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VOLUME AVERAGED TWO-PHASE (GAS SOLID) INTERIOR BALLISTICS EQUATIONS

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September 1984

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US ARMY BALLISTIC RESEARCH LABORATORY
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20. ABSTRACT *(Continue on reverse side if necessary and identify by block number)*

This report presents a complete mathematical derivation of governing equations for two-phase (gas-solid) interior ballistic flows. The derivation is based on instantaneous weighted volume averaging of local conservation equations, and it contains a complete discussion of errors that are introduced by the averaging. Initial conditions and boundary conditions that are consistent with the averaging procedure are discussed. The final form of the equations is chosen to facilitate their numerical solution.

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For the compressible gas phase, the three-dimensional average equations model the transient effects of viscosity, heat conduction and turbulence, and for the incompressible solid phase they model the intergranular stress, ignition and burning. The interaction between the phases is reflected by models for drag, heat transfer and source terms. Commonly used and new experimental and theoretical correlations are listed and discussed. These correlations complete the set of equations for the numerical modeling of interior ballistics flows.

The exposition of the theoretical basis of averaged equations shows that for the resolution of interior ballistic boundary layers the model is applicable only to two-phase flows with minute particles (smaller than the gas boundary layer). When large particles exist in the flow, then the resolution of boundary layers could possibly be performed by phenomenological engineering approximations.

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1. INTRODUCTION

The flowing medium in a gun tube typically is a mixture of a compressible gas with burning solid propellant grains. Details of the flow are important for weapons development, but only bulk properties can be routinely measured, such as the trajectory of the projectile, the pressure history at a fixed station, the heating of the gun tube, etc. Therefore, a need exists for a detailed mathematical model of interior ballistics two-phase flows.

A complete mathematical description of the flow could provide the motion and combustion history of each propellant grain and of the gas flow between the grains. The corresponding local governing equations are easily established, but they cannot be solved numerically because of the great number of grid points needed to describe a flow with many moving interfaces. The computational work can be reduced only be sacrificing the detailed description of the flow. To that end one considers mean values of the two-phase flow that are derived from the local properties of the gas and grains. The governing equations for these average properties are established by averaging the local governing equations.

This report presents a complete and consistent mathematical model of three-dimensional, transient interior ballistics (gas-solid) phenomena in which the total effects of the gas phase viscosity, turbulence, and heat conduction on the average variables are included. In contrast, most existing models neglect viscous and heat conduction effects, and, thus, can characterize only the wave propagation in a two-phase flow. The theory of the model is complete and consistent in that all the averaged variables, equations, initial and boundary conditions, regions of definition of the variables and correlations are precisely defined and derived using the same averaging. The need for such an approach is due to the complexity of the multiphase, multidimensional viscous flow field and a lack of detailed experimental data. Under such conditions, models formulated on phenomenological arguments are often unreliable. Also a phenomenological derivation seldom provides precise error bounds. A theoretically derived model permits one to investigate with more confidence ballistic processes that cannot be observed in detail because error bounds are precisely formulated and can be tested. Furthermore, a careful mathematical derivation of the model can reveal restrictions on the model itself. The presented mathematical model possesses the following features: (1) The averaging process insures a sufficient differentiability of the average variables so that the governing partial differential equations are defined. (2) Appropriate averages are used for quantities that are defined over volume and for those that are defined over a surface. (3) The regions of definition of the average variables are given. (4) The necessary auxiliary conditions to the governing equations, e.g., initial conditions and boundary conditions, are consistent with the averaging process used to derive the governing equations. (5) Terms that are modeled by correlations possess simple physical interpretations. Estimates are given for the difference between the theoretical definitions of the correlations and the expressions actually used. (6) Whenever the contribution of a term is neglected in an equation, a corresponding error term is established. (7) Because the equations are to be solved numerically, attention is given to an appropriate form for numerical solution. (8) The model represents a two-phase (gas-solid) flow in which the solid ignites and burns, and it also simulates other phenomena which occur in a viscous, heat conducting interior ballistic flow.

Previous work on two-phase equations for interior ballistics has been done by Gough,[1] Kuo et al.,[2] Fisher and Trippe,[3] and Krier et al.[4] The primary purpose of these works was the investigation of the wave propagation within the gun tube during the early phases of the interior ballistic phenomenon. Gough's equations were later augmented to include gas-phase viscosity and heat conduction, and used in a computer program developed by Gibeling et al.[5] Our equations are different because we have used a different averaging process, chosen a different set of dependent variables, and changed some correlation models that provide experimental input to the theory. Furthermore, our approach differs from the ones mentioned above because it is based solely on a consistent mathematical theory.

The averages in this report are computed by weighted averaging over a finite volume. Gough[1] used instead a weighted averaging over an infinite space-time domain with an unspecified weight function. The rationale of our choice is based on the observation that any averaging smooths out local details. In order not to lose too many details, one should, therefore, use

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[1] *P.S. Gough, "The Flow of a Compressible Gas Through an Aggregate of Mobile, Reacting Particles," Ph.D. Thesis, Department of Mechanical Engineering, McGill University, Montreal, 1974.*

[2] *K.K. Kuo, J.H. Koo, T.R. Davis, and G.R. Coates, "Transient Combustion in Mobile, Gas-Permeable Propellants,"* Acta. Astron.*, Vol. 3, No. 7-8, pp. 574-591, 1976.*

[3] *E.B. Fisher and A.P. Trippe, "Mathematical Model of Center Core Ignition in the 175mm Gun," Calspan Report VQ-5163-D-2, 1974.*

[4] *H. Krier, W.F. van Tassell, S. Rajan, and J. Vershaw, "Model of Flamespreading and Combustion Through Packed Beds of Propellant Grains," University of Illinois at Urbana-Champaign Report, TR-AAE-74-1, 1974.*

[5] *H.J. Gibeling, R.C. Buggeln, and H. McDonald, "Development of a Two-Dimensional Implicit Interior Ballistics Code," USA ARDC AMCCOM/Ballistic Research Laboratory Contractor Report, ARBRL-CR-00411, APG, MD, January 1980, AD No. AD 387 458.*

the smallest averaging domain that is compatible with the requirements of the problem at hand. One requirement of the averages is that they should be differentiable as many times as the ensuing governing equations indicate. It has been shown by Delhaye and Achard[6] that line or surface averages of a gas/particle mixture do not possess the required differentiability properties. Therefore, the smallest domain for averaging is a three-dimensional volume. Time averaging is not needed to insure differentiability, if the weight function for space averaging is chosen properly (see Section 2.2). If one, nevertheless, chooses to time average, then the time average interval would have to be very small because we are interested in an accurate characterization of a rapidly changing flow field.

The size of the averaging volume is important. The use of an infinite volume for averaging is not appropriate in confined flows because for such a volume the sum of the volume fractions of the two phases is not equal to one. This creates problems for the formulation of the governing equations and the boundary conditions, and for the interpretation of the results. The problem with the formulation of the equations is eliminated by using an appropriate finite volume average, while the others become more easily tractable. We discuss the problems in Sections 4.4 and 4.6. If the weight function in any infinite volume average is zero outside some finite distance from the point at which the average is taken, then the resulting average is obviously equivalent to a finite volume average. If the value of the weight function is zero outside some distance which depends on the location of the point at which the average is taken, then the resulting average is equivalent to a variable finite volume average. In this type of average additional terms in the partial differential equations for the average quantities appear that represent the effects of the change of the averaging volume in time and space. This complication is avoided in the present report by restricting the attention to a fixed finite volume average with a fixed weight function.

The average equations which are derived in Section 3 include the effects of gas viscosity and of turbulence. Furthermore, the choice of equations for averaging and the choice of dependent variables has a bearing on the numerical solution of the equations. We have chosen a set of variables that eliminates some possible numerical singularities, enhances the accuracy of numerical differentiation, and separates important physical processes for easier modeling. The choice of variables is discussed in Section 4.2. We also have chosen the internal energy equation for averaging

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[6] *J.M. Delhaye and J.L. Achard, "On the Use of Averaging Operators in Two-Phase Modeling," in Thermal and Hydraulic Aspects of Nuclear Reactor Safety, Vol. 1: Light Water Reactors, O.C. Jones and S.G. Bankoff, eds., pp. 289-332, ASME, New York, 1977.*

instead of the commonly used total energy equation. The reasons for this choice are that it produces a clear separation of physical effects and a more lucid modeling of two-phase phenomena. They are discussed in Sections 3.2.3 and 4.7.3, respectively. As a result of the consideration of viscous effects and the choice of equations and variables, our governing equations differ from those derived by Gough. Each set of equations has different approximation errors and some of the required models of experimental correlations are different.

The experimental correlations in interior ballistics are characterized by a scarcity of data. This is one reason why corresponding mathematical models have not been firmly established. In Section 4.7 we list a set of correlations, most of which are included in Gough's work. Some improvements and changes reflect the difference of our approach.

Even with the reduction of the problem size by the change from local to average functions, one is faced with a formidable numerical problem. Typically, in a two-phase flow one has a set of eleven non-linear partial differential equations. (Up to thirteen equations if a turbulence model is included). In order to describe the three-dimensional flow in reasonable detail one has to specify the eleven variables at a minimum of about 54,000 grid points. If the flow is specialized to axially symmetric, then the number of grid points may be reduced to about 1,500. Therefore, one should exploit the axial symmetry of the gun whenever possible. The proper coordinates for flows with axial symmetry are cylindrical coordinates. Therefore, we have listed in Appendix A all equations in cylindrical coordinates for flows that are independent of the circumferential coordinate.

2. ANALYTICAL BASIS

2.1 Assumptions

In the next three Sections (2.2, 2.3, and 2.4) we shall discuss some properties of averaged functions and develop general formulas that are needed for the derivations in Section 3. The averages to be discussed are weighted space averages over a finite averaging volume. We do not try to establish general properties of such averages but rather concentrate on what is needed for a specific interior ballistics modeling. For that application, the quantities to be averaged are the local properties of a gas and of propellant particles within the averaging volume. We assume that no other material is present in the tube.

The gas is assumed to be non-reacting and obeying a set of algebraic equations of state that permits one to express all thermodynamic variables in terms of two such quantities. The particular set of equations of state considered are the Noble-Abel equation and a constant ratio of specific heats.

However, most of the results are independent of the particular set of equations of state chosen.

We will assume that the gas is viscous and in a state without shocks within the averaging volume. This is necessary to have average equations with the proper differentiability conditions. Particular differentiability conditions of the local gas properties will be enumerated in Section 2.2.

If shocks are present in the gas flow, then one could average only over the shock free regions and treat the shocks as explicit boundaries. However, this approach has serious drawbacks because of the uncertainty of the corresponding boundary conditions (see Section 4.6). Space or time averaging is not the appropriate technique for the treatment of interior ballistics flows with shocks or other internal discontinuities.

The propellant particles are assumed to be incompressible and elastic. We shall neglect all effects of the rotation of the solid particles, and shall assume that the grains do not fracture. Like in the gas, the local material properties within and on the surface of each particle are assumed to be differentiable functions of time and space. Particulars of the differentiability conditions will be enumerated in Section 2.2.

2.2 Averaging Integrals and Their Derivatives

2.2.1 Averaging Volume Integrals.

We define the averaging volume V(x) as the inside of a closed surface S(x). Both are independent of time and dependent on a spacial coordinate vector x as a parameter. For instance, if V(x) is a sphere, then x may be chosen as the center of the sphere. About the surface S(x), we assume that it has a well defined normal almost everywhere. The shape and the size of the averaging volume are assumed to be constant.

The particles are defined by corresponding surfaces, s_{pi}. Because the particles are moving and burning, the s_{pi} are functions of time, but they are independent of the parametric coordinate vector x. We assume that the particle surfaces, too, have well defined normals almost everywhere. We define as S_p the union of all those particle surfaces s_{pi} that are within the averaging volume V, including its surface S_v. Accordingly, the intersection $S_p \cap S_v$ can have a finite area. Most often, the area of the intersection will be zero (Figure 1).

All averages will be defined by integrals over the space occupied either by gas or by particles. In order to have a convenient notation for the corresponding integrals, we define a phasic function β as follows

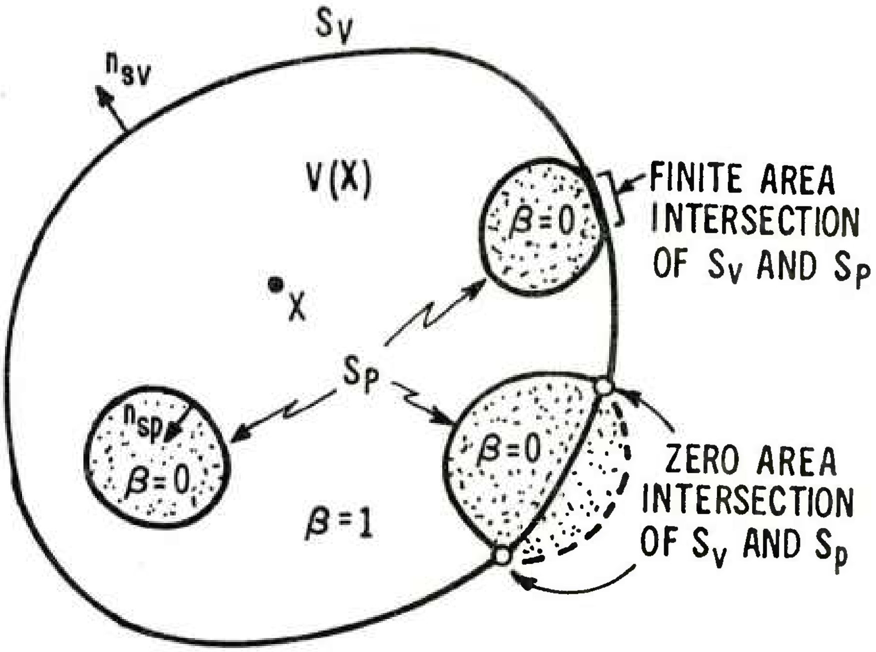

Figure 1. Averaging Volume

$$\beta(t,\xi) = \begin{cases} 0 \text{ if } \xi \text{ is inside a particle at time } t \\ 1 \text{ if } \xi \text{ is outside particles or on a particle surface at time } t. \end{cases} \tag{2.1}$$

We will also use a non-negative weight function g for the calculation of averages. Let

$$VG = \int_{V(x)} g(\xi-x)\, dV(\xi) = \text{constant} \tag{2.2}$$

be the integral of the weight function ("the weighted averaging volume"). Then the weighted volume fraction occupied by gas is

$$\alpha(t,x) = \frac{1}{VG} \int_{V_{gas}(t,x)} g(\xi-x)\, dV(\xi) = \frac{1}{VG} \int_{V(x)} \beta(t,\xi)\, g(\xi-x)\, dV(\xi) \quad . \tag{2.3}$$

The intrinsic average $\phi(t,x)$ of a function $\check{\phi}(t,x)$ that is defined in the regions occupied by gas is defined by

$$\alpha(t,x)\;\phi(t,x) = \frac{1}{VG}\int_{V_{gas(t,x)}} g(\xi-x)\;\check{\phi}(t,\xi)\;dV(\xi)$$

$$= \frac{1}{VG}\int_{V(x)} \beta(t,\xi)\;g(\xi-x)\;\check{\phi}(t,\xi)\;dV(\xi) \quad . \tag{2.4}$$

Notice that, whereas $\check{\phi}(t,x)$ is defined only within regions occupied by gas, the average $\phi(t,x)$ is defined for all values of x (within limits outlined in Section 2.3).

A corresponding average $\overset{*}{\phi}(t,x)$ of a function $\check{\overset{*}{\phi}}(t,x)$ that is defined only inside the particles is given by

$$[1-\alpha(t,x)]\overset{*}{\phi}(t,x) = \frac{1}{VG}\int_{V(x)} [1-\beta(t,\xi)]g(\xi-x)\check{\overset{*}{\phi}}(t,\xi)dV(\xi) \quad . \tag{2.5}$$

Sufficient conditions for the existence of the average function are the piecewise continuity with respect to x of the functions $\check{\phi}(t,x)$ and $\check{\overset{*}{\phi}}(t,x)$ within their regions of definition. Obviously, the average of any function of time only is the function itself.

2.2.2 Time Derivative of Volume Integrals. The averaging integrals (2.3), (2.4), and (2.5) define functions of t and x. In this section we formulate differentiability conditions of the average functions with respect to time t.

Applying Leibnitz formula (Truesdell and Toupin)[7] to an averaging integral (2.4) over V_{gas} we obtain

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[7] *C. Truesdell and R. Toupin, "The Classical Field Theories," in Encyclopedia of Physics, S. Flugge, ed., Vol. III/1, Springer-Verlag, 1960.*

$$\frac{\partial}{\partial t} \int_{V_{gas}(t,x)} \psi(t,x,\xi)\, dV(\xi) = \int_{V_{gas}(t,x)} \frac{\partial}{\partial t} [\psi(t,x,\xi)]\, dV(\xi)$$

$$+ \int_{S_p(t,x)} [\psi(t,x,\xi(\zeta))(\tilde{u}_{sp} \cdot n_{sp})]\, dS(\zeta) \quad , \qquad (2.6)$$

or

$$\frac{\partial}{\partial t} \int_{V(x)} \beta(t,\xi)\, \psi(t,x,\xi)\, dV(\xi)$$

$$= \int_{V(x)} \beta \frac{\partial}{\partial t} \psi\, dV(\xi) + \int_{S_p(t,x)} \psi(t,x,\xi(\zeta))\, (\tilde{u}_{sp} \cdot n_{sp})\, dS(\zeta) \quad ,$$

where $\tilde{u}_{sp}$ is the velocity of a point of S_p and n_{sp} is the outward unit normal of S_p at the same point. (The "outward" normal points by definition into the grains, Figure 1.) The surface integral is only over S_p and not over S_v because the latter surface is assumed to be stationary.

The first integral on the right-hand side of Eq. (2.6) exists and is a continuous function of x and t if $\partial\psi/\partial t$ is a continuous function of x and t and a piecewise continuous function of ξ. The surface integral over S_p in Eq. (2.6) exists if the surface velocity is finite. However, the area of the surface S_p has discontinuities with respect to x and, possibly, with respect to t, whenever the intersection $S_p \cap S_v$ has a finite area. Therefore, the surface integral is a continuous function of x and t only if $\psi = 0$ on S_v.

Because in our case

$$\psi(t,x,\xi) = g(\xi - x)\, \tilde{\phi}(t,\xi) \quad , \qquad (2.7)$$

we may formulate the following sufficient conditions for the continuity of the time derivative of the averaging integral in terms of g and $\tilde{\phi}$:

$$\left.\begin{array}{ll} \dfrac{\partial\tilde{\phi}(t,\xi)}{\partial t} & \text{is continuous with respect to t and piecewise continuous with respect to } \xi \text{ in the domain of definition of } \tilde{\phi}, \\ g(\xi - x) & \text{is continuous in V,} \\ g(\xi - x) = 0 & \text{on the surface } S_v. \end{array}\right\} \quad (2.8)$$

If $\tilde{\phi}$ denotes a gas phase local variable, then the first condition in Eq. (2.8) applies only when (ξ,t) designates a point in the gas phase. If $\tilde{\phi}$ denotes a solid phase local variable, then the first condition in Eq. (2.8) applies only when (ξ,t) designates a point in the solid phase.

The differentiation formula (2.6) is in terms of g and $\tilde{\phi}$

$$\int_V \beta g \frac{\partial\tilde{\phi}(t,\xi)}{\partial t} dV(\xi) = \frac{\partial}{\partial t} \int_V \beta g\tilde{\phi}\, dV - \int_{S_p} g\tilde{\phi}\, (\tilde{u}_{sp} \cdot n_{sp})\, dS \quad . \qquad (2.9)$$

The corresponding formula for functions $\tilde{\overset{*}{\phi}}$ that are defined within the solid grains is

$$\int_V (1-\beta)\, g \frac{\partial\tilde{\overset{*}{\phi}}}{\partial t} dV - \frac{\partial}{\partial t} \int_V (1-\beta)\, g\tilde{\overset{*}{\phi}}\, dV + \int_{S_p} g\tilde{\overset{*}{\phi}}\, (\tilde{u}_{sp} \cdot n_{sp})\, dS \quad . \qquad (2.10)$$

In the latter formula, the surface normal n_{sp} again points into the grains. Because now we are integrating over the inside of the grains, the sign of the last integral in Eq. (2.10) is opposite to that of the corresponding integral in Eq. (2.9).

2.2.3 **Spacial Derivatives of Volume Integrals.** Applying Leibnitz type formula to an averaging integral (2.4) over V_{gas} one obtains*

$$\nabla_x \int_{V(x)} \beta(t,\xi)\, \psi(t,x,\xi)\, dV(\xi) = \int_V \beta\, \nabla_x \psi dV + \int_{S_v - S_p} \psi n_s dS + \int_{S_v\, S_p} \psi n_{sp} dS \qquad (2.11)$$

Gauss theorem (Fulks[8] p. 354) applied to the same integration volume is

$$\int_V \beta\, \nabla_\xi \psi dV = \int_{S_v - S_p} \psi\, n_s dS + \int_{S_p} \psi\, n_{sp} dS \quad . \qquad (2.12)$$

**We note that ψ and ϕ could be scalars, vectors, or second order tensors. For example, if ψ is a vector, dots signifying the divergence of ψ and the dot product of ψ should be used in Eq. (2.11). For simplicity, the use of dots is omitted in Section 2 wherever ψ and ϕ are not specified. The understood presence or absence of a dot should be clear form the context.*

[8] *W. Fulks, Advanced Calculus, 2nd Ed., John Wiley and Sons, Inc., New York, 1969.*

Subtracting Eq. (2.12) from Eq. (2.11) one obtains

$$\nabla_x \int_V \beta\, \psi\, dV = \int_V \beta\, (\nabla_x + \nabla_\xi)\psi\, dV - \int_{S_p} \psi n_{sp} dS + \int_{S_p \cap S_v} \psi n_{sp} dS \quad . \tag{2.13}$$

Sufficient conditions for the continuity of the right-hand side of Eq. (2.13) are

$$\left.\begin{array}{ll} (\nabla_x + \nabla_\xi)\, \psi(t,x,\xi) & \text{is continuous with respect to} \\ & x \text{ and } t\text{, and piecewise continuous} \\ & \text{with respect to } \xi \text{ in the domain} \\ & \text{of definition of } \psi. \\ \psi = 0 & \text{on } S_v \quad . \end{array}\right\} \tag{2.14}$$

In our application we want some of the average functions to be differentiable twice with respect to the spacial variables. By a formal differentiation of Eq. (2.13) we obtain, assuming that $\psi = 0$ on S_v,

$$\nabla_x \nabla_x \int_V \beta\psi dV = \nabla_x \int_V \beta(\nabla_x + \nabla_\xi)\psi\, dV - \nabla_x \int_{S_p} \psi n_{sp} dS \quad . \tag{2.15}$$

Next, we apply the formula (2.13) to the first integral on the right-hand side of Eq. (2.15) obtaining

$$\begin{aligned} \nabla_x \int_V \beta(\nabla_x + \nabla_\xi)\psi\, dV &= \int_V \beta(\nabla_x + \nabla_\xi)\, (\nabla_x + \nabla_\xi)\psi\, dV \\ &\quad - \int_{S_p} (\nabla_x + \nabla_\xi)\psi n_{sp} dS + \int_{S_p \cap S_v} (\nabla_x + \nabla_\xi)\psi n_{sp}\, dS \quad . \end{aligned} \tag{2.16}$$

The surface integral in (2.15) is

$$\nabla_x \int_{S_p} \psi n_{sp} dS = \int_{S_p} \nabla_x \psi\, n_{sp}\, dS \quad . \tag{2.17}$$

Sufficient continuity conditions for (2.16) are

$$\left.\begin{array}{ll} (\nabla_x + \nabla_\xi)\,(\nabla_x + \nabla_\xi)\psi & \text{is piecewise continuous with respect to} \\ & \xi\text{, and continuous with respect to } t \\ & \text{and } x \text{ in the domain of definition of } \psi\text{ ,} \\ (\nabla_x + \nabla_\xi)\psi = 0 & \text{on } S_V \quad . \end{array}\right\} \quad (2.18)$$

Sufficient for the continuity of (2.17) is that

$$\begin{array}{ll} \nabla_x \psi & \text{is continuous with respect to } t \text{ and} \\ & x \text{ and piecewise continuous with} \\ & \text{respect to } \xi \quad . \end{array} \qquad (2.19)$$

Because $\psi(t,x,\xi) = g(\xi - x)\check{\phi}(t,\xi)$, we may express the continuity conditions in terms of $g(\xi - x)$ and $\check{\phi}(t,\xi)$ as follows.

Sufficient for the continuity of first order spacial derivatives of the averaging integral is that (see Eq. (2.14))

$$\left.\begin{array}{ll} \nabla_\xi \check{\phi}(t,\xi) & \text{is piecewise continuous with respect} \\ & \text{to } \xi \text{ and continuous with respect to} \\ & t \text{ in the domain of the definition of } \check{\phi}\text{ ,} \\ g(\xi - x) & \text{is continuous in } V\text{ ,} \\ g(\xi - x) = 0 & \text{on } S_V \quad . \end{array}\right\} \quad (2.20)$$

The integration formula (2.13) in terms of g and $\check{\phi}$, if the conditions (2.20) are satisfied, is

$$\int_{V(x)} \beta g \nabla_\xi \check{\phi}(t,\xi)\,dV(\xi) = \nabla_x \int_V \beta g \check{\phi}\,dV + \int_{S_p} g \check{\phi}\, n_{sp}\,dS \quad . \qquad (2.21)$$

The corresponding formula to (2.21) for functions $\check{\overset{*}{\phi}}$ defined within the solid grains is

$$\int_{V(x)} [1-\beta] g\, \nabla_\xi \check{\overset{*}{\phi}}(t,\xi)\,dV(\xi) = \nabla_x \int_{V(x)} [1-\beta] g\, \check{\overset{*}{\phi}}\,dV - \int_{S_p} g\, \check{\overset{*}{\phi}}\, n_{sp}\,dS \quad . \qquad (2.22)$$

The continuity conditons (2.18) and (2.19) for second order derivatives are in terms of g and $\check{\phi}$ as follows

$\nabla_\xi \nabla_\xi \breve{\phi}(t,\xi)$ is piecewise continuous with respect to ξ and continuous with respect to t in the domain of definition of $\breve{\phi}$,

$\nabla_x g(\xi - x)$ is piecewise continuous (This suffices because $\breve{\phi}$ is continuously differentiable due to the first condition, Eq. (2.20)). (2.23)

$g(\xi - x) = 0$ on S_v .

The integration formula (2.15) is, if these conditions are satisfied,

$$\int_{V(x)} \beta g \nabla_\xi \nabla_\xi \breve{\phi}(t,\xi) dV(\xi) = \nabla_x \nabla_x \int_{V(x)} \beta g \breve{\phi} dV + \int_{S_p} g \nabla_\xi \breve{\phi} n_{sp} dS - \int_{S_p} (\nabla_\xi g) \breve{\phi} n_{sp} dS . \quad (2.24)$$

In summary, if the weight function g is chosen such that its first derivatives are piecewise continuous, $g > 0$ in V, and $g = 0$ on S_v, then the averaging integrals are continuously differentiable at least once if $\breve{\phi}$ is differentiable, and at least twice if $\breve{\phi}$ is twice differentiable within its region of definition.

2.2.4 Averaging Surface Integrals.

Some flow properties are only defined on the surface of the propellant grains, e.g., the burning rate, the regression distance, and the surface temperature. The corresponding averages are computed by surface integrals.

The weighted area of the grain surface that is contained in the averaging volume is

$$SG = \int_{S_p(t,x)} g(s(t,\zeta) - x) \, dS(\zeta) \quad , \qquad (2.25)$$

where $x = s(t,\zeta)$ defines the surface and ζ represents surface coordinates. Contrary to the weighted averaging volume VG, the weighted surface area SG is not a constant but a function of t and x.

Average surface functions are defined by

$$\phi(t,x) = \frac{1}{SG} \int_{S_p(t,x)} g\big(s(t,\zeta) - x\big) \breve{\phi}(t,\zeta) \, dS(\zeta) \quad . \qquad (2.26)$$

We discuss the differentiability of the surface averages by considering a single grain. Let its surface $s(t,\zeta)$ be defined in Cartesian coordinates by

$$s(t,\zeta) = \begin{pmatrix} x_s(t,\zeta) \\ y_s(t,\zeta) \\ z_s(t,\zeta) \end{pmatrix} \quad . \tag{2.27}$$

Then the surface element $dS(\zeta)$ is defined by (Courant and John)[9]

$$dS = Z(t,\zeta)d\zeta \quad , \tag{2.28}$$

where $d\zeta$ is the product of the differentials of the components of ζ, $Z(t,\zeta) = \left(\det\left[\left(\frac{\partial s}{\partial \zeta}\right)^T \left(\frac{\partial s}{\partial \zeta}\right)\right]\right)^{1/2}$, and $\partial s/\partial\zeta$ is the Jacobian matrix of the function $s(t,\zeta)$.

The contributions of the single grain to the weighted grain surface area is according to Eq. (2.25)

$$SG_i = \iint_{\zeta_1}^{\zeta_2} g\big(s(t,\zeta)-x\big)\; Z(t,\zeta)\; d\zeta \quad . \tag{2.29}$$

The time derivative of SG_i is

$$\frac{\partial}{\partial t}(SG_i) = \int_s (-\nabla_x g)\cdot\frac{\partial s}{\partial t}\, Z\, d\zeta + \int_s g\,\frac{\partial Z}{\partial t}\, d\xi + \Big[\int_{s\cap S_v} gZ\, dC\Big]\frac{\partial C}{\partial t} \quad . \tag{2.30}$$

The integral in the last term in Eq. (2.30) is to be taken over the intersection C of the grain surface s with the boundary S_v of the averaging volume. If we assume that $g = 0$ on S_v then the integral is identically zero, and we do not have to specify conditions for $\partial C/\partial t$.

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[9] *R. Courant and F. John, <u>Introduction to Calculus and Analysis</u>, Vol. II, pp. 459-462, John Wiley and Sons, Inc., New York, 1974.*

Sufficient conditions for the right-hand side of Eq. (2.30) to be a continuous function of x and t are

$$\left.\begin{array}{ll} \frac{\partial^2 s}{\partial\zeta\partial t} & \text{is piecewise continuous with respect to } \zeta \\ & \text{and continuous with respect to } t \quad , \\ \nabla_x g & \text{is continuous, with possible exception of} \\ & \text{isolated singular points} \quad , \\ g = 0 & \text{on } S_V \\ \nabla_x g = 0 & \text{on } S_V \quad . \end{array}\right\} \qquad (2.31)$$

The first condition in Eq. (2.31) is satisfied if the grain surface has a normal almost everywhere. The next two conditions on $g(\xi - x)$ are essentially the same as encountered before in the discussion of volume averages. The last condition on g is new, and it needs to be introduced if $\partial s/\partial t$ is not equal to zero and the intersection $s \cap s_V$ has a finite area. (See the comment to Eq. (2.6).)

Next, we consider the spacial derivatives of SG_i. One obtains according to Leibnitz type rule

$$\nabla_x(SG_i) = \int_s \nabla_x g \; Z \; d\zeta + \Big[\int_{s \cap S_V} g \; Z \; dC \Big] \frac{\partial C}{\partial x} \quad . \qquad (2.32)$$

The right-hand side of Eq. (2.32) obviously is continuous if the conditions (2.31) are satisfied.

If the averaging volume contains several grains then SG is the sum of the individual SG_i. The sum is continuously differentiable if each of the grains satisfies the first condition in Eq. (2.31), and g satisfies the other three conditions.

We now turn to the surface average function $\phi(t,x)$, defined by Eq. (2.26). We notice that ϕ is a continuous function of all its arguments, if the conditions (2.31) are satisifed and the surface function $\breve{\phi}(t,\zeta)$ is continuous with respect to time and piecewise continuous with respect to ζ. We assume that $\breve{\phi}$ possesses these properties and reformulate Eq. (2.26) as follows

$$\phi \sum_i (SG_i) = \sum_i \Big(\int_{s_{pi}} g \, \breve{\phi} \; dS \Big) \quad . \qquad (2.33)$$

The time derivative of the left-hand side of Eq. (2.33) is

$$L_t = \phi \frac{\partial}{\partial t}(SG) + (SG)\frac{\partial \phi}{\partial t} \quad . \tag{2.34}$$

The first term in this expression is continuous under our assumptions. Therefore, also the second term (and $\partial\phi/\partial t$) is continuous, if the time derivative of the right-hand side of Eq. (2.33) is continuous. The contribution of each term on the right-hand side of Eq. (2.33) to the time derivative is, via Eq. (2.30)

$$\begin{aligned} R_{ti} = & \int_{s_{pi}} (-\nabla_x g) \frac{\partial s}{\partial t} \tilde{\phi}\, Z\, d\zeta + \int_{s_{pi}} g \frac{\partial \tilde{\phi}}{\partial t} Z\, d\zeta \\ & + \int_{s_{pi}} g\tilde{\phi} \frac{\partial Z}{\partial t} d\zeta + \Big[\int_{s_{pi}\cap S_v} g\, \tilde{\phi}\, Z\, dC \Big] \frac{\partial C}{\partial t} \quad . \end{aligned} \tag{2.35}$$

R_{ti} is a continuous function of x and t if in addition to the condition (2.31) $\tilde{\phi}$ also satisfies the condition

$\frac{\partial \tilde{\phi}}{\partial t}$ is a continuous function of t and a piecewise continuous function of ζ on each s_{pi}. (2.36)

Because ϕ and $(SG)_t$, in Eq. (2.34), are continuous functions if (2.31) and (2.36) are satisfied, these conditions are sufficient to insure that $\phi(t,x)$ is continuously differentiable with respect to time.

In order to investigate the spacial differentiability of $\phi(t,x)$ we differentiate Eq. (2.33) with respect to x. On the left-hand side we obtain

$$L_x = \phi \nabla_x (SG) + (SG)\nabla_x \phi \quad . \tag{2.37}$$

On the right-hand side of Eq. (2.33), each summand produces the expression

$$R_{xi} = \int_{s_{pi}} (\nabla_x g)\, \breve{\phi}\, Z\, d\zeta + \Big[\int_{s_{pi} \cap S_v} g \breve{\phi}\, Z\, dC \Big] \nabla_x C \quad . \tag{2.38}$$

R_{xi} is continuous if the conditions (2.31) are satisfied. Because $\phi \nabla_x (SG)$ is continuous, the conditions are sufficient for continuous differentiability of ϕ with respect to the spacial coordinate.

Second order spacial derivatives of surface averaged quantities do not enter the governing equations. Therefore, we do not formulate existence condition for these derivatives.

2.2.5 Differential Equation for Surface Averages.

All surface averages satisfy a differential equation for material properties. We shall derive the equation in this section.

Let $U(t,x)$ be an arbitrary velocity vector and let g satisfy the conditions (2.31). Then one can combine Eqs. (2.30) and (2.32) obtaining for the sum SG of all individual SG_i.

$$\frac{\partial}{\partial t}(SG) + U \nabla_x (SG) = \int_{S_p} (\nabla_x g) \cdot \Big(U - \frac{\partial s}{\partial t}\Big) Z\, d\zeta + \int_{S_p} g \frac{\partial Z}{\partial t}\, d\zeta \quad . \tag{2.39}$$

The integrals on the right-hand side are taken over S_p, i.e., over all grain surfaces contained in the averaging volume.

A corresponding formula can be derived for the product $(SG)\,\phi$ from Eqs. (2.34), (2.35), (2.37), and (2.38) with the result

$$\begin{aligned} \frac{\partial}{\partial t}\big((SG)\,\phi\big) + U \nabla_x\big((SG)\,\phi\big) &= \int_{S_p} (\nabla_x g) \cdot \Big(U - \frac{\partial s}{\partial t}\Big) \breve{\phi}\, Z\, d\zeta \\ &\quad + \int_{S_p} g\, \breve{\phi} \frac{\partial Z}{\partial t}\, d\zeta + \int_{S_p} g \frac{\partial \breve{\phi}}{\partial t} Z\, d\zeta \quad . \end{aligned} \tag{2.40}$$

Next, we eliminate the derivatives of SG between Eqs. (2.39) and (2.40), obtaining the differential equation

$$\begin{aligned} \frac{\partial \phi}{\partial t} + U \nabla_x \phi &= \frac{1}{SG} \int_{S_p} g \frac{\partial \breve{\phi}}{\partial t} Z\, d\zeta - \frac{1}{SG} \int_{S_p} (\breve{\phi} - \phi) \Big(U - \frac{\partial s}{\partial t}\Big) \cdot (\nabla_\xi g)\, Z\, d\zeta \\ &\quad + \frac{1}{SG} \int_{S_p} (\breve{\phi} - \phi) g \frac{\partial Z}{\partial t}\, d\zeta \quad . \end{aligned} \tag{2.41}$$

The first integral on the right-hand side of Eq. (2.41) is by definition the surface average of $\partial\tilde{\phi}/\partial t$. The other two integrals are generally assumed to be small and neglected for interior ballistics problems. We notice that both integrals vanish if $\phi = \tilde{\phi}$ on the propellant surface, i.e., if the property $\tilde{\phi}$ is identical for all grains. If U is taken as the average grain velocity, the term $U-\partial s/\partial t$ may be small, e.g., if all grains have the same velocity and do not burn, because $\partial s/\partial t$ is equal to the sum of the local grain velocity and local surface regression velocity. The term $\partial Z/\partial t$ is zero if the grains are not burning.

If we neglect the last two integrals in Eq. (2.41) and use Eq. (2.26) to define

$$\dot{\phi} = \frac{1}{SG} \int_{S_p} g \frac{\partial\tilde{\phi}}{\partial t} dS(\zeta) \tag{2.42}$$

then the differential equation, Eq. (2.41) simplifies to

$$\frac{\partial\phi}{\partial t} + U \nabla_x \phi = \langle\phi\rangle \quad , \tag{2.43}$$

where $\langle\phi\rangle$ is a model for $\dot{\phi}$.

For the velocity U one chooses the average grain velocity, assuming that by this choice one of the neglected terms can be kept small while not introducing another dependent variable.

2.3 Regions of Definition of Average Variables

In this section we describe regions of definition of the average functions. In principle, the averaging volume V can be of any shape and size. However, in order to preserve an axial symmetry of the averaged quantities, the volume V, the weight function g, and the reference point x associated with the location of the volume, all must be chosen with certain symmetry properties. Instead of trying to formulate a general averaging volume with the desired properties, we give two examples of admissible averaging volumes.

The simplest example of an averaging volume is a sphere with the reference point x in its center and a weight function that depends only on the distance from its center. Let the diameter of the sphere be ℓ.

Another example is an orthogonal circular cylinder with the reference point at its center and with an axis parallel to the axis of the gun tube. To be specific, we assume that the height of the cylinder is $2\ell/3$ if ℓ is the diameter of the cylinder. In this example, the weight function depends on the radial as well as on the axial coordinates within the cylinder, and the volume of the averaging volume is the same as that of the spherical averaging volume.

In both examples, the quantity ℓ is equal to a diameter of the averaging volume. In general, we may assume a characteristic length ℓ associated with any particular averaging volume. The size of the volume and, therefore, the size of ℓ, is restricted by two requirements. First, the averaging volume must fit inside the gun barrel and, second, we want it to be larger than the largest grain in order to insure that gas is present within every averaging volume. Let $\overset{*}{D}_p$ be the largest diameter of a grain and let D_{gun} be the inner diameter of the gun tube. Then in the two examples ℓ must satisfy the conditions

$$(\overset{*}{D}_p)_{max} < \ell < (D_{gun})_{min} \quad . \tag{2.44}$$

One would obtain similar restrictions for the characteristic length of any averaging volume. We assume that $\overset{*}{D}_p$ and D_{gun} are such that the inequalities in Eq. (2.44) can be satisfied by a margin if ℓ is properly chosen.

The position of the averaging volume (and its reference point) inside the gun tube is restricted. If a constant averaging volume intersects a boundary, then the sum of the gas volume fraction α, as defined by Eq. (2.3), and of the corresponding particle volume fraction is not equal to one. Consequently, the definition of averages by Eqs. (2.2) through (2.5) cannot be used if a non-zero intersection occurs, and the location of the averaging volume is restricted to positions without intersections between the averaging volume and boundaries. (See also Section 4.6) This means that the reference point x cannot be moved arbitrarily close to all boundaries. If the averaging volume is a sphere with the diameter ℓ, then x is restricted to locations that are at least $\ell/2$ away from the breech, the walls, and projectile base. In the second example (cylinder), x may be located at points that are at least $\ell/2$ away from the tube walls and $\ell/3$ away from the breech and from the projectile base. Consequently, because of the finite size of the averaging volume, none of the averaged quantities are defined in the boundary regions. If the grain diameter $\overset{*}{D}_p$ is large, then the regions where the averaged quantities are not defined can be a significant part of the interior of the gun tube.

In the remaining regions, the porosity α and all averages pertaining to gas properties are everywhere defined by Eqs. (2.3) and (2.4), respectively.

Average properties of propellant grains are defined by Eq. (2.5). The definition provides a value for the average function only if $\alpha < 1$, i.e., if there are grains within the averaging volume. The limitation also holds for surface averaged quantities, defined by Eq. (2.26). The surface averaged quantities are grain properties and they are defined only if there are grains within the averaging volume.

Another average dependent variable which is introduced in Section 4.2 is the weighted number $\overset{*}{m}$ of grains in the averaging volume that is defined by

$$\overset{*}{m}(t,x) = VG\,(1-\alpha)/v_p(\overset{*}{d}) \quad , \tag{2.45}$$

where $\overset{*}{d}$ is the average regression distance of the grains and $v_p(\overset{*}{d})$ is the corresponding grain volume, given by a correlation function. According to the definition, $\overset{*}{m}$ is indeterminate in regions without grains, because $\overset{*}{d}$ is not defined in those regions. We notice, however that $\overset{*}{m} \to 0$ and $\nabla_x \overset{*}{m} \to 0$ as x moves to a position where the averaging volume contains no grains. Therefore, we may define a continuation $\overset{*}{m} \equiv 0$ in regions without grains. With this extension, $\overset{*}{m}$ is defined in all those regions where gas properties are defined, i.e., everywhere, except in boundary regions.

2.4 Averaging Weight Function

The averaging weight function g(y) is defined inside the averaging volume V and on its boundary S_v. It has the following properties (see Sections 2.2.2, 2.2.3, and 2.2.4)

$$\left.\begin{array}{ll} g > 0 & \text{in } V \;, \\ g = 0 & \text{on } S_v \;, \\ \nabla g & \text{continuous in } V \text{ with possible exception of isolated} \\ & \text{singular points} \;, \\ \nabla g = 0 & \text{on } S_v \;. \end{array}\right\} \tag{2.46}$$

Next, we give examples of functions g(y) that satisfy these conditions for the two examples of averaging volumes mentioned in the previous section. Let $y = \xi - x$, i.e., let the point of origin of the coordinate vector y be at the center of the averaging volume. (In both our examples the center coincides with the reference point x.)

If V is a sphere with the diameter ℓ, then we may define the weight function by

$$g(y) = \frac{(2+n)\ (3+n)\ (4+n)}{6} \left(1 - \frac{|y|}{\ell/2}\right)^{1+n} \quad , \text{ for } -\frac{\ell}{2} < y < \ell/2 \qquad (2.47)$$

with an arbitrary n > 0. The weighted averaging volume VG is for this g(y)

$$VG = \int_V g\ dV = 4\pi \int_0^{\ell/2} g(y) y^2 dy = \frac{4}{3}\pi \left(\frac{\ell}{2}\right)^3 \quad . \qquad (2.48)$$

As a second example we chose a cylinder with the diameter ℓ and height $2\ell/3$. Let r and z be the radial and axial coordinates within the cylinder, with the point of origin at the center of the cylinder Then we may define with arbitrary positive m and n

$$g(r,z) = \frac{1}{2}\ (2+m)\ (2+n)\ (3+n) \left(1 - \frac{|z|}{\ell/3}\right)^{1+m} \left(1 - \frac{|r|}{\ell/2}\right)^{1+n} \quad . \qquad (2.49)$$

The weighted averaging volume VG is for this choice of g

$$VG = \int_V g\ dV = 4\pi \int_0^{\ell/3} \int_0^{\ell/2} g(r,z) r\ drdz = \frac{4}{3}\pi \left(\frac{\ell}{2}\right)^3 \quad , \qquad (2.50)$$

i.e., equal to the volume $|V|$ of the cylinder itself.

In both examples, we have weight functions with a maximum at the center of the averaging volume. The functions are continuous but their gradients possess discontinuities. The weight function for the spherical averaging volume has a discontinuous point at the center of the sphere. The second weight function has a singular gradient along the line r = 0 and on the plane z = 0. Therefore, if the flow includes phenomena that require surface averaging one should use a different weight function for the cylindrical averaging volume. (For volume averaging, piecewise continuity of ∇g is sufficient.)

The following two weight functions have no discontinuities. They are chosen such that the weighted averaging volume is the same as before, i.e., equal to the volume of a sphere with diameter ℓ.

A weight function example for a sphere is

$$g(r) = \frac{\pi^2}{\pi^2-4} [\cos (\pi \frac{r}{\ell/2}) + 1] \quad . \tag{2.51}$$

A weight function for the cylindrical averaging volume is

$$g(r,z) = \frac{\pi^2}{\pi^2-4} [\cos (\frac{r}{\ell/2}) + 1] [\cos (\frac{z}{\ell/3}) + 1] \quad . \tag{2.52}$$

Numerous other examples can be constructed, e.g., based on the functions

$$g(r) \approx (1 - (\frac{r}{\ell/2})^{2m})^{1+n} \tag{2.53}$$

$$g(r) \approx [\cos (\frac{\pi}{2} \frac{r}{\ell/2})]^{1+n} \tag{2.54}$$

and corresponding for the dependence on z. Particularly, functions of the type (2.53) with large integer m and small positive n have properties that are desirable according to Section 4.2.1.

3. CONSERVATION EQUATIONS

The mathematical description of a two-phase flow field is composed of two sets of local conservation equations (one for each phase), a set of local constitutive relations for each phase, and interfacial or jump conditions which relate locally the two phases only on the interfaces. As in other two-phase models of interior ballistics, all chemical reactions are excluded. Burning of the grains is represented by a transfer of mass, momentum, and energy from the solid phase to the gas phase. Furthermore, the effects of body forces on both phases are assumed to be negligible. By averaging the local conservation equations according to the definitions and formulas determined in Section 2, and by using the local interfacial conditions, we derive the coupled set of average two-phase equations. The details of this procedure are given in this section. The average equations in vector form are derived in three spatial dimensions and time. The governing equations for axially symmetric flow in cylindrical coordinates are listed in Appendix A.

3.1 Local Equations

3.1.1 Local Conservation Equations.

The flow field is assumed to be composed of two disjoint phases: gas and solid grains. The gas is assumed to be compressible, viscous and heat conducting. The local conservation equations for the gas are the Navier-Stokes equations (Tsien, pp. 3-16)[10]

$$\frac{\partial \check{\rho}}{\partial t} + \nabla\cdot(\check{\rho}\check{u}) = 0 \quad , \tag{3.1}$$

$$\frac{\partial (\check{\rho}\check{u}\check{e})}{\partial t} + \nabla\cdot(\check{\rho}\check{u}\check{u}) = -\nabla\check{p} + \nabla\cdot\check{\Pi} \quad , \tag{3.2}$$

$$\frac{\partial (\check{\rho}\check{e})}{\partial t} + \nabla\cdot(\check{\rho}\check{u}\check{e}) = -\check{p}\,\nabla\cdot\check{u} + \check{\Phi}_1 - \nabla\cdot\check{Q} \quad , \tag{3.3}$$

where $\check{\rho}$, $\check{e}$, and $\check{u}$ are the density, specific internal energy, and the velocity vector, respectively. The constitutive laws for the viscous stress tensor $\check{\Pi}$, the heat dissipation function $\check{\Phi}_1$, and the heat conduction vector $\check{Q}$ are

$$\check{\Pi} = 2\check{\mu}\check{E} + (\check{\lambda} - \frac{2}{3}\check{\mu})\,\nabla\cdot\check{u}\ I \quad , \tag{3.4}$$

$$\check{\Phi}_1 = 2\check{\mu}\ \check{E}:\check{E} + (\check{\lambda} - \frac{2}{3}\check{\mu})\ (\nabla\cdot\check{u})^2 \quad , \tag{3.5}$$

$$\check{Q} = -\check{\kappa}\ \nabla\check{T} \quad , \tag{3.6}$$

where

$$\check{E} = 0.5\ [\nabla\check{u} + (\nabla\check{u})^T] \quad , \tag{3.7}$$

and $\check{\mu}$, $\check{\lambda}$, $\check{\kappa}$ are the shear viscosity coefficient, the bulk viscosity coefficient and the heat conduction coefficient, respectively, that may depend on the local temperature $\check{T}$. The local pressure and temperature are given by equations of state of the form $\check{p} = \check{p}(\check{\rho},\check{e})$ and $\check{T} = \check{T}(\check{\rho},\check{e})$.

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[10] *H.S. Tsien, "The Equations of Gas Dynamics," in Fundamentals of Gas Dynamics," H.W. Emmons, ed., Princeton University Press, Princeton, NJ, 1958.*

Each solid grain is assumed to be incompressible (the density of a grain $\breve{\overset{*}{\rho}}$ = constant) but deformable. The local conservation equations for the solid phase can be expressed in a form similar to those of Eqs. (3.1) and (3.2) (Prager)[11]

$$\frac{\partial}{\partial t}(\breve{\overset{*}{\rho}}) + \nabla\cdot(\breve{\overset{*}{\rho}}\,\breve{\overset{*}{u}}) = 0 \quad , \tag{3.8}$$

$$\frac{\partial}{\partial t}(\breve{\overset{*}{\rho}}\,\breve{\overset{*}{u}}) + \nabla\cdot(\breve{\overset{*}{\rho}}\,\breve{\overset{*}{u}}\,\breve{\overset{*}{u}}) = \nabla\cdot\breve{\overset{*}{\Pi}} \quad , \tag{3.9}$$

where $\breve{\overset{*}{u}}$ is the local velocity vector of the grain. For our purposes, the solid phase stress tensor $\breve{\overset{*}{\Pi}}$ represents the total stress within the solid grain. A constitutive law for $\breve{\overset{*}{\Pi}}$ could be based on Hooke's law. Although the local angular momentum of the grains could be significant, it is assumed that the average effect of the angular momentum is small and can be neglected. Consequently, the local conservation equation for the angular momentum of a grain is omitted.

3.1.2 Local Interfacial Conditions. The interfacial conditions relate the two disjoint phases. The interface between the gas and solid is considered a singular surface across which mass, momentum and energy is transferred. The conditions that are valid on the interface can be expressed as (Truesdell and Toupin)[7]:

$$n\cdot\breve{\rho}(\breve{u} - \breve{u}_{sp}) = n\cdot\breve{\overset{*}{\rho}}(\breve{\overset{*}{u}} - \breve{u}_{sp}) \quad , \tag{3.10}$$

$$n\cdot\breve{\rho}(\breve{u} - \breve{u}_{sp})\,\breve{u} + n\,\breve{p} - n\cdot\breve{\Pi} = n\cdot\breve{\overset{*}{\rho}}(\breve{\overset{*}{u}} - \breve{u}_{sp})\,\breve{\overset{*}{u}} - n\cdot\breve{\overset{*}{\Pi}} \quad , \tag{3.11}$$

$$\begin{aligned} &n\cdot\breve{\rho}(\breve{u} - \breve{u}_{sp})\,[\breve{e} + \tfrac{1}{2}\breve{u}\cdot\breve{u}] + \breve{p}\,n\cdot\breve{u} + n\cdot\breve{Q} - n\cdot\breve{\Pi}\cdot\breve{u} \\ &\qquad = n\cdot\breve{\overset{*}{\rho}}(\breve{\overset{*}{u}} - \breve{u}_{sp})\,[\breve{\overset{*}{e}} + \tfrac{1}{2}\breve{\overset{*}{u}}\cdot\breve{\overset{*}{u}}] + n\cdot\breve{\overset{*}{Q}} - n\cdot\breve{\overset{*}{\Pi}}\cdot\breve{\overset{*}{u}} \quad , \end{aligned} \tag{3.12}$$

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[11] *W. Prager, Introduction to Mechanics of Continua, Ginn and Company, New York, 1961.*

where $\breve{u}_{sp}$ is the local interface velocity, n is a unit normal, and $\overset{*}{\breve{Q}}$ is the local heat conduction vector within the grain.

The local interface velocity $\breve{u}_{sp}$ is defined in terms of the local regression rate $\dot{\breve{d}}$ of the grain surface

$$\breve{u}_{sp}\big(t,\xi(\zeta)\big) = \overset{*}{\breve{u}}\big(t,\xi(\zeta)\big) + n_{sp}\,\dot{\breve{d}}\big(t,\xi(\zeta)\big) \quad , \tag{3.13}$$

where ζ is the surface coordinate vector, $\dot{\breve{d}} > 0$ and n_{sp} is the unit normal to the grain, outward with respect to the gas.

3.2 Averaging of the Local Conservation Equations

3.2.1 Derivations of the Average Gas Continuity Equation and Porosity Equation.

To derive the average gas phase continuity equation, we multiply Eq. (3.1) by $\beta(t,\xi)g(\xi-x)$, integrate over the averaging volume $V(x)$ and obtain

$$\int_{V(x)} \beta(t,\xi)g(\xi-x)\,\frac{\partial\breve{\rho}(t,\xi)}{\partial t}\,dV(\xi) + \int_{V(x)} \beta(t,\xi)g(\xi-x)\,\nabla_\xi\cdot[\rho(t,\xi)\breve{u}(t,\xi)]\,dV(\xi) = 0 \quad . \tag{3.14}$$

Using formulas (2.9) and (2.21) with respect to the first and second integrals of (3.14), respectively, we have

$$\frac{\partial}{\partial t}\int_V \beta g\breve{\rho}\,dV + \nabla_x\cdot\int_V \beta g\breve{\rho}\breve{u}\,dV + \int_{S_p} g\,\breve{\rho}\,(\breve{u}-\breve{u}_{sp})\cdot n_{sp}\,dS = 0 \quad . \qquad ((3.15)$$

By the definition of a volume averaged quantity (2.4) and the interfacial mass flux condition (3.10), Eq. (3.15) can be written as

$$\frac{\partial}{\partial t}\big(\alpha(t,x)\rho(t,x)\big) + \nabla\cdot\big(\alpha(t,x)\boxed{\rho u}(t,x)\big) + \frac{\overset{*}{\rho}}{VG}\int_{S_p} g(\overset{*}{\breve{u}}-\breve{u}_{sp})\cdot n_{sp}\,dS = 0 \quad , \tag{3.16}$$

because $\check{\overset{*}{\rho}} = \overset{*}{\rho}$ = constant and VG = constant. In Eq. (3.16) ρ is the average gas density and the quantity $\boxed{\rho u}$ is the average of the gas momentum density $\check{\rho}\check{u}$. We define the average gas velocity vector u as the ratio

$$u(t,x) \equiv \frac{\boxed{\rho u}\ (t,x)}{\rho(t,x)} \quad . \tag{3.17}$$

Using this definition of u, the local regression rate, defined by Eq. (3.13), and the definition of the average surface function (2.26), we can rewrite the average gas continuity Eq. (3.16) as

$$\frac{\partial}{\partial t}\,[\alpha(t,x)\rho(t,x)] + \nabla\cdot[\alpha(t,x)\rho(t,x)u(t,x)] = \overset{*}{\rho}\,\frac{SG(t,x)}{VG}\,\dot{d}(t,x)\,. \tag{3.18}$$

The derivation of the average solid phase continuity equation proceeds in a similar fashion to that of the average gas continuity equation. Multiplying Eq. (3.8) by $(1-\beta)g$, integrating over V(x), invoking formulas (2.10) and (2.22), and using the definition (2.5) of an average solid grain property, and (3.13) of the local regression rate, we have

$$\frac{\partial}{\partial t}\left(VG(1-\alpha)\overset{*}{\rho}\right) + \nabla\cdot\left(VG(1-\alpha)\ \boxed{\overset{**}{\rho u}}\right) - \overset{*}{\rho}\int_{S_p} g\ \check{\dot{d}}\ dS = 0 \quad . \tag{3.19}$$

Using the surface average definition (2.26) and the fact that $\overset{*}{\rho}$ is a constant, Eq. (3.19) can be written as

$$\frac{\partial}{\partial t}\,(1-\alpha) + \nabla\cdot[(1-\alpha)\overset{*}{u}] = \frac{SG}{VG}\,\dot{d} \quad . \tag{3.20}$$

Hence, for incompressible solid grains, the average continuity equation for the solid phase, Eq. (3.20), is the governing equation for the porosity α.

We notice that, if the density is constant or depends only on time, then the average velocity is given directly by Eq. (2.5), e.g., $\overset{*}{u}$. The different definition of the average gas velocity via the average momentum density by Eq. (3.17) is advantageous when the density depends on the spatial coordinate.

The average gas continuity equation, Eq. (3.18), is coupled to the solid phase by the source term $\overset{*}{\rho}(SG/VG)\dot{d}$. As expected, the amount of mass added to the gas phase is exactly the amount liberated from the solid phase. If the grains are not regressing (not burning), then the average regression rate $\dot{d}$ and the source term are zero. The surface average

SG and the surface average regression rate $\dot{d}$ are two new unknowns. To restrict the number of unknowns, $\dot{d}$ is replaced by a correlation (denoted by $\langle \dot{d} \rangle$) which is obtained from experiments (see Section 4.7.7). To understand the error involved in such a substitution, we rewrite Eq. (3.18) as

$$\begin{aligned} \frac{\partial}{\partial t}[\alpha\rho] + \nabla\cdot[\alpha\rho u] &= \overset{*}{\rho}\,\frac{SG}{VG}\,\langle \dot{d}(t,x)\rangle \\ &\quad + \overset{*}{\rho}\,\frac{SG}{VG}\Big[\frac{1}{SG}\int_{S_p} g(\xi(\zeta)-x)\,\dot{d}(t,\xi(\zeta))\,dS(\zeta) - \langle \dot{d}(t,x)\rangle\Big] \quad . \end{aligned} \tag{3.21}$$

The bracketed term on the right-hand side of Eq. (3.21) is the error term and is equal to

$$\frac{1}{SG}\sum_i \Big[\check{\dot{d}}\,(t,\xi(\hat{\zeta}_i)) \int_{s_{pi}} g(\xi(\zeta)-x)\,dS(\zeta)\Big] - \langle \dot{d}(t,x)\rangle \tag{3.22a}$$

by the mean value theorem for multiple integrals (Apostol)[12] and where $\hat{\zeta}_i$ is some point on s_{pi}. From expression (3.22a), the following inequality can be derived:

$$\Big|\frac{1}{SG}\int_{S_p} g\,\check{\dot{d}}\,dS(\zeta) - \langle \dot{d}\rangle\Big| \leqslant \max_i\Big|\check{\dot{d}}(t,\xi(\zeta_i)) - \langle \dot{d}(t,x)\rangle\Big| \quad . \tag{3.22b}$$

Thus, a sufficient condition for the error to be small is that the difference between the local regression rate $\dot{d}$ over each surface and the value of the correlation $\langle \dot{d} \rangle$ at point x is small. A common expression for $\langle \dot{d} \rangle$ is given by Eq. (4.100). If the error given by Eq. (3.22a) is not small, another correlation for $\langle \dot{d} \rangle$ must be used. In practice, the error is assumed small and Eqs. (3.18) and (3.20) are written with $\dot{d}$ replaced by $\langle \dot{d} \rangle$. Furthermore, an additional formal error could be introduced by the modeling of SG. However, this is avoided by the definition of $\overset{*}{m}$ in terms of SG (see Section 4.7.8).

3.2.2 Derivations of the Average Gas and Solid Momentum Equations.

The average gas momentum equation is derived by multiplying the local momentum equation, Eq. (3.2), by the function βg, by integrating over the

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[12] *T. Apostol, Mathematical Analysis, 1st, Ed., Addison-Wesley Publishing Co., Inc., New York, 1957.*

averaging volume V(x) and by applying formulas (2.9) and (2.21). The results of these operations can be written as

$$\frac{\partial}{\partial t}\int_V \beta g\, \breve{\rho}\breve{u}\; dV - \int_{S_p} g\, \breve{\rho}\breve{u} n_{sp}\cdot \breve{u}_{sp}\; dS + \nabla_x \cdot \int_V \beta g\, \breve{\rho}\breve{u}\breve{u}\; dV$$

$$+ \int_{S_p} g\; n_{sp}\cdot\breve{\rho}\breve{u}\breve{u}\; dS = -\nabla_x \int_V \beta g\; \breve{p}\; dV + \nabla_x\cdot\int_V \beta g\; \breve{\Pi}\; dV \qquad (3.23)$$

$$- \int_{S_p} g\; (n_{sp}\breve{p} - n_{sp}\cdot\breve{\Pi})\; dS \quad .$$

We use the definition of an average gas property (2.4) and the definition of u (3.17) in Eq. (3.23) to obtain

$$\frac{\partial}{\partial t}\,[\alpha(t,x)\rho(t,x)u(t,x)] + \nabla\cdot[\alpha(t,x)\;\boxed{\rho u u}\,(t,x)]$$

$$= -\nabla\left\{\frac{1}{VG}\int_V \beta g\breve{p}\; dV\right\} + \nabla\cdot\left\{\frac{1}{VG}\int_V \beta g\breve{\Pi}\; dV\right\} \qquad (3.24)$$

$$- \frac{1}{VG}\int_{S_p} g\left\{n_{sp}\breve{p} - n_{sp}\cdot\breve{\Pi} + n_{sp}\cdot\breve{\rho}\,[\breve{u} - \breve{u}_{sp}]\;\breve{u}\right\}\; dS \quad .$$

The term $\boxed{\rho u u}\,(t,x)$ represents the average of the tensor $\breve{\rho}\breve{u}\breve{u}$. Because the average quantities ρ and u are already defined, we can denote the fluctuations of the values of the local variables from the value of the average variables as

$$\breve{\rho}'(t,\xi,x) = \breve{\rho}(t,\xi) - \rho(t,x) \quad ,$$

and (3.25)

$$\breve{u}'(t,\xi,x) = \breve{u}(t,\xi) - u(t,x) \quad .$$

If we substitute formulas (3.25) into the integral representation of $\alpha\boxed{\rho u u}$, we obtain

$$\frac{1}{VG}\int_V \beta g\; \breve{\rho}\breve{u}\breve{u}\; dV = \alpha\rho u u + \frac{1}{VG}\int_V \beta g\; \breve{\rho}\breve{u}'\breve{u}'\; dV \quad . \qquad (3.26)$$

The difference between the first term on the right-hand side of Eq. (3.26) and the left-hand side, involves a volume average of the product of velocity fluctuations. We define this difference as the turbulent stress tensor of the flow. Thus, turbulence in this report is defined as volume averaged fluctuations. The turbulent stress tensor Π_T models the quantity

$$-\frac{1}{\alpha}\frac{1}{VG}\int_V \beta g\, \check{\rho}\check{u}'\check{u}'\, dV = \rho uu - \boxed{\rho uu} \quad . \tag{3.27}$$

We shall not discuss particular turbulence models in this report. A model is proposed in Gibeling et al.[5] Using the integral representation of $\boxed{\rho uu}$ and applying the mean value theorem for multiple-integrals (Apostol),[12] we can rewrite the right-hand side of Eq. (3.27) when V_{gas} is a connected set as

$$[u(t,x)u(t,x) - \check{u}(t,\xi)\check{u}(t,\xi)]\,\rho(t,x) \quad , \tag{3.28}$$

where ξ lies in V_{gas} and is different for each component of the tensor $\check{u}\check{u}$. From Eq. (3.28), a good model of the turbulent stress tensor for compressible flows is one which models the significant differences between the tensors uu and $\check{u}\check{u}$. With respect to the errors generated by such a model Π_T in Eq. (3.24), we want the errors in the vector

$$\nabla\cdot\left\{\alpha\Pi_T - \left[\alpha\rho uu - \alpha\boxed{\rho uu}\right\}\right. \tag{3.29}$$

to be minimized by the model.

Substituting Eq. (3.27) into Eq. (3.24), using Eq. (3.13), and algebraically manipulating the result, we have

$$\begin{aligned}
\frac{\partial}{\partial t}[\alpha\rho u] + \nabla\cdot[\alpha\rho uu] = {} & -\alpha\nabla p + \nabla\cdot(\alpha\Pi) + \nabla\cdot(\alpha\Pi_T) \\
& + \overset{*}{\rho}\,\frac{SG}{VG}\,\overset{*}{u}\langle\dot{d}\rangle - \Big[\frac{1}{VG}\int_{S_p} g(n_{sp}\breve{p} - n_{sp}\cdot\breve{\Pi})dS + p\,\nabla\alpha\Big] \\
& - \Big\{\frac{1}{VG}\int_{S_p} g\big[n_{sp}\cdot\breve{\rho}(\breve{u}-\breve{u}_{sp})\breve{u} - n_{sp}\cdot\breve{\overset{*}{\rho}}(\breve{\overset{*}{u}}-\breve{u}_{sp})\breve{\overset{*}{u}}\big]\,dS\Big\} \\
& + \Big\{\frac{1}{VG}\int_{S_p} \overset{*}{\rho}\,\breve{\dot{d}}\,\breve{\overset{*}{u}}\,dS - \frac{SG}{VG}\,\overset{*}{u}\langle d\rangle\Big\} \qquad (3.30) \\
& + \Big\{\nabla\cdot\Big[\frac{1}{VG}\int_{V} \beta g(\rho uu - \breve{\rho}\breve{u}\breve{u})\,dV - \alpha\Pi_T\Big]\Big\} \\
& - \Big\{\nabla\Big[\frac{1}{VG}\int_{V} \beta g\breve{p}\,dV - \alpha p\Big]\Big\} \\
& + \nabla\cdot\Big[\frac{1}{VG}\int_{V} \beta g\breve{\Pi}\,dV - \alpha\Pi\Big]\Big\} \quad ,
\end{aligned}$$

where p and Π are the constitutive models for the average pressure defined by $[\int_V \beta g\breve{p}dV]/[\alpha\cdot VG]$ and the average viscous stress tensor defined by $[\int_V \beta g\breve{\Pi}dV]/(\alpha\cdot VG]$, respectively. In general, it is simpler to model the average pressure and viscous stress tensor than to actually integrate the local constitutive laws. Each term in Eq. (3.30) which is enclosed by braces is an error term. We now shall discuss each error.

The errors in the models p, Π, Π_T, and those introduced by $\overset{*}{u}\langle\dot{d}\rangle$ are represented by the last four terms on the right-hand side of Eq. (3.30). If V_{gas} is connected, the errors in the last two terms can be written as

$$\nabla_x\Big[\frac{1}{VG}\int_V \beta g p\,dV - \alpha p\Big] = \nabla\big\{\alpha(t,x)\,\big[p\big(t,\hat{\xi}(x)\big) - p\big(t,x\big)\big]\big\} \qquad (3.31)$$

and

$$\nabla_x\cdot\Big[\frac{1}{VG}\int_V \beta g\breve{\Pi}\,dV - \alpha\Pi\Big] = \nabla\cdot\big\{\alpha(t,x)\big[\breve{\Pi}\big(t,\hat{\xi}(x)\big) - \Pi\big(t,x\big)\big]\big\} \quad , \qquad (3.32)$$

where $\hat{\xi}(x)$ are the mean value points in $V_{gas}(t,x)$ which, in general, are different for p and for each components of the tensor $\breve{\Pi}$. The models p and Π as well as the errors (3.31) and (3.32) are discussed in Sections 4.7.1

and 4.7.2, respectively. For the gas momentum equation, the best approximations for p and Π are the ones which minimize both the differences in their values and their derivatives.

The error in the turbulence model was discussed previously in this section.

The second braced term in Eq. (3.30) can be written as

$$\overset{*}{\rho}\,\frac{SG}{VG}\left\{\sum_i \frac{1}{SG}\int_{sp_i} g\,\breve{\overset{*}{u}}(t,\xi(\zeta))\,\breve{\dot{d}}(t,\xi(\zeta))\,dS(\zeta) - \overset{*}{u}(t,x)\,\langle\dot{d}(t,x)\rangle\right\} \quad .(3.33)$$

If both, $\breve{\overset{*}{u}}$ and $\breve{\dot{d}}$ which are defined on the grain surface are functions of t only, then expression (3.33) is zero and no error exists. When this is not the case, one can bound (3.33) using the mean value theorem for multiple integrals by

$$\left|\overset{*}{\rho}\,\frac{SG}{VG}\right| \max_i \left|\breve{\overset{*}{u}}(t,\xi(\zeta_i))\,\dot{d}(t,x) - \overset{*}{u}(t,x)\,\langle\dot{d}(t,x)\rangle\right| \quad , \qquad (3.34)$$

where ζ_i is different on each surface sp_i. Expression (3.34) can be bounded by

$$\left|\overset{*}{\rho}\,\frac{SG}{VG}\right| \left\{\dot{d}(t,x)\max_i\left|\breve{\overset{*}{u}}(t,\xi(\zeta_i)) - \overset{*}{u}(t,x)\right| + \left|\overset{*}{u}(t,x)\right|\left|\langle\dot{d}(t,x)\rangle - \dot{d}(t,x)\right|\right\} \; . \qquad (3.35)$$

Thus, the error in replacing $\frac{1}{SG}\int_{Sp} g\breve{\overset{*}{u}}\,\dot{d}\;dS$ with $\overset{*}{u}\langle\dot{d}\rangle$ consists of two parts. One error involves the approximation of $\dot{d}$ with $\langle\dot{d}\rangle$ and is discussed in Section 3.2.1. The other term is small if the values of the local particle velocity at the grain surfaces are near that of the average particle velocity at x; that is if the fluctuations are small. If both terms are not small, then a correlation of the fluctuations $\breve{\overset{*}{u}}\,\breve{\dot{d}}'$ must be modeled and included in Eq. (3.30).

The term

$$\frac{1}{VG}\int_{S_p} g\left[n_{sp}\cdot\breve{\rho}(\breve{u}-\breve{u}_{sp})\breve{u} - n_{sp}\cdot\breve{\overset{*}{\rho}}(\breve{\overset{*}{u}}-\breve{u}_{sp})\breve{\overset{*}{u}}\right] dS \qquad (3.36)$$

can be rewritten using the mass flux jump Eq. (3.10) and regression rate definition (3.13) as

$$-\overset{*}{\rho}\,\frac{1}{VG}\int_{S_p} g\,(\check{u}-\check{\overset{*}{u}})\,\check{\dot{d}}\,dS \quad , \tag{3.37}$$

or using the momentum flux jump Eq. (3.11) as

$$\frac{1}{VG}\int_{S_p} g\left[(n_{sp}\cdot\check{\Pi} - n_{sp}\,\check{p}) - n_{sp}\cdot\check{\overset{*}{\Pi}}\right] dS \quad . \tag{3.38}$$

On the interface between the gas and the particles, we assume either that the normal stresses are equal (the integrand in Eq. (3.38) is zero), or equivalently, that the gas and particle velocities are equal (the difference in the integrand in Eq. (3.37) is zero). In the special case of no burning $\check{\dot{d}} = 0$, the error is zero. When the above assumption is not true, the expression (3.36) must be modeled by a correlation.

From Eq. (2.21) with $\check{\phi} = 1$, we have the relationship

$$\nabla\alpha = -\frac{1}{VG}\int_{S_p} g n_{sp}\,dS \quad . \tag{3.39}$$

Using the formula (3.39), we have the equality

$$\begin{aligned} &\frac{1}{VG}\int_{S_p} g[n_{sp}\check{p} - n_{sp}\cdot\check{\Pi}]\,dS + p\nabla\alpha \\ &= \frac{1}{VG}\int_{S_p} g[n_{sp}(\check{p} - p) - n_{sp}\cdot\check{\Pi}]\,dS \quad . \end{aligned} \tag{3.40}$$

We define the surface integral on the right-hand side of Eq. (3.40) as the drag force. The drag force is modeled by the correlation D which is discussed in Section 4.7.5. The error incurred by this approximation is

$$\left\{\int_{S_p} g[n_{sp}(\check{p} - p) - n_{sp}\cdot\check{\Pi}]\,dS - D(t,x)\right\} \quad . \tag{3.41}$$

This definition is consistent with Ishii's[13] development but is different from Gibeling et al.[5] and Gough's[1] which is defined in terms of the surface integral of the weighted fluctuation of the normal total gas stress tensor; $n_{sp}\cdot(\Pi-\breve{\Pi}) - n_{sp}(p-\breve{p})$. For the special case when the average viscous stress tensor is zero (the inviscid two-phase model), our definition and those of Gibeling et al.[5] and Gough[1] agree. We recognize the fact that Eq. (3.41) is a formal definition which may not correspond to an experimentally determined drag force. In such a case, other effects included in the experimental drag force would have to be subtracted to obtain the correlation corresponding to D.

The derivation of the average solid phase momentum equation parallels that for the average gas momentum equation. We multiply Eq. (3.9) by $(1-\beta)g$, integrate over the averaging volume V, use formulas (2.10) and (2.22) and the definition of the average of a solid grain property (2.5) to obtain

$$\frac{\partial}{\partial t}\left[\left(1-\alpha(t,x)\right)\boxed{\overset{**}{\rho u}}(t,x)\right] + \nabla\cdot\left[\left(1-\alpha\right)\boxed{\overset{***}{\rho uu}}(t,x)\right]$$

$$= \nabla_x\cdot\left\{\frac{1}{VG}\int_V (1-\beta)g\breve{\overset{*}{\Pi}}(t,\xi)\,dV\right\} \tag{3.42}$$

$$+\int_{S_p} g\, n_{sp}\cdot\breve{\overset{*}{\rho}}(\breve{\overset{*}{u}}-\breve{u}_{sp})\breve{\overset{*}{u}}\,dS - \int_{S_p} g\, n_{sp}\cdot\breve{\overset{*}{\Pi}}\,dS \quad .$$

Because $\overset{*}{\rho}$ is a constant, $\boxed{\overset{**}{\rho u}}(t,x) = \overset{*}{\rho}\,\overset{*}{u}(t,x)$ and $\boxed{\overset{***}{\rho uu}}(t,x) = \overset{*}{\rho}\,\boxed{\overset{**}{uu}}(t,x)$. By adding and subtracting $\nabla[(1-\alpha)p]$, by using Eq. (3.39), and replacing $n_{sp}\cdot\breve{\overset{*}{\Pi}}$ on the surface with its equivalent via the momentum flux interfacial jump condition (3.11), we can rewrite Eq. (3.42) as

---

[13] M. Ishii, *Thermo-Fluid Dynamic Theory of Two-Phase Flow,* Eyrolles, France 1975.

$$
\begin{aligned}
\frac{\partial}{\partial t}[(1-\alpha)\overset{**}{\rho u}] + \nabla\cdot[(1-\alpha)\overset{*}{\rho}\boxed{\overset{**}{uu}}] &= -(1-\alpha)\nabla p \\
&+ \nabla_x\cdot\{\frac{1}{VG}\int_V (1-\beta)g\breve{\overset{*}{\Pi}}\, dV + (1-\alpha)\, pI\} \\
&+ \frac{1}{VG}\int_{S_p} g\; n_{sp}\cdot\breve{\overset{*}{\rho}}(\breve{\overset{*}{u}}-\breve{u}_{sp})\breve{\overset{*}{u}}\, dS \\
&+ \frac{1}{VG}\int_{S_p} g[n_{sp}\breve{p} - n_{sp}p - n_{sp}\cdot\breve{\Pi}]\, dS \\
&+ \frac{1}{VG}\int_{S_p} g[n_{sp}\cdot\breve{\rho}(\breve{u}-\breve{u}_{sp})\breve{u} - u_{sp}\cdot\breve{\overset{*}{\rho}}(\breve{\overset{*}{u}}-\breve{u}_{sp})\breve{\overset{*}{u}}]\, dS \quad ,
\end{aligned}
\tag{3.43}
$$

where I is the identity tensor. Eq. (3.43) can be rewritten as

$$
\begin{aligned}
\frac{\partial}{\partial t}[(1-\alpha)\overset{**}{\rho u}] + \nabla\cdot[(1-\alpha)\overset{***}{\rho uu}] &= -(1-\alpha)\nabla p + \nabla\cdot[(1-\alpha)\overset{*}{\Pi}] \\
&+ \nabla\cdot[(1-\alpha)\overset{*}{\Pi}_T] - \overset{*}{\rho}\,\frac{SG}{VG}\,\overset{*}{u}\,\langle\dot{d}\rangle + \frac{1}{VG}\, D \\
&+ \{\frac{1}{VG}\int_{S_p} g[n_{sp}\cdot\breve{\rho}(\breve{u}-\breve{u}_{sp})\breve{u} - n_{sp}\cdot\breve{\overset{*}{\rho}}(\breve{\overset{*}{u}}-\breve{u}_{sp})\breve{\overset{*}{u}}]\, dS\} \\
&+ \{\frac{1}{VG}\int_{S_p} gn_{sp}\cdot\breve{\overset{*}{\rho}}(\breve{\overset{*}{u}}-\breve{u}_{sp})\breve{\overset{*}{u}}\, dS + \overset{*}{\rho}\,\frac{SG}{VG}\,\overset{*}{u}\langle\dot{d}\rangle\} \\
&+ \{\nabla\cdot[\overset{*}{\rho}(1-\alpha)\;(\overset{**}{uu}-\boxed{\overset{**}{uu}}\,) - (1-\alpha)\,\overset{*}{\Pi}_T]\} \\
&+ \{\nabla\cdot[(\frac{1}{VG}\int_V (1-\beta)g\,\breve{\overset{*}{\Pi}}\, dV + (1-\alpha)pI - (1-\alpha)\overset{*}{\Pi}]\} \\
&+ \{\nabla\cdot[(\frac{1}{VG}\int_{S_p} g[n_{sp}(\breve{p}-p) - n_{sp}\cdot\breve{\Pi}]\, dS - \frac{1}{VG}\, D\}
\end{aligned}
\tag{3.44}
$$

where $\overset{*}{\Pi}$ is the constitutive model for the average stress tensor for the solid phase and represents

$$
\frac{1}{1-\alpha}\,\frac{1}{VG}\int_V (1-\beta)g\,\breve{\overset{*}{\Pi}}\, dV + pI \quad ,
\tag{3.45}
$$

and $\overset{*}{\Pi}_T$ is the constitutive model for the average solid phase turbulent stress tensor. In analogy to Π_T, $\overset{*}{\Pi}_T$ models the tensor (see Eq. (3.27))

$$\overset{*}{u}(t,x)\overset{*}{u}(t,x) - \boxed{\overset{**}{uu}}(t,x) = -\frac{1}{1-\alpha}\frac{1}{VG}\int_V (1-\beta)g\,\overset{\sim}{\overset{*}{u}}{}'\,\overset{\sim}{\overset{*}{u}}{}'\,dV \quad . \qquad (3.46)$$

We recall that by definition $\overset{\sim}{\overset{*}{\Pi}}$ denotes the total stress tensor for the solid grain. The quantity defined by Eq. (3.45) is the difference between the average total stress in the solid phase (the integral of $(1-\beta)g\overset{\sim}{\overset{*}{\Pi}}/VG$ over the averaging volume) and the stress caused by the average gas pressure ($-pI$). The resulting stress is the stress caused by the grains themselves, for example, by the compactification of the propellant bed. Consequently, we call the expression (3.45), the average intergranular stress, and $\overset{*}{\Pi}$ the average intergranular stress model. As with the average pressure, viscous stress tensor, and turbulent gas stress tensor, it is simpler to separately model the intergranular stress, the solid phase turbulent stress, and the drag. The errors incurred by these models are represented by the last three braced terms in Eq. (3.44).

The remaining error terms in Eq. (3.44) (those enclosed by braces) are the surface integral involving the velocity or stress jump, and the surface integral representing the source term. These terms are discussed in the derivation of the average gas momentum equation (see the analyses beginning near Eqs. (3.36) and (3.33), respectively).

3.2.3 <u>Derivation of the Average Gas Internal Energy Equation</u>. The average internal energy is needed to compute certain quantities, e.g., the pressure and temperature via the equations of state for the average quantities. The average internal energy can be obtained in either of two ways. First, by adding the local internal energy equation to the equation for the local kinetic energy, an equation for the local total energy can be written. Following a similar procedure to those given in Sections 3.2.1 and 3.2.2, we then can derive an average total energy equation. Finally, the average internal energy value is obtained as the difference between the average total energy, and the average kinetic energy determined from the average velocities. The second way is to average the local internal energy equation, Eq. (3.3), directly. The former procedure is the most common. However, we use the latter approach because several terms which must be assumed small or modeled by additional correlations can be avoided, and the terms which must be modeled, have simpler physical interpretations, and therefore, are easier to model. An example of a term that can be eliminated by the second method but is present in the first is

$$\int_V \beta(t,\xi)\, g(\xi-x)\, \left[\check{\rho}(t,\xi)\check{u}(t,\xi)\cdot\check{u}(t,\xi) - \rho(t,x)u(t,x)\cdot u(t,x)\right]\, dV$$

$$= \int_V \beta g\, \check{\rho}\, \check{u}'\cdot\check{u}'\, dV \quad . \tag{3.47}$$

The non-negative integral (3.47) is the average difference between the local kinetic energy and the dot product of the average velocity times the density. An example of a term that can be modeled more easily in the average internal energy equation is the dissipation term. In the average internal energy equation, the term Φ represents the average conversion of viscous work by the fluid into heat only, whereas, in the average total energy equation, the corresponding term $\nabla\cdot(\Pi\cdot u)$ models the average conversion of viscous work of the fluid into <u>two</u> quantities, heat and kinetic energy.

The average internal energy equation is derived in a similar fashion as the average gas continuity equation and gas momentum equations. We multiply Eq. (3.3) by βg, integrate over the averaging volume $V(x)$ and use formulas (2.9) and (2.21) to obtain

$$\frac{\partial}{\partial t} \int_V \beta g\, \check{\rho}\check{e}\, dV + \nabla\cdot \int_V \beta g\, \check{\rho}\check{u}\check{e}\, dV = - \int_{S_p} g n_{sp}\cdot\check{\rho}(\check{u}-\check{u}_{sp})\check{e}\, dS$$

$$- \int_V \beta g\, \check{p}\nabla\cdot\check{u}\, dV \; + \int_V \beta g\, \check{\Phi}_1\, dV - \nabla\cdot \int_V \beta g\, \check{Q}\, dV \tag{3.48}$$

$$- \int_{S_p} g\, \check{Q}\cdot n_{sp}\, dS \quad .$$

We define the average specific internal energy e similar to the average gas velocity, that is, as the quotient of the average internal energy density $\boxed{\rho e}$ and the average mass density ρ :

$$e = \frac{\boxed{\rho e}(t,x)}{\rho(t,x)} \; . \tag{3.49}$$

Using Eqs. (3.13) and (3.49), Eq. (3.48) can be written, after some manipulation, as

$$
\begin{aligned}
\frac{\partial}{\partial r}(\alpha\rho e) + \nabla\cdot(\alpha\rho e u) = &- \alpha p\nabla\cdot u + \alpha\Phi_L + \alpha\Phi_T - \nabla\cdot(\alpha Q) \\
&+ \overset{*}{\rho}\,\frac{SG}{VG}\,e\,\langle\dot{d}\rangle - \frac{1}{VG}\int_{S_p} g\breve{Q}\cdot n_{sp}\,dS \\
&+ \nabla\cdot\left[\alpha\rho e u - \alpha\boxed{\rho e u}\right] + \left[\frac{1}{VG}\int_V \beta g\breve{\Phi}_1\,dV - \alpha\Phi_L - \alpha\Phi_T\right] \qquad (3.50) \\
&+ \nabla\cdot\left[\alpha Q - \frac{1}{VG}\int_V \beta g\breve{Q}\,dV\right] + \left[\alpha p\nabla\cdot u - \frac{1}{VG}\int_V \beta g\breve{p}\nabla\cdot\breve{u}\,dV\right] \\
&- \overset{*}{\rho}\,\frac{SG}{VG}\,\hat{e}\,\langle\dot{d}\rangle - \frac{1}{VG}\int_{S_p} \breve{g}\breve{e}\breve{\dot{d}}\,dS\Big] \quad ,
\end{aligned}
$$

where Φ_L, Φ_T, and Q are the constitutive models for the average dissipation function, turbulent dissipation function, and the average heat conduction, respectively. The average energy release by the propellant during burning is denoted by $\hat{e}(t,x)$. The term $\alpha\rho e u-\alpha\boxed{\rho e u}$, which is $-(1/VG)\int\beta g\breve{\rho}\breve{e}'\breve{u}'\,dV$, is analogous to that in Eq. (3.26). This term is zero if either $\breve{e}' \equiv 0$, or $\breve{u}' \equiv 0$, i.e., if $\breve{e}$ or $\breve{u}$ is a function of time only. However, in turbulent flows, this term can be significant. A model of the term as the gradient of the energy variable is given by Cebeci and Smith.[14] In interior ballistics the term is probably large, because for moving and burning grains the extrema of $\breve{e}'$ and $\breve{u}'$ are likely to correlate. We denote the model of this term by Q_T. The term $\int_{S_p}(g\breve{Q}\cdot n_{sp}/SG)dS$ represents the average heat flux into the particle from the gas and is modeled by the correlation $\langle\dot{e}\rangle$. The models for Φ_L and Φ_T, Q and Q_T, and e and $\langle\dot{e}\rangle$ are discussed in Sections 4.7.3, 4.7.4, and 4.7.8, respectively.

We now can rewrite Eq. (3.50) as

---

[14] *T. Cebeci and A. Smith, Analysis of Turbulent Boundary Layers, Academic Press, New York, 1974.*

$$
\begin{aligned}
\frac{\partial}{\partial t}(\alpha\rho e) + \nabla\cdot(\alpha\rho e u) = {} & -\alpha p\,\nabla\cdot u + \alpha\Phi_L + \alpha\Phi_T - \nabla\cdot(\alpha Q) - (\alpha Q_T) \\
& + \overset{*}{\rho}\,\frac{SG}{VG}\,\hat{e}\,\langle\dot{d}\rangle - \frac{SG}{VG}\langle\dot{e}\rangle \\
& + \left\{\frac{1}{VG}\int_V \beta g\left[\breve{\Phi}_1(t,\xi) - \Phi_L(t,x) - \Phi_T(t,x)\right] dV\right\} \\
& - \left\{\nabla\cdot\frac{1}{VG}\int_V \beta g[\breve{Q}(t,\xi) - Q(t,x)]\, dV\right\} - \left\{\nabla\cdot\left[(\alpha\,[\rho e u] - \alpha\rho e u) - \alpha Q_T\right]\right\} \\
& - \left\{\frac{1}{VG}\int_{S_p} g[\breve{Q}(t,\xi)\cdot n_{sp} - \langle\dot{e}\rangle]\, dS\right\} \\
& + \left\{\frac{1}{VG}\int_V \beta g[p(t,x)\nabla\cdot u(t,x) - \breve{p}(t,\xi)\nabla\cdot\breve{u}(t,\xi)]\, dV\right\} \\
& + \left\{\overset{*}{\rho}\,\frac{SG}{VG}\left[\hat{e}\,\langle\dot{d}\rangle - \frac{1}{VG}\int_{S_p} \breve{g}\breve{e}\breve{\dot{d}}\, dS\right]\right\} \quad ,
\end{aligned}
\tag{3.51}
$$

where the terms enclosed by braces are error-type terms.

The first four error terms depend on a model and are discussed in the appropriate model section (see Section 4). The remaining two terms can be written by following similar analyses to these in the average gas momentum equation derivation as

$$
\begin{aligned}
\frac{1}{VG}\int_V \beta g\,[p\nabla\cdot u - \breve{p}\nabla\cdot\breve{u}]\, dV = {} & \alpha(t,x)\; p(t,x)\;[\nabla\cdot u(t,x) - \nabla\cdot\breve{u}(t,\xi(x))] \\
& + \alpha(t,x)\;\; \nabla\cdot\breve{u}(t,\xi(x))\;[p(t,x) - \breve{p}(t,\xi(x))]
\end{aligned}
\tag{3.52}
$$

and

$$
\begin{aligned}
& \left|\overset{*}{\rho}\,\frac{SG}{VG}\left[\hat{e}\,\langle\dot{d}\rangle - \frac{1}{SG}\int_{S_p} g\,\breve{e}\,\breve{\dot{d}}\, dS\right]\right| \\
& < \left|\overset{*}{\rho}\,\frac{SG}{VG}\right|\,\left\{\hat{e}\,\left|\,\langle\dot{d}\rangle - \dot{d}\right| + \dot{d}\,\max_i \left|\hat{e}(t,x) - \breve{e}(t,\xi(\zeta_i))\right|\right\}
\end{aligned}
\tag{3.53}
$$

where $\xi(x)$ is a point in V_{gas}(V_{gas} is assumed connected) and ζ_1 is a point on the surface s_{pi}.

The error represented by Eq. (3.52) consists of two parts: the error made by using the divergence of the average velocity for the divergence of the local velocity, and the error made by using the average pressure correlation for the local pressure. If both $\tilde{p}$ and $\nabla\cdot\tilde{u}$ were functions of time only, the error would be zero. If the term is not negligible, then a correlation that models the average fluctuations of $\tilde{p}\nabla\cdot\tilde{u}$ from $p\nabla\cdot u$ must be included. Most often the term is neglected, but a model may be necessary in some turbulent flows. The error generated by replacing the surface integral of $\widetilde{g\dot{e}d}/SG$ with the product of correlations $\hat{e}\langle\dot{d}\rangle$, Eq. (3.53), also consists of two parts. The first involves the approximation of $\dot{d}$ by $\langle\dot{d}\rangle$ which is discussed in Section 3.2.1. The second is small if the fluctuations are small of the local internal energy from the specific internal energy of the gas at flame temperature, e. In practice, both errors are assumed small.

If not, a correlation which models the fluctuation of $\widetilde{\dot{e}d}$ from $\hat{e}\langle\dot{d}\rangle$ over the surface of the grains must be included.

3.2.4 Derivations of the Surface Average Equations. On the surface of the particles, the average normal regression distance $\overset{*}{d}$ and the average surface temperature $\overset{*}{T}$ can be defined according to the definition (2.26),

where $\tilde{\overset{*}{d}}$ and $\tilde{\overset{*}{T}}$ denote the local values, respectively. For a spherical particle, for example, $\overset{*}{d}$ is the local difference between the original radius of the particle and its current radius. According to Section 2.2.5, the variables $\overset{*}{d}$ and $\overset{*}{T}$ satisfy the differential Eq. (2.41) so that the average regression distance equation is

$$\begin{aligned}\frac{\partial \overset{*}{d}}{\partial t} + \overset{*}{u}\cdot\nabla\overset{*}{d} = \langle\dot{d}\rangle &+ \left\{\frac{1}{SG}\int_{S_p} g\left(\frac{\partial \tilde{\overset{*}{d}}}{\partial t} - \langle\dot{d}\rangle\right) dS\right\} \\ &+ \left\{\frac{1}{SG}\int_{S_p} \left(\tilde{\overset{*}{d}} - \overset{*}{d}\right)\left(\overset{*}{u} - \tilde{u}_{sp}\right)\cdot\nabla_x g\ dS\right\} \\ &+ \left\{\frac{1}{SG}\int_{S_p} \left(\tilde{\overset{*}{d}} - \overset{*}{d}\right) g\,\frac{\partial Z}{\partial r}\, d\zeta\right\} \quad ,\end{aligned} \tag{3.54}$$

and the average surface temperature equation is

$$\frac{\partial \overset{*}{T}}{\partial t} + \overset{*}{u}\cdot\nabla\overset{*}{T} = \langle\dot{T}\rangle + \Big\{\frac{1}{SG}\int_{S_p} g\Big(\frac{\partial \check{\overset{*}{T}}}{\partial t} - \langle\dot{T}\rangle\Big)\, dS\Big\}$$

$$+ \Big\{\frac{1}{SG}\int_{S_p} \big(\check{\overset{*}{T}} - \overset{*}{T}\big)\big(\overset{*}{u} - \check{u}_{sp}\big)\cdot\nabla_x g\, dS\Big\} \qquad (3.55)$$

$$+ \Big\{\frac{1}{SG}\int_{S_p} \big(\check{\overset{*}{T}} - \overset{*}{T}\big)\, g\,\frac{\partial Z}{\partial t}\, d\zeta\Big\} \quad ,$$

where $\check{u}_{sp} = \frac{\partial s}{\partial t}$, $\langle\dot{d}\rangle$ is the correlation for the regression rate, and $\langle\dot{T}\rangle$ is the correlation for the rate of change of grain surface temperature.

The last three terms in each of the Eqs. (3.54) and (3.55) are error type terms. The first error terms in Eqs. (3.54) and (3.55) are the surface averages of the fluctuations between the local values and its corresponding correlation values of the regression rate and surface temperature, respectively. The regression rate term is discussed in Section 3.2.1 and similar error estimates and comments can be made concerning the surface temperature term. The remaining error terms involve fluctuations from formally defined averages. The last terms in Eqs. (3.54) and (3.55) involve fluctuations of $\check{\overset{*}{d}}$ and $\check{\overset{*}{T}}$ from their average values, respectively. Because the integrands of these surface integrals include other terms, these integrals are not surface averages of fluctuations, and, thus, are not necessarily zero. The other set of error terms include the product of the fluctuations of the local interface velocity from the volume average particle velocity $\overset{*}{u}$ with the fluctuations of $\check{\overset{*}{T}}$ and $\check{\overset{*}{d}}$ from their average values. As before, the integrals involving these products are not surface average integrals. If the fluctuations are small over the surface of all the particles, then the terms can be neglected. Such cases occur when the regression distance and/or the surface temperature of all the grains are equal. If these surface integrals represent significant contributions to the rate of change of the variables, correlations for them must be formulated and included in the governing Eqs. (3.54) and (3.55).

3.3 Summary and Discussion of the Conservation Equations Without Error Terms

In this section, we will list and discuss the equations derived in Section 3.2 without error terms. We are aware that some of the neglected terms may be significant in some flows. In such cases, it (they) can be appended to the governing equation(s) and modeled. A good way to decide whether a term should be neglected or included in a set of equations is to compare the accurate solution of the equations with data from well-defined, carefully done experiments. Furthermore, we realize that some of the constitutive laws and correlations quite possibly can be coupled to each other and terms in the governing equations could be grouped differently. Thus, the formal and physical meaning of some of the constitutive laws and correlations can change. Therefore, the form of the equations, correlates, and constitutive laws for interior ballistic applications listed in this report should not be considered as final.

The porosity Eq. (3.20) (the average solid phase continuity equation) can be written as

$$\frac{\partial}{\partial t}(1-\alpha) + \nabla\cdot\left[(1-\alpha)\overset{*}{u}\right] = -\Gamma_1 \quad , \tag{3.56}$$

where the source term is given by

$$\Gamma_1 = \frac{SG}{VG}\langle\dot{d}\rangle \quad . \tag{3.57}$$

The average solid phase momentum Eq. (3.44) expresses the conservation of the solid phase momentum density, and is

$$\begin{aligned}\frac{\partial}{\partial t}\left[(1-\alpha)\overset{**}{\rho u}\right] + \nabla\cdot\left[(1-\alpha)\overset{***}{\rho u u}\right] = &- (1-\alpha)\nabla p + (1-\alpha)\overset{*}{\rho}\, A_{stress} \\ &+ (1-\alpha)\rho\, A_{drag} - \overset{**}{\rho u}\Gamma_1 \quad ,\end{aligned} \tag{3.58}$$

where

$$(1-\alpha)\overset{*}{\rho}A_{stress} = \nabla\cdot\left[(1-\alpha)\overset{*}{\Pi} + (1-\alpha)\overset{*}{\Pi}_T\right] \quad , \tag{3.59}$$

and

$$(1-\alpha)\rho\, A_{drag} = \frac{1}{VG}D \quad . \tag{3.60}$$

The average gas phase continuity Eq. (3.21) is

$$\frac{\partial}{\partial t}(\alpha\rho) + \nabla\cdot(\alpha\rho u) = \overset{*}{\rho}\Gamma_1 \quad . \tag{3.61}$$

The average gas phase momentum Eq. (3.30) expresses the conservation of the momentum density and, with the definition of drag (3.40), can be written as

$$\frac{\partial}{\partial t}(\alpha\rho u) + \nabla\cdot(\alpha\rho uu) = -\alpha\nabla p + \alpha\rho\ A_{visc} + \alpha\rho\ A_{turb}$$
$$+ \overset{**}{\rho u}\Gamma_1 - (1-\alpha)\rho\ A_{drag} \quad , \tag{3.62}$$

where

$$\alpha\rho\ A_{visc} = \nabla\cdot(\alpha\Pi) \quad , \tag{3.63}$$

and

$$\alpha\rho\ A_{turb} = \nabla\cdot(\alpha\Pi_T) \quad . \tag{3.64}$$

The average gas phase energy Eq. (3.51) expresses the conservation of the gas phase internal energy density, and is

$$\frac{\partial}{\partial t}(\alpha\rho e) + \nabla\cdot(\alpha\rho e u) = -\alpha p\nabla\cdot u + \alpha\Phi_1 + \alpha\Psi_1 + \overset{*\hat{}}{\rho e}\Gamma_1 \quad , \tag{3.65}$$

where

$$\Phi_1 = \Phi_L + \Phi_T \quad , \tag{3.66}$$

and

$$\alpha\Psi_1 = -\nabla\cdot(\alpha Q) - \frac{SG}{VG}\langle\dot{e}\rangle - \nabla\cdot(\alpha Q_T) \quad . \tag{3.67}$$

The term Φ_1 contains all the models for the heat dissipation functions and the term Ψ_1 contains those for the heat conduction within the gas and to the particles, and the turbulent heat flux. The average specific energy released by the burning of the propellant is denoted by $\hat{e}(t,x)$.

The governing equations for the surface average regression rate (3.54) and for the surface average surface temperature (3.55) are

$$\frac{\partial \overset{*}{d}}{\partial t} + \overset{*}{u}\cdot\nabla\, \overset{*}{d} = \langle \dot{d} \rangle \quad , \qquad (3.68)$$

and

$$\frac{\partial \overset{*}{T}}{\partial t} + \overset{*}{u}\cdot\nabla\, \overset{*}{T} = \langle \dot{T} \rangle \quad . \qquad (3.69)$$

Because the left-hand sides of these equations represent material derivatives, one can interpret the equations as state equations for the surface material.

The source term is modeled by $\frac{SG}{VG}\langle \dot{d} \rangle$ which appears in every volume averaged equation. Recalling the definition of the source term

$$\frac{SG}{VG}\,\dot{d}(t,x) = \frac{1}{VG}\int_{S_p} g\,\check{\dot{d}}\,dS, \qquad \check{\dot{d}} \geqslant 0 \quad , \qquad (3.70)$$

we see that the model must be zero when no particle is burning within the averaging volume at point (t,x) (regression rate $\check{\dot{d}}$ is zero). When no particles exist within the averaging volume we want the value of the source term to be zero. This is reasonable because for the case of uniformly regressing particles, the integral in Eq. (3.70) approaches zero as the porosity approaches one. Furthermore, the value of the model must be always non-negative. Comparing Eq. (3.61) and $\overset{*}{\rho}$ times Eq. (3.56), we see that the value of the averge mass flux per volume added to the gas phase is exactly that being taken away from the solid phase within the averaging volume. The average balance can also be seen in the momentum equations and involves the momentum flux model $\rho u \Gamma_1$. The drag force per volume, D/VG, is also balanced on the average in the momentum Eqs. (3.58) and (3.62). We note that the model for the drag force D should be zero when no particles exist ($\alpha = 1$) in the flow because then the drag force Eq. (3.40) is zero (S_p has zero surface area). Appropriate types of average stress tensors are also included in the average momentum equations. The average stress tensors Π, Π_T, $\overset{*}{\Pi}$, $\overset{*}{\Pi}_T$ in Eqs.

(3.62) and (3.58) are defined via volume averages in contrast to the surface average definitions of the source and drag terms. These average stress tensors are weighted by the appropriate phase volume fractions, i.e., by α for Π and Π_T and by $(1-\alpha)$ for $\overset{*}{\Pi}$ and $\overset{*}{\Pi}_T$. Consequently, the contribution of the average gas stress tensors to the change of gas momentum consists of the two terms $\alpha\nabla\cdot(\Pi + \Pi_T)$ and $\nabla\alpha\cdot(\Pi + \Pi_T)$. An analogous statement holds with respect to the solid phase. The internal energy of the gas phase, Eq. (3.65), is augmented by the source term $\overset{*}{\rho}\hat{e}\Gamma_1$. The appropriately weighted volume averaged heat dissipation functions Φ_L and Φ_T (the contribution from turbulence) are grouped together. The average work done by the gas pressure is denoted by $-p\nabla\cdot u$ and is weighted by the porosity. The average heat flux between the gas and the solid is represented by $\frac{SG}{VG}\langle\dot{e}\rangle$. The correlation $\langle\dot{e}\rangle$ should be positive when the temperature of the gas is higher than that of the solid, negative in the opposite case and zero when the temperatures are the same or when no particles exist in the averaging volume. The average heat conduction in the gas is modeled by $\nabla\cdot(\alpha Q)$. The turbulent heat flux vector is modeled similarly by $\nabla\cdot(\alpha Q_T)$. The last three terms are grouped in one term Ψ_1. The surface averaged equation for the average regression distance, Eq. (3.68), has a non-negative valued right-hand side represented by the correlation $\langle\mathring{d}\rangle$. The governing equation for the average surface temperature, Eq. (3.69), has a right-hand side that usually should have the same algebraic sign as $\langle\mathring{e}\rangle$.

The limiting case of no particles within a region is of particular interest in interior ballistics applications because such regions do exist inside a gun tube. The other limiting case of no gas does not exist in our applications and, thus, is of no practical interest. In the case of no particles (α=1), the set of conservation equations greatly simplify. The source terms are zero and the drag and interface heat transfer terms are also zero. However, it is important to notice that, first, the gas phase equations do not reduce to the local equations, Eqs. (3.1) through (3.3). The simplified set (α=1) differs in <u>form</u> from the local equations because it includes the turbulence terms, that is, $\nabla\cdot(\Pi_T)$, $\alpha\Phi_T$, and $\nabla\cdot(Q_T)$. This fact reminds us that the resulting set of equations is still a set of average equations for a finite averaging volume V. Secondly, even if the averages of all the products of fluctuations were zero (no turbulence), then the set of equations for the gas flow would have the same form as the local equations, but the solutions would not be the same in general. This is so because the quantities ρ, u, and e are averaged, and their initial and boundary conditions are not the same as the initial and boundary conditions for $\tilde{\rho}$, $\tilde{u}$, and $\tilde{e}$ in general. Thirdly, if we let the averaging volume go to zero in the simplified set (with α=1), the turbulence terms would be zero because the fluctuations are averaged over the averaging volume which has zero volume. In this case ($\alpha \to 1$ and $V(x) \to 0$) the averaged equations reduce in form to the local equations and the initial and boundary conditions should reduce to the local conditions. Thus, the solutuions of the two sets would be identical. Fourthly, in the case of $\alpha=1$, the equations for $\overset{*}{d}$ and $\overset{*}{T}$, Eqs. (3.68) and (3.69), are homogenous ($\langle\dot{d}\rangle = \langle\dot{T}\rangle = 0$) but a value of $\overset{*}{d}$ and $\overset{*}{T}$ can be computed from these equations if $\overset{*}{u}$ is defined. Although these values would be physically meaningless, they allow the solution to be computed numerically everywhere without tracing the internal boundaries of gas and mixture. Because these internal boundaries cannot be predicted ahead of time in a two-dimensional flow field, this provides a distinct numerical advantage. Fifthly, the average solid phase momentum equation is identically satisfied when $\alpha=1$. Thus, the components of the vector $\overset{*}{u}$ cannot be determined from Eq. (3.58), and the numerical advantages discussed with respect to $\overset{*}{d}$ and $\overset{*}{T}$ are lost. In fact, when an implicit numerical algorithm is used to solve Eqs. (3.56) through (3.69) directly for the variables ρ, α, u, $\overset{*}{u}$, e, $\overset{*}{d}$, and $\overset{*}{T}$, it can be shown that the matrix equation which must be solved for a new time level of values is singular (the rank of the matrix is deficient) when $\alpha=1$. To avoid this situation, we can algebraically manipulate the porosity and solid phase momentum equations into a non-conservative form when $\partial\overset{*}{u}/\partial t$ has a coefficient one. Then the components of $\overset{*}{u}$ can be defined everywhere. Another advantage of solving for the values of $\overset{*}{u}$, $\overset{*}{d}$, and $\overset{*}{T}$ directly from their governing partial differential equations when $\alpha=1$ is that their values should be continuous at $\alpha=1$ if the equations approach a non-singular form at $\alpha=1$.

In Section 4.1, 4.2, and 4.3, we discuss better forms of the partial differential equations and another choice of dependent variables for numerical treatment.

4. GOVERNING EQUATIONS

4.1 Basic System of Governing Equations

A system of conservation equations for average flow properties was derived in Section 3. One obtains an equivalent system of differential equations by solving the conservation Eqs. (3.56) through (3.69) for the time derivatives of the dependent variables. Let the ensuing system be called governing equations of the flow. It consists of the following set of equations

$$
\begin{aligned}
\frac{\partial \rho}{\partial t} &= -\nabla\cdot(\rho u) - \frac{\rho}{\alpha}\left[(1-\alpha)\nabla\cdot\overset{*}{u} - (u-\overset{*}{u})\cdot\nabla(1-\alpha)\right] + \left(\frac{\overset{*}{\rho}-\rho}{\alpha}\right)\Gamma_2 \quad ,\\
\frac{\partial e}{\partial t} &= -u\cdot\nabla e - \frac{p}{\rho}\nabla\cdot u + \left(\frac{e-e}{\alpha}\right)\frac{\overset{*}{\rho}}{\rho}\Gamma_2 + \frac{1}{\rho}(\Phi_1+\psi_1) \quad ,\\
\frac{\partial u}{\partial t} &= -(u\cdot\nabla)u - \frac{1}{\rho}\nabla p - \frac{1}{\alpha}(u-\overset{*}{u})\frac{\overset{*}{\rho}}{\rho}\Gamma_2 - \frac{1-\alpha}{\alpha}A_{drag} + A_{visc} + A_{turb} \quad ,\\
\frac{\partial \overset{*}{u}}{\partial t} &= -(\overset{*}{u}\cdot\nabla)\overset{*}{u} - \frac{1}{\overset{*}{\rho}}\nabla p + \frac{\rho}{\overset{*}{\rho}}A_{drag} + A_{stress} \quad , \qquad (4.1)\\
\frac{\partial \alpha}{\partial t} &= \nabla\cdot\left((1-\alpha)\overset{*}{u}\right) + \Gamma_2 \quad ,\\
\frac{\partial \overset{*}{d}}{\partial t} &= -\overset{*}{u}\cdot\nabla\overset{*}{d} + \langle\dot{d}\rangle \quad ,\\
\frac{\partial \overset{*}{T}}{\partial t} &= -\overset{*}{u}\cdot\nabla\overset{*}{T} + \langle\dot{T}\rangle \quad .
\end{aligned}
$$

The system is closed by a number of correlation models that will be discussed in detail in Section 4.7. Presently, we merely give a short exposition of the corresponding terms in Eq. (4.1). The listed arguments of the correlation functions are only representative, indicating the most obvious dependences. The actual models may depend on fewer or on more arguments. Also, all models depend implicitly or explicitly on the averaging volume and on the averaging weight function.

The equations of state enter the system in form of a relation for the pressure, viz.,

$$p = p(\rho, e) \quad , \quad (\mathrm{Pa}) \quad . \qquad (4.2)$$

The mass source due to the phase change by combustion is presented by

$$\dot{\Gamma}_2 = (1 - \alpha)\,\frac{s_p(\overset{*}{d})}{v_p(\overset{*}{d})}\,\langle\dot{d}\rangle \quad , \quad (1/s) \quad , \tag{4.3}$$

where we define $\frac{SG}{VG} = (1-\alpha)s_p(\overset{*}{d})/v_p(\overset{*}{d})$, and $v_p(\overset{*}{d})$ and $s_p\langle\overset{*}{d}\rangle$ are the volume and surface correlations, respectively, for propellant grains with the regression distance $\overset{*}{d}$. The quantity $\langle\dot{d}\rangle$ represents the regression rate correlation. Generally it is a function of the type

$$\langle\dot{d}\rangle = \langle\dot{d}\rangle\,(p, |\overset{*}{u} - u|, \partial p/\partial t) \quad , \quad (m/s) \quad . \tag{4.4}$$

The heat dissipation is modeled by the function

$$\Phi_1 = \Phi_1(u, T, \alpha, \overset{*}{u}, \dot{d}) \quad , \quad (W/m^3) \tag{4.5}$$

where $T(\rho, e)$ is provided by the equation of state correlation. The heat conduction is represented by the function

$$\Psi_1 = \Psi_1(T, \nabla T, \nabla \cdot \nabla T, \langle\dot{T}\rangle) \quad , \quad (W/m^3) \quad . \tag{4.6}$$

The last argument of Ψ_1 in Eq. (4.6) is the rate of change of the grain surface temperature, which may be modeled, e.g., by

$$\langle\dot{T}\rangle = \langle\dot{T}\rangle\,(\overset{*}{T}, T, |\overset{*}{u} - u|) \quad , \quad (K/s) \quad . \tag{4.7}$$

The term A_{drag} represents the acceleration due to the drag between gas and particles

$$A_{drag} = A_{drag}\,((\overset{*}{u} - u), \overset{*}{d}, T) \quad , \quad (m/s^2) \quad . \tag{4.8}$$

The velocity governing equations contain three more acceleration terms. They are, the acceleration by the laminar viscosity

$$A_{visc} = A_{visc} = (T, \nabla u, \nabla \cdot \nabla u, \alpha) \quad , \quad (m/s^2) \quad , \tag{4.9}$$

the acceleration due to turbulence

$$A_{turb} = A_{turb}\,(T, \nabla u, \nabla \cdot \nabla u, \ldots) \quad , \quad (m/s^2) \quad , \tag{4.10}$$

and the acceleration due to intergranular stress and solid phase turbulence

$$A_{stress} = A_{stress}\,(\alpha, \overset{*}{d}, \nabla \overset{*}{u}, \ldots) \quad , \quad (m/s^2) \quad . \tag{4.11}$$

The system of governing equations, Eqs. (4.1), is for numerical solution more advantageous than the system of conservation Eqs. (3.56) through (3.69) because none of the Eqs. (4.1) become identically satisfied as $\alpha \to 1$. This permits one to carry out the calculations throughout the interior of the gun tube without tracking the boundaries of regions with $\alpha = 1$.

We can further improve the equations system by selecting a new set of dependent variables. The choice of the new variables and the corresponding new system of governing equations are described in Sections 4.2 and 4.3, respectively.

4.2 Choice of Dependent Variables

4.2.1 Particle Number Function. If the source term Γ_2 is computed using Eq. (4.3), then one can expect numerical difficulties as $v_p(\overset{*}{d})$ approaches zero. Interpreting the equation physically, it is plausible that $1 - \alpha \sim v_p$, so that Γ_2 vanishes at the limit. However, because α and $\overset{*}{d}$ (and, consequently, $v_p(\overset{*}{d})$) are separate variables, their numerical values will, in general, approach the corresponding limits at different times and locations. In a computer program, the situation requires special safeguards to prevent overflow.

The special programming can be avoided if the number of particles is introduced as a dependent variable. This can be done by different approaches. In one approach, one assumes that the governing equations, Eqs. (4.1) for α and $\overset{*}{d}$, and the source term correlation (4.3) hold exactly. Then the number of particles, $\overset{*}{m}(t,x)$, can be introduced by a formal definition in terms of already defined functions. In a second approach, one avoids the use of the correlation (4.3) and defines $\overset{*}{m}(t,x)$ concurrently with the particle volume function $v_p(\overset{*}{d})$ such that the equation for α in the equation system (4.1) is satisfied approximately. Finally, one can define $\overset{*}{m}(x,t)$

by a specific "reasonable" formula and then seek to determine a corresponding function $v_p(\overset{*}{d})$ such that the equation for α is approximately satisfied. Each of the approaches requires some approximations. The last approach has the advantage that it provides guidelines how to chose the particle volume function $v_p(\overset{*}{d})$.

We start with the first approach and define $\overset{*}{m}$ in terms of α and $v_p(\overset{*}{d})$ as in Eq. (2.45) by

$$\overset{*}{m}(t,x) = VG\ (1-\alpha)/v_p(\overset{*}{d}) \quad . \tag{4.12}$$

The two governing equations for α and $\overset{*}{d}$ in Eqs. (4.1) are, if the definition of Γ_2 by Eq. (4.3) is used,

$$\left.\begin{aligned} &\frac{\partial(1-\alpha)}{\partial t} = -\nabla\cdot\left((1-\alpha)\overset{*}{u}\right) - (1-\alpha)\frac{s_p(\overset{*}{d})}{v_p(\overset{*}{d})}\langle\dot{d}\rangle \\ &\text{and} \\ &\frac{\partial\overset{*}{d}}{\partial t} = -\overset{*}{u}\cdot\nabla\overset{*}{d} + \langle\dot{d}\rangle \quad . \end{aligned}\right\} \tag{4.13}$$

Next, we express α in terms of $\overset{*}{m}$ and v_p using Eq. (4.12), and obtain

$$\alpha = 1 - \frac{\overset{*}{m}}{VG}\, v_p(\overset{*}{d}) \quad . \tag{4.14}$$

The expression (4.14) is substituted into the first Eq. (4.13). After simple manipulations, whereby the relation

$$\frac{dv_p(\overset{*}{d})}{d\overset{*}{d}} = -\ s_p(\overset{*}{d}) \tag{4.15}$$

is assumed, one obtains from the system (4.13) the new system

$$\left.\begin{aligned} &\frac{\partial\overset{*}{m}}{\partial t} = -\nabla\cdot(\overset{*}{m}\ \overset{*}{u}) \quad , \\ &\frac{\partial\overset{*}{d}}{\partial t} = -\overset{*}{u}\cdot\nabla\overset{*}{d} + \langle\dot{d}\rangle \quad . \end{aligned}\right\} \tag{4.16}$$

Thus, one can replace the two governing Eqs. (4.13) by the two Eqs. (4.16) and the relation (4.14). If $\overset{*}{m}$ is used instead of α as dependent variable, then the source term Γ_2 in the equation system (4.1) is calculated by

$$\Gamma_2 = \frac{\overset{*}{m}}{VG} s_p(\overset{*}{d}) \langle\dot{d}\rangle \quad , \tag{4.17}$$

instead of using Eq. (4.3). The expression (4.17) has no numerical singularities. In addition, the new Eqs. (4.16) are simpler than the previously used set (4.13). Physically interpeted, the first Eq. (4.16) means conservation of the number of particles, independently of their size, whereas the second equation governs the average size of the particles, independently of their number in the averaging volume.

The weak point of the described formal introduction of $\overset{*}{m}(t,x)$ (the first approach) is that $\overset{*}{m}$ and the governing equation for $\overset{*}{m}$ contain inaccuracies that depend on the quality of the formula (4.3) for the source term Γ_2. In order to make the definition of $\overset{*}{m}$ independent of these inaccuracies, one can define $\overset{*}{m}$ concurrently with $v_p(\overset{*}{d})$ and $s_p(\overset{*}{d})$ by the relation (4.12), which we write in the form

$$\overset{*}{m}(t,x)\ v_p(\overset{*}{d}) = \int_V (1-\beta)\ g\ dV \quad , \tag{4.18}$$

the Eq. (4.15), and

$$\overset{*}{m}(t,x) s_p(\overset{*}{d}) = \int_{S_p} g\ dS = SG \quad . \tag{4.19}$$

The Eqs. (4.15), (4.18), and (4.19) are consistent in the sense that Eq. (4.19) is a consequence of Eqs. (4.15) and (4.18).

The exact expression for the source term Γ_2 is

$$\Gamma_2 = \frac{1}{VG} \int_{S_p} g\ \breve{\dot{d}}\ dS = \frac{SG}{VG} \dot{d} \quad . \tag{4.20}$$

Therefore, if Eq. (4.19) holds

$$\Gamma_2 = \frac{\overset{*}{m}}{VG} s_p(\overset{*}{d})\ \dot{d} \quad . \tag{4.21}$$

If we also use the exact average value $\dot{d}$ instead of the correlation $\langle\dot{d}\rangle$ in the governing equation for $\overset{*}{d}$, then one obtains from these relations and from the two Eqs. (4.13) by formal manipulation as above

$$\left.\begin{aligned} \frac{\partial \overset{*}{m}}{\partial t} &= - \nabla\cdot(\overset{**}{mu}) \quad , \\ \frac{\partial \overset{*}{d}}{\partial t} &= - \overset{*}{u}\cdot\nabla\overset{*}{d} - \dot{d} \quad . \end{aligned}\right\} \quad (4.22)$$

Eqs. (4.21) and (4.22) are derived without any simplifying approximations for the source term. When the equations are incorporated into the equation system (4.1) for numerical solution, then the average $\dot{d}$ will, of course, be replaced by the corresponding correlation $\langle\dot{d}\rangle$.

The weak point of the second approach is that the two functions $\overset{*}{m}$ and v_p with the desired properties do not exist in general, and, therefore, one has to use functions that satisfy the Eqs. (4.15), (4.18), and (4.19) only approximately. The non-existence can be seen, e.g., by considering the ratio s_p/v_p, which according to Eqs. (4.18) and (4.19) is equal to

$$s_p(\overset{*}{d})/v_p(\overset{*}{d}) = \int_{S_p} g \, dS \Big/ \int_V (1-\beta)\, g \, dV \quad . \qquad (4.23)$$

The right-hand side of Eq. (4.23) obviously depends not only on the average $\overset{*}{d}$, but also explicitly on t and x. Even in the special case where all particles are equal, i.e., $\breve{\overset{*}{d}} \equiv \overset{*}{d} = \text{constant}$, the ratio depends on the position of the grains, i.e., explicitly on t and x. On the other hand, if g is a constant, then Eq. (4.23) can be, indeed, a function of $\overset{*}{d}$ only, and a proper function $v_p(\overset{*}{d})$ might be found. (Actually, g can be only approximately a constant in order to insure the differentiability of the average flow variables, see Section 2.4).

Because the Eqs. (4.15), (4.18), and (4.19) cannot be satisfied exactly, one might as well define, as a third approach, $\overset{*}{m}(x,t)$ by a reasonable formula and then seek such a function $v_p(\overset{*}{d})$ that satisfies the above mentioned equations approximately. (The other possibility, to choose $v_p(\overset{*}{d})$ and then define $\overset{*}{m}$ by Eq. (4.18) amounts to the definition by Eq. (4.12). The corresponding $\overset{*}{m}$ has undesirable limit properties when some grains in the averaging volume are reduced by combustion to zero.)

Either of the following two formulas define functions $\overset{*}{m}(t,x)$ with reasonable limit properties:

$$\overset{*}{m} = \sum_{i=1}^{m} \{\frac{1}{s_{pi}} \int_{S_i \Omega V} gdS\} \quad , \tag{4.24}$$

$$\overset{*}{m} = \sum_{i=1}^{m} \{\frac{1}{v_{pi}} \int_{V_i \Omega V} gdV\} \quad . \tag{4.25}$$

In these equations, m is the number of grains or grain parts in V, s_{pi} are the surface areas of the grains, S_i are their surfaces, v_{pi} are the magnitudes of their volumes, and V_i are their volumes. The contribution of a grain that is reduced to zero volume is $g(\xi_i(t) - x)$, where $\xi_i(t)$ is the location of the grain. When all grains are reduced to zero, then either of the formulas produces

$$\overset{*}{m}(t,x) = \sum_{i=1}^{m} g\{\xi_i(t) - x) \quad . \tag{4.26}$$

If all grains have the same finite size, then the formulas reduce to Eqs. (4.18) and (4.19), respectively. Finally, if g is constant then the contribution to $\overset{*}{m}$ of each grain that is completely inside V is one, and the contribution of a grain partially in V is less than one, in accordance with its location. Only for constant g, and all grains located inside V, the function $\overset{*}{m}$ is independent of $\overset{*}{d}$. Therefore, the factorization as postulated by Eqs. (4.18) and (4.19) can be best approximated if the weight function is constant over most of the averaging volume.

If $\overset{*}{m}$ is defined by either of the Eqs. (4.24) or (4.25), then one may select the volume correlation $v_p(\overset{*}{d})$ to fit the choice of $\overset{*}{m}$. The surface area correlation $s_p(\overset{*}{d})$ is then obtained by the formula (4.15). The selection of $v_p(\overset{*}{d})$ is discussed in Section 4.7.9.

4.2.2 Pressure Logarithm and Entropy.

The equation system (4.1) contains two thermodynamic quantities as dependent variables, namely, the density ρ and the specific internal energy e. One can replace this pair of variables by a different pair of thermodynamic quantities and replace the first two equations in Eq. (4.1) by corresponding governing equations for the new pair. The variables can be chosen such that the new system of equations is better suited for numerical treatment.

First, we notice that up to six equations contain the gradient of the pressure. The handling of the gradient terms can be simplified considerably if the pressure p itself is chosen as a dependent variable instead of ρ. The replacement reduces the total number of terms in the equation system.

Second, one may replace e by another variable, e.g., by the specific entropy s, the specific enthalpy h, or the temperature T. These choices do not simplify the equations. The number of terms does not change if s is used instead of e, but it does increase if h is used instead of e. Choosing T as a dependent variable, one obtains the most complicated equations.

Based on these considerations, we have chosen s as a second thermodynamic variable. First, it does not complicate the equation system. Second, s is proportional to the logarithm of the temperature, whereas e is proportional to the temperature itself. Therefore, if the flow contains large temperature variations, its representation in terms of s is much smoother and more amenable to numerical differentiation. (One can expect large temperature variations in certain interior ballistics problems.)

The relation between, s, p, and T is for Noble-Abel gases

$$s = A_1 \ln(T) - A_2 \ln(p) \qquad (4.27)$$

with constant A_1 and A_2. The Eq. (4.27) suggests that $q=\ln(p)$ would be an even better choice than p as the other thermodynamic variable. If q is a function of p only, then this replacement does not introduce any new complications in the governing equations. Our final choice of thermodynamic variables is, therefore, the specific entropy s [J/(kg•K)] and a pressure logarithm function q, which we define as

$$q(p) = q_1[\ln(p/p_1) + 1] \quad , \quad (\mathrm{Pa}) \qquad (4.28)$$

with constant q_1 and p_1.

The first two equations in the system of governing Eqs. (4.1), if expressed in terms of s and q, are

$$\begin{aligned} \frac{\partial s}{\partial t} &= - u\cdot\nabla s + \frac{p}{\rho T} B + H\,\Gamma + (\Phi + \psi) \\ & \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad (4.29) \\ \frac{\partial q}{\partial t} &= - u\cdot\nabla q - \frac{\rho}{\rho_q}\left[\nabla\cdot u + \frac{e_s}{T} B\right] + \frac{1}{e_q}\left[e - e - e_s H\right]\Gamma - \frac{\rho_s}{\rho_q}(\Phi + \psi) \quad , \end{aligned}$$

where

$$\left.\begin{aligned}
B &= \frac{1}{\alpha}\left[(1-\alpha)\,\nabla\cdot\overset{*}{u} - (u-\overset{*}{u})\cdot\nabla(1-\alpha)\right] \quad ,\\
H &= \frac{1}{T}\left[(\hat{e} + p/\overset{*}{\rho}) - (e + p/\rho)\right] \quad ,\\
\Gamma &= \frac{1}{\alpha}\frac{\overset{*}{\rho}}{\rho}\Gamma_2 = \frac{1}{\alpha}\frac{\overset{*}{\rho}}{\rho}\frac{\overset{*}{m}}{VG}\,s_p(\overset{*}{d})\,\langle\dot{d}\rangle \quad ,\\
\Phi &= \frac{1}{T\rho}\Phi_1 \quad ,\\
\Psi &= \frac{1}{T\rho}\Psi_1 \quad ,
\end{aligned}\right\} \tag{4.30}$$

and

$$\left.\begin{aligned}
\rho_q &= \frac{\partial\rho(p,s)}{\partial p}\frac{dp}{dq} \quad ,\\
\rho_s &= \frac{\partial\rho(p,s)}{\partial s} \quad ,\\
e_q &= \frac{\partial e(p,s)}{\partial p}\frac{dp}{dq} \quad ,\\
e_s &= \frac{\partial e(p,s)}{\partial s} \quad .
\end{aligned}\right\} \tag{4.31}$$

In the derivation of the equation for q, we used the relationship $\rho^2 e_q = p\rho_q$ which can be obtained from the second law of thermodynamics (Hund).[15] In Eq. (4.31), $dp/dq = p/q_1$ by Eq. (4.28), and the derivatives of the thermodynamic functions are modeled by the equation of state correlation, described in Section 4.7.1.

4.3 Final System of Governing Equations

The governing Eqs. (4.1) can be expressed as follows in term of the new set of variables that were introduced in Section 4.2.

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[15] F. Hund, *Einführung in die Theoretische Physik*, Bd. 4, "Theorie der Wärme," p. 135 ff, Bibliographisches Institut, Leipzig, 1950.

$$\left.\begin{aligned}
\frac{\partial s}{\partial t} &= - u\cdot\nabla s + \frac{p}{\rho T}\, B + H\Gamma + (\Phi + \Psi) , \\
\frac{\partial q}{\partial t} &= - u\cdot\nabla q - \frac{\rho}{\rho_q}\left(\nabla\cdot u + \frac{e_s}{T}\, B\right) + \frac{1}{e_q}\,(\hat{e} - e - e_s H)\Gamma - \frac{\rho_s}{\rho_q}\,(\Phi + \Psi) , \\
\frac{\partial u}{\partial t} &= - (u\cdot\nabla)\, u - \frac{p_q}{\overset{*}{\rho}}\,\nabla q - (u - \overset{*}{u})\Gamma - \frac{1-\alpha}{\alpha}\, A_{drag} + A_{visc} + A_{turb} , \\
\frac{\partial \overset{*}{u}}{\partial t} &= - (\overset{*}{u}\cdot\nabla)\, \overset{*}{u} - \frac{p_q}{\overset{*}{\rho}}\,\nabla q + \frac{\rho}{\overset{*}{\rho}}\, A_{drag} + A_{stress} , \\
\frac{\partial \overset{*}{m}}{\partial t} &= - \nabla\cdot(\overset{*}{m}\, \overset{*}{u}) , \\
\frac{\partial \overset{*}{d}}{\partial t} &= - \overset{*}{u}\cdot\nabla \overset{*}{d} + \langle \dot{d} \rangle , \\
\frac{\partial \overset{*}{T}}{\partial t} &= - \overset{*}{u}\cdot\nabla \overset{*}{T} + \langle \dot{T} \rangle
\end{aligned}\right\}\quad (4.32)$$

with

$$\left.\begin{aligned}
B &= \frac{1}{\alpha}\left[(1-\alpha)\,\nabla\cdot\overset{*}{u} - (u - \overset{*}{u})\cdot\nabla(1-\alpha)\right] , \\
\alpha &= 1 - v_p(\overset{*}{d})\, \overset{*}{m}/VG , \\
H &= \frac{1}{T}\left[(\hat{e} + p/\overset{*}{\rho}) - (e + p/\rho)\right] , \\
\Gamma &= \frac{1}{\alpha}\,\frac{\overset{*}{\rho}}{\rho}\,\frac{\overset{*}{m}}{VG}\, s_p(\overset{*}{d})\, \langle \dot{d} \rangle .
\end{aligned}\right\}\quad (4.33)$$

The partial derivatives ρ_s, ρ_q, e_s, and e_q are defined by Eq. (4.31). The derivative $p_q = dp/dq$ is equal to p/q_1 if q is the pressure logarithm defined by Eq. (4.28).

Models of the various correlation terms in Eq. (4.32) are discussed in Section 4.7. Their physical meaning is as follows: Γ represents the mass source due to combustion, Φ represents the heat dissipation, Ψ contains the heat conduction terms, $e(s,p)$, $T(s,p)$, and $\rho(s,p)$ are thermodynamic state functions, A_{drag} is the acceleration due to drag, A_{visc} is the acceleration due to vicosity, A_{turb} is the acceleration due to turbulence, A_{stress} is the acceleration due to intergranular stress and solid phase turbulence, $\langle \dot{d} \rangle$ is the regression rate correlation, $\langle \dot{T} \rangle$ is a correlation for the heat conduction between gas and particles, e is e at flame temperature, $s_p(\overset{*}{d})$ is the average surface area of a single grain, and $v_p(\overset{*}{d})$ is the average volume of a single grain. The variable $\langle \dot{T} \rangle$ enters also the first two Eqs. (4.32) as an argument of the term ψ.

The correlations are defined in terms of volume or surface averages. Therefore, the models of the correlations should be different for different averaging volumes and/or different weight functions. However, because experimentally determined correlation models are usually reported without reference to any averaging, their relation to specific averaging procedures are difficult to determine. Therefore, the influence of their relationship on the overall accuracy of the interior ballistics model has not been established.

4.4 Regions of Definition

According to Section 2.3, the average quantities describing gas properties are defined at all interior points of the gun tube, except for boundary regions the shape of which depends on the averaging volume. The average quantities are the density $\alpha\rho$, the energy density $\alpha\rho e$, and the momentum density vector $\alpha\rho u$. Consequently, all other quantities that are defined in terms of these quantities are defined in the same regions. Such quantities are, e.g., e, u, s, q, T, etc. The porosity α has the same region of definition. The grain number function $\overset{*}{m}$ also can be defined in the same region by using the extension $\overset{*}{m} = 0$ if the averaging volume contains no grains.

Average quantities describing grain properties are defined only at reference points for which the averaging volume contains grains. Therefore, the set of average conservation equations for $(1-\alpha)\overset{*}{\rho}\overset{*}{u}$, $(1-\alpha)\overset{*}{\rho}$, $\overset{*}{d}$, and $\overset{*}{T}$ is not defined in regions without grains (see Section 3.3). By a reformulation of the conservation equations, we obtained in Section 4.3 an equivalent set of governing equations (4.32). This set has no singularities at $\alpha = 1$ and it enables one to calculate nominal grain properties at all interior points where the gas properties are defined. Therefore, one can extend the definition of average grain properties as follows. The grain properties are defined by the averaging integrals (see Section 2.2), if the averaging volume contains grains. In other regions, the grain properties are defined as the solution of Eqs. (4.32). In interior ballistics problems this definition amounts to an interpolation of $\overset{*}{u}$, $\overset{*}{d}$, and $\overset{*}{T}$ across regions without grains. When the grains have been reduced to zero volume, one can still calculate their motion, which now corresponds to a so-called "dusty gas" model. In such a gas, the dust follows the gas flow according to a drag law, but it does not influence the gas flow itself. Using the set (4.32) as governing equations one obtains regions of "dusty gas" where $\overset{*}{m} > 0$ and $v_p(\overset{*}{d}) = 0$. In regions with $\overset{*}{m} = 0$ and $v_p(\overset{*}{d}) > 0$ the equations provide an interpolation of $\overset{*}{u}$, $\overset{*}{T}$ and $\overset{*}{d}$ in space and time between regions with grains.

In the boundary regions discussed in Section 2.3, none of the average quantities are defined and, consequently, the differential Eqs. (4.32) have no meaning in these regions. Strictly speaking, one should provide boundary conditions for Eqs. (4.32) at the boundaries $\ell/2$ away from the tube walls and $\ell/2$ or $\ell/3$ away from the breech and projectile, if the average volume is defined as a sphere (2.47) or cylinder (2.49). The meaning of the solution of the equations in the boundary regions is not obvious if one prescribes boundary conditions on the solid boundaries instead. Section 4.6 contains a discussion of the boundary condition problem.

4.5 Initial Conditions

Typical local initial conditions for the local dependent variables in interior ballistics problems are constant state conditions over the entire region. Because averaging of a constant produces the same constant, the intial averages in most cases are simply equal to the local values.

Deviation from a constant initial state typically involves either a porosity $\overset{*}{\alpha}$ that is not uniform, or a non-uniform grain size, i.e., a non-uniform $\overset{*}{d}$. In these cases, one cannot use the local values of $\overset{*}{m}$ and $\overset{*}{d}$ as initial values. Instead, the initial profiles must be computed by averaging the local values, whereby the same averaging volume V and weight function g should be used as for the correlation models and boundary conditions.

In regions where intially the grain number $\overset{*}{m}$ is zero one has to extrapolate or interpolate the values of $\overset{*}{u}$, $\overset{*}{d}$, and $\overset{*}{T}$. The initial grain velocity is normally identically zero and one can use $\overset{*}{u} = 0$ for the extrapolation. Likewise, the initial grain surface temperature is usually constant, and the same constant can be used for extrapolation. The regression distance may not be constant if different sizes of grains are located in different regions. In such cases, one has to use a common sense extrapolation that produces a smooth initial surface $\overset{*}{d}\,(0,x)$.

In the boundary regions, "correct" initial values cannot be specified for reasons explained in Section 4.4. The proper choice of these initial values depends on the method of treatment of the boundary regions. However, one can assume that any reasonable treatment will produce uniform values, if the local function values are uniform. Therefore, one may specify in the boundary regions the same uniform initial values as in the interior region. If the initial conditions are not uniform, then one has to design such an extrapolation of the averages to the boundary that is consistent with the treatment of boundary conditions.

4.6 **Boundary Conditions**

A theory that could provide guidelines for the formulation of boundary conditions for averaged equations has not been developed. Therefore, interior ballistics calculations usually are done with plausible ad hoc assumptions about boundary values. In this section, we shall outline the requirements for a boundary condition theory and suggest a possible approach to the formulation of such a theory. Because the theory has not been developed, we shall also discuss ad hoc boundary conditions.

Discussing boundary conditions for averaged differential equations in confined volumes, we have to distinguish between two boundaries. For the purpose of the present discussions, we call them the outer boundary and the inner boundary, respectively. The outer boundary consists of the solid walls of the volume. In interior ballistics the solid walls are the tube walls, the breech, and the base of the projectile. The inner bundary is the limit of validity of the average differential equations. As discussed in Sections 2.3 and 4.4, the inner boundary is located a finite distance inward from the outer boundary. The magnitude of the distance depends on the size of the averaging volume. If the averaging volume is a sphere with the diameter ℓ, then the inner boundary is located $\ell/2$ away from the tube walls, breech, and projectile. If the averaging volume is the cylinder described in Section 2.3, then the inner boundary is $\ell/2$ away from the tube walls and $\ell/3$ away from the breech and projectile base. Let the region between the outer and inner boundaries be called the boundary region, and the region inside the inner boundary be called the inner region.

Classical theory for the discussion of necessary boundary conditions, well-posedness, and existence can be only applied to the inner boundary. Gough (1974) presents some of the discussion, implicitly assuming that the conditions on both boundaries are identical. The assumption is permissible if the size of the boundary region is small compared to the size of salient structures of the flow field. Because the size of the boundary region must be large compared to the size of propellant grains (see Section 2.3), it is generally not small compared to, e.g., the gas boundary layer. For interior ballistics flows, therefore, one cannot assume that boundary conditions on the inner and outer boundaries are identical.

Physical boundary conditions, such as $u\text{-}\mathbf{u}_{wall}$, are only given for the local gas phase functions on the outer boundary. The only physical boundary condition for the particles is that no single particle can penetrate the wall. In addition, one may also formulate collision conditions for single particles impacting on the wall, i.e., on the outer boundary.

A boundary condition theory for average equations has to bridge the gap between the outer and inner boundaries. It should provide a complete set of boundary conditions for the average quantities on the inner boundary in terms of the local physical boundary conditions on the outer boundary.

One possible approach to the problem is by construction of a continuation of the solution into the boundary region. If such a continuation is established, then one has reduced the problem to the formulation of boundary conditions on the outer boundary only. The simplest method to obtain a continuation is to define it as the solution of the same differential equations and correlations that are valid in the inner region. Then one needs only conditions on the outer boundary and disregards the existence of the inner boundary. This is the usual approach in two-phase flow calculations. It has the deficiency the one has no guidelines how to formulate the boundary conditions for the continued functions, because they are neither the local functions nor the average functions.

A more promising continuation may be obtained by changing the definition of the averages such that it includes the boundary region. This requires that the averaging volume V has a shape that depends on the position x of the reference point. The conservation equations of Section 3 are derived under the assumption of a fixed size and shape of V. The averages defined for a variable V satisfy a different set of differential equations. The continuation into the boundary region could be computed by solving Eqs. (4.32) in the inner region and the new set in the boundary region, and by matching both solutions at the inner boundary. The boundary conditions on the outer boundary then represent conditions for averaged functions and can be modeled accordingly.

Because a theory of the described type is not available, we now formulate ad hoc conditions that may be used for the differential equation system (4.32).

The local boundary conditions for the gas are: $U = u_{wall}$, a condition for the temperature prescribing either $T = T_{wall}$ or $\partial T/\partial n = (\partial T/\partial n)_{wall}$, where n is the normal to the wall, and the mass conservation equation. In the spirit of interpreting the solutions of the differential equations as averages, one would not directly use these conditions as boundary conditions. Instead, some interpolation is needed that reflects the averaging. We propose the following approach.

Let $\ell/2$ be the distance between the inner and outer boundary and let ε be an estimate of the thickness of the gas boundary layer. Let ϕ be a function with prescribed local boundary value $\breve{\phi}_{wall}$ and n_i be the unit normal to the inner boundary, pointing outward with respect to the interior. We then use the following boundary condition on the outer boundary for gas properties

$$\phi_{outerb} = [\tfrac{\ell}{2} (\phi_{innerb} + (\nabla\phi_{innerb} \cdot n_i) + \varepsilon\breve{\phi}_{wall}]/(\tfrac{\ell}{2} + \varepsilon) . \qquad (4.34)$$

Because ℓ is larger than a particle diameter (see Section 2.3), the boundary value on the outer boundary, when computed by Eq. (4.34), will approach the local boundary value only if the particles are small compared to the thickness of the boundary layer ($\varepsilon >> \ell/2$). This may be the case, e.g., when the flow of wear reducing additives is investigated. If the particles are large compared to the thickness of the boundary layer ($\ell/2 >> \varepsilon$), then the outer boundary value given by Eq. (4.34) approaches an extrapolated value from the inner boundary.

Eq. (4.34) may used to determine the boundary values of u, and T or $\partial T/\partial n$. The average gas continuity equation may be used to close the set of boundary conditions for gas properties.

The formulation of a boundary condition for the average particle velocity presents a dilemma. On one hand, the condition should prevent the particles from penetrating the wall. On the other hand, the average particle velocity at the outer boundary may very well point into the wall, merely indicating an accumulation of particles within the averaging volume. As an ad hoc measure we disregard the second possibility and suggest for the average particle velocity at the outer boundary the following formula. Let $\overset{*}{u}_{DE}$ be the solution obtained from the differential equation system (4.32) at the outer boundary, $\breve{u}_{wall}$ be the velocity of the wall, and n_{wall} be the unit normal to the wall pointing outward. Then the outer boundary value of $\overset{*}{u}$ is

$$\overset{*}{u}_{outerb} = \overset{*}{u}_{DE} - n_{wall} \max(0,(\overset{*}{u}_{DE} - \breve{u}_{wall})\cdot n_{wall}) \quad . \tag{4.35}$$

The resulting $\overset{*}{u}_{outerb}$ satisfies the condition

$$(\overset{*}{u}_{outerb} - u_{wall})\cdot n_{wall} < 0 \quad , \tag{4.36}$$

which on the average prevents the particles from flowing through the wall and permits at the same time the particles to leave the region near to the wall or projectile.

The quantities $\overset{*}{m}$, $\overset{*}{d}$, and $\overset{*}{T}$ are computed by solving the corresponding governing equations at the outer boundary.

4.7 Models of Correlation

4.7.1 Equations of State.

For the derivation of the average equations in Section 3, we used the averages of two thermodynamic quantities, namely, the density ρ and the specific internal energy e. The conservation equations contain two other thermodynamic quantities, the pressure p and the temperature T. (The latter enters the heat conduction term and may be also used in other correlations.) They were assumed to be related to e and ρ by equations of state, i.e., by

$$\left.\begin{aligned} & p = p(\rho, e) \\ & \text{and} \\ & T = T(\rho, e) \quad . \end{aligned}\right\} \qquad (4.37)$$

Generally, one uses in Eq. (4.37) the same functions that hold locally. This introduces errors in several terms of the average conservation equations.

As an example, let us consider the error term in the average momentum equation. The error made by approximating the volume average of the local pressure by the first equation in (4.37) is from Eq. (3.31), Section 3.2.2,

$$C_m = \frac{1}{\alpha\rho} \nabla\left[\alpha(t,x)\left(\breve{p}(t,\xi(x)) - p(t,x)\right)\right] \quad . \qquad (4.38)$$

As discussed in Section 3.2.2, to minimize the error by a proper choice of the function p, we need to minimize the errors in the functional values as well as in the gradient values. However, the pressure function enters the equation system in various places and in different combinations. Therefore, the use of the local equations of state is probably as good an approximation as any. Correspondingly, one also uses the local equations of state when the entropy s is introduced as a dependent variable.

All thermodynamic variables (temperature, pressure, density, energy entropy, and enthalpy) are completely determined in terms of two variables if two "equations of state" are provided by postulate or measurement. Using the two given equations, all other relations can be derived from the laws of thermodynamics, which provide the following three systems of differential equations (Hund):[15]

$$\left.\begin{aligned} & \frac{\partial c_v(\rho, T)}{\partial \rho} = -\frac{1}{\rho^2} T \frac{\partial^2 p(\rho, T)}{\partial T^2} \quad , \\ & c_p - c_v = \frac{T}{\rho^2} \left(\frac{\partial p(\rho, T)}{\partial T}\right)^2 \Big/ \left(\frac{\partial p(\rho, T)}{\partial \rho}\right) \quad , \end{aligned}\right\} \qquad (4.39)$$

(c_p and c_v are the specific heats (J/(kg•K) for constant pressure and volume respectively),

$$\left.\begin{aligned}\frac{\partial e(\rho,T)}{\partial\rho} &= -\frac{1}{\rho^2}\left(T\frac{\partial p(\rho,T)}{\partial T}-p\right) \quad ,\\[2ex] \frac{\partial e(\rho,T)}{\partial T} &= c_v \quad ,\end{aligned}\right\} \tag{4.40}$$

and

$$\left.\begin{aligned}\frac{\partial s(\rho,T)}{\partial\rho} &= -\frac{1}{\rho^2}\frac{\partial p(\rho,T)}{\partial T} \quad ,\\[2ex] \frac{\partial s(\rho,T)}{\partial T} &= \frac{1}{T}c_v \quad .\end{aligned}\right\} \tag{4.41}$$

An equation of state that is often used in interior ballistics is the Noble-Abel equation

$$p(\rho,T) = \frac{R}{M}T\frac{\rho}{1-\eta\rho} \quad , \tag{4.42}$$

where R = 8.3143 J/(mol•K) is the universal gas constant, M (kg/mol) is the molar mass, and η (m^3/kg) is the covolume. From Eqs. (4.39) and (4.42) one finds that for a Noble-Abel gas

$$\left.\begin{aligned}c_v &= c_v(T)\\ &\text{and}\\ c_p &= c_v(T)+\frac{R}{M} \quad .\end{aligned}\right\} \tag{4.43}$$

Therefore, in order to completely specify the gas, one has to provide, in addition to Eq. (4.42), a temperature function $c_v(T)$. Alternatively one can specify instead of $c_v(T)$ a function $c_p(T)$, or a function $\gamma(T)$ that gives the ratio $c_p/c_v = \gamma(T)$. In the latter case, the specific heat functions are

$$\left.\begin{aligned} c_v(T) &= \frac{1}{\gamma(T)-1}\frac{R}{M} \\ &\text{and} \\ c_p(T) &= \frac{\gamma(T)}{\gamma(T)-1}\frac{R}{M} \quad . \end{aligned}\right\} \quad (4.44)$$

We assume that $\gamma(T)$ is constant, and obtain with this assumption the functions $e(\rho,T)$ and $s(\rho,T)$ by integration of Eqs. (4.40) and (4.41). After some manipulations, one can express the quantities of interest in terms of p and s, as required by the system of governing Eqs. (4.32). The results are listed below. T_R and p_R are reference values which determine the integration constant for the entropy.

$$\left.\begin{aligned} T(p,s) &= T_R\left(\frac{p}{p_R}\right)^{\frac{\gamma-1}{\gamma}} \exp\left(\frac{M}{R}\frac{\gamma-1}{\gamma}s\right) && , \quad \mathrm{K} \quad , \\ e &= \frac{1}{\gamma-1}\frac{R}{M}T && , \quad \mathrm{J/kg} \quad , \\ \rho &= \left(\frac{R}{M}\frac{T}{p}+\eta\right)^{-1} && , \quad \mathrm{kg/m^3} \quad , \end{aligned}\right\} \quad (4.45)$$

$$\left.\begin{aligned} \frac{\partial T(p,s)}{\partial p} &= \frac{\gamma-1}{\gamma}\frac{T}{p} \quad , \\ \frac{\partial T(p,s)}{\partial s} &= \frac{\gamma-1}{\gamma}\frac{M}{R}T \quad , \end{aligned}\right\} \quad (4.46)$$

$$\left.\begin{aligned} \frac{\partial e(p,s)}{\partial p} &= \frac{\gamma-1}{\gamma}\frac{e}{p} \quad , \\ \frac{\partial e(p,s)}{\partial s} &= \frac{1}{\gamma}T \quad , \end{aligned}\right\} \quad (4.47)$$

and

$$\left.\begin{aligned} \frac{\partial \rho(p,s)}{\partial p} &= \frac{1}{\gamma}\frac{\rho}{p}(1-\eta\rho) \quad , \\ \frac{\partial \rho(p,s)}{\partial s} &= -\frac{M}{R}\frac{\gamma-1}{\gamma}\rho\,(1-\eta\rho) \quad . \end{aligned}\right\} \quad (4.48)$$

The square of the sound speed is

$$a^2 = \gamma \frac{p}{\rho} \frac{1}{1-\eta\rho} \quad m^2/s^2 \quad . \tag{4.49}$$

The specific entropy, expressed in terms of pressure and temperature, is

$$s = \frac{R}{M} \frac{\gamma}{\gamma-1} \ell n \left[\frac{T}{T_R} \left(\frac{p}{p_R}\right)^{\frac{1-\gamma}{\gamma}} \right] \quad , \quad J/(kg \cdot K) \quad . \tag{4.50}$$

4.7.2 **Acceleration by Gaseous Stresses.** The governing equation for the average gas velocity in the equation system (4.32) contains the terms A_{visc} and A_{turb}. The former term represents the acceleration due to laminar viscosity. The latter term represents the acceleration due to turbulence. A simple turbulence model is a Reynolds stress model with viscosity coefficients depending, e.g., on temperature. Then the forms of A_{visc} and A_{turb} are identical (see Eqs. (B.9) and (B.34)). We restrict our discussion to the term A_{visc}. More complicated turbulence models are possible (see Gibeling et al.)[3] but will not be discussed in this report.

According to Section 3.3, Eq. (3.63), the viscous acceleration term is

$$A_{visc} = \frac{1}{\alpha\rho} \nabla (\alpha\Pi) \quad , \tag{4.51}$$

where Π models the gas volume average of the local viscous stress tensor $\breve{\Pi}$. The local tensor is given in terms of the strain rate tensor $\breve{E}$ by (Tsien, p. 13)[10]

$$\breve{\Pi} = 2 \breve{\mu} \breve{E} + (\breve{\lambda} - \frac{2}{3} \breve{\mu}) \text{ trace } (\breve{E}) \; I \quad , \tag{4.52}$$

where $\breve{\mu}$ and $\breve{\lambda}$ are the shear viscosity coefficient and the bulk viscosity coefficient, respectively. Both are assumed to be functions of temperature. The strain rate tensor is defined by

$$\breve{E} = \frac{1}{2} \left(\nabla\breve{u} + (\nabla\breve{u})^T \right) \quad . \tag{4.53}$$

The modeling of the average viscous acceleration term involves models of the average viscosity coefficients and a model of the average strain rate tensor E.

The models of the average viscosity coefficients are purely empirical. A convenient set of formulas is the following generalization of the so-called Sutherland formula:

$$\left.\begin{aligned} \mu(T) &= \mu_o + \mu_1 \frac{T^{1.5}}{\mu_2+T} \quad , \quad \mathrm{Pa \cdot s} \quad , \\ &\text{and} \\ \lambda(T) &= \lambda_o + \lambda_1 \frac{\lambda^{1.5}}{\lambda_2+T} \quad , \quad \mathrm{Pa \cdot s} \quad . \end{aligned}\right\} \qquad (4.54)$$

The generalization consists of the addition of the parameters μ_o and λ_o, thereby including in the model the constant functions.

The average strain rate tensor E is usually modeled by applying the local formula (4.53) to the average velocities. Then Π is obtained by using Eqs. (4.52) without the tildes and (4.54) with temperature $T(\rho, e)$ calculated from the average values of ρ and e. The approximation error is Eq. (3.32), Section 3.2.2, divided by $\alpha\rho$, i.e.,

$$C_m = \frac{1}{\alpha\rho} \nabla \cdot \int_V \beta g \left[\breve{\Pi}(\breve{u}, \breve{\rho}, \breve{e}) - \Pi(u, \rho, e)\right] \, dV \quad . \qquad (4.55)$$

The error part that comes from the replacement of $\breve{\rho}$ and $\breve{e}$ and ρ and e is probably smaller than the uncertainties of the empirical formulas (4.54). However, the error part that comes from the use of the average velocity in Eq. (4.53), can be large because the formula involves derivatives of the velocity and in a viscous two-phase flow the local derivatives can be quite large. The integration in (4.55) does not necessarily cancel out corresponding large local undulations of the integrand. An empirical correlation based on careful experiments certainly could enhance the usefulness of the described model of the viscous acceleration term.

4.7.3 Heat Dissipation. All the heat dissipation terms are denoted by Φ and they enter the governing Eqs. (4.32) for the specific entropy s and for the pressure logarithm function q. According to Sections 3.2.3, 3.3, 4.1, 4.2, and 4.3 the term Φ models

$$\frac{1}{\alpha\rho T} \frac{1}{VG} \int_V \beta g \, \breve{\Phi} \, dV \quad , \qquad (4.56)$$

where the local heat dissipation function Φ is given by (Tsien[10], p. 15)

$$\check{\Phi} = 2\,\check{\mu}\ \text{trace}\ (\check{E}^2) + (\check{\lambda} - \frac{2}{3}\check{\mu})\ (\text{trace}\ \check{E})^2 \quad , \quad W/m^3 \quad , \qquad (4.57)$$

$\check{E}$ is the local strain rate tensor defined by Eq. (4.53), and $\check{\mu}$ and $\check{\lambda}$ are the local shear and bulk viscosity coefficients, respectively.

Usually Φ is defined in the same fashion as the equations of state (Section 4.7.1), i.e., by calculating a $\bar{\Phi}$ with the same formula as $\check{\Phi}$, but using the average quantities instead of the local quantities. The modeling of the viscosity coefficients is discussed in Section 4.7.2. In Cartesian coordinates, the formula is (Tsien[10], p. 15)

$$\frac{1}{\rho T}\,\bar{\Phi}(E) = \frac{1}{\rho T}\left[\frac{1}{2}\,\mu\,\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)^2 + (\lambda - \frac{2}{3}\,\mu)\left(\frac{\partial u_i}{\partial x_i}\right)^2\right] \quad , \qquad (4.58)$$

whereby summation over i and j is assumed.

Even without considering turbulence, Eq. (4.58) likely underestimates the value of the expression (4.56) because local undulations will generally greatly increase the value of the integrand. If a difference exists between the average velocities of the phases, then local velocity gradients entering Eq. (4.56) are particularly large, but are neglected in Eq. (4.58).

In order to estimate the effect of local gradient variations, we compute the heat dissipation term in a linear flow field superimposed by an undulation. Particularly, we assume the following velocity components in Cartesian coordinates:

$$\left.\begin{aligned} u_1 &= U + \frac{\Delta u}{L}\,x + \hat{u}(x,y,z) \quad , \\ u_2 &= \hat{u}(x,y,z) \quad , \\ u_3 &= \hat{u}(x,y,z) \quad , \end{aligned}\right\} (4.59)$$

where the undulating part is given by the formula

$$\hat{u}(x,y,z) = \hat{U}\,\sin\left(\frac{2\pi}{L}\,x\right)\,\sin\left(\frac{2\pi}{L}\,y\right)\,\sin\left(\frac{2\pi}{L}\,z\right) \quad . \qquad (4.60)$$

The local heat dissipation for this flow field is according to Eq. (4.57)

$$\tilde{\Phi} = \frac{1}{\rho T}\Big[\frac{1}{2}\mu\,(\phi_{xx}^2 + \phi_{yy}^2 + \phi_{zz}^2 + 2\phi_{xy}^2 + 2\phi_{xz}^2 + 2\phi_{yz}^2) + (\lambda - \frac{2}{3}\mu)\,\frac{1}{4}\,(\phi_{xx} + \phi_{yy} + \phi_{zz})^2\Big] \quad , \tag{4.61}$$

where

$$\phi_{xx} = \hat{U}\,\frac{2\pi}{L}\,2\cos\left(\frac{2\pi}{L}x\right)\sin\left(\frac{2\pi}{L}y\right)\sin\left(\frac{2\pi}{L}z\right) + 2\,\frac{\Delta u}{L} \quad ,$$

$$\phi_{yy} = \hat{U}\,\frac{2\pi}{L}\,2\sin\left(\frac{2\pi}{L}x\right)\cos\left(\frac{2\pi}{L}y\right)\sin\left(\frac{2\pi}{L}z\right) \quad ,$$

$$\phi_{zz} = \hat{U}\,\frac{2\pi}{L}\,2\sin\left(\frac{2\pi}{L}x\right)\sin\left(\frac{2\pi}{L}y\right)\cos\left(\frac{2\pi}{L}z\right) \quad , \tag{4.62}$$

$$\phi_{xy} = \hat{U}\,\frac{2\pi}{L}\sin\left(\frac{2\pi}{L}(x+y)\right)\sin\left(\frac{2\pi}{L}z\right) \quad ,$$

$$\phi_{xz} = \hat{U}\,\frac{2\pi}{L}\sin\left(\frac{2\pi}{L}(x+z)\right)\sin\left(\frac{2\pi}{L}y\right) \quad ,$$

$$\phi_{yz} = \hat{U}\,\frac{2\pi}{L}\sin\left(\frac{2\pi}{L}x\right)\sin\left(\frac{2\pi}{L}(y+z)\right) \quad ,$$

Next, we assume that the averaging volume is a cube with side lengths nL and that the weight function g is constant. For that case, the integral (4.56) yields

$$\Phi = \frac{1}{\rho T}\Big[\left(\frac{\Delta u}{nL}\right)^2\left(\frac{4}{3}\mu+\lambda\right) + \left(\frac{\hat{U}}{L}\right)^2\pi^2\left(5\mu+\frac{3}{2}\lambda\right)\Big] \quad . \tag{4.63}$$

The first term in the brackets in Eq. (4.63) is the contribution of the linear field to Φ. The second term is the contribution of the superposed undulations. One sees that for $\Delta u/(nL) \approx \hat{U}/L$ the contribution of the undulations is about 40 times larger than that of the linear flow field. Interestingly, the contribution of the undulations does not depend on the number of periods in the averaging volume, but only on the amplitude $\hat{U}$ and wave length L. The example shows that the usual approximation of Φ by the formula (4.58) can be grossly in error.

A model of the contributions of undulations in two-phase flow due to the difference between u and $\overset{*}{u}$ can be derived in the same manner as Eq. (4.63). To simplify the formulas let us chose the coordinate system such that the x-direction coincides with the direction of $u-\overset{*}{u}$. Then the velocity undulations may be approximated by

$$\left.\begin{aligned} \hat{u}_1 &= (u-\overset{*}{u})\ \sin\left(\frac{2\pi}{D}x\right)\ \sin\left(\frac{2\pi}{D}y\right)\ \sin\left(\frac{2\pi}{D}z\right) \quad , \\ \hat{u}_2 &= 0 \quad , \\ \hat{u}_3 &= 0 \quad , \end{aligned}\right\} \quad (4.64)$$

where D is the distance between the centers of the particles.

Let m be the number of particles in the averaging volume. We associate each maximum of the function $\hat{u}_1$ with a particle. Then there are four particles in the elemental volume D^3 and $m = 4V/D^3$. Therefore,

$$D = (4V/m)^{1/3} \quad . \qquad (4.65)$$

The contribution of the undulations (4.64) to the dissipation function is one third of the contribution of the undulations (4.59) in all velocity coordinates, as can be verified. Therefore, a reasonable model for the contribution due to velocity differences is

$$\langle\Phi\rangle = \frac{1}{\rho T}\,(u-\overset{*}{u})^2\left(\frac{m}{4V}\right)^{2/3}\pi^2\left(\frac{5}{3}\mu+\frac{1}{2}\lambda\right) \quad , \quad \mathrm{W\cdot(kg\cdot K)} \quad . \qquad (4.66)$$

In a computer program where m and V are not available, one can use in Eq. (4.66) the quotient $\overset{*}{m}/(VG)$ instead of m/V without changing the magnitude of $\langle\Phi\rangle$. The correlation (4.66) probably gives only the order of magnitude of the contribution due to velocity differences in the flow. However, it certainly is better than the usual assumption $\langle\Phi\rangle = 0$. In relation to the error term involving the dissipation function in Eq. (3.51), Section 3.2.3, the function $\langle\Phi\rangle$ approximates the error between the volume average of the local dissipation function and the average dissipation function $\bar{\Phi}(E)$.

The models for the turbulent dissipation function vary widely. A simple model for Φ_T is one which has an identical form to $\bar{\Phi}$ (Eq. (4.58)) but with different viscosity coefficients. Gibeling et al.,[5] suggest a model based on the algebraic relationship among a turbulent length scale, turbulent viscosity, and turbulent kinetic energy.

The complete dissipation term that enters the governing equation is the sum of Eqs. (4.58), (4.66), and the model for Φ_T:

$$\Phi = \frac{1}{\rho T}\,\bar{\Phi}(E) + \langle\Phi\rangle + \frac{1}{\rho T}\,\Phi_T \quad , \quad \mathrm{W/(kg\cdot K)} \quad . \tag{4.67}$$

The approximation error is the difference between the expressions (4.56) and (4.67).

4.7.4 Heat Conduction. The heat conduction term Ψ enters the governing equation, Eq. (4.32), in two places. The term itself models at least two phenomena: the heat conduction within the gas defined in terms of the average quantities, and the heat conduction from the gas to the solid. Depending on the model for the deviations of $\check{\rho}\check{e}\check{u}$ from $\rho e u$, we also can have a turbulent heat flux vector defined in a similar manner as the average heat conduction. We shall discuss each of these models in turn.

Locally, the heat conduction within the gas is assumed to be governed by Fourier's law

$$\check{Q} = -\,\check{\kappa}(\check{T})\nabla\check{T} \quad , \quad \mathrm{W/m^2} \quad , \tag{4.68}$$

where $\check{\kappa}(\check{T})$ is the thermal conductivity coefficient which depends on the local temperature. The corresponding average heat conduction term in Eq. (4.32) is a model of

$$-\,\frac{1}{\alpha\rho T}\,\nabla\cdot\left[\frac{1}{VG}\int_V \beta g\check{Q}\,dV\right] = \frac{1}{\alpha\rho T}\,\nabla\cdot\left[\frac{1}{VG}\int_V \beta g\check{\kappa}(\check{T})\,\nabla\check{T}\,dV\right] \quad . \tag{4.69}$$

The volume average in expression (4.69) is usually modeled as Eq. (4.68) without the tildes; that is, the local temperature $\check{T}$ is replaced by the average T (obtained from the average values of s and q by the equation of state correlation, Section 4.7.1), and the local thermal conductivity coefficient $\check{\kappa}(\check{T})$ is replaced by the average coefficient $\kappa(T)$. The latter can be modeled by a generalized Sutherland-type correlation,

$$\kappa(T) = \kappa_o + \kappa_1\,\frac{T^{1.5}}{\kappa_2+T} \quad , \quad \mathrm{W/(m\cdot K)} \quad . \tag{4.70}$$

An estimate of the error incurred by using the model instead of expression (4.69) can be obtained as follows when V_{gas} is connected:

$$\left.\begin{aligned} C_Q &= \frac{-1}{\alpha\rho T}\nabla\cdot\Big[\frac{1}{VG}\int_V \beta g\check{Q}\,dV - \alpha Q\Big] = \frac{1}{\alpha\rho T}\nabla\cdot\Big[\frac{1}{VG}\int_V \beta g\check{\kappa}\nabla\check{T}\,dV - \alpha\kappa\nabla T\Big] \\ &= \frac{1}{\alpha\rho T}\nabla\cdot\big[\alpha\hat{\kappa}\nabla\hat{T} - \alpha\kappa\nabla T\big] \qquad , \end{aligned}\right\} \quad (4.71)$$

where $\hat{T} = \check{T}(\hat{s},\hat{q})$ and $\hat{k} = \check{k}(\hat{T})$ are mean value points of the integrand. Expanding Eq. (4.71) further one obtains

$$C_Q = \frac{1}{\alpha\rho T}\nabla\cdot\big[\alpha(\hat{\kappa}-\kappa)\,\nabla T + \alpha\kappa\nabla(\hat{T}-T)\big] \tag{4.72}$$

and

$$|C_Q| \leqslant \max_V \Big|\frac{\beta}{\alpha\rho T}\nabla\cdot\big[\alpha(\check{\kappa}-\kappa)\nabla\check{T} + \alpha\kappa\nabla(\check{T}-T)\Big| \ . \tag{4.73}$$

The term involving the difference $\check{\kappa}-\kappa$ can be reduced if the model parameters κ_o, κ_1, and κ_2 in the correlation (4.70) are chosen such that

$$\kappa(T)\ \frac{1}{\alpha VG}\int_V \beta g\,\check{\kappa}\,dV \qquad . \tag{4.74}$$

The term involving $\nabla(\check{T}-T)$ reflects the modeling error due to local undulations of the gas temperature.

The heat conduction between the gas and the particles is represented in Eq. (4.32) by a model of

$$-\frac{1}{\alpha\rho T}\frac{1}{VG}\int_{S_p} g\check{Q}\cdot n_{sp}\,dS = \frac{1}{\alpha\rho T}\frac{1}{VG}\int_{S_p} g\,\check{\kappa}\,\nabla\check{T}\cdot n_{sp}\,dS \qquad . \tag{4.75}$$

The integrand in Eq. (4.75) is the heat flux into the particles. We define the surface averaged heat flux by

$$\dot{e} = \frac{1}{SG}\int_{S_p} g\,\check{\kappa}\,\nabla\check{T}\cdot n_{sp}\,dS \quad , \quad W/m^2 \quad , \tag{4.76}$$

and rewrite expression (4.75) as

$$-\frac{1}{\alpha\rho T}\frac{SG}{VG}\dot{e} \quad . \qquad (4.77)$$

The quantity $\dot{e}$ has been modeled by various different experimental correlations. A relatively simple formula is (Gibeling et al.)[5]

$$\langle\dot{e}\rangle = \frac{\overset{*}{m}}{SG}\, s_p\, [h_c(T-\overset{*}{T}) + h_r(T-\overset{*}{T})] \quad , \quad W/m^2 \quad , \qquad (4.78a)$$

where $\overset{*}{T}$ is the average grain surface temperature. The coefficients h_c and h_r in Eq. (4.78) model heat transfer by conduction and radiation, respectively. Gibeling et al.[5] suggest the following expression for the coefficients in case of spherical particles and Nobel-Abel gas:

$$h_c = \frac{\kappa}{\overset{*}{D}_p/2} + 0.2\left(\frac{\gamma}{\gamma-1}\,\frac{R}{M}\,\frac{(\kappa 2\rho)^2|u-\overset{*}{u}|^2}{\mu\overset{*}{D}_p/2}\right)^{1/3} \quad , \quad W/(m^2K) \quad , \qquad (4.78b)$$

where $\overset{*}{D}_p$ is the diameter of the particles, and μ is the shear viscosity coefficient (Section 4.7.2), and

$$h_r = \overset{*}{\varepsilon}\,\sigma_{SB}(T+\overset{*}{T})\,(T^2+\overset{*}{T}^2) \quad , \quad W/(m^2K) \quad , \qquad (4.78c)$$

where $\overset{*}{\varepsilon}$ is the particle emissivity and $\sigma_{SB} = 5.67032 \cdot 10^{-8}$ $Wm^{-2}K^{-4}$ is the Stephan-Boltzmann constant.

The model $\langle\dot{e}\rangle$ should be consistent with the model $\langle\dot{T}\rangle$ of the grain surface temperature rate of change. The relation between both models is discussed in Section 4.7.10.

The model of the significant deviations of $\breve{\rho}\breve{e}\breve{u}$ from $\rho e u$ (denoted by Q_T, see Section 3.3) can have different forms. One model of the turbulent heat flux vector, given by Ishii[13] and Gibeling et al.,[5] is

$$Q_T = -\kappa_T\left[\nabla T - \frac{\nabla\alpha}{\alpha}(T_i - T)\right] \quad , \quad W/m^2 \quad , \qquad (4.79)$$

where T_i is an average temperature on the interface (a function of T and $\overset{*}{T}$) and κ_T is given by an algebraic formula involving an effective viscosity and Prandtl number.

The heat conduction term Ψ is the sum of the three described models, i.e.,

$$\begin{aligned}\Psi &= \Psi_{gas} + \Psi_{particle} + \Psi_{turb} \\ &= \frac{1}{\alpha\rho T}\nabla\cdot(\alpha\kappa\nabla T) - \frac{1}{\alpha\rho T}\frac{SG}{VG}\langle\dot{e}\rangle - \frac{1}{\alpha\rho T}\nabla\cdot(\alpha Q_T) \quad , \quad W/(kg\cdot K) \quad .\end{aligned} \tag{4.80}$$

4.7.5 **Acceleration by Drag.** The acceleration by drag between gas and particles enters the governing Eqs. (4.32) for the velocities u and $\overset{*}{u}$. The term is defined by (Section 3.3)

$$A_{drag} = \frac{1}{(1-\alpha)\rho}\,\frac{1}{VG}\,D \quad , \tag{4.81}$$

where D models

$$\frac{1}{VG}\int_{S_p} g[n_{sp}(\tilde{p} - p) - n_{sp}\cdot\tilde{\Pi}]\,dS \quad , \tag{4.82}$$

$\tilde{p}$ and $\tilde{\Pi}$ are the local pressure and viscous stress tensor, and p is the average pressure. In interior ballistics applications, the term is modeled by experimental correlations that are available for single particles (e.g., spheres) and for packed beds of particles. For situations between these extremes one has to interpolate.

In order to see how the drag coefficient c_D for a single sphere relates to A_{drag}, we consider a situation where the m identical particles do not interfere with each other. Then the absolute value of the drag force acting on a single particle is

$$\left.\begin{aligned}|F| &= \frac{1}{\overset{*}{m}}\left|\iint_{S_p} g[n_{sp}(\tilde{p}-p) - n_{sp}\cdot\tilde{\Pi}]\,dS\right| \\ &= \frac{VG}{\overset{*}{m}}(1-\alpha)\,\rho\,|A_{drag}| \quad .\end{aligned}\right\} \tag{4.83}$$

In terms of the drag coefficient c_D, the force is (Schlichting, p. 15)[16]

$$|F| = \frac{1}{2} c_D \, |u-\overset{*}{u}|^2 \, a_p \, \rho \quad , \qquad (4.84)$$

where a_p is the frontal area of the particle. Eliminating $|F|$ between Eqs. (4.83) and (4.84) one obtains

$$|A_{drag}| = \frac{1}{2} c_D \, |u-\overset{*}{u}|^2 \, a_p \, \frac{\overset{*}{m}}{VG} \, \frac{1}{1-\alpha} \quad , \qquad (4.85)$$

or, using Eq. (4.12), Section 4.2.1,

$$|A_{drag}| = \frac{1}{2} c_D \, |u-\overset{*}{u}|^2 \, \frac{a_p(\overset{*}{d})}{v_p(\overset{*}{d})} \quad . \qquad (4.86)$$

The drag coefficient for a single sphere can be approximated by

$$c_D = 24/R_e + 0.4 \quad , \qquad (4.87)$$

where

$$R_e = |u-\overset{*}{u}| \; \rho \, D_p(\overset{*}{d})/\mu \qquad (4.88)$$

is the particle Reynolds number and $D_p(\overset{*}{d})$ is the average particle diameter. (About the approximation (4.87), see Figure 1.5 in Schlichting, p. 16).[16]

Substituting the expression (4.87) into (4.86) and observing that the acceleration is in the direction of $u-\overset{*}{u}$ one obtains for non-interfering spheres the Reynolds formula

$$A_{Reynolds} = (u-\overset{*}{u}) \, \frac{a_p(\overset{*}{d})}{v_p(\overset{*}{d})} \left(0.2|u-\overset{*}{u}| + 12 \, \frac{\mu}{\rho D_p(\overset{*}{d})}\right) \quad . \qquad (4.89)$$

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[16] *H. Schlichting, Boundary Layer Theory, 4th Ed., McGraw-Hill Book Co., New York, 1960.*

For a packed bed one finds, e.g., the Ergun correlation (Gibeling et al., pp. 15 and 30)[5]

$$A_{Ergun} = (u-\overset{*}{u})\,\frac{a_p(\overset{*}{d})}{v_p(\overset{*}{d})}\,\frac{2}{3}\,\frac{1}{\alpha^2}\left(1.75\left|u-\overset{*}{u}\right| + 150(1-\alpha)\,\frac{\mu}{\rho D_p(\overset{*}{d})}\right) \qquad (4.90)$$

In order to interpolate between both formulas one may assign limits for their validity. For instance, one could assume that the dispersed sphere formula holds for $\alpha > 0.9$, and the compacted sphere formula holds for $\alpha < 0.65$. Then the acceleration term is

$$A_{drag} = \begin{cases} A_{Reynolds} & \text{for } \alpha \geqslant 0.9 \quad , \\ 4[(\alpha - 0.65)\,A_{Reynolds} + (0.9-\alpha)A_{Ergun}] & \text{for } 0.65<\alpha<0.9 \quad , \\ A_{Ergun} & \text{for } \alpha \leqslant 0.65 \quad . \end{cases} \qquad (4.91)$$

The quoted limits are arbitrary and may be changed, if experiments are available. Also, other than the Ergun formula may be used, if experimental data indicate a better approach.

4.7.6 Acceleration by Granular Stresses. Acceleration by granular stresses enters the governing Eq. (4.32) for the particle velocity $\overset{*}{u}$. The term is formally defined by (see Section 3.3)

$$A_{stress} = \frac{1}{(1-\alpha)\overset{*}{\rho}}\,\nabla\cdot\left[(1-\alpha)\overset{*}{\Pi}\right] + \frac{1}{(1-\alpha)\overset{*}{\rho}}\,\nabla\cdot\left[(1-\alpha)\overset{*}{\Pi}_T\right] \quad . \qquad (4.92)$$

The second term of Eq. (4.92) represents the acceleration of the particulate phase by solid phase turbulence which is defined by Eq. (3.46), Section 3.2.2, and may be modeled by a solid phase turbulent stress tensor $\overset{*}{\Pi}_T$. Because the density of the solid phase is much larger than that of the gas phase and the sizes of the propellant grains are large, the turbulence of the solid phase is assumed negligible and $\overset{*}{\Pi}_T$ is set equal to zero.

In the first term of Eq. (4.92) the variable $\overset{*}{\Pi}$ models

$$\frac{1}{1-\alpha}\,\frac{1}{VG}\int_V (1-\beta)\,g\,(\check{\overset{*}{\Pi}} + pI)\,dV \qquad (4.93)$$

(see Eq. (3.44)). It is interpreted physically as the effect of grain interaction with grains. Without such an interaction the stresses $\overset{*}{\Pi}$ inside the grains would be equal to the negative of the surrounding gas pressure or nearly so, and the acceleration term A_{stress} could be neglected, except for turbulence considerations.

Generally in interior ballistics, one makes two assumptions about the model $\overset{*}{\Pi}$ of the average integranular stresses. First, one assumes that it is a function of α only and, second, one assumes that it is a diagonal matrix i.e.,

$$\overset{*}{\Pi} = I\, R_p(\alpha) \quad . \tag{4.94}$$

The second assumption means that the stresses have the effect of a pressure that acts on the particles in addition to the gas pressure. With these assumptions, one obtains from Eq. (4.92) for the acceleration

$$A_{stress} = \frac{1}{1-\alpha}\frac{d}{d\alpha}\left[\frac{1-\alpha}{\overset{*}{\rho}} R_p(\alpha)\right] \nabla(1-\alpha) \quad . \tag{4.95}$$

The derivative term in Eq. (4.95) is interpreted as the square of the sound speed $\overset{*}{a}$ in the dispersed phase, and A_{stress} is expressed as

$$A_{stress} = -\,\overset{*}{a}{}^{2}(\alpha)\,\frac{1}{1-\alpha}\,\nabla(1-\alpha) \quad . \tag{4.96}$$

The modeling of A_{stress} is reduced by these assumptions to the modeling of a sound speed function $a(\alpha)$. The sound speed can be measured in packed beds and in suspended particle flows, so that the model can be tested in these special cases.

The function $\overset{*}{a}(\alpha)$ should increase with higher particle density $(1-\alpha)\overset{*}{\rho}$, i.e., with decreasing α. Also, as α approaches one, the function should approach zero. Let a_{sp} be the sound speed within a particle and let us assume that for $\alpha = \alpha_1$ all particles touch each other, so that $\overset{*}{a}(\alpha_1) = a_{sp}$. Let $\overset{*}{a}(\alpha)$ become zero at $\alpha = \alpha_2 < 1$. Then a reasonable model for $\overset{*}{a}(\alpha)$ is

$$\overset{*}{a}(\alpha) = \begin{cases} a_{sp}\left(\dfrac{\alpha_1 - \alpha_o}{\alpha - \alpha_o}\right)\left(\dfrac{\alpha_2-\alpha}{\alpha_2-\alpha_1}\right) & \text{for } \alpha_o < \alpha < \alpha_2 \;, \\ 0 & \text{for } \alpha_2 < \alpha \quad . \end{cases} \tag{4.97}$$

In Eq. (4.97), the value $\alpha = \alpha_o$ corresponds to a highest density $(1-\alpha_o)\overset{*}{\rho}$ that can be achieved by compacting the particles. If $\alpha_o = 0$ then one assumes that the particles can be crushed and compacted to a solid mass with the density $\overset{*}{\rho}$. The last factor in Eq. (4.97) merely lets $\overset{*}{a}$ approach zero as α approaches α_2. Thus, one assumes that for $\alpha > \alpha_2$ particle interaction can be neglected. Gibeling et al.,[5] uses a similar formula in which $\alpha_o = 0$ and the second factor is set equal to one. Using that formula, one sets $a(\alpha) \equiv 0$ for $\alpha > \alpha_1$. It seems that a continuous transition to zero, as provided by our formula (4.97), is more realistic.

4.7.7 Burning Rate. The burning or regression rate directly enters the governing equation for the regression distance $\overset{*}{d}$ in Eqs. (4.32). The corresponding term is defined as the surface average of the local regression rate $\partial\overset{*}{d}/\partial t = (\tilde{u}_{sp} - \tilde{\overset{*}{u}})\cdot n_{sp}$ (see Sections 3.1.2 and (3.2.1) and is approximated by

$$\langle\dot{d}\rangle \approx \frac{1}{SG} \int_{S_p} g \frac{\partial \tilde{\overset{*}{d}}}{\partial t}\, ds \quad . \tag{4.98}$$

The linear regression rate can be measured, e.g., in closed bomb or strand burner experiments. The experiments show a dependence of the burning rate on the gas pressure, on gas velocity (erosive burning) and on the time derivative of the pressure (dynamic burning). Best established is the dependence of the burning rate on pressure, which is modeled by the equation

$$\dot{d}_s = B_o + B_1 p^{B_2} \tag{4.99}$$

with constant B_o, B_1, and B_2. The dependence on the relative velocity $|u-\overset{*}{u}|$ and on the pressure change $\partial p/\partial t$ can be incorporated into the model equation either as additive terms or as a factor. The simplest model $\langle\dot{d}\rangle$ is obtained by neglecting these dependence and setting $\langle\dot{d}\rangle$ equal to $\dot{d}_s$, i.e.,

$$\langle\dot{d}\rangle = \begin{cases} 0 & \text{for } \langle\overset{*}{T}\rangle < T_{ignition} \\ B_o + B_1 p^{B_2} & \text{for } \langle\overset{*}{T}\rangle > T_{ignition} \end{cases} \quad . \tag{4.100}$$

The largest uncertainty of this model comes from the experimentally determined model parameters, and from the assumptions that erosive and/or dynamic burning is, or is not important. An averaging error is also introduced by the use of the equation of state function p(s,q) in Eq.

(4.100). However, the error is likely to be negligible compared to the general inaccuracy of the model function. These errors are included in the error estimate (3.22), Section 3.2.1.

4.7.8 Source Terms. In this section, we discuss terms in Eq. (4.32) that are associated with the burning of the propellant. They are characterized by the factor $\langle \dot{d} \rangle$, which represents the regression rate correlation and is discussed in Section 4.7.7. Because of this factor, the source terms are equal to zero if no burning takes place, and they represent sources of mass, energy, and momentum if the grains are burning. In the governing Eqs. (4.32), the terms have the common factor Γ and they enter the equations for s, q and u. The factor Γ models (Section 3.3)

$$\frac{1}{\alpha}\frac{\overset{*}{\rho}}{\rho}\frac{1}{VG}\int_{S_p} g(\breve{u}_{sp} - \breve{\overset{*}{u}})\cdot n_{sp}\, dS \quad , \quad 1/s \quad , \tag{4.101}$$

and is defined by

$$\Gamma = \frac{1}{\alpha}\frac{\overset{*}{\rho}}{\rho}\frac{SG}{VG}\langle \dot{d} \rangle \quad . \tag{4.102}$$

In Eq. (4.102), SG can be eliminated using the relation (4.19), Section 4.2.1. The result is

$$\Gamma = \frac{1}{\alpha}\frac{\overset{*}{\rho}}{\rho}\frac{\overset{*}{m}}{VG}\, s_p(\overset{*}{d})\, \langle \dot{d} \rangle \quad , \tag{4.103}$$

as stated by Eq. (4.33).

The approximation error in Eq. (4.102) is that of the correlation $\langle \dot{d} \rangle$ (see Section 3.2.1). In the expression (4.103) one has, in addition, errors associated with the representation of the weighted surface SG by the product $\overset{*}{m}s_p$. Because the representation is part of the definition of $\overset{*}{m}$ (see Section 4.2.1), it does not formally introduce new errors.

The governing Eq. (4.32) for the gas velocity contains the source term $(\overset{*}{u}-u)\Gamma$. The term models

$$\frac{1}{\alpha}\frac{\overset{*}{\rho}}{\rho}\frac{1}{VG}\int_{S_p} (\breve{\overset{*}{u}}-u)\, g\, [(\breve{u}_{sp} - \breve{\overset{*}{u}})\cdot n_{sp}]\, dS \quad , \quad m/s^2 \quad . \tag{4.104}$$

The error in the governing equation caused by the model (4.103) is

$$\frac{1}{\alpha}\frac{\overset{*}{\rho}}{\rho}\frac{1}{VG}\int_{S_p}(\check{\overset{*}{u}}-\overset{*}{u})\,g\,[(\check{u}_{sp}-\check{\overset{*}{u}})\cdot n_{sp}].dS\,\cdot \qquad (4.105)$$

The error is zero if all grains have the same velocity and do not rotate.

The governing Eq. (4.32) for the entropy contains the source term HΓ. The term is derived under the assumption that the approximation

$$\int_{S_p} g\,\check{e}\,(\check{u}_{sp}-\check{\overset{*}{u}})\cdot n_{sp}\,dS \approx \hat{e}\int_{S_p} g\,(\check{u}_{sp}-\check{\overset{*}{u}})\cdot n_{sp}\,dS \qquad (4.106)$$

holds. Eq. (4.106) is indeed an identity if the local specific energy $\check{e}$ of the gas released from the burning propellant surface is equal to a constant e. This is a common assumption in interior ballistics. The constant e is the specific energy of the gas at "flame temperature", i.e.,

$$\hat{e} = \frac{1}{\gamma-1}\frac{R}{M}T_{flame} = \frac{1}{\gamma-1}g_a I_p \quad , \quad J/kg \quad , \qquad (4.107)$$

where g_a is the standard acceleration 9.80665 m/s^2 and

$$I_p = T_{flame}\,R/(g_a M) \quad , \quad m \quad , \qquad (4.108)$$

is the "force" or "impetus" of the propellant. (Sometimes also the product $g_a I_p (m^2/s^2)$ is called the "impetus" of the propellant.)

In some cases, a modeling of $\hat{e}$ may be better than the assumption of a constant e. For instance, if the propellant contains a retardant then one could assume that the flame temperature is a function of the regression distance, and consequently, $\hat{e} = \hat{e}(\overset{*}{d})$. Of course, the modeling then involves averaging errors, because the local $\hat{e}(\check{\overset{*}{d}})$ would be replaced by a function $\hat{e}(\overset{*}{d})$ of the average $\overset{*}{d}$.

The factor H is defined by

$$H = \frac{1}{T}\,[(\hat{e}+p/\overset{*}{\rho}) - (e+p/\rho)] \quad , \quad J/(kg\cdot K) \quad , \qquad (4.109)$$

i.e., H is the difference between the enthalpy of the gas emerging from the flame and of the surrounding gas, divided by the gas temperature.

The approximations that effect this term are those of the equations of state (see Section 4.7.1).

The source term in the governing equation (4.32) for the pressure logarithm function q has as a factor of Γ the expression $(e-e-e_s H)/e_q$, where $e_s(s,q)$ and $e_q(s,q)$ are the partial derivatives of the specific internal energy with respect to s and q, respectively. The factor is derived by formal manipulation and the approximations involved in the derivation are the same as discussed above.

4.7.9 **Grain Volume and Surface**. We recall the discussions in Section 4.2.1 about the definition of the grain number function $\overset{*}{m}$. The formal definition of the average grain volume function $v_p(\overset{*}{d})$ and of the average grain surface function $s_p(\overset{*}{d})$ should be consistent with the definition of $\overset{*}{m}$. In this section, we shall discuss definitions that are consistent with Eqs. (4.18) and (4.19), respectively.

For convenience, we repeat the pertinent equations and definitions in this section. Our goal is to find such functions $\overset{*}{m}$, v_p, s_p, that satisfy the following set of relations

$$\overset{*}{d}(t,x) = \frac{1}{SG} \int_{S_p} g \, \check{\overset{*}{d}} \, dS \quad . \tag{4.110}$$

$$\frac{dv_p(\overset{*}{d})}{d\overset{*}{d}} = - s_p(\overset{*}{d}) \quad , \tag{4.111}$$

$$\overset{*}{m}(t,x) \; s_p(\overset{*}{d}) = \int_{S_p} g \, dS \quad , \tag{4.112}$$

$$\overset{*}{m}(t,x) \; v_p(\overset{*}{d}) = \int_V (1-\beta) \, g \, dV \; . \tag{4.113}$$

We found in Section 4.2.1, that such functions in general do not exist and, therefore, suggested to define $\overset{*}{m}$ by either of the following two equations:

$$\overset{*}{m} = \sum_{i=1} \left\{\frac{1}{s_{pi}} \int_{S_p \cap V} g \, dS\right\} \quad , \tag{4.114}$$

or

$$\overset{*}{m} = \sum_{i=1}^{m} \left\{\frac{1}{v_{pi}} \int_{V_i \cap V} g \, dV\right\} \quad . \tag{4.115}$$

Once $\overset{*}{m}$ is defined, then one can define either s_p or v_p by Eqs. (4.112) or (4.113), respectively, and find the other function from Eq. (4.111).

The approximations involved are, first, due to the assumption that $\overset{*}{m}$, as defined, is independent of $\overset{*}{d}$. The accuracy of the approximation is improved if the weight function g is almost constant over the averaging volume. A second approximation is due to the assumption that s_p or v_p, defined by Eqs. (4.112) or (4.113), respectively do not depend explicitly on t and x. Again, an almost constant g may improve the accuracy of this approximation.

The modeling of the functions v_p and s_p practically is done at a limit, assuming constant g, and identical particles. In this case, the functions simply represent a single particle.

If there is a variation of particle sizes within the averaging volume, then by either of the described formalisms one obtains average n_p and s_p that are slanted towards the larger particles. Investigations of the significance of this bias have not been done for interior ballistics problems.

4.7.10. <u>Grain Surface Heating Rate</u>. The grain surface heating rate enters the governing equation, Eq. (4.32), for the grain surface temperature

$$\frac{\partial \overset{*}{T}}{\partial t} = - \overset{*}{u}\cdot\nabla\overset{*}{T} + \langle\dot{T}\rangle \quad . \tag{4.116}$$

The term $\langle\dot{T}\rangle$ is the correlation model for

$$\dot{T} = \frac{1}{SG} \int_{S_p} \frac{\partial \overset{*}{T}}{\partial t}\, g \; dS \quad , \tag{4.117}$$

i.e., for the average rate of change of the surface temperature. The change is related to the heat flux to the particles, $\dot{e}$, discussed in Section 4.7.4. Therefore, the model $\langle\dot{T}\rangle$ should be consistent with the model $\langle\dot{e}\rangle$.

Like the grain surface and grain volume functions, the surface temperature model function is usually established by considering the limiting case of identical grains, i.e., by treating a single grain. Typically, if the grain has a simple geometry, one calculates the temperature field within the grain corresponding to the energy transfer $\langle\dot{e}\rangle$. This involves the solution of a differential equation that is valid within the grain and the determination of the corresponding surface temperature. However, the solution of Eq. (4.116) is the surface temperature itself and the temperature field within the grain is not needed (if a model $\langle\dot{T}\rangle$ is available. Once the surface temperature is known, it is used to determine the energy transfer at the next time step or the commencement of ignition. This type of calculation is used if one is particularly interested in the ignition process. After ignition, all heat transfer is assumed to be zero, because then the energy flow phenomena are dominated by the combustion and the associated heat release. The continued heating of the grains is assumed to be of no consequence for the combustion.

In order to illustrate the relation between $\langle\dot{T}\rangle$ and the heat transfer from the gas to the particle, Section 4.7.4, Eq. (4.77), we consider a very simple model in which the temperature in each grain is assumed to be uniform. (The model is not recommended for simulation of interior ballistics, but it shows the salient features of the relation.) Let $\overset{*}{c}_p$ be the specific heat of the particle material. Then the heat capacity of one particle is $\overset{*}{c}_p v_p \overset{*}{\rho}$, (J/K), and the relation between the energy transfer models $\langle\dot{e}\rangle$ and $\langle\dot{T}\rangle$ is

$$\overset{*}{m}\,\overset{*}{c}_p\overset{*}{\rho}v_p\langle\dot{T}\rangle = \langle\dot{e}\rangle SG \quad . \tag{4.118}$$

From Eq. (4.118) and expression (4.77), Section 4.7.4, the model for the heat conduction between the gas and particles can be written in terms of $\langle\dot{T}\rangle$ as

$$\Psi_{\text{particle}} = \frac{1}{\alpha\rho T}\,\frac{\overset{*}{m}}{VG}\left[\overset{*}{c}_p\overset{*}{\rho}v_p\langle\dot{T}\rangle\right] \quad . \tag{4.119}$$

The important result is the existence of a relation like Eq. (4.118) between $\langle\dot{T}\rangle$ and $\langle\dot{e}\rangle$. It would be replaced by a different relation if the heat flow within the particle were taken into account, as described above. In that case, the expression in the brackets in Eq. (4.119) would be changed correspondingly.

5. SUMMARY AND CONCLUSIONS

Interior ballistics models are mostly based on engineering approximations and insight, like Lagrange's model. Alternatively, one can assume that the gas and particles locally satisfy all conservation equations, and obtain the model by an averaging process. In this report, we follow the latter approach and present a complete mathematical derivation of weighted volume averaged equations including all error terms, sufficient conditions for the necessary differentiability of the average variables, and regions of definition of the average variables. Initial and boundary conditions that are consistent with the volume averaged equations are discussed. Correlations that are used to close the system of partial differential equations are examined. Some of these correlations are different from those commonly used in interior ballistic applications.

The average governing equations that are derived in this report model the transient effects of viscosity, heat conduction, and turbulence in the compressible gas phase; the ignition, intergranular stress, and burning in the incompressible solid phase; and the corresponding interactions between the phases, e.g., drag, heat transfer, and source terms. Turbulence is defined in terms of volume averages with only elementary models presented for completeness of the report. In the average model, quantities appear that are defined only on the surfaces of the grains. We show that these quantities satisfy a general partial differential equation. The relationships between the volume average equations and the local equations for individual phases are discussed as the volume approaches zero. Because these equations must be solved via a computer, an appropriate form and choice of dependent variables for numerical solution are discussed. Thus, this report presents a complete and consistent mathematical model of interior ballistics for non-reacting burning particle-gas flows.

The exposition of the theoretical basis of averaged equations permits us to draw the following conclusions:

First, the proper averaging domain is a finite volume that is larger than the propellant grains. Line and surface averaging cannot be used because the corresponding averages do not have the necessary differentiability properties. Infinite volume averaging is not appropriate for interior ballistics (or other confined flows) because in such a volume the phases do not occupy complementary spaces. Time averaging is not applicable in interior ballistics because of the unsteady and rapidly changing flow conditions, including moving boundaries.

Second, the average equations are valid only for cases where the averaging volume consists of gas and particles or just gas and where the local functions have no discontinuities within their respective domains. Therefore, average governing equations are not suitable for describing flows with shocks, contact discontinuities, etc. On the other hand, by a proper formulation of the governing equations, we obtain a system that can be solved numerically without explicitly following the boundaries of regions without particles.

Third, the average equations are not valid in the boundary region, the thickness of which is equal to a radius of the averaging volume. Consequently, the formulation of proper boundary conditions is problematic, and has not been solved satisfactorily. (We do not consider ad hoc treatments of special cases an adequate solution of the general problem.) Also, resolution of interior ballistics boundary layers based on volume average two-phase equations is only possible in exceptional cases, when particles are smaller than the typical boundary layer. The study of two-phase flow fields with small additive particles that are associated with wear and erosion of gun tubes may be such as exceptional case.

Fourth, one-dimensional interior ballistics models based on volume averaging are less problematic than two-dimensional models, because the averaging volume occupies a finite thickness cross-section of the tube and is large compared to the particles. The only problems with such models are the formulation of boundary conditions at the breech and projectile.

Fifth, a mathematical basis for two-dimensional interior ballistic models could possibly be obtained by an extension of the theory of average equations. Such an extension may be possible by generalizing to a variable volume averaging or by using statistical averages instead of volume averages. The first approach will alleviate some problems, but it cannot remove the basic cause of problems in two-dimensional modeling: the particle sizes that are large compared to the gas boundary layer. The second approach (statistical averaging) has not been tried successfully for two-phase flows. There the encountered problems are mathematical, requiring a major investment in the development of the theory. Also, it is not certain if the problems associated with boundary conditions will be alleviated by statistical averaging.

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APPENDIX A

GOVERNING EQUATIONS FOR AXIALLY SYMMETRIC FLOWS IN CYLINDRICAL COORDINATES

APPENDIX A

GOVERNING EQUATIONS FOR AXIALLY SYMMETRIC FLOWS IN CYLINDRICAL COORDINATES

This appendix contains a list of the governing equations in component form in cylindrical coordinates for the case of axially symmetric flow. The subscripted variables denote the components of a vector and not the derivative of these variables. All derivatives are written in a non-abbreviated form. The listed equations are in a form which is compatible with Eq. (4.32), Sect. 4.3. The components of the gas average velocity and the particle average velocity are

$$u = (u_r, u_\theta, u_z) \quad , \quad (\mathrm{m/s}) \quad , \tag{A.1}$$

$$\overset{*}{u} = (\overset{*}{u}_r, \overset{*}{u}_\theta, \overset{*}{u}_z) \quad , \quad (\mathrm{m/s}) \quad , \tag{A.2}$$

where the subscripts r, θ, and z refer to the radial, angular, and axial coordinate directions, respectively. The components of the gradient of a scalar f are

$$\nabla f = \left\{\left(\frac{\partial f}{\partial r}\right)_r, (0)_\theta, \left(\frac{\partial f}{\partial z}\right)_z\right\} \quad . \tag{A.3}$$

The divergence of a vector $F = (F_r, F_\theta, F_z)$ is

$$\nabla \cdot F = \frac{1}{r}\,\frac{\partial (rF_r)}{\partial r} + \frac{\partial F_z}{\partial z} \quad . \tag{A.4}$$

The independent variables are time t, radial position r, and axial position z. The dependent average variables which are computed from the governing partial differential equations are: the specific entropy s, the pressure logarithm function q, the radial gas velocity u_r, the circumferential gas velocity u_θ, the circumferential particle velocity $\overset{*}{u}_\theta$, the axial particle velocity $\overset{*}{u}_z$, the number of particles within the averaging volume $\overset{*}{m}$, the regression distance $\overset{*}{d}$, and the surface temperature of the particles $\overset{*}{T}$.

The entropy equation is

$$\frac{\partial s}{\partial t} = - u_r \frac{\partial s}{\partial r} - u_z \frac{\partial s}{\partial z} + \frac{p}{\rho T} B + H \Gamma + \Phi + \Psi \tag{A.5}$$

where p, ρ, T, H, Γ, are given by Eqs. (B.6), (B.4), (B.2), (B.27), and (B.26), respectively. The expression for B is

$$B = \frac{1}{\alpha} \left\{ (1-\alpha) \left[\frac{1}{r} \frac{\partial (r\overset{*}{u}_r)}{\partial r} + \frac{\partial \overset{*}{u}_z}{\partial z}\right] - (u_r - \overset{*}{u}_r) \frac{\partial (1-\alpha)}{\partial r} - (u_z - \overset{*}{u}_z) \frac{\partial (1-\alpha)}{\partial z} \right\} , \tag{A.6}$$

and the porosity α is given by Eq. (B.1). The dissipation function Φ is

$$\Phi = \frac{1}{\rho T} \bar{\Phi}(E) + \frac{1}{\rho T} \Phi_T + \langle \phi \rangle \quad , \tag{A.7}$$

where

$$\begin{aligned} \bar{\Phi}(E) = {} & \frac{4}{3} \mu \left[\left(\frac{\partial u_r}{\partial r}\right)^2 + \left(\frac{u_r}{r}\right)^2 + \left(\frac{\partial u_z}{\partial z}\right)^2 - \left(\frac{u_r}{r} \frac{\partial u_r}{\partial r} + \frac{\partial u_r}{\partial r} \frac{\partial u_z}{\partial z} + \frac{u_r}{r} \frac{\partial u_z}{\partial z}\right) \right] \\ & + \mu \left[\left(r \frac{\partial}{\partial r} \left(\frac{u_\theta}{r}\right)\right)^2 + \left(\frac{\partial u_z}{\partial r} + \frac{\partial u_z}{\partial r}\right)^2 + \left(\frac{\partial u_\theta}{\partial z}\right)^2 \right] \\ & + \lambda \left[\frac{\partial u_r}{\partial r} + \frac{u_r}{r} + \frac{\partial u_z}{\partial z}\right]^2 \quad , \end{aligned} \tag{A.8}$$

and μ, λ, ⟨ϕ⟩, and Φ_T, are given by Eqs. (B.7), (B.8), (B.13), and (B.35), respectively. The heat conduction term Ψ is given by Eq. (B.15) as

$$\Psi = \Psi_{gas} + \Psi_{particle} + \Psi_{turb} \quad , \tag{A.9}$$

where

$$\Psi_{gas} = \frac{1}{\alpha\rho T}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\alpha\kappa\frac{\partial T}{\partial r}\right) + \frac{\partial}{\partial z}\left(\alpha\kappa\frac{\partial T}{\partial z}\right)\right] \quad , \tag{A.10}$$

$$\Psi_{turb} = \frac{1}{\alpha\rho T}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\alpha\kappa_T\frac{\partial T}{\partial r}\right) + \frac{\partial}{\partial z}\left(\alpha\kappa_T\frac{\partial T}{\partial z}\right)\right. \tag{A.11}$$

$$\left. - \frac{1}{r}\frac{\partial}{\partial r}\left(r\kappa_T(T_i - T)\frac{\partial\alpha}{\partial r}\right) - \frac{\partial}{\partial z}\left(\kappa_T(T_i - T)\frac{\partial\alpha}{\partial z}\right)\right] \quad ,$$

$\Psi_{particle}$, κ are given by Eqs. (B.17), (B.14), respectively, and κ_T, T_i are discussed near Eq. (B.36).

The pressure logarithm function equation is

$$\frac{\partial q}{\partial t} = -u_r\frac{\partial q}{\partial r} - u_z\frac{\partial q}{\partial z} - \frac{\rho}{\frac{\partial\rho}{\partial q}}\left(\frac{1}{r}\frac{\partial(ru_r)}{\partial r} + \frac{\partial u_z}{\partial z} + \frac{\partial e}{\partial s}\frac{1}{T}B\right) \tag{A.12}$$

$$+ \frac{1}{\frac{\partial e}{\partial q}}\left(\hat{e} - e - \frac{\partial e}{\partial s}H\right)\Gamma - \frac{\partial\rho}{\partial s}\frac{1}{\frac{\partial\rho}{\partial q}}(\Phi + \Psi) \quad ,$$

where ρ, e, T, B, $\hat{e}$, H, Γ, Φ, and Ψ are given by Eqs. (B.4), (B.3), (B.2), (A.6), (B.28), (B.27), (B.26), (A.7), and (A.9), respectively.

The radial gas velocity equation is

$$\frac{\partial u_r}{\partial t} = -u_r\frac{\partial u_r}{\partial r} - u_z\frac{\partial u_r}{\partial z} + \frac{u_\theta^2}{r} - \frac{dp}{dq}\frac{1}{\rho}\frac{\partial q}{\partial r} - (u_r - \overset{*}{u}_r)\,\Gamma \tag{A.13}$$

$$- \frac{(1-\alpha)}{\alpha}(A_{drag})_r + (A_{visc})_r + (A_{turb})_r \quad ,$$

where

$$\begin{aligned}(A_{visc})_r = \frac{1}{\alpha\rho}\Big\{&\frac{\partial}{\partial r}\Big[\alpha\mu\,\frac{2}{3}\Big(2\,\frac{\partial u_r}{\partial r} - \frac{u_r}{r} - \frac{\partial u_z}{\partial z}\Big) + \alpha\lambda\Big(\frac{1}{r}\,\frac{\partial}{\partial r}(r u_r) + \frac{\partial u_z}{\partial z}\Big)\Big] \\ &+ \frac{\partial}{\partial z}\Big[\alpha\mu\Big(\frac{\partial u_r}{\partial z} + \frac{\partial u_z}{\partial r}\Big)\Big] + 2\alpha\mu\,\frac{\partial}{\partial r}\Big(\frac{u_r}{r}\Big)\Big\} \quad ,\end{aligned} \tag{A.14}$$

and p, ρ, Γ, α, μ, and λ are given by Eqs. (B.6), (B.4), (B.26), (B.1), (B.7), and (B.8), respectively. The radial component of the drag $(A_{drag})_r$ is given by the radial component of Eq. (B.20). The radial component of acceleration due to turbulence $(A_{turb})_r$ could be given by the radial component of Eq. (B.34) which is Eq. (A.14) with μ and λ replaced by μ_T and λ_T.

The circumferential gas velocity equation is

$$\begin{aligned}\frac{\partial u_\theta}{\partial t} = &- u_r\,\frac{\partial u_\theta}{\partial r} - u_z\,\frac{\partial u_\theta}{\partial z} - \frac{u_r u_\theta}{r} - (u_\theta - \overset{*}{u}_\theta)\Gamma \\ &- \frac{(1-\alpha)}{\alpha}\,(A_{drag})_\theta + (A_{visc})_\theta + (A_{turb})_\theta \quad ,\end{aligned} \tag{A.15}$$

where

$$(A_{visc})_\theta = \frac{1}{\alpha\rho}\Big\{\frac{\partial}{\partial r}\Big[\alpha\mu\; r\,\frac{\partial}{\partial r}\Big(\frac{u_\theta}{r}\Big)\Big] + \frac{\partial}{\partial z}\Big[\alpha\mu\,\frac{\partial u_\theta}{\partial z}\Big] + 2\alpha\mu\,\frac{\partial}{\partial r}\Big(\frac{u_\theta}{r}\Big)\Big\} \tag{A.16}$$

and α, Γ, μ, λ, and ρ are given by Eqs. (B.1), (B.26), (B.7), (B.8), and (B.4), respectively. The circumferential component of the drag $(A_{drag})_\theta$ is given by the circumferential component of Eq. (B.20). The circumferential component of the acceleration due to turbulence $(A_{turb})_\theta$ could be given by the circumferential components of Eq. (B.34) which is Eq. (A.16) with μ and λ replaced by μ_T and λ_T.

The axial gas velocity equation is

$$\begin{aligned}\frac{\partial u_z}{\partial t} = &- u_r\,\frac{\partial u_z}{\partial r} - u_z\,\frac{\partial u_z}{\partial z} - \frac{dp}{dq}\,\frac{1}{\rho}\,\frac{\partial q}{\partial z} - (u_z - \overset{*}{u}_z)\Gamma \\ &- \frac{(1-\alpha)}{\alpha}\,(A_{drag})_z + (A_{visc})_z + (A_{turb})_z \quad ,\end{aligned} \tag{A.17}$$

where

$$(A_{visc})_z = \frac{1}{\alpha\rho}\{\frac{\partial}{\partial r}[\alpha\mu(\frac{\partial u_r}{\partial z} + \frac{\partial u_z}{\partial r})] + \frac{\alpha\mu}{r}[\frac{\partial u_r}{\partial z} + \frac{\partial u_z}{\partial r}]$$

$$+ \frac{\partial}{\partial z}[\alpha\mu\frac{2}{3}(2\frac{\partial u_z}{\partial z} - \frac{\partial u_r}{\partial r} - \frac{u_r}{r}) + \alpha\lambda(\frac{\partial u_z}{\partial z} + \frac{\partial u_r}{\partial r} + \frac{u_r}{r})]\} \quad , \qquad (A.18)$$

and p, ρ, Γ, α, μ, and λ are given by Eqs. (B.6), (B.4), (B.26), (B.1), (B.7), and (B.8), respectively. The axial component of the drag $(A_{drag})_z$ is given by the axial component of Eq. (B.20). The axial component of the acceleration due to turbulence $(A_{turb})_z$ could be given by the axial component of Eq. (B.34) which is Eq. (A.18) with μ and λ replaced by μ_T and λ_T .

The components of the solid phase velocity equation are the radial solid phase velocity equation

$$\frac{\partial \overset{*}{u}_r}{\partial t} = -\overset{*}{u}_r\frac{\partial u_r}{\partial r} - \overset{*}{u}_z\frac{\partial \overset{*}{u}_r}{\partial z} + \frac{\overset{*}{u}_\theta^{\,2}}{r} - \frac{dp}{dq}\frac{1}{\overset{*}{\rho}}\frac{\partial q}{\partial r} + \frac{\rho}{\overset{*}{p}}(A_{drag})_r + (A_{stress})_r \quad , \qquad (A.19)$$

the circumferential solid phase velocity equation

$$\frac{\partial \overset{*}{u}_\theta}{\partial t} = -\overset{*}{u}_r\frac{\partial u_\theta}{\partial r} - \overset{*}{u}_z\frac{\partial \overset{*}{u}_\theta}{\partial z} - \frac{\overset{*}{u}_r\overset{*}{u}_\theta}{r} + \frac{\rho}{\overset{*}{\rho}}(A_{drag})_\theta \quad , \qquad (A.20)$$

and the axial solid phase velocity equation

$$\frac{\partial \overset{*}{u}_z}{\partial t} = -\overset{*}{u}_r\frac{\partial \overset{*}{u}_z}{\partial r} - \overset{*}{u}_z\frac{\partial \overset{*}{u}_z}{\partial z} - \frac{dp}{dq}\frac{1}{\overset{*}{\rho}}\frac{\partial q}{\partial z} + \frac{\rho}{\overset{*}{\rho}}(A_{drag})_z + (A_{stress})_z \qquad (A.21)$$

where p and ρ are given by Eqs. (B.6) and (B.4), respectively. The density of the solid phase $\overset{*}{\rho}$ is assumed constant. The components of the accelerations due to drag, A_{drag}, and intergranular stress, A_{stress}, are given by the components of Eqs. (B.20) and (B.23), respectively.

The particle number equation is

$$\frac{\partial \overset{*}{m}}{\partial t} = -\frac{1}{r}\frac{\partial}{\partial r}(r\overset{*}{m}\overset{*}{u}_r) - \frac{\partial}{\partial z}(\overset{*}{m}\overset{*}{u}_z) \quad . \qquad (A.22)$$

The regression distance equation is

$$\frac{\partial \overset{*}{d}}{\partial t} = - \overset{*}{u}_r \frac{\partial \overset{*}{d}}{\partial r} - \overset{*}{u}_z \frac{\partial \overset{*}{d}}{\partial z} + \langle \dot{d} \rangle \quad , \tag{A.23}$$

where the burning rate correlation $\langle \dot{d} \rangle$ is given by Eq. (B.25).

The surface temperature equation is

$$\frac{\partial \overset{*}{T}}{\partial t} = - \overset{*}{u}_r \frac{\partial \overset{*}{T}}{\partial r} - \overset{*}{u}_z \frac{\partial \overset{*}{T}}{\partial z} \langle \dot{T} \rangle \quad , \tag{A.24}$$

where the correlation $\langle \dot{T} \rangle$ for the rate of change of grain surface temperature is discussed in Section 4.7.10.

APPENDIX B

CORRELATION MODEL FORMULAS

APPENDIX B

CORRELATION MODEL FORMULAS

This appendix contains a list of correlation model formulas. The formulas are discussed in detail in Section 4.7. The terms listed in this appendix are in a form compatible with Eq. (4.32), Section 4.3, and Appendix A.

The porosity or gas volume fraction (Section 4.2.1) is given by

$$\alpha = 1 - v_p(\overset{*}{d})\overset{*}{m}/VG \quad . \qquad (B.1)$$

The equations of state (Section 4.7.1) are

$$T(p,s) = T_R\left(\frac{p}{p_R}\right)^{(\gamma-1)/\gamma} \exp\left(\frac{M}{R}\,\frac{\gamma-1}{\gamma}\,s\right) \quad , \quad K \quad , \qquad (B.2)$$

$$e = \frac{1}{\gamma-1}\,\frac{R}{M}\,T \quad , \quad J/kg \quad , \qquad (B.3)$$

$$\rho = \left(\frac{R}{M}\,\frac{T}{p} + \eta\right)^{-1} \quad , \quad kg/m^3 \quad , \qquad (B.4)$$

$$a^2 = \gamma\frac{p}{\rho}\,\frac{1}{1-\eta\rho} \quad , \quad m^2/s^2 \quad , \qquad (B.5)$$

where $R = 8.3143$ J/(mol·K) is the universal gas constant, M (kg/mol) is the molar mass and η (m^3/kg) is the covolume. The pressure logarithm function q is defined by (Section 4.2.2)

$$q = q_1[\ln(p/p_1) + 1] \quad , \quad Pa, \quad \text{or} \quad p = p_1\exp\left(\frac{q}{q_1} - 1\right) \quad , \quad Pa \quad . \qquad (B.6)$$

The shear viscosity coefficient μ and the bulk viscosity coefficient λ are (Section 4.7.2)

$$\mu = \mu_o + \mu_1\,\frac{T^{1.5}}{\mu_2 + T} \quad , \quad Pa\cdot s \quad , \qquad (B.7)$$

$$\lambda = \lambda_o + \lambda_1\,\frac{T^{1.5}}{\lambda_2 + T} \quad , \quad Pa\cdot s \quad . \qquad (B.8)$$

The *acceleration by viscosity* is modeled by (Section 4.7.2)

$$A_{visc} = \frac{1}{\alpha\rho} \nabla \cdot \left\{\alpha\left[2\mu E + (\lambda - \frac{2}{3}\mu)\ (\text{trace } E)\ I\right]\right\}, \quad m/s^2 \ , \qquad (B.9)$$

where E is the strain rate tensor computed using the average velocities, i.e.,

$$E = 0.5\ \left(\nabla u + (\nabla u)^T\right) \quad . \qquad (B.10)$$

The *heat dissipation function* term is modeled by (Section 4.7.3)

$$\Phi = \frac{1}{\rho T}\,\bar{\Phi}(E) + \langle\Phi\rangle + \frac{1}{\rho T}\,\Phi_T \quad , \quad W/(kg\cdot K) \quad , \qquad (B.11)$$

where

$$\bar{\Phi}(E) = 2\mu\ \text{trace}(E^2) + (\lambda - \frac{2}{3}\mu)\ (\text{trace } E)^2 \quad , \quad W/m^3 \quad , \qquad (B.12)$$

$$\langle\Phi\rangle = \frac{1}{\rho T}\ |u-\overset{*}{u}|^2\left(\frac{\overset{*}{m}}{4 \cdot VG}\right)^{2/3} \pi^2\left(\frac{5}{3}\mu + \frac{1}{2}\lambda\right) \quad , \quad W/(kg\cdot K) \quad , \qquad (B.13)$$

and Φ_T is given by Eq. (B.35).

The *thermal conductivity coefficient* κ is modeled by (Section 4.7.4)

$$\kappa = \kappa_o + \kappa_1 \frac{T^{1.5}}{\kappa_2 + T} \quad , \quad W/(m\cdot K) \quad . \qquad (B.14)$$

The *heat conduction term* in the governing equations is modeled by (Section 4.7.4)

$$\Psi = \Psi_{gas} + \Psi_{particle} + \Psi_{turb} \quad , \quad W/(kg\cdot K) \quad , \qquad (B.15)$$

where

$$\Psi_{gas} = \frac{1}{\alpha\rho T}\ \nabla\cdot(\alpha\ \kappa\ \nabla T) \qquad (B.16)$$

and

$$\Psi_{\text{particle}} = \begin{cases} -\dfrac{1}{\alpha\rho T}\dfrac{\overset{*}{m}}{VG}\, s_p\left[h_c(T-\overset{*}{T}) + h_r(T-\overset{*}{T})\right] & , \quad \text{before ignition} \\ 0 & , \quad \text{after ignition} \end{cases}$$

(B.17)

with

$$h_c = \frac{\kappa}{\overset{*}{D}_p/2} + 0.2\left(\frac{\gamma}{\gamma-1}\,\frac{R}{M}\,\frac{(\kappa 2\rho)^2\,|u-\overset{*}{u}|^2}{\mu\,\overset{*}{D}_p/2}\right)^{1/3} \quad , \ \mathrm{W/(m^2\cdot K)} \quad , \qquad \text{(B.18)}$$

and

$$h_r = \overset{*}{\varepsilon}\,\sigma_{SB}(T+\overset{*}{T})\,(T^2+\overset{*}{T}{}^2) \quad , \ \mathrm{W/(m^2\cdot K)} \quad . \qquad \text{(B.19)}$$

In Eq. (B.19), $\overset{*}{\varepsilon}$ is the particle emissivity, $\sigma_{SB} = 5.67032\cdot 10^{-8}\ \mathrm{W\cdot m^{-2}K^{-4}}$ is the Stephan-Boltzman constant, and $\overset{*}{T}$ is the average grain surface temperature. The turbulent heat flux within the gas, Ψ_{turb} is given by Eqs. (B.36) and (B.37).

The acceleration term due to the drag between gas and particles is modeled by (Section 4.7.5).

$$A_{drag} = \begin{cases} A_{Ergun} & \text{for } \alpha \leq 0.65 \quad , \\ 4\left[(\alpha-0.65)A_{Reynolds} + (0.9-\alpha)A_{Ergun}\right] & \text{for } 0.65<\alpha<0.9 \quad , \\ A_{Reynolds} & \text{for } 0.9 \leq \alpha \quad , \end{cases}$$

(B.20)

where

$$A_{Ergun} = (u-\overset{*}{u})\,\frac{a_p}{v_p}\,\frac{2}{3}\,\frac{1}{\alpha^2}\left[1.75\,|u-\overset{*}{u}| + 150\,(1-\alpha)\,\frac{\overset{*}{\mu}}{\rho\,\overset{*}{D}_p}\right] \quad , \quad \mathrm{m/s^2} \quad , \qquad \text{(B.21)}$$

and

$$A_{\mathrm{Reynolds}} = (u-\overset{*}{u})\,\frac{a_p}{v_p}\left[0.2\,\left|u-\overset{*}{u}\right| + 12\,\frac{\mu}{\rho\,\overset{*}{D}_p}\right] \quad , \quad \mathrm{m/s^2} \quad . \tag{B.22}$$

The acceleration term due to intergranular stress is modeled by (Section 4.7.6)

$$A_{\mathrm{stress}} = -\,\overset{*}{a}{}^{2}\,\frac{1}{1-\alpha}\,\nabla(1-\alpha) \quad , \quad \mathrm{m^2/s^2} \quad , \tag{B.23}$$

where $\overset{*}{a}(\alpha)$ is a sound speed function for the particulate phase. The function is modeled by

$$\overset{*}{a}(\alpha) = \begin{cases} a_{sp}\left(\dfrac{\alpha_1 - \alpha_o}{\alpha - \alpha_o}\right)\left(\dfrac{\alpha_2 - \alpha}{\alpha_2 - \alpha_1}\right) & \text{for } \alpha_o < \alpha < \alpha_2 \\ 0 & \text{for } \alpha_2 \leq \alpha \end{cases} \quad . \tag{B.24}$$

The burning rate is modeled by (Section 4.7.7)

$$\langle\dot{d}\rangle = \begin{cases} 0 & \text{for } \langle\overset{*}{T}\rangle < T_{\mathrm{ingition}} \\ B_o + B_1 p^{B_2} \quad , \quad \mathrm{m/s,} & \text{for } \langle\overset{*}{T}\rangle \geq T_{\mathrm{ignition}} \end{cases} \quad . \tag{B.25}$$

The source term Γ is (Section 4.7.8)

$$\Gamma = \frac{1}{\alpha}\,\frac{\overset{*}{\rho}}{\rho}\,\frac{\overset{*}{m}}{VG}\,s_p\,\langle\dot{d}\rangle \quad , \quad \mathrm{1/s} \quad . \tag{B.26}$$

The enthalpy factor H of the source term (Section 4.7.8) is defined by

$$H = \frac{1}{T}\left[(\hat{e} + p/\overset{*}{\rho}) - (e + p/\rho)\right] \quad , \quad \mathrm{J/(kg\cdot K)} \quad , \tag{B.27}$$

where $\hat{e}$ is

$$\hat{e} = \frac{1}{\gamma-1}\,\frac{R}{M}\,T_{flame} = \frac{1}{\gamma-1}\,g_a I_p \quad . \quad J/kg \quad , \qquad (B.28)$$

with $g_a = 9.80665\ m/s^2$ being the standard acceleration.

The <u>particle geometry</u> enters the equations as the four functions $v_p(\overset{*}{d})$, $s_p(\overset{*}{d})$, $\overset{*}{D}_p(\overset{*}{d})$ and $a_p(\overset{*}{d})$. We provide the formulas that define these functions for spherical, cylindrical, and tubular grains.

For a <u>spherical grain</u> with initial diameter $\overset{*}{D}_o$ one defines

$$\left.\begin{aligned}
R &= \max\,(0,\ ((\overset{*}{D}_o - 2\overset{*}{d})/2) \quad , \\
v_p &= \frac{4}{3}\,\pi\,R^3 \quad , \\
s_p &= 4\,\pi\,R^2 \quad , \\
a_p &= \pi\,R^2 \quad , \\
\overset{*}{D}_p &= 2R \quad ,
\end{aligned}\right\} (B.29)$$

A <u>solid cylindrical grain</u> may be described by its initial diameter, $\overset{*}{D}_o$, and height, L_o. Let

$$\left.\begin{aligned}
R &= (\overset{*}{D}_o - 2\overset{*}{d})/2 \quad , \\
L &= L_o - 2\overset{*}{d} \quad .
\end{aligned}\right\} (B.30)$$

If either $R < 0$ or $L < 0$, then the grain has been burnt. If both quantities are positive, then we define

$$\left.\begin{aligned} v_p &= \pi\ LR^2 \quad , \\ s_p &= 22\pi R(R+L) \quad , \\ a_p &= (2RL + \pi R^2)/2 \ , \\ \overset{*}{D}_p &= (2R+L)/2 \quad . \end{aligned}\right\} (B.31)$$

A tubular grain may be defined by its initial height and the initial outer and inner diameters, $\overset{*}{D}_o$ and $\overset{*}{d}_o$, respectively. Let

$$\left.\begin{aligned} R &= (\overset{*}{D}_o - 2\overset{*}{d})/2 \quad , \\ r &= (\overset{*}{d}_o + 2\overset{*}{d})/2 \quad , \\ L &= \overset{*}{L}_o - 2\overset{*}{d} \quad . \end{aligned}\right\} (B.32)$$

The grain is completely burnt if either $R-r< 0$ or $L< 0$. If both of these quantities are positive, then the grain geometry functions are

$$\left.\begin{aligned} v_p &= \pi(\overset{*}{D}_o + \overset{*}{d}_o)\ (R-r)L/2 \quad , \\ s_p &= \pi\ (\overset{*}{D}_o + \overset{*}{d}_o)\ (R-r+L) \quad , \\ a_p &= \ (2RL + \pi(R^2 - r^2))/2 \quad , \\ \overset{*}{D}_p &= (2R+L)/2 \ . \end{aligned}\right\} (B.33)$$

We consider a detailed study of turbulence models for interior ballistics flows to be outside the scope of this report. Hence, the correlation models are quite elementary and are listed in this report only for completeness. The acceleration by the gas phase turbulent stress tensor A_{turb} and the turbulent heat dissipation function Φ_T, could have the same form as A_{visc} (Eq. (B.9)) and $\bar{\Phi}(E)$, (Eq. (B.12)), respectively, but different viscosity coefficients, that is,

$$A_{turb} = \frac{1}{\alpha\rho} \nabla\cdot\left\{\alpha\left[2\,\mu_T E + \left(\lambda_T - \frac{2}{3}\mu_T\right)\left(\text{trace } E\right) I\right]\right\} \quad , \text{ m/s}^2 \quad , \text{(B.34)}$$

$$\Phi_T = 2\,\mu_T \text{ trace } (E^2) + \left(\lambda_T - \frac{2}{3}\mu_T\right)\left(\text{trace } E\right)^2 \quad , \text{ W/m}^3 \quad , \text{(B.35)}$$

where μ_T and λ_T denote the viscosity coefficients for turbulent flows. The manner in which these coefficients are determined strongly depends on the particular turbulence model one uses and, hence, will not be given. As discussed in Section 4.7.6, the solid phase turbulent stress tensor $\overset{*}{\Pi}_T$ is set to zero. The turbulent heat flux vector Q_T is modeled by Ishii[13] and Gibeling et al.[5] as

$$Q_T = -\,\kappa_T\left[\nabla T - \frac{\nabla\alpha}{\alpha}\,(T_i - T)\right] \quad , \quad \text{W/m}^2 \quad , \qquad \text{(B.36)}$$

where T_i is an average temperature on the interface (a function of T and $\overset{*}{T}$) and κ_T is given by an algebraic formula involving an effective viscosity and Prandtl number. The corresponding model of Ψ_{turb} in Eq. (B.15) is

$$\Psi_{turb} = -\,\frac{1}{\alpha\rho T}\,\nabla\cdot(\alpha\,Q_T) \quad , \quad \text{W/(kg}\cdot\text{K)} \quad . \qquad \text{(B.37)}$$

LIST OF SYMBOLS

This list contains symbols that are frequently used in the report. Symbols that are defined and used only locally are not included in the list.

Function symbols in general indicate average quantities. A tilde over a function symbol is used to indicate the local value of a function. An asterisk over a symbol indicates that it represents a property of the propellant grains.

a – sound speed in gas, m/s

a_{sp} – sound speed of particle material, m/s

$\overset{*}{a}$ – sound speed in the particulate phase, m/s

a_p – average frontal area of a particle, m^2

a_{drag} – acceleration term due to drag, m/s^2

A_{Ergun} – Ergun correlation for A_{drag}, m/s^2

$A_{Reynolds}$ – Reynolds correlation for A_{drag}, m/s^2

A_{stress} – acceleration term due to intergranular stress, m/s^2

c_v – specific heat capacity at constant volume, J/(kg•K)

c_p – specific heat capacity at constant pressure, J/(kg•K)

$\overset{*}{d}$ – regression distance, m

$\dot{d}_s$ – stationary burning rate, m/s

$\langle\dot{d}\rangle$ – burning rate correlation function, m/s

D – drag force correlation, N

$\overset{*}{D}_p$ – average particle diameter, m

e – specific internal energy, J/kg

$\hat{e}$ – e at flame temperature, J/kg

e_s, e_q – partial derivatives of e, K and m^3/kg, respectively

$\langle \dot{e} \rangle$ - correlation for surface averaged heat flux between the particles and gas, W/m^2

E - strain rate tensor, $1/s$

g - averaging weight function

H - specific enthalpy difference (4.109), $J/(kg \cdot K)$

I - identity tensor of second order

I_p - "force" or impetus of the propellant, m

ℓ - diameter of averaging volume, m

m - number of grains in averaging volume

$\overset{*}{m}$ - weighted number of grains in averaging volume

M - molar mass, kg/mol

n_{sp} - unit outward normal with respect to the gas on S_p

n_{sv} - unit outward normal to S_v

p - pressure, Pa

p_q - derivative of the function $p(q)$

Q - gas phase heat conduction, W/m^2

Q_T - gas phase turbulent heat flux, W/m^2

q - pressure logarithm function, Eq. (4.28), Sect. 4.2.2, Pa

r - radial coordinate, m

R - universal gas constant, 8.3143 $J/(mol \cdot K)$

s - specific entropy, $J/(kg \cdot K)$

s_p - average surface area of a single grain, m^2

S_p - union of all grain surfaces in V

SG - weighted area of S_p, m^2

S_v - surface of averaging volume V

t - time, s

T - gas temperature, K

T_{flame} - flame temperature, K

$\overset{*}{T}$ - grain surface temperature, K

$\langle \dot{T} \rangle$ - correlation for rate of change of grain surface temperature, K/s

u - gas velocity, m/s

u_r, u_θ, u_z - the radial, circumferential and axial components of u, m/s

$\overset{*}{u}$ - particle velocity, m/s

$\overset{*}{u}_r, \overset{*}{u}_\theta, \overset{*}{u}_z$ - the radial, circumferential, and axial components of, $\overset{*}{u}$, m/s

$\breve{u}_{sp}$ - velocity of a point of S_p, m/s

v_p - average value of the volume of a single particle, m^3

V - averaging volume

VG - weighted value of V, m^3

x - spacial coordinate vector, m

z - axial coordinate, m

Z - surface element metric

α - gas volume fraction (porosity)

β - phasic function (Section 2)

γ - ratio of specific heats

Γ - source term, (4.33), Section 4.3, 1/s

Γ_1 - $SG\langle \dot{d} \rangle / VG$, 1/s

Γ_2 - $\frac{\alpha\rho}{\overset{*}{\rho}}\Gamma$, 1/s

ζ - surface coordinate vector

η - covolume in equation of state, m^3/kg

κ - thermal conductivity coefficient, W/(m• K)

λ - bulk viscosity coefficient, Pa• s

μ - shear viscosity coefficient, Pa• s

ξ - spacial coordinate vector, m

Π - viscous stress tensor, Pa

Π_T - gas phase turbulent stress tensor, Pa

$\overset{*}{\Pi}$ - intergranular stress tensor, Pa

$\overset{*}{\Pi}_T$ - solid phase turbulent stress tensor, Pa

ρ - gas density, kg/m^3

$\overset{*}{\rho}$ - particle density, kg/m^3

ρ_s, ρ_q - partial derivatives of $\rho(s,q)$, $(kg/m^3)\cdot(kg\cdot K/J)$, and s^2/m^2, respectively

ϕ - function describing a gas property, Section 2

$\overset{*}{\phi}$ - function describing a particle property, Section 2

Φ - dissipation term, W/(kg• K)

$\bar{\Phi} = \Phi_L$ - dissipation function, W/m^3

Φ_T - gas phase turbulent dissipation function, W/m^3

$\langle\Phi\rangle$ - dissipation correlation term, W/(kg• K)

Φ_1 - $\rho T \Phi$, W/m^3

$\psi(t,x,\xi)$ - general function, Section 2

Ψ - heat conduction term, W/(kg• K)

Ψ_{gas} - heat conduction due to gas conductivity, W/(kg• K)

$\Psi_{particle}$ - heat conduction due to heat loss to particles, W/(kg• K)

Ψ_{turb} - turbulent heat conduction, W/(kg• K)

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