}}$. For an ideal gas because of Eq. (1.17a),

$$a^2 = \gamma \frac{p}{\rho} = \gamma RT \qquad (1.19)$$

Adding and subtracting from the continuity equation the momentum equation multiplied by a yield the following equivalent system:

$$\left.\begin{aligned} \frac{\partial p}{\partial t} + (u + a) \frac{\partial p}{\partial x} + \rho a \left\{\frac{\partial u}{\partial t} + (u + a) \frac{\partial u}{\partial x}\right\} &= -\frac{\rho u a^2}{x} \epsilon \\ \frac{\partial p}{\partial t} + (u - a) \frac{\partial p}{\partial x} - \rho a \left\{\frac{\partial u}{\partial t} + (u - a) \frac{\partial u}{\partial x}\right\} &= -\frac{\rho u a^2}{x} \epsilon \\ \frac{\partial S}{\partial t} + u \frac{\partial S}{\partial x} &= 0 \end{aligned}\right\} \qquad (1.20)$$

Apparently, these equations contain total derivatives of the unknown functions along the following directions, respectively:

$$(\lambda_1) \qquad \frac{dx}{dt} = u + a \tag{1.21}$$

$$(\lambda_2) \qquad \frac{dx}{dt} = u - a \tag{1.22}$$

$$(\lambda_3) \qquad \frac{dx}{dt} = u \tag{1.23}$$

Hence, these directions are the required "characteristic directions". The rate of change of the unknown functions along these directions are:

$$\text{along} \qquad \lambda_1; \ \frac{dp}{dt} + \rho a \frac{du}{dt} = -\frac{\rho u a^2}{x} \epsilon \tag{1.24}$$

$$\text{along} \qquad \lambda_2; \ \frac{dp}{dt} - \rho a \frac{du}{dt} = -\frac{\rho u a^2}{x} \epsilon \tag{1.25}$$

$$\text{along} \qquad \lambda_3; \ \frac{dS}{dt} = 0 \tag{1.26}$$

The characteristic directions λ_i define three families of curves in the physical plane (x, t). By recalling the property of characteristics as loci of possible discontinuities for the first- and high-order derivatives of the unknown functions (see Appendix A), it becomes apparent from Eqs. (1.21), (1.22) and (1.23) that such possible discontinuities propagate in three different ways with respect to the gas.

Discontinuities occurring across the first two families of characteristics propagate with the local speed of sound with respect to the gas and are relative to first- (or higher-order) derivatives of pressure and velocity only. In particular, discontinuities across the first family of characteristics (Eq. (1.21)) represent waves travelling with the flow and are often referred to as forward sound (or Mach) waves. Discontinuities across the second family of characteristics (Eq. (1.22)) travel against the flow and are often called backward sound (or Mach) waves. Discontinuities occurring across the third family of characteristics are stationary with respect to the fluid (Eq. (1.23) describes the path line of a particle) and are relative to first-(or higher-) order derivatives of the entropy only.

Along each family of characteristics a well-defined relation holds for the rate of change of the dependent variables. In the literature the corresponding equations (Eqs. (1.24) to (1.26)) are indifferently referred to as either characteristics equations in the (u, p) plane or as regularity conditions (see also Appendix A). Notice that along a path line the regularity condition imposes the constancy of the entropy. This indeed should have been expected since the entropy variation of a particle must be zero for a non-viscous, non-conducting fluid. In the case of an isentropic flow, the entropy being by hypothesis everywhere constant, the families of characteristics reduce themselves to the first two families.

The system of the six total differential equations (1.21) through (1.26) is completely equivalent to the original system (1.18). Every solution of the original system satisfies the characteristic equations. Conversely, every solution of the characteristic system generally satisfies the original system.

B.3. *Quasi-one-dimensional unsteady continuous motion of an ideal fluid*[17–24]

The condition that all the flow variables be functions of only one space co-ordinate is approximately realized in flows within ducts with slowly varying cross-sectional area. Indeed if the slope of the cross-sectional area function $A(x)$ is not too large and if, in addition, the curvature of the center line of the duct is not too large compared to the height of the section itself, the velocity along the normal to the direction of the flow will not change appreciably in magnitude nor in direction. In this case the axial component of the velocity and its derivatives are larger than the transverse component and its derivatives by at least one order of magnitude.* It is then plausible to define at each station x an average value of the velocity which is constant throughout the section. The averaging process must be such as to satisfy the continuity equation integrated along the cross-section's height. The flow in these conditions is usually referred to as quasi-one-dimensional because all the flow properties are assumed to be a function of only one space co-ordinate. The approximations involved in the mathematical treatment of quasi-one-dimensional flow derive from the averaging process previously described and from the fact that the averaged constant flow properties thus derived are substituted in the momentum and entropy equations.

In this approximation, the flow properties at any point of the flow can be expressed as a summation of two parts.

$$\rho(x,y,z) = \boldsymbol{\rho}(x) + \epsilon r(x,y,z)$$
$$u(x,y,z) = \mathbf{u}(x) + \epsilon v(x,y,z)$$
$$p(x,y,z) = \mathbf{p}(x) + \epsilon \pi(x,y,z)$$

where the coefficient ϵ is a small number. The quantities $\boldsymbol{\rho}(x)$, $\mathbf{u}(x)$, $\mathbf{p}(x)$ are independent of the co-ordinates y and z, and therefore are constant at each cross-section A, and are defined by:

$$\boldsymbol{\rho}(x) = \frac{1}{A}\iint \rho \, dA$$

$$\mathbf{u}(x) = \frac{1}{A}\iint u \, dA$$

$$\mathbf{p}(x) = \frac{1}{A}\iint p \, dA$$

* Obviously the regions of the boundary layer in the immediate vicinity of the wall are to be excluded. Nevertheless if the height of these dissipative regions is much smaller than the height of the cross-section of the stream tube, then the averaging process described in the main text is still physically plausible.