

SOLUTIONS OF
THE KINETIC COAGULATION EQUATION
AND
PREDICTIONS FOR GAS-PARTICLE FLOW

A thesis submitted for the degree of
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by

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D E C L A R A T I O N

I declare that the material contained in this thesis is the result of my own work, performed at Imperial College since registration for the Ph.D. degree, and that none of it has been submitted for any other degree.

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A B S T R A C T

Coagulation of suspended droplets or particles is introduced as a phenomenon common to several fields in science and engineering, which due to its special characteristics of stochasticity and determinism is shown to represent a complex modelling problem.

Some of the vast coagulation-related literature is reviewed, with emphasis on the so-called kinetic coagulation equation, a deterministic nonlinear integro-differential equation describing conservation of particle mass in a developing size distribution. Shortcomings, problems and assumptions involved in previous attempts to solve that equation are discussed.

Based on a pseudo-Lagrangian coagulation model, i.e. one whose solution follows the "particle" size evolution (instead of the mass or number density as a function of size), and by means of a nonlinear integral transformation on the kinetic equation, a set of two integro-differential equations for coagulation is derived. For any specified collision mechanism, i.e. for any given coagulation kernel (but unit collection efficiency), these equations are capable in principle of overcoming most problems associated with previous solutions of the more traditional equation.

A semi-discretized numerical solution employing shape-preserving quadratic splines is developed and results therefrom are compared with analytical

solutions for two particular coagulation kernel: constant and proportional to the sum of the volumes, and with a numerical solution for Brownian coefficient, in all cases exhibiting a good agreement.

A further model is described which incorporates the coagulation calculation into a flux model, in order to predict the spatial variation of particle size and velocity distribution in a flowing suspension, where collisions result from the differing response of distinctly-sized particles to the acceleration of the continuous phase. Coagulation in such a case (e.g. for solid-propellant rocket motor nozzles, nuclear high-pressure wet steam turbines) is more difficult to evaluate because of the "two-dimensional" particle number distribution, a function of both size and velocity. The present model attempts to overcome some of the simplifications in previously reported models.

An application is made to linear kinetic coagulation in a one-dimensional gas-particle flow along a variable cross-section passage, representing crudely a high-pressure turbine blade passage in a nuclear wet steam turbine, and the resulting predictions, with good agreement for 10 and 20 classes of particles, are analysed and discussed. The importance of nonequilibrium two-phase flow models, such as the present flux model, for this kind of problem has been concluded from the results.

Advantages and limitations of the general model are put in perspective, and the possibilities open for future work are considered.

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Finally I dedicate, with love, this work to

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Daniel

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NOMENCLATURE

Faithful to our policy of self-containment, we have, throughout the text, tried to keep the definition of any quantity close to the expressions in which that quantity appears. Here we list only the variables we consider important enough to be listed, such as the key ones for the Figures. Some names (e.g. A, B, C) have been employed, without any ambiguity, for more than one entity, usually internal to a Chapter.

LATIN LETTERS

A (A_0)	(initial) cross-section of passage (m^2).
$\bar{d}$ ($\bar{d}$)	(initial mass average) particle diameter (m).
f	volumetric number density function (m^{-6}).
K	coagulation kernel.
L	length of passage (m).
M	nondimensional mass rate density = $Q(x,y) x$.
M_n	moment of order n = $\int_0^\infty v^n f(v,t) dv$.
N (N_0)	(initial) total number concentration (m^{-3}).
q	volumetric number rate density ($m^{-3}s^{-1}$).

Q	nondimensional number rate density = $(N_o U_o A_o / \bar{v}) q$.
$r (\bar{r})$	(initial mass average) particle radius (m).
t	time (s).
T	nondimensional time $\propto N_o t$, the proportionality constant depending on the kernel definition.
$u (u_g)$	(gas) particle velocity (m/s).
U_o	initial gas velocity (m/s).
$U (U_g)$	nondimensional (gas) particle velocity = u/U_o .
$v (\bar{v})$	(initial mass average) particle volume (m^3).
x	nondimensional particle volume = $v/\bar{v}$.
$\bar{x}$	nondimensional average volume = $\int_0^\infty x Q(x,y) dx / \int_0^\infty Q(x,y) dx$.
y	nondimensional streamwise position = z/L .
z	streamwise position along the passage (m).
$w_p (w_{p_o})$	(initial) particle-mass fraction (wetness fraction, for steam).
W	nondimensional number concentration density = $(N_o / \bar{v}) f$.

GREEK LETTERS

ρ_g	material gas density (Kg/m^3).
ρ_p	material particle density (Kg/m^3).
μ	gas viscosity ($\text{Kg m}^{-1}\text{s}^{-1}$).
η	self-similarity variable = (M_o/M_1) v.
ψ	self-similarity variable = $(M_1/[M_o]^2)$ f.

CHAPTER 1

INTRODUCTION

1.1 THE COAGULATION PHENOMENON

When two (or more) macroscopic particles in a suspension come close enough to each other so that they collide with a finite sticking probability, they give rise, even temporarily, to a new particle or agglomerate. Thus, a phenomenon generally called "coagulation" is taking place.

Since several mechanisms might be able, alone or in combination, to draw the particles together, "coagulation" represents a broad class of phenomena, whose modelling depends on the detailed description of the interaction and the surroundings, as well as the behaviour of the resulting agglomerates. It is hardly surprising, therefore, that one can detect the occurrence of coagulation in widely varying fields in science and engineering, the corresponding literature easily attesting to that fact.

From the beginning, researchers have understood coagulation as a non-deterministic phenomenon, not only owing to the sheer number of particles involved, but also because particles lose their identities as the process evolves. So, considerable efforts have been exerted to formulate a suitable probabilistic model for coagulation. The first results in the context of Brownian and shear coagulation were due to Smoluchowski (Drake [1]), whose kinetic coalescence equation has become the main, if not the only,

coagulation model. His idea of separating the kinetic from the physical effects, confining the latter to suitably defined kernels, has been of the fundamental importance for the advances in coagulation studies. Since Smoluchowski's works, coagulation research can be divided as follows.

- Studies on the particle-particle interactions, in order to obtain a better understanding of collision and coalescence mechanisms.
- Studies on stochastic models for coagulation, in order to replace or substantiate the kinetic equation.
- Studies on the solutions, analytic or numerical, for the kinetic equation itself, either in discrete or continuous form.

Smoluchowski, assuming Brownian motion of the aerosol and initially monodisperse distribution, developed a discrete form of the kinetic coagulation equation

$$\partial N_i(t)/\partial t = - \sum_{j=1}^{\infty} a_{ij} N_i(t) N_j(t) + 1/2 \sum_{i-j=k}^i a_{kj} N_k(t) N_j(t) , \quad (1.1)$$

where N_i is the number concentration of i -particles and a_{ij} is the non-negative and symmetrical collision (coagulation) frequency between i - and j -particles.

Supposing a_{ij} constant, Smoluchowski solved the equation (1.1). The classic result for the total number of particles is

$$N(t) = N_0/(1 + t/T) , \quad (1.2)$$

where $N(t)$ is the total number of particles at time t , N_0 is the initial number of particles the same size and T is a constant related to the particle diffusivity and N_0 .

Over several decades many workers (e.g. Corner et al [2] in 1951) have tried to compare Smoluchowski's theory with actual data. An experimental apparatus has been employed in [3] but unfortunately, in common with most works at that time, only the total number concentration was determined. They, and many other authors found good agreement at the beginning of the process, the results worsening with time, because of the increasing polydispersity.

Realizing that constant coagulation coefficient (or kernel) (to be defined) does not represent a good hypothesis for strong polydispersions, and that for a very large number of differently sized particles the summations in (1.1) can be replaced by integrals, Muller (Drake [1]) developed the well-known continuum form of the kinetic equation

$$\begin{aligned} \partial f(v,t)/\partial t = & - \int_0^{\infty} K(v,u) f(v,t) f(u,t) du + \\ & 1/2 \int_0^v K(v-u,u) f(v-u,t) f(u,t) du , \end{aligned} \quad (1.3)$$

where $f(v,t) dv$ is the number concentration of particles whose volume lie between v and $v + dv$ and $K(v,x)$ is the coagulation kernel, assumed nonnegative and symmetrical.

The first integral in (1.3) expresses the disappearance of particles of

volume v from the interval $v, v+dv$ due to coagulation between them and any other particle of volume u . The second integral says that the coagulation between particles of size u and $(v-u)$ gives rise to a particle of volume v . The one-half is necessary to avoid doubly counting the combinations.

Given an initial distribution $f(v, t_0)$, it is obvious that the collection (or kinetic) equation (1.3) is not truly stochastic. In fact, under this deterministic aspect it is a very complex partial integrodifferential equation and the existence and uniqueness of solutions have to be proved. Melzak [4] and McLeod [5] have accomplished that only for a particular choice of collection (or coagulation) kernels, some of them considered physically unrealistic (Drake [1]), a viewpoint under criticism nowadays [6]. Although a general solution has never been found, we will see later that for some mathematically convenient kernels and initial conditions, analytic results have been obtained (Scott [7]).

In particular, the kinetic equation describes the mean behaviour of the size distribution as expressed by the time dependence of the average $f(v, t)$ (it will become apparent later what is meant by the term "average"). In this sense, the equation is unable to describe the deviations from that mean behaviour and is stochastically incomplete. However, considering that the collision-coalescence phenomenon is itself stochastic, it is legitimate to ask if and when the kinetic (or collection) equation yields meaningful results. This question, as will be seen, has indeed been addressed by many authors on the subject.

1.2 THE THESIS OUTLINE

In Chapter 2 we discuss briefly the validity of the kinetic equation, as

well as presenting some of its analytical and numerical solutions and corresponding shortcomings and advantages. Finally, for the sake of completeness, the concept of coagulation kernel and some related works are exposed.

In Chapter 3 we develop, starting from the classical continuous kinetic equation, the theoretical basis of our pseudo-Lagrangian model, which aims to overcome some shortcomings of previous solutions.

In Chapter 4, we formulate a numerical scheme based on splines for the system of equations originated from Chapter 3.

We present in Chapter 5 some cases, through which we put our previously developed numerical formulation to test. Those cases consist of Scott's analytical solutions for Gamma initial distributions and kernels either constant or proportional to the sum of particle volumes [7], and a numerical solution for exponential initial distribution and Brownian kernel [8]. The outcomes are also discussed in this Chapter.

We dedicate Chapter 6 to the development of the flux model, in order to take into account particle and continuum-phase velocities and velocity-related coagulation. Results from an application to a two-phase flow through a one-dimensional equivalent blade passage of a high-pressure steam turbine [9] are presented and discussed.

Our general conclusions and recommendations for future developments can be found in Chapter 7. For completeness, the codes for the flux model (the general model is similar) is presented in the Appendices.

References are listed separately for each Chapter in order to make each Chapter as self-contained as possible. Also, it is very important to notice

that, throughout this work, the equations are written using single-line notation, i.e. numerator and denominator in the same line. Therefore, to avoid ambiguity, expressions should be interpreted from left to right, precedence being given to terms within brackets, very much like in a computer Language.

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CHAPTER 2

PRELIMINARY CONSIDERATIONS

2.1 INTRODUCTION

In this Chapter we define some concepts and survey the literature related to each one of the three aspects of the classical approach for coagulation, presented earlier: the validity of the kinetic model, the solutions for the kinetic equation and the physics of the coagulation kernels.

2.2 THE VALIDITY OF THE KINETIC MODEL

Marcus [1], employing probabilistic arguments, uncovered the so-called infinite closure problem (of which more below) and concluded that the kinetic equation (1.3) represents a consequence of the simplest closure assumption: uncorrelated distribution densities for differently sized particles. From then on, an exhaustive and passionate argument about the validity of the kinetic equation (1.1) or (1.3) developed, involving many researchers. Along the same lines as Marcus', and in the context of cloud droplets, Scott [2] has tried to develop a model for coagulation, using Poisson statistics. Consider $g(u,v,t)$ $du dv$ the uniform number concentration of droplets of mass u to $u + du$ and v to $v + dv$ simultaneously. Also consider $N(t)$ the stochastic total number of particles of all sizes. The following development is based on Scott [2].

The expected total number of droplets is

$$\bar{N}(t) = \int_0^{\infty} f(v,t) dv \quad . \quad (2.1)$$

The variance of $N(t)$ can be shown as to be

$$E[(N(t) - \bar{N}(t))^2] = \int_0^{\infty} \int_0^{\infty} g(v,u,t) dv du - \left[\int_0^{\infty} f(v,t) dv \right]^2 + \int_0^{\infty} f(v,t) dv \quad . \quad (2.2)$$

If there is no correlation between the particle densities, their joint distribution can be expressed as

$$g(u,v,t) = f(u,t) f(v,t) \quad . \quad (2.3)$$

Thus, substituting (2.3) into (2.2) we conclude that

$$\text{var}(N(t)) = \bar{N}(t) \quad , \quad (2.4)$$

that is, $N(t)$ behaves very much like a Poisson distribution.

However, let us now consider coalescence with low but non-zero correlation, which may be caused by turbulence mixing, by bringing together groups of particles of distinctly different sizes, or by competition for mass in a small volume. Therefore, we write

$$g(v_1, v_2, t) = f(v_1, t) f(v_2, t) + R_2(v_1, v_2, t) , \quad (2.5)$$

where R_2 measures the degree of correlation. Also needed is a three-droplet correlation $h(v_1, v_2, v_3, t)$, expressed as

$$\begin{aligned} h(v_1, v_2, v_3, t) = & f(v_1, t) f(v_2, t) f(v_3, t) + \\ & R_2(v_1, v_2, t) f(v_3, t) + \\ & R_2(v_2, v_3, t) f(v_1, t) + R_2(v_1, v_3, t) f(v_2, t) + \\ & R_3(v_1, v_2, v_3, t) . \end{aligned} \quad (2.6)$$

This is the situation in which we have more unknowns than equations and always one correlation more is needed: the so-called closure problem. If it is possible to neglect the correlation among triplets, R_3 will be set to zero.

The integro-differential equations for f and g as extensions of the usual collection equation can be written as

$$\partial f(v,t)/\partial t = 1/2 \int_0^v g(v-u,u,t) K(v-u,u) du - \int_0^\infty g(v,u,t) K(v,u) du , \quad (2.7)$$

$$\begin{aligned} \partial g(v_1,v_2,t)/\partial t = & 1/2 \int_0^{v_2} h(v_1,v_2-u,u) K(v_2-u,u) du + \\ & 1/2 \int_0^{v_1} h(v_1-u,v_2,u) K(v_1-u,u) du - \\ & \int_0^\infty h(v_1,v_2,u,t) [K(v_1,u) + K(v_2,u)] du . \end{aligned} \quad (2.8)$$

Using (2.5) in (2.7)

$$\begin{aligned} \partial f(v,t)/\partial t = & 1/2 \int_0^v f(v-u,t) f(u,t) K(v-u,u) du - \\ & \int_0^\infty f(v,t) f(u,t) K(v,u) du + \\ & 1/2 \int_0^v R_2(v-u,u,t) K(v-u,u) du - \\ & \int_0^\infty R_2(v,u,t) K(v,u) du . \end{aligned} \quad (2.9)$$

Now using (2.5) and (2.6) with $R_3 = 0$ in (2.8) and simplifying with (2.9)

$$\begin{aligned}
\partial R_2(v_1, v_2, t) / \partial t = & \int_0^{v_2} R_2(v_1, v_2 - u, t) f(u, t) K(v_2 - u, u) du + \\
& \int_0^{v_1} R_2(v_1 - u, v_2, t) f(u, t) K(v_1 - u, u) du - \\
& \int_0^\infty R_2(v_2, u, t) f(v_1, t) K(v_1, u) du - \\
& \int_0^\infty R_2(v_1, u, t) f(v_2, t) K(v_2, u) du - \\
& \int_0^\infty R_2(v_1, v_2, t) f(u, t) [K(v_1, u) + K(v_2, u)] du .
\end{aligned} \tag{2.10}$$

It is important to realize that with no correlation, the already known kinetic (or collection) equation (1.3) is obtained from (2.9). The coupled equations (2.9) and (2.10) are in principle sufficient to determine f and R_2 in terms of their initial values $f(v, t_0)$ and $R_2(u, v, t_0)$. Hence, it is possible to determine the variance (2.2) as a function of time using the expression

$$\text{var}(N(t)) = \int_0^\infty \int_0^\infty R_2(v_1, v_2, t) dv_1 dv_2 + \int_0^\infty f(v, t) dv , \tag{2.11}$$

or the system could be solved by finding $f(v, t)$ using the kinetic equation and calculating $R_2(u, v, t)$ in (2.10), the result being applied in (2.11) determining a new $f(v, t)$ and so on. However, closing the system by neglecting R has only heuristic justification. It is a kind of first order approximation (FOST) widely employed in turbulence theory but in instances, as stressed by Lerche & Parker [3], dangerous enough to invalidate the outcome.

Warshaw [4] has derived the kinetic equation and discussed the validity of this equation under the most common assumptions (for cloud physics). He has concluded that the equation should not be used for very small number of droplets or for small cloud volumes. In reply to Scott [2] and Berry [5], Warshaw [6] has put in question the validity of the Poisson statistics considered by Scott [2]. Long [7], studying the use of finite-difference methods for the kinetic equation, has concluded that the results depend on the relative number of droplets of different sizes in a population and were less reliable for certain intermediate droplet sizes. Scott [8] has put in doubt Long's analysis but Long [9] replied showing Scott's mistakes in his Poisson statistics. Bayewitz et al. [10] have tried to clear up the debate among Scott, Warshaw, Long and others, about the validity of the kinetic equation, by developing what they claimed to be the real stochastic coalescence model, including a correlation function of particle densities. Their results showed again that under certain assumptions the kinetic equation can be used, but for small population and small cloud volume the results could differ substantially from the stochastic model. More recently, Sampson and Ramkrishna [11] have discussed a number of possibilities of closure for the problem of product of density functions.

Despite all discussions and perhaps because of the apparently insurmountable problem of infinite closure, the kinetic equation, in one of its guises in the form of equations (1.1) or (1.3), established itself firmly in the literature dedicated to coagulation.

2.3 SOLUTIONS FOR THE KINETIC EQUATION

Friedlander [12], in order to explain the long-time behaviour of

experimental aerosol distributions, developed a similarity formulation for the kinetic equation, by defining the following variable transformations onto the number density and the volume:

$$f(v,t) = M_0^2(t)/M_1(t) \psi(\eta) , \quad (2.12)$$

$$\eta = M_0(t)/M_1(t) v , \quad (2.13)$$

with

$$M_n(t) = \int_0^\infty v^n f(v,t) dv , \quad (2.14)$$

as the n-order central moment of $f(v,t)$.

If the coagulation kernel is a homogeneous function of u and v , i.e

$$K(hu,hv) = h^\mu K(u,v) , \quad (2.15)$$

where μ is the degree of homogeneity, then the kinetic equation (1.3) can be transformed into an ordinary equation for $\psi(\eta)$, of which a (time-independent) solution, if obtainable, is called a self-preserving spectrum.

Later, a number of coagulation mechanisms (some of which we describe below), for many kinds of disperse phase, were investigated both theoretically and experimentally by several authors, e.g. Swift and Friedlander [13], in search of self-preserving distributions, with varying degrees of success. In particular, kernels proportional to the sum and the product of the volumes were shown not to generate self-preserving solutions.

Although there is no general solution for the kinetic equation, some workers, with a careful choice of kernels and initial conditions, have succeeded in finding analytic solutions. The most classic example is Scott [14], who has solved analytically, with the help of the Laplace transforms, the kinetic equation, for initial Gamma distributions and three collection kernels: proportional to the sum and product of particle volumes and constant. His results are still being used to test numerical solutions, e.g. Bleck [15] and the present work. More recently, Spouge [16] has presented some implicit series solutions for the same kernels, that, although interesting, are not simpler than Scott's, despite the author's claims.

For general kernels, however, a numerical formulation is likely to be the only hope to solve the kinetic equation. In this sense, the most straightforward way is by means of finite differences, and even simpler, the use of equation (1.1), since equation (1.3) implies the need for quadratures. For the discrete equation (1.1) both class definition (in terms of an adequate spectrum representation with a reasonable number of classes), and spectrum stretching (generation of larger and larger particles by coagulation) represent the main problems to be solved.

Realizing that for broader initial distributions, linearly dividing the size interval would imply an unmanageably large number of size ranges, Berry [17] has discretized the coagulation (or kinetic) equation (in terms of particle size distribution) using equal logarithmic intervals, by means of the expression

$$r(j) = \bar{r} \exp[(j-1)/6 \ln 2] , \quad (2.16)$$

where r stands for particle radius, with $\bar{r}$ being the radius of the particle whose volume is $\bar{v} = M_1/M_0$ (average volume of the number distribution density).

By incorporating new classes, according to an arbitrary extrapolation procedure, Berry [17] has taken into account the increasing size range reached by the growing particles. He has investigated the behaviour of his scheme for various collection kernels. For some time, Berry's formulation became standard, although there were some doubts with respect to the accuracy and stability of the schemes employed for the interpolation (for finding function values between data points) and the quadratures (for evaluating the integrals) used in his paper. Later, acknowledging that fact, Berry and Reinhardt [18],[19],[20] and [21] have improved upon the resolution of the kinetic equation by using better interpolation formulas and integration schemes, and discussed the results for "hydrodynamic" kernel (see below) and single as well as double-peaked initial size distributions, checking the numerical results through the conservation of total mass.

Realizing that Berry's method could be cumbersome and time consuming, some workers have devised alternative procedures. Bleck [15] has developed a scheme to discretize and solve the kinetic equation, employing an approximate averaging process to the integrals, in order to avoid altogether the quadratures. Even though his method seemed fast, the preliminary evaluation of the coefficients (that replace the integrals) and preconditioning of data could work as disadvantages. In another attempt to circumvent the quadrature evaluations, Williams [22] has developed an ingenious scheme to attribute particles to logarithmically discretized size classes, assigning uniform or linear particle distribution for each class, and evaluating the coalescence probability for a pair of particles from either the same or distinct classes, and using the result, and mass conservation, in order to reclassify the outcomes of each coalescence. Unfortunately, not only his time integration scheme was rather crude, but he has not presented comparisons with standard analytical solutions, e.g. Scott [14]. Brown [23] has used Bleck's method implemented into an implicit scheme for the solution of the kinetic equation with breakup terms, which according to him are responsible for stability problems. Breakup terms are additional integral terms in which the kernels account for the possibility of particles splitting into several fragments, either as an outcome of the coalescence itself or due to the particle dynamics. One of the first experimental results in droplet breakup is found in McTaggart-Cowan and List [24]. Projecting droplets onto a stationary droplet-target, they have found that they could divide the breakup fragments into four basic types: "neck", "sheet", "disk" and "bag". However, due to the experimental limitations, they have used rather large droplets.

Srivastava [25] has tried to solve the kinetic equation with breakup terms fitted using the little experimental data available at the time. He has shown a possibility of a stationary distribution.

Brown [26] has investigated the stability of a finite-difference scheme to the kinetic equation. He has assumed a trapezoidal rule for the integrals. Later on, he discussed [27] the problems of computational instability in numerical solutions of the kinetic equation. Brown [28] returned again to this instability problem and tried to find by heuristic methods a bound for the time step. His problems were certainly associated to the algorithm chosen for the time integration. Much more recently, J. D. R. Stock et al. have reported the use of Bleck's method in aerosol modelling [29].

Polynomial fittings are being used nowadays to avoid the arbitrariness and data conditioning associated to schemes such as Williams' and Bleck's, although spectrum stretching (producing finite domain errors) and the need for extrapolation, still present some difficulty. Finite-domain errors are fractions of the total number and volume of particles contained in the finite computational domain, and can be written as (Gelbard and Seinfeld [30]):

$$E_0(t) = \int_{v_a}^{v_b} f(v,t) dv / M_0(t) , \quad (2.17)$$

$$E_1(t) = \int_{v_a}^{v_b} v f(v,t) dv / M_1(t) . \quad (2.18)$$

Computationally, v_a and v_b would never be 0 and ∞ , and the departure of

$E_0(t)$ and $E_1(t)$ from unity gives us a measure of the errors associated to this finite domain.

Some examples of polynomial representations for the kinetic equation are the method of weighted residuals over the entire domain, employed by Sampson and Ramkrishna [31], or the method of collocation on finite elements, such as orthogonal collocation (Legendre polynomials) or cubic splines, studied by Gelbard and Seinfeld [30], as well as the osculating quadratic splines, used in the present work.

There have been many solutions based on the moments of the discretized size (or volume) distribution. Tambour and Seinfeld [32] have presented some approximate analytic solutions for a new range of kernels, by solving a discrete equation for the total number of particles, assuming certain moments of the distribution as constant during the time interval. For a large number of classes such solution might become cumbersome. Frenklach [33] has developed differential equations for the first moments of the discrete size distribution, for the case of constant kernel. Ernst et al. [34] have studied the evolution of the moments of the size distribution for mass-product kernels, assuming the possibility of gelation, i.e. the formation of an infinite cluster. Unfortunately, the solutions employing moments are not, in general, more easily solvable than the kinetic equation itself.

There have been very few works on the all important subject of particle coalescence in nonequilibrium two-phase flow involving particle velocities, due mostly to the difficulty of developing the proper two-phase flow equations. We will discuss this case in more detail in a later Chapter.

2.4 THE COAGULATION KERNELS

As before, let $f(v,t) dv$ be the average number concentration of particles, whose volume is between v and $v + dv$. Invoking the uncorrelated-distribution assumption, we write for the average number of collisions

$$P(v_1, v_2, dt) (V f(v_1, t) dv_1) (V f(v_2, t) dv_2) , \quad (2.19)$$

where $P(x,y,dt)$ is the probability that a particle of volume x collides (and coalesces) with a particle of volume y , in the time interval dt per unit volume, and V is the total volume.

Let us define $K(v_1, v_2)$ such that

$$P(v_1, v_2, dt) = (K(v_1, v_2)/V) dt , \quad (2.20)$$

where $K(x,y)$ represents the number of collisions (and coalescence) per unit time, that is, the collision-coagulation frequency function. From the kinetic equation, we notice that $K(x,y)$ acts as a kernel inside the integral terms, hence the name "coagulation kernel" that we employ for $K(x,y)$ throughout the present work. In reality, $K(x,y)$ is related to coagulation by means of the assumption that the coalescence frequency is a fraction $E(x,y)$ of the collision frequency (the coalescence efficiency), and the collision frequency is a fraction $F(x,y)$ of all possible particle

pairing (the collision efficiency), both parameters frequently combined in one collection efficiency.

Once assuming the uncorrelated hypothesis and adopting the kinetic equation, the physics of coagulation is confined exclusively to the coagulation kernel $K(x,y)$. From Smoluchowski on, many authors have dedicated a lot of time and effort in the quest for expressions for $K(x,y)$ able to represent selected aspects of real phenomena, and, having been given a (theoretical) $K(x,y)$, to find the coefficients $E(x,y)$ and $F(x,y)$.

In this work, we use some mathematically convenient kernels, that, up to a constant, may be expressed as

$$K(x,y) = 1 , \tag{2.21}$$

$$K(x,y) = x + y , \tag{2.22}$$

$$K(x,y) = x y , \tag{2.23}$$

and, again up to a constant, the Brownian kernel

$$K(x,y) = 2 + (x/y)^{1/3} + (y/x)^{1/3} , \tag{2.24}$$

when coagulation of spherical particles is controlled by Brownian diffusion (e.g Drake [35]).

From meteorological studies we borrow the "hydrodynamical" kernel, resulting from the scavenging process developed by the larger particles (droplets) falling through air more rapidly than the smaller ones. From the Figure 2.1 we deduce that the maximum volume swept by a larger particle per unit time is equal to (up to a constant)

$$(r_1 + r_2)^2 |u_1 - u_2| , \quad (2.25)$$

where r_i and u_i is the radius and velocity of the particles of volume v_i . Since the smaller drops tend to be carried around the large ones, only a fraction inside that previously defined volume will be collected. Besides, once the particles collide, they might not coalesce. Taking these facts into account, we again define the coagulation kernel as

$$K(v_1, v_2) = E(v_1, v_2) F(v_1, v_2) (r_1 + r_2)^2 |u_1 - u_2| , \quad (2.26)$$

where $E(x, y)$ is the collision efficiency and $F(x, y)$ is the coalescence efficiency. The collision efficiency is defined by

$$E(v_1, v_2) = y_b^2 / (r_1 + r_2)^2 , \quad (2.27)$$

where y_b is the limiting distance from the axis of the larger drop within which the smaller droplets must be found, in order to be collected.

Although in the present work, for simplicity, we assume those efficiencies equal to unity, their importance is attested by the number of works, mostly experimental in character, dealing with the determination of correlations for them. The classic example is the work by Hocking [36], in which he established that no droplet less than $19 \mu\text{m}$ in radius would be capable of colliding with smaller ones, when settling in still air, a result contradicted by many authors afterwards, Davis [37] among them.

Lin and Lee [38] have studied the collision efficiency by superposing the flow field around one drop onto the flow field of another, and compared their results against the ones available in the Literature. They considered gravity, inertia and drag forces. Levin and Machnes [39] have designed an experimental apparatus in order to determine the coalescence efficiency. Their results showed that the droplet distribution was affected by the various correlations. Arbel and Levin [40],[41] developed a coalescence model, taking into account some forces related to the approach of the droplets, as well as the possibility of bouncing after collisions, and compared their results with the Literature. Podvysotsky and Shraiber [42] have presented an experimental study of the effect of the impact angle of colliding droplets on coalescence and breakup.

Zinchenko [43] has calculated the gravitational coagulation efficiency, by analysing the relative trajectories of two liquid drops, assuming Stokes

flow, although this assumption is not valid but for particle Reynolds number very much less than the unity.

Leo and List [44],[45] have developed an experiment to determine coalescence efficiencies and size distributions for very large droplets, considering breakup. Beard and Ochs [46] have measured the coalescence efficiency for various pairs of uncharged drops of distinct sizes, comparing their results with the Literature. Beard [47] has formulated an energy model to compare the collisional kinetic energy with the viscous dissipation for oscillating raindrops as functions of size, droplet distribution and rainfall rate. More recently, Chen [48] has developed a model able to predict the evolution of the dimpled film between two drops or bubbles in close contact.

2.5 CONCLUSION

Although we have shown that all three aspects of coagulation studies are important, from now on we restrict drastically our discussion, by assuming that the kinetic equation and some modified forms do represent an adequate model for the coagulation phenomena. Moreover, for simplicity sake, in the coagulation kernels selected, we will consider the collection efficiency as unity.

In the next Chapter, we will develop and discuss our pseudo-Lagrangian (variable size-class) approach for particle coagulation, which in later chapters we will put to test and finally employ to solve some problems related to coagulation in gas-particle flows.

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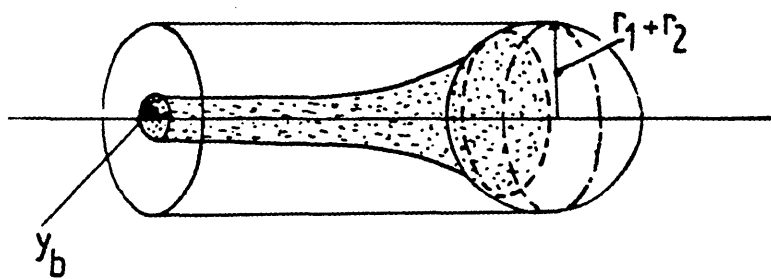


FIGURE 2.1 - Collision efficiency between large and small drops.

CHAPTER 3

THE THEORETICAL FOUNDATIONS OF THE MODEL

3.1 INTRODUCTION

In this chapter, we define and discuss a special coordinate transformation onto the classical coagulation equation, and show that this transformation is the basis of the so-called pseudo-Lagrangian models and their simplifications.

3.2 THE PSEUDO-LAGRANGIAN MODEL

Let us consider the kinetic equation (1.3):

$$\begin{aligned} \partial f(v,t)/\partial t = & - \int_0^{\infty} K(v,u) f(v,t) f(u,t) du + \\ & 1/2 \int_0^v K(v-u,u) f(v-u,t) f(u,t) du . \end{aligned} \quad (3.1)$$

All discretized versions of this equation represent "true particles" no more than the continuous version, for we have seen that a necessary (but by no means sufficient) condition for its validity is the large number of particles involved in the process, in order that fluctuations smooth out

discontinuities. In addition, we should remember that even the continuous equation will end up discretized for computational reasons.

Now let us define the parametric transformation

$$v = v(v_o, t) , \quad (3.2)$$

specified by the expression

$$\partial v(v_o, t) / \partial t = \int_0^v K(v(v_o, t), u) f(u, t) u \, du , \quad (3.3)$$

which could represent the rate of change of volume suffered by a particle of volume $v(v_o, t)$, whose initial volume was v_o , by absorption of smaller particles.

The parametrization (3.2) is depicted in Figure 3.1, where it can be seen that the coordinate lines are naturally generated by the coagulation itself, according to the equation (3.3).

In terms of the differential of v in (3.2), we write

$$dv = \partial v(v_o, t) / \partial v_o \, dv_o + \partial v(v_o, t) / \partial t \, dt . \quad (3.4)$$

Now, consider the distribution density function $f(v,t) = f(v(v_o,t),t) = f^*(v_o,t)$, in terms of differentials

$$df = \partial f(v,t)/\partial v \, dv + \partial f(v,t)/\partial t \, dt \quad . \quad (3.5)$$

Substituting (3.4) in (3.5) we get

$$df = \partial f(v,t)/\partial v \left[\partial v(v_o,t)/\partial v_o \, dv_o + \partial v(v_o,t)/\partial t \, dt \right] + \partial f(v,t)/\partial t \, dt. \quad (3.6)$$

For constant v_o , (3.6) becomes

$$df_{v_o} = \left[(\partial f(v,t)/\partial v) (\partial v(v_o,t)/\partial t) + \partial f(v,t)/\partial t \right] dt , \quad (3.7)$$

that is the same as

$$\partial f^*(v_o,t)/\partial t = (\partial f(v,t)/\partial v) (\partial v(v_o,t)/\partial t) + \partial f(v,t)/\partial t . \quad (3.8)$$

Substituting (3.1) and (3.3) into (3.8), we write

$$\begin{aligned} \frac{\partial f^*}{\partial t}(v_0, t) = & - \int_0^\infty K(v(v_0, t), u) f(v(v_0, t)) f(u, t) du + \\ & 1/2 \int_0^v K(v(v_0, t)-u, u) f(v(v_0, t)-u, t) f(u, t) du + \\ & \int_0^v K(v(v_0, t), u) (\partial f(v(v_0, t))/\partial v) f(u, t) u du . \end{aligned} \quad (3.9)$$

We now show that the transformation (3.2) is invertible, i.e. one-to-one. To accomplish that we differentiate (3.3) with respect to v_0 , obtaining, with a little help from a Leibniz-type formula [1]:

$$\begin{aligned} \partial^2 v(v_0, t)/\partial v_0 \partial t = & \int_0^v (\partial v(v_0, t)/\partial v_0) (\partial K(v, u)/\partial v) f(u, t) u du + \\ & K(v, v) f(v, t) v (\partial v(v_0, t)/\partial v_0) , \end{aligned} \quad (3.10)$$

which after rearranging becomes

$$\begin{aligned} \partial^2 v(v_0, t)/\partial v_0 \partial t = & (\partial v(v_0, t)/\partial v_0) \left\{ \int_0^v (\partial K(v, u)/\partial v) f(u, t) u du + \right. \\ & \left. K(v, v) f(v, t) v \right\} . \end{aligned} \quad (3.11)$$

We define, neglecting the function of v_0 for simplicity of notation:

$$g(t) = \partial v(v_0, t) / \partial v_0 , \quad (3.12)$$

and

$$\begin{aligned} F(v(t), t) = \int_0^v (\partial K(v(t), u) / \partial v) f(u, t) u \, du + \\ K(v(t), v(t)) f(v(t), t) v(t). \end{aligned} \quad (3.13)$$

Recasting (3.11) into the form

$$dg(t)/dt = g(t) (F(v(t), t) , \quad (3.14)$$

$$g(0) = 1 , \text{ for any } v_0, \quad (3.15)$$

and consequently

$$g(t) = \exp\left\{ \int_0^t F(v(s), s) \, ds \right\} . \quad (3.16)$$

From the fact that

$$g(t) = \partial v(v_o, t) / \partial v_o > 0, \text{ for any } (v_o, t), v_o \neq 0, \quad (3.17)$$

we are able to conclude that the transformation (3.2) makes sense globally, i.e, it is well defined for all nonzero v .

We rearrange (3.9) into the form

$$\begin{aligned} \partial f^*(v_o) / \partial t = & - \int_v^\infty K(v(v_o, t), u) f(v(v_o, t), t) f(u, t) du + \\ & I(v(v_o, t), t), \end{aligned} \quad (3.18)$$

where

$$\begin{aligned} I(v(v_o, t), t) = & \int_0^v \{ 1/2 K(v(v_o, t) - u, u) f(v(v_o, t) - u, t) + \\ & K(v(v_o, t), u) [(\frac{\partial f}{\partial v}(v(v_o, t), t) u - \\ & f(v(v_o, t))] \} f(u, t) du. \end{aligned} \quad (3.19)$$

The integral term in (3.18) might be interpreted as the rate of change of the number density of particles with volume $v(v_0, t)$, whose initial volume was v_0 , by absorption by larger particles.

Multiplying (3.18) by $v(v_0, t)$ and integrating for all volumes, and defining $s = v(v_0, t)$, we get

$$\int_0^{\infty} s \left(\frac{\partial f(s, t)}{\partial t} \right) \left(\frac{\partial s}{\partial v_0} \right) dv_0 = - \int_0^{\infty} \int_v^{\infty} K(s, u) f(s, t) f(u, t) s du ds + \int_0^{\infty} I(s, t) s ds, \text{ for any } (v_0, t). \quad (3.20)$$

Multiplying (3.3) by $f(v(v_0, t), t)$ and integrating for all volumes, and using the previously defined s , we express

$$\int_0^{\infty} f(s, t) \left(\frac{\partial s}{\partial t} \right) \left(\frac{\partial s}{\partial v_0} \right) dv_0 = \int_0^{\infty} \int_v^{\infty} K(s, u) f(s, t) f(u, t) u du ds, \quad (3.21)$$

for any (v_0, t) .

Now, adding (3.20) to (3.21) gives us

$$\frac{\partial}{\partial t} \int_0^{\infty} f(s, t) s \left(\frac{\partial^2 s}{\partial t \partial v_0} \right) dv_0 = \int_0^{\infty} I(s, t) s ds, \text{ for any } (v_0, t), \quad (3.22)$$

because the first integrals in the expressions (3.20) and (3.21) can be seen to cancel each other.

However, by mass conservation

$$\partial/\partial t \int_0^{\infty} f(s,t) s \, ds \equiv 0 ,$$

and consequently, substituting (3.14) in (3.22), we find that

$$\int_0^{\infty} \{I(s,t) + f(s,t) F(s,t)\} s \, ds = 0 , \text{ for any } (v_0, t) . \quad (3.23)$$

We conclude that $|I(s,t) + f(s,t) F(s,t)|$ must decrease faster than s increases for the integral to be bounded. In particular, if one assumes $I(s,t) = 0$ for any (v_0, t) , it is possible to obtain an approximate continuous pseudo-Lagrangian model for coagulation, in the form of the system

$$\partial f(v(v_0, t), t) / \partial t = - \int_v^{\infty} K(v(v_0, t), u) f(v(v_0, t), t) f(u, t) \, du , \quad (3.24)$$

$$\partial v(v_0, t) / \partial t = \int_0^v K(v(v_0, t), u) f(u, t) u \, du , \quad (3.25)$$

or, in discretized fashion

$$dN_i/dt = -\sum_{j=1}^p d_{ij} C(v_i, v_j) N_i N_j , \quad (3.26)$$

$$dv_i/dt = \sum_{j=1}^i d_{ij} C(v_i, v_j) N_j v_j , \quad (3.27)$$

where N_i represents the total concentration of particles of class i , $C(v_i, v_j)$ the discrete coagulation kernel, p is the total number of suitably defined classes and $d_{ij} = 1/2 (2 - \delta_{ij})$, (to avoid double counting).

Although not specially difficult, we have never found the previous derivation, leading to (3.3) and (3.9) and even to (3.26) and (3.27), anywhere else.

Pseudo-Lagrangian models, frequently cited in the Russian Literature, are apparently due to Sternin (Palatnik & Azhibekov [2]), although Tolfo [3] has it attributed to Fuchs and Sutugin [4]. Tolfo [3] has tried to assess the validity of the system (3.26),(3.27) as an alternative model for coagulation. After presenting a very simple development of (3.26),(3.27) by splitting the discretized mass conservation equation, he has compared, for several kernels and initial conditions, the solutions obtained by employing a numerical formulation for the classic equation

(3.1) [5] (what he called "exact solution"), the system (3.26) and (3.27), and similarity transformations (see Chapter 2), when possible. He has observed that the approximate pseudo-Lagrangian description could be useful for the cases in which the distributions are neither too concentrated in few classes nor the coagulation kernels too large.

Replacing the equation (3.1) by the system (3.24) and (3.25) or (3.26) and (3.27) offers some advantages for coagulation calculations. It can be seen that not only the total mass is conserved throughout, but its allocation to each class is determined by the process itself. In fact, one may interpret those equations as if following the evolution of particles with given initial volume, whose number concentration decreases by absorption by the larger particles, and whose volume increases by absorbing the smaller ones (hence the name pseudo-Lagrangian description).

The already mentioned mass (or volume) self-allocation is appealing since it is possible to reach larger and larger volumes while keeping the number of classes low. There is no need to redistribute, more or less arbitrarily, the mass in the classes to cope with the ever increasing volumes, as is the case with fixed-size class models. Another interesting feature can be made apparent in the pseudo-Lagrangian model if in the place of an initial number concentration, an initial number flux or number rate, incorporating particle velocities, is considered instead. This idea was informally taken up in a work by Crowe and Willoughby [6], in which they have tried to develop a coagulation model for a solid-fuel rocket nozzle, able to take into account the relative velocities between the particles, although there the definition of a class is not at all clear and, unlike all the other models, their system of equations is algebraic, developed from a fairly crude integration scheme.

Our development of equation (3.18) shows for the first time the approximate nature of (3.26) and (3.27), given by the term $I(v(v_0, t), t)$, (Eq. 3.19). Unfortunately, the assumption that this term is identically null, essential for (3.24) and (3.25) or (3.26) and (3.27), cannot in general be made. Consider for a moment a constant coagulation kernel. Assuming that $I(s, t)$ is zero for all (v_0, t) implies from (3.23) that $F(s, t) = 0$, since $f(s, t)$ is always positive or zero and, from the definition (3.13), $F(r, t)$ cannot be negative when the kernel is constant.

3.3 CONCLUSION

Even though the system (3.24) and (3.25) or (3.26) and (3.27) is inherently approximate, the newly developed system formed by the equations (3.3) and (3.9) is exact and retains most of the features of the more simplified approach. Its extra terms, however, seem to introduce considerable difficulty into its solution. A numerical solution for the complete system employing splines on finite elements is analysed in the next chapter.

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On this diagram, subscript t (and v) denotes the partial derivative with respect to time (and volume).

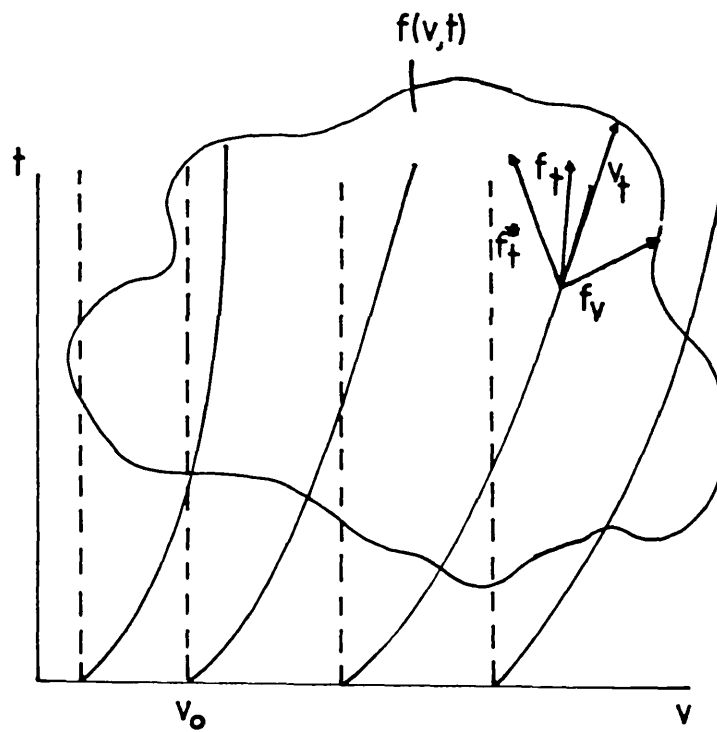


FIGURE 3.1 - Density function f parameterized in terms of initial volume v_0 and time t .

CHAPTER 4

A NUMERICAL FORMULATION FOR THE MODEL

4.1 INTRODUCTION

Having developed an exact pseudo-Lagrangian description for coagulation and considered its advantages and shortcomings, we dedicate this chapter to the numerical solution of those equations in terms of splines.

4.2 PRELIMINARIES FOR A NUMERICAL SOLUTION

We repeat here the system of equations that we have developed in the previous chapter.

$$\begin{aligned} \partial f^*(v_0, t) / \partial t = & - \int_0^{\infty} K(v(v_0, t), u) f(v(v_0, t), t) f(u, t) du + \\ & 1/2 \int_0^v K(v(v_0, t) - u, u) f(v(v_0, t) - u, t) f(u, t) du + \\ & (\partial f(v, t) / \partial v) (\partial v(v_0, t) / \partial t) , \end{aligned} \quad (4.1)$$

$$\partial v(v_0, t) / \partial t = \int_0^v K(v(v_0, t), u) f(u, t) u du . \quad (4.2)$$

The distinguishing feature of such a system is that the quadratures must be evaluated using variable and unequal width intervals between each two points (classes), although the number of classes is fixed and defined by the discretized initial distribution. Therefore a class is not defined by size of its particles, but by its place among the other classes. We discretize the initial number density distribution $f(v_0)$ by sampling that function at a finite number p of pre-determined volumes v_{o_i} , such that $v_{o_i} < v_{o_{i+1}} < v_{o_{i+k}}$. Thus, as we have seen earlier, $v(v_{o_i}, t) < v(v_{o_{i+1}}, t) < v(v_{o_{i+k}}, t)$, and consequently we are allowed to attribute the i -class to v_{o_i} without any ambiguity. We assume also that p classes can adequately "cover" the initial number distribution $f(v_0)$ ($f(v, t)$ must decrease very fast while v increases because of mass conservation). Substituting the integrals by quadratures, we replace our system of two integro-partial differential equations by an initial-value system of nonlinear ordinary differential ones. Any suitable scheme, e.g. an explicit Runge-Kutta, can be employed to integrate the resulting system and update both the number density and the volumes.

We have seen that most finite difference schemes (with respect to volume) imply some arbitrary assumptions on the particle distribution within a class and on the outcome of each coagulation, which becomes clear not only from simple schemes, such as Williams' [1], in which the insistence on attributing particle-like properties to mathematical entities brings about most of the problems, but also from more sophisticated ones, such as Bleck's [2], in which averages are determined based on some arbitrary relationships for the number distribution within a class. In order to represent exactly a distribution, the number of classes in a finite-

difference scheme must be very large. In addition, substantial errors might appear due to the finite representation of the integral terms. In order to allow for the unequal intervals and to avoid the troublesome aspects previously discussed, we decided on a finite-element scheme, in which the number density function is replaced by splines defined on each interval (v_i, v_{i+1}) . "Splines" are piecewise-interpolating functions, usually but not exclusively polynomials, such that not only their values at some intermediate nodes obey some relationship with the values of the function at the same nodes but also the n -continuity of the derivatives at every v_i is granted. In the classical case of cubic splines, one cubic polynomial is defined for each finite element (with no intermediate node) such that the four free parameters are determined by the interpolated function and its derivative at the nodes. It turns out that at these points the second derivative is also continuous. Because of their smoothness, cubic splines tend to oscillate around sharp corners, generating an unrealistic fit, and worse yet causing catastrophic effects on the first derivatives. In our case, that means a potentially unstable behaviour, such as the build-up of negative values for the number concentration. Although calculating the derivatives apart from the splines helps to solve the problem, we describe next a much more radical approach, based on a very special spline.

4.3 THE SHAPE-PRESERVING QUADRATIC SPLINES

Shape-preserving quadratic splines are based on a remarkable property of the quadratic Bernstein polynomials. For a continuous function f defined in the interval $[0,1]$, without loss of generality, the Bernstein polynomial of n -order is defined by [3]

$$B_n(f) = \sum_{k=1}^n f(k/n) P_{n,k} , \quad (4.3)$$

with

$$P_{n,k}(x) = \binom{n}{k} x^k (1-x)^{n-k} . \quad (4.4)$$

Therefore, the quadratic polynomial is

$$B_2(f) = f(0) (1-x)^2 + 2f(1/2) x (1-x) + f(1) x^2 , \quad (4.5)$$

and the derivative is written

$$B_2'(f)(x) = 2 (f(0) - 2f(1/2) + f(1)) x + 2f(1/2) - 2 f(0) ,$$

with the following properties:

$$(1) \quad B_2(f)(0) = f(0) ,$$

$$B_2(f)(1) = f(1) ; \quad (4.6)$$

$$(2) \quad B_2'(f)(0) = 2 (f(1/2) - f(0)) ,$$

$$B_2'(f)(1) = 2 (f(1) - f(1/2)) ; \quad (4.7)$$

$$(3) \quad f(x) \geq 0 \text{ implies } B_2(f) \geq 0, \text{ } x \text{ in } [0,1],$$

$$f'(x) \geq 0 \text{ implies } B_2'(f) \geq 0, \text{ } x \text{ in } [0,1] . \quad (4.8)$$

Now let us consider an $f(x)$, x in $[0,1]$, composed of two straight lines, one through $x = 0$ and slope M_1 and the other through $x = 1$ and slope M_2 , such that their intersection occur at $x = 1/2$ (Figure 4.1). It can be seen that

$$M_1 = 2 (f(1/2) - f(0)), \quad (4.9)$$

$$M_2 = 2 (f(1) - f(1/2)); \quad (4.10)$$

and the property (2) becomes

$$B_2'(f)(0) = M_1 , \quad (4.11)$$

$$B_2'(f)(1) = M_2 . \quad (4.12)$$

Hence we conclude that not only $B_2(f)$ preserves the shape of f , but it has a continuous first derivative on $[0,1]$, while $f(x)$ does not. Using this property, we construct a piecewise-linear function f in $[0,1]$, which has slope M_1 at 0 and M_2 at 1, and such that the interval $[0,1]$ can be partitioned into subintervals in such way that the piecewise-quadratic polynomial S , satisfying $S = B_2(f)$ on each subinterval, is a quadratic spline S . Of course, there are many possibilities for partitioning the interval $[0,1]$, and consequently such splines are unique only upon the partition. The following algorithm, from [4], offers just one solution.

Let us consider as given the pairs of data (x_j, y_j) , $j = 1, \dots, N$, strictly increasing x , and the slopes M_j at x_j (Figure 4.2). We write the obvious normalization formulas, for any pair, with $y_1 = f(0)$ and $y_2 = f(1)$:

$$r = (x - x_1)/(x_2 - x_1) , \quad (4.13)$$

$$M_1^* = M_1 (x_2 - x_1) , \quad (4.14)$$

$$M_2^* = M_2 (x_2 - x_1) . \quad (4.15)$$

We determine r' such that r' represents the intersection of the lines

through y_1 , slope M_1^* and y_2 , slope M_2^* .

$$r' = (y_2 - y_1 - M_2^*) / (M_1^* - M_2^*) \quad . \quad (4.16)$$

If $0 \leq r' \leq 1$ then let $r_0 = r'$, otherwise let $r_0 = 1/2$.

After some easy calculations, the expressions for the normalized quadratic splines become

(a) if $r \leq r_0$:

$$q = r/r_0 \quad ,$$

$$S(q) = y_1 (1 - q)^2 + 2 P_1 q (1 - q) + P_3 q^2 \quad ; \quad (4.17)$$

(b) if $r > r_0$:

$$q = (r - r_0) / (1 - r_0) \quad ,$$

$$S(q) = P_3 (1 - q)^2 + 2 P_2 q (1 - q) + y_2 q^2 \quad ; \quad (4.18)$$

with

$$P_1 = 1/2 M_1^* r_0 + y_1 , \quad (4.19)$$

$$P_2 = 1/2 M_2^* (r_0 - 1) + y_2 , \quad (4.20)$$

$$P_3 = P_1 - r_0 (P_1 - P_2) . \quad (4.21)$$

The slope at an interior point is determined using the two neighbouring data points, while at an endpoint, the two points immediately preceding (or succeeding) it. Let us define S_i as

$$S_i = (y_i - y_{i-1})/(x_i - x_{i-1}) , \quad i = 2, \dots, N . \quad (4.22)$$

Consider an interior point i , $1 < i < N$. If $S_i S_{i+1} \leq 0$, then we set $M_i = 0$. Otherwise, let

$$M_i = 2 S_i S_{i+1} / (S_i + S_{i+1}) . \quad (4.23)$$

As for the endpoints, we have two cases to be considered:

(a) $i = N$:

if $S_{N-1} S_N < 0$ then $M_N = 2 S_N$. Otherwise, let

$$M_N = 2 S_N - M_{N-1} . \quad (4.24)$$

(b) $i = 1$:

if $S_2 S_3 < 0$ then $M_1 = 2 S_2$. Otherwise, let

$$M_1 = 2 S_2 - M_2 . \quad (4.25)$$

In the scheme above the derivatives are determined at once from the data, and the quadratic shape-preserving splines are calculated for each interval.

4.4 THE REFORMULATED SYSTEM

Let us proceed to the nondimensionalization of the variables. Because of the mass conservation

$$\int_0^{\infty} f(v,t) v \, dv = N_0 \bar{v} , \quad (4.26)$$

that, in a more convenient form becomes

$$\int_0^{\infty} W(x,T) x \, dx = 1 , \quad (4.27)$$

where $W(x,T)$ is defined as

$$W(x,T) = \bar{v}/N_0 \, f(v,t) . \quad (4.28)$$

We define, also

$$T = A N_0 t , \quad (4.29)$$

$$x = v/\bar{v} , \quad (4.30)$$

where $\bar{v}$ is the mass averaged volume

$$\bar{v} = \int_0^{\infty} f(v,t) v \, dv / \left(\int_0^{\infty} f(v,t) \, dv \right) , \quad (4.31)$$

and A is a constant conveniently defined according to the kernel specification. For instance, A is proportional to $\bar{v}$ for the kernel proportional to the sum of volumes.

Finally we recast the system (4.1), (4.2), with the help of (4.28–31) into the nondimensional semi-discretized form on the finite-elements:

$$\begin{aligned} d\bar{w}_i^*(T)/dT = & - \int_{x_1}^{x_p} K(x_i, r) W(x_i, T) W(r, T) dr + \\ & 1/2 \int_{x_1}^{x_i} K(x_i - r, r) W(x_i - r, T) W(r, T) dr + \\ & (d\bar{w}(x_i, T)/dx) dx_i/dT \quad , \end{aligned} \quad (4.32)$$

$$dx_i(T)/dT = \int_{x_1}^{x_i} K(x_i, r) W(r, T) r dr \quad , \quad (4.33)$$

where $i = 1, 2, \dots, p$, p particle classes.

In (4.32) and (4.33), the integrals are to be replaced by quadratures for each interval between x_j and x_{j+1} , and the derivative by its spline counterpart for each x_i . There is one spline evaluation for the nondimensional number concentration density W , used for the interpolations at the values of $x_i - r$, in the integrands. Using a Lagrange interpolation formula [5], we obtain the Simpson's quadrature for unequal intervals (which reduces to the conventional Simpson' Rule, in the case $x_2 - x_1 = x_3 - x_2$):

$$\int_{x_1}^{x_3} f(x) dx = (x_3 - x_1)/6 \{ (3s - 1)/s f(x_1) + f(x_2)/(s(1 - s)) + (2 - 3s)/(1 - s) f(x_3) \} , \quad (4.34)$$

with

$$s = (x_2 - x_1)/(x_3 - x_1) . \quad (4.35)$$

The system is now ready for the time integration.

4.5 THE TIME INTEGRATION

We perform the integration in time by means of a Runge-Kutta scheme, based on the calculation of a five-stage fourth-order formula, using the first five K_i of a six-stage fifth-order method. That procedure, known as Runge-Kutta-Fehlberg or RKF45 [6], for $dy_j/dx = F_j(x, y)$, $y = (y_1, y_2, \dots, y_{2p})$ and $h = x_i - x_0$, is described below, where

$y_1, \dots, y_p$ account for the number distribution variables, $F_1, \dots, F_p$ being the R.H.S. of (4.32), and

$y_{p+1}, \dots, y_{2p}$ account for the size (or volume) variables, $F_{p+1}, \dots, F_{2p}$ representing the R.H.S. of (4.33).

The coefficients are determined by the expressions

$$K_{1,j} = F_j(x_0, y_0) , \quad (4.36)$$

$$K_{2,j} = F_j(x_0 + h/4, y_0 + h/4 K_1) , \quad (4.37)$$

$$K_{3,j} = F_j(x_0 + 3h/8, y_0 + h/32 [3 K_1 + 9 K_2]) , \quad (4.38)$$

$$K_{4,j} = F_j(x_0 + 12h/13, y_0 + h/2197 [1932 K_1 - 7200 K_2 + 7296 K_3]) , \quad (4.39)$$

$$K_{5,j} = F_j(x_0 + h, y_0 + h [439/216 K_1 - 8 K_2 + 3680/513 K_3 - 845/4104 K_4]) , \quad (4.40)$$

$$K_{6,j} = F_j(x_0 + h/2, y_0 + h [-8/27 K_1 + 2 K_2 - 3544/2565 K_3 + 1859/4104 K_4 - 11/40 K_5]) . \quad (4.41)$$

where $y_0 = (y_{0_1}, \dots, y_{0_{2p}})$ and $K_i = (K_{i_1}, \dots, K_{i_{2p}})$, $i = 1, \dots, 6$.

The fourth-order update is

$$y_j^{(4)} = y_{o_j} + h \left[\frac{25}{216} K_{1_j} + \frac{1408}{2565} K_{3_j} + \frac{2197}{4104} K_{4_j} - \frac{1}{5} K_{5_j} \right] , \quad (4.42)$$

and the fifth-order formula is

$$y_j^{(5)} = y_{o_j} + h \left[\frac{16}{135} K_{1_j} + \frac{6586}{12825} K_{3_j} + \frac{28561}{56437} K_{4_j} - \frac{9}{50} K_{5_j} + \frac{2}{55} K_{6_j} \right] . \quad (4.43)$$

The local truncation error of the method is given by the absolute value of

$$y_j^{(4)} - y_j^{(5)} = h \left[\frac{1}{360} K_{1_j} - \frac{128}{4275} K_{3_j} - \frac{2197}{75240} K_{4_j} + \frac{1}{50} K_{5_j} + \frac{2}{55} K_{6_j} \right] . \quad (4.44)$$

We define the relative error by

$$E_{R_j} = |y_j^{(4)} - y_j^{(5)}| / y_j^{(4)} , \quad y_j^{(4)} \neq 0 , \quad (4.45)$$

and, based on the L_1 Norm, we define the average error as

$$E_R = \sum_i E_{R_i} . \quad (4.46)$$

The L_1 Norm was finally selected because trials employing the L_{∞} Norm (Max Error) revealed it to behave unpredictably. An error tolerance E must be supplied (e.g. 10^{-8}) as well as the maximum integration interval, which is duly normalized to 1. The step length is halved if E_R is greater than E/h^{*2} , and doubled if E_R is less than or equal to $E/(25 h^{*2})$ (because this is a fourth-order method) [6], where h^* is a fraction of the normalized full step. Additionally, in the case of h^* becoming smaller than a minimum (e.g. 2^{-10}), the procedure is halted and a warning is emitted.

The main advantages of the scheme above become apparent when one considers the fact that the coagulation is very fast at the beginning, slowing down as the total number concentration diminishes. Allowing for large time-saving integration steps is only possible with adaptive-length step procedures. Besides that, such schemes can cater for the wide changes in the coagulation rate that occur with distinct coagulation kernels and/or initial conditions, while keeping (for tolerance of 10^{-8}) the maximum relative error E_R at about 10^{-5} , no matter under which circumstances, although the penalty for larger steps is a far smaller error tolerance.

4.6 THE CODE

All algorithms were coded in Standard Pascal, for a 68000-based

microcomputer. Pascal, although a rather old Programming Language, was chosen because of its data-type definition facilities, as well as its inherent safety, readability and portability, which have allowed for substantial changes without too much difficulty. In terms of time, it can be shown that the resulting program is a N^2 Code, i.e the running time is proportional to the square of the number of classes.

4.7 CONCLUSION

A collocation method using osculatory quadratic splines for the pseudo-Lagrangian system previously obtained in the previous Chapter was developed, with a special adaptative interval for the time integration. Since this is not an orthogonal collocation (optimal) method, in the next Chapter we shall submit the model to some standard tests in order to analyse its behaviour.

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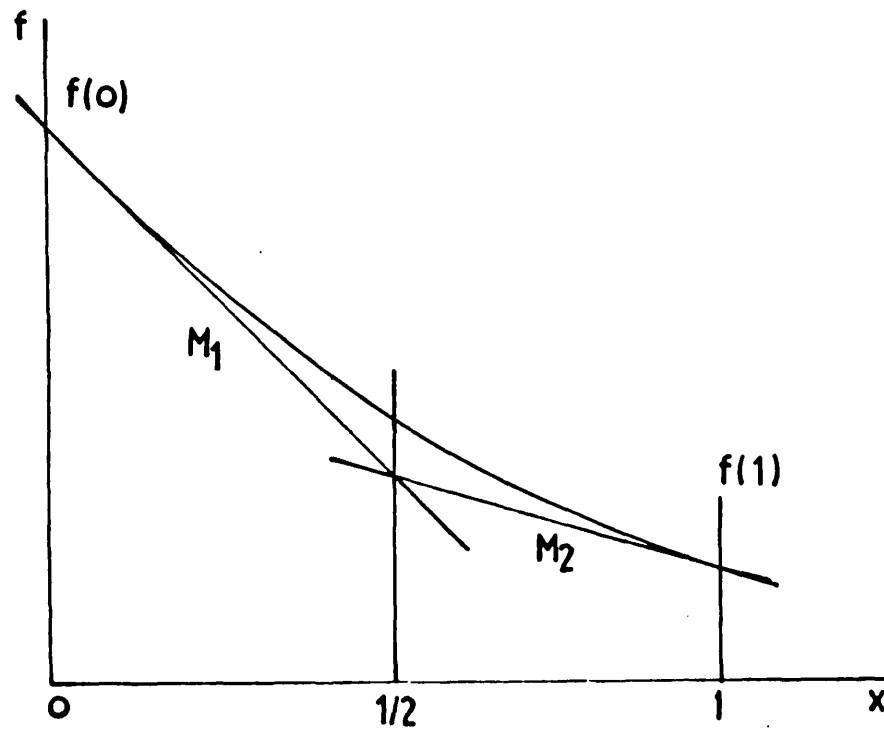


FIGURE 4.1 - Representation of the osculatory properties of the quadratic Bernstein polynomial.

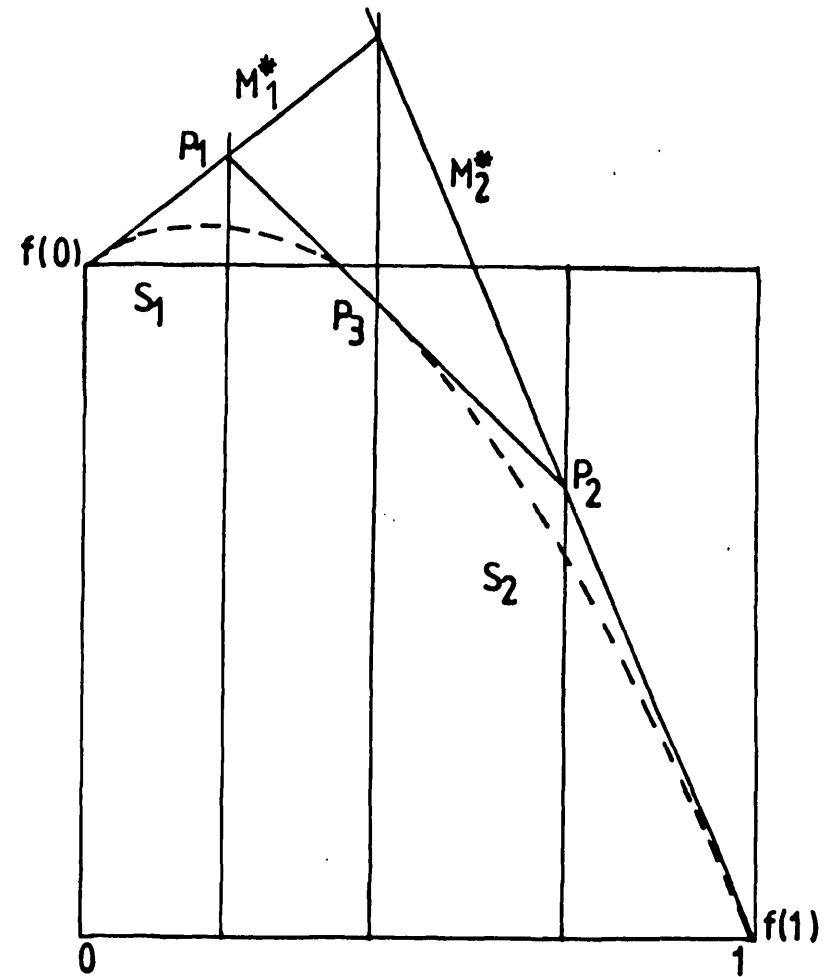


FIGURE 4.2 - The scheme for the determination of the quadratic splines for each normalized interval $[0, 1]$.

CHAPTER 5

TEST CASES

5.1 INTRODUCTION

The numerical scheme for the coagulation problem in terms of the system (4.1), (4.2) developed in the previous chapter is now submitted to some standard tests for which analytical solutions are available, and one additional test (Brownian kernel) for which the comparison is made with another numerical solution, since there is no analytical solution.

5.2 COMPARISON WITH ANALYTICAL SOLUTIONS

Classic analytical results were developed by Scott [1], although these are subject to some limitations exposed by Drake [2]. Employing Laplace transforms, Scott evaluated the infinite series solutions for three special kernels: constant, proportional to the sum of volumes, and proportional to the product of volumes, for the following family of initial conditions:

$$w_0(x) = [(s + 1)^{(s + 1)} / \Gamma(s + 1)] x^s e^{-x (s + 1)} , \quad (5.1)$$

with

$$W_0(x) = (\bar{v}/N_0) f_0(v) , \quad (5.2)$$

$$x = v/\bar{v} , \quad (5.3)$$

where s is a positive real number, N_0 is the initial total number concentration of particles, $\bar{v}$ is the initial mass average particle size (or volume), $f_0(v)$ is the initial number distribution as a function of particle volume v , and $\Gamma(y)$ is the Gamma function.

However exact the series solutions are, their usefulness is, for computational reasons, usually conditioned to the determination of their equivalent closed forms. By means of the saddle-point method [1], [2], Scott found approximate closed solutions that unfortunately in most cases exhibited large errors (e.g. negative number concentrations) for smaller volumes. For some of them, however, such closed forms are exact. That is the case for constant kernel and s equals to 0 and 1 in the equation (5.1) [2]. For those cases the solutions are

$$W(x,T) = [4e^{-2x/(T+2)}]/(T+2)^2 , \text{ for } s = 0, \quad (5.4)$$

$$W(x,T) = [8e^{-2x/(T+2)^{1/2}} (T+2)^{3/2}] \sinh\{2x [T/(T+2)]^{1/2}\}, \text{ for } s = 1, (5.5)$$

with

$$T = B N_0 t , \quad (5.6)$$

and

$$K(x,y) = B , \quad (5.7)$$

where t is time, and x and y are nondimensional volumes.

For the kernel proportional to the sum of volumes and s equals to 0 (exponential initial condition), the series is sufficiently simple to be programmed, if Stirling's Formula for factorials [3] is used. This series is the following:

$$W(x,T) = [(1 - r)/(x r^{1/2})] e^{-x(r + 1)} I_1(2 x r^{1/2}) , \quad (5.8)$$

with

$$T = b_0 N_0 t , \quad (5.9)$$

$$r = 1 - e^{-T} , \quad (5.10)$$

$$K(x,y) = b_0 \bar{v} (x + y) , \quad (5.11)$$

where again t is time, x and y are nondimensional volumes and $I_1(x)$ is the modified Bessel function of the first order [3].

Figures 5.1 to 5.5 show at the selected time intervals of 100, 200 and 1000 seconds, the analytical and numerical solutions for constant kernel and $s = 0$ (exponential) for both the number density (Fig. 5.1, 5.2 and 5.3) and the mass distribution (Fig. 5.4 and 5.5). Note that Figure 5.2 depicts a detail of Fig. 5.1, representing the number density after 1000 seconds. Analogously, Figures 5.6 to 5.10 represent the results after the same intervals, for constant kernel and $s = 1$ (nearly Normal). Again, a rescaled number density at 1000 seconds is represented in Figure 5.7.

The coagulation process at 100, 500 and 1000 seconds for a kernel proportional to the sum of volumes and $s = 0$ as initial condition can be found in Figures 5.11 to 5.14.

The evolution of the nondimensional total particle number concentration $N(T)/N_0$, against nondimensional time T , can be seen in Figure 5.15, for constant kernel ($s = 0$ and $s = 1$), and Figure 5.16, for kernel proportional to the sum of volumes. In the same Figures, the extent of conservation of

mass for each case can be analysed. The analytical results for the total number concentration is, for constant kernel, given by

$$N(T)/N_0 = 2/(T + 2) \quad , \quad (5.12)$$

and, for proportional-to-the-sum kernel and $s = 0$ in Eq. 5.1, by

$$N(T)/N_0 = e^{-T} \quad . \quad (5.13)$$

We have used Scott's data [1] for the results in Figures 5.1-5.16, i.e.

$\bar{d} = 20 \mu\text{m}$, and coefficients b_0 and B such that, for constant kernel

$$T = 0.0429 \, t \quad , \quad (5.14)$$

and, for proportional-to-the-sum kernel and $s = 0$,

$$T = 0.00153 \, t \quad . \quad (5.15)$$

The equivalence between real time t , nondimensional time T and the resulting $N(T)/N_0$, for both constant and proportional-to-the-sum kernels,

can be found in the Table I below, assuming Scott's data [1].

CONSTANT KERNEL:

t (sec)	T	N(T)/N ₀ (%)
100	4.29	31.79
200	8.58	18.90
1000	42.9	4.45

PROPORTIONAL TO THE SUM (s = 0):

t (sec)	T	N(T)/N ₀ (%)
100	0.153	85.8
500	0.765	46.5
1000	1.53	21.6

TABLE I - Equivalence of t, T and the value of N(T)/N₀, according to Scott's data [1]

5.2.1 DISCUSSION

Preparing data for manipulation (e.g. solving equations) and presentation of results, is not a trivial task. An improper selection of dimensional and nondimensional variables might imply awkward equations to deal with or the need for re-evaluation every time a parameter is altered. Throughout this work, we have used the Scott's format [1] in terms of nondimensional

number density $W(x,T)$, ratio of volume ratio $x = v/\bar{v}$ and time T , because we consider it to be natural and selfconsistent. As we will see in Chapter 6, entirely new variables have been defined, number rate density, for instance, just by applying the same basic principles. On the other hand, due to the wide range of numerical values involved, it is impossible to meaningfully represent all data from any one case in just one Figure. Taking constant kernel and $s = 1$, for instance, one should use Figures 5.6 and 5.7 to interpret the medium range of volumes (Fig. 5.7, for 1000 seconds), while consulting Figure 5.8 to learn about the behaviour of the tail end of the distribution (larger particle volumes), and similarly for mass. It is only from the analysis of Figures 5.11 and 5.12 that one can conclude that, in the case of the kernel proportional to the sum of volumes, the numerical results for larger particle volumes are decreasing much faster than the analytic counterparts, symptom that the model is not generating larger particles at the correct rate. Significantly, there is an increasing discrepancy between the analytical and numerical values of the total number concentration, for this kernel (Fig. 5.16) while for constant kernel, the agreement is very good indeed (Fig. 5.15). Gelbard [4] has presented a numerical method based on orthogonal collocation on finite elements [5], for exponential initial distribution ($s = 0$) and the same kernels we have been discussing. Unfortunately, his results are presented in such a way that is not possible to observe the detailed behaviour of the tail end of the distributions, although we can safely say that the results using the present (nonoptimal) model are at least as good as the ones in [4].

Although the analytical solutions make the previously presented kernels mathematically convenient, those kernels are unrealistic in the sense that,

as a result of the coagulation, the mass conservation eventually no longer holds. For kernels proportional to the sum of volumes, this increase is actually very fast. On the other hand, such fast growth offers an enormous challenge for any numerical formulations, which, because of their inner limitations (e.g. the finite domain error previously explained), are expected to break down after some time interval. Also, the integro-differential character of the coagulation equation, that is, the local behaviour of the density function depending on its global description with respect to all volume values, might give rise to further difficulties. That fact may explain why the results for constant kernel are better than those for kernel proportional to the sum of volumes (the same occurring in [4]).

5.3 COMPARISON WITH A NUMERICAL SOLUTION

A somewhat more realistic situation was the object of discussion in [6], in which the Brownian kernel for $Kn \ll 1$ was used:

$$K(x,y) = 2 + (x/y)^{1/3} + (y/x)^{1/3} \quad . \quad (5.16)$$

In [6], one representative of the Method of Weighted Residuals (orthogonal collocation) [5] was implemented into a perturbation solution for the difference between the accurate solution and an analytical solution for an "approximate problem" (constant kernel). In other words, the method employed in [6] was carefully cast for the solution to the Brownian coagulation with exponential initial distribution. On the other hand, in our model we needed simply a redefinition of the kernel to the one in (5.5),

and of the nondimensionalizing constants.

The comparison between the results using [6] and our model for exponential initial condition can be examined in Figure 5.17, the nondimensional total number and mass concentration as functions of nondimensional time T , being depicted in Figure 5.18.

5.3.1 DISCUSSION

For this case, the computation time for one cycle (see Chapter 4) has increased substantially, undoubtedly due to the kernel calculations: there are two exponential functions for each kernel to be evaluated, and most exponential implementations tend to be very slow and unoptimized.

We have superimposed the results from the present model onto the curves presented in [6], since the actual data was not available. Even considering those limitations, there is a very good agreement between the "dots" and the curves, at least up to $T = 10$ (Fig. 5.17), resulting in a reduction in the total number concentration to a few percent of N_0 (Fig. 5.18). It must be remarked that the relaxation method described in [6], besides needing fine tuning by changing two parameters, is only applicable to the special case of Brownian coagulation, while the present model is quite general, although, because of cumulative inaccuracies, we cannot claim that it produces correct results for very long coagulation times, as can be seen from the Figures.

5.4 CONCLUSION

Either for analytical solutions or numerical ones, for kernels as widely

distinct as constant and Brownian, the quality of the comparisons attested by the Figures 5.1-5.18 is quite remarkable. However we can conclude from the increasing inaccuracy of the results for larger times, that even a model designed to overcome the limitations of the fixed size classes such as ours is not immune to the finite domain errors.

Next, we want to employ the model to predict the coagulation induced by the relative particle velocities in gas-particle flows. For that, we have to perform some modifications to the original equations.

5.5 REFERENCES

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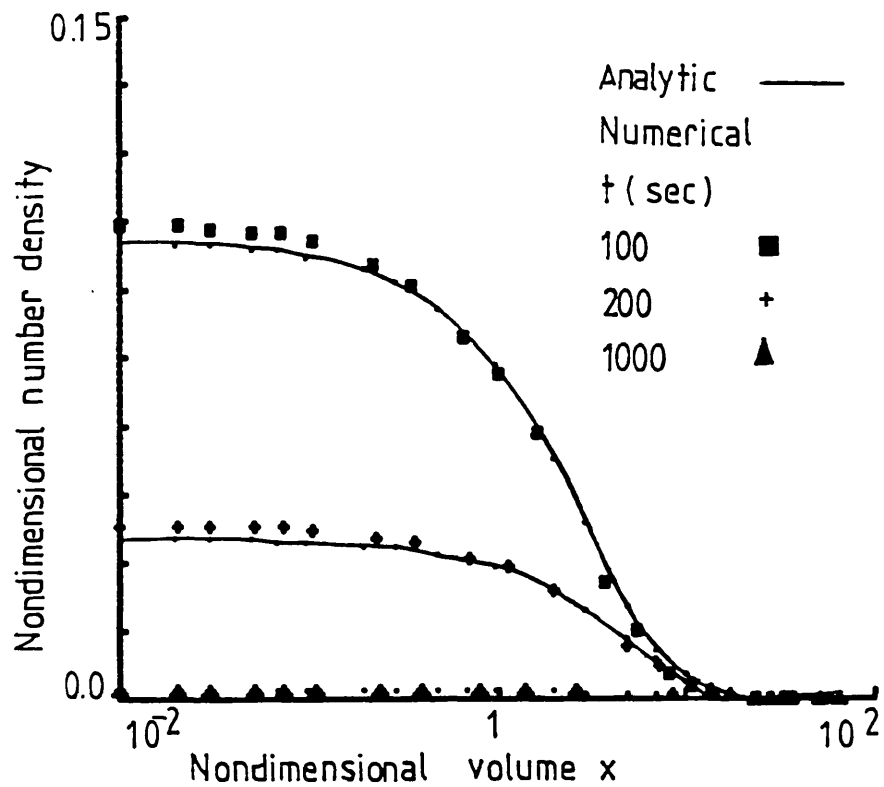


FIGURE 5.1 - Evolution of the nondimensional number density as a function of the volume ratio $x = v/\bar{v}$, with time, for constant kernel and initial condition $s = 0$ in the equation (5.1). Comparison between the analytic solution [1] and the present model.

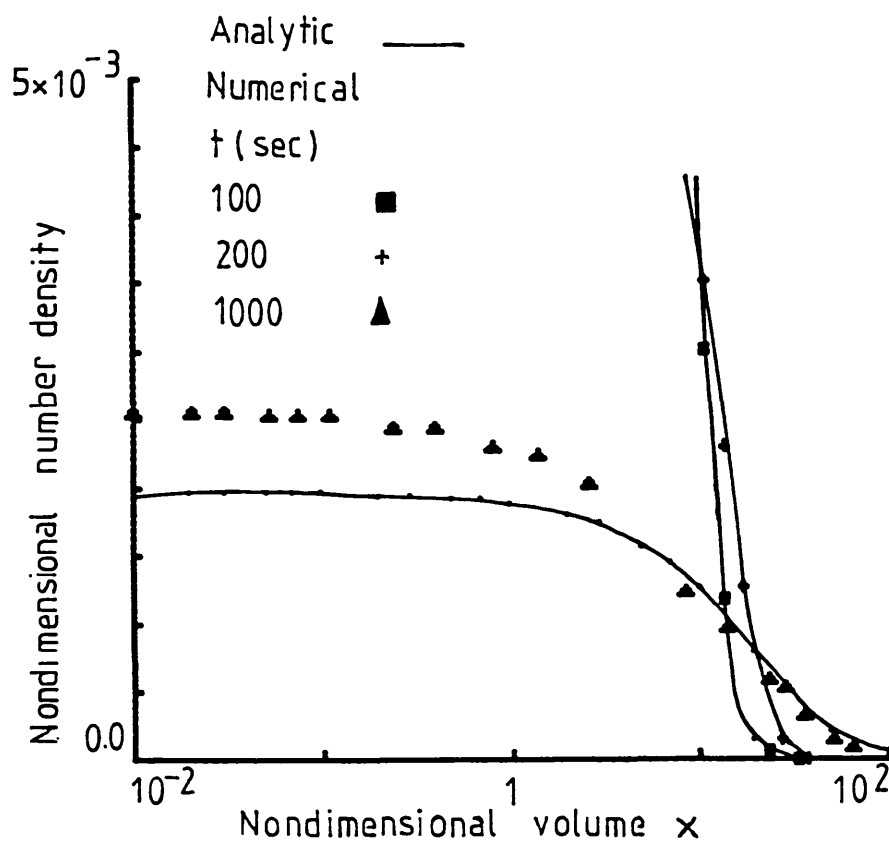


FIGURE 5.2 - Detail of Fig. 5.1, for the time of 1000 seconds.

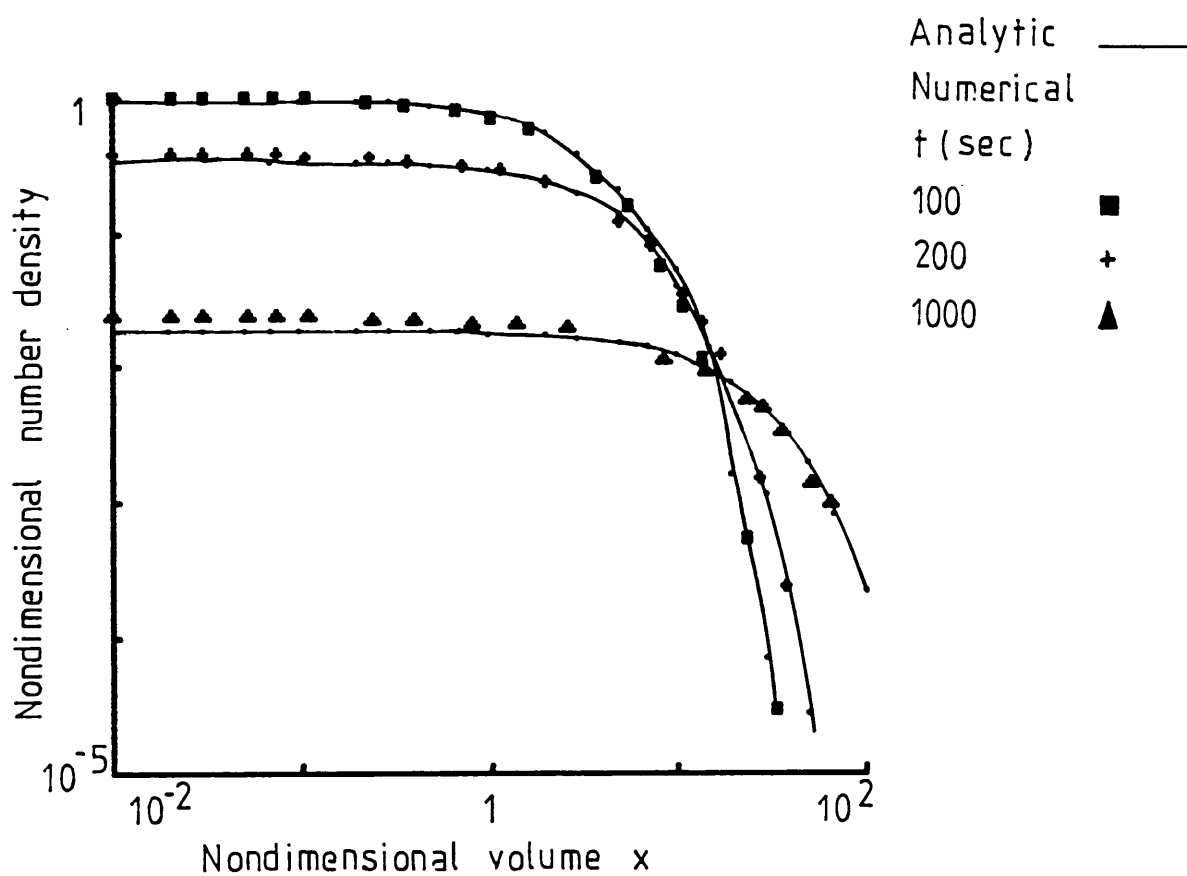


FIGURE 5.3 – The same as Fig. 5.1, but in log scaling, in order to emphasize the behaviour for larger particles.

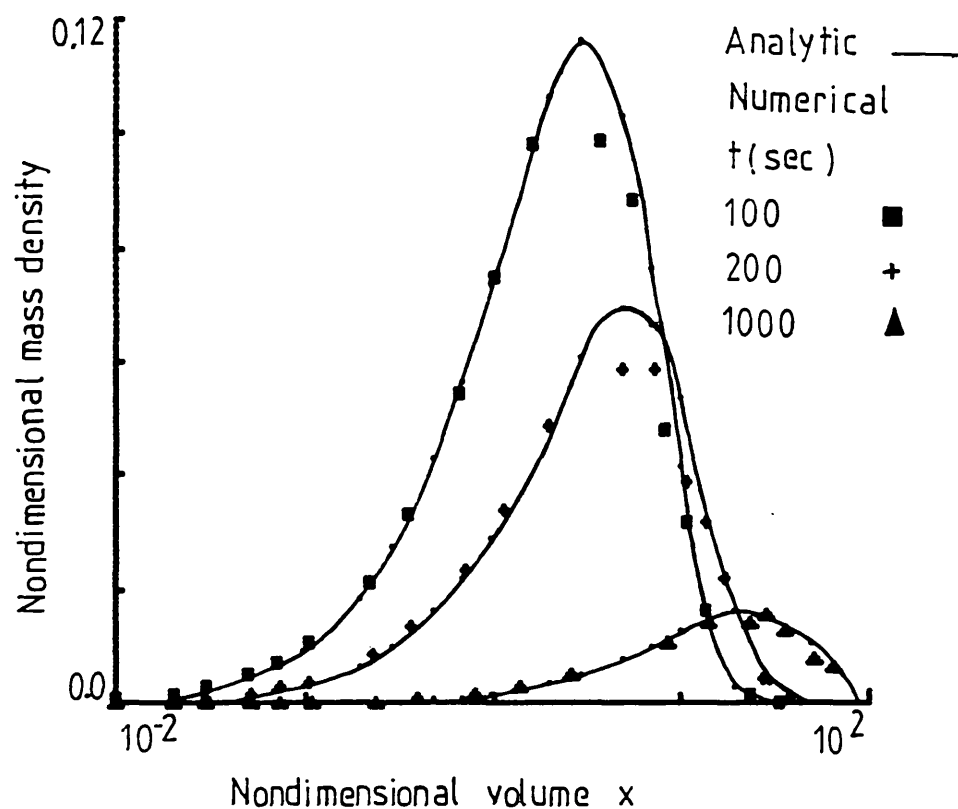


FIGURE 5.4 - Evolution of the nondimensional mass density as a function of the volume ratio $x = v/\bar{v}$, with time, for constant kernel and initial condition $s = 0$ in the equation (5.1). Comparison between the analytic solution [1] and the present model.

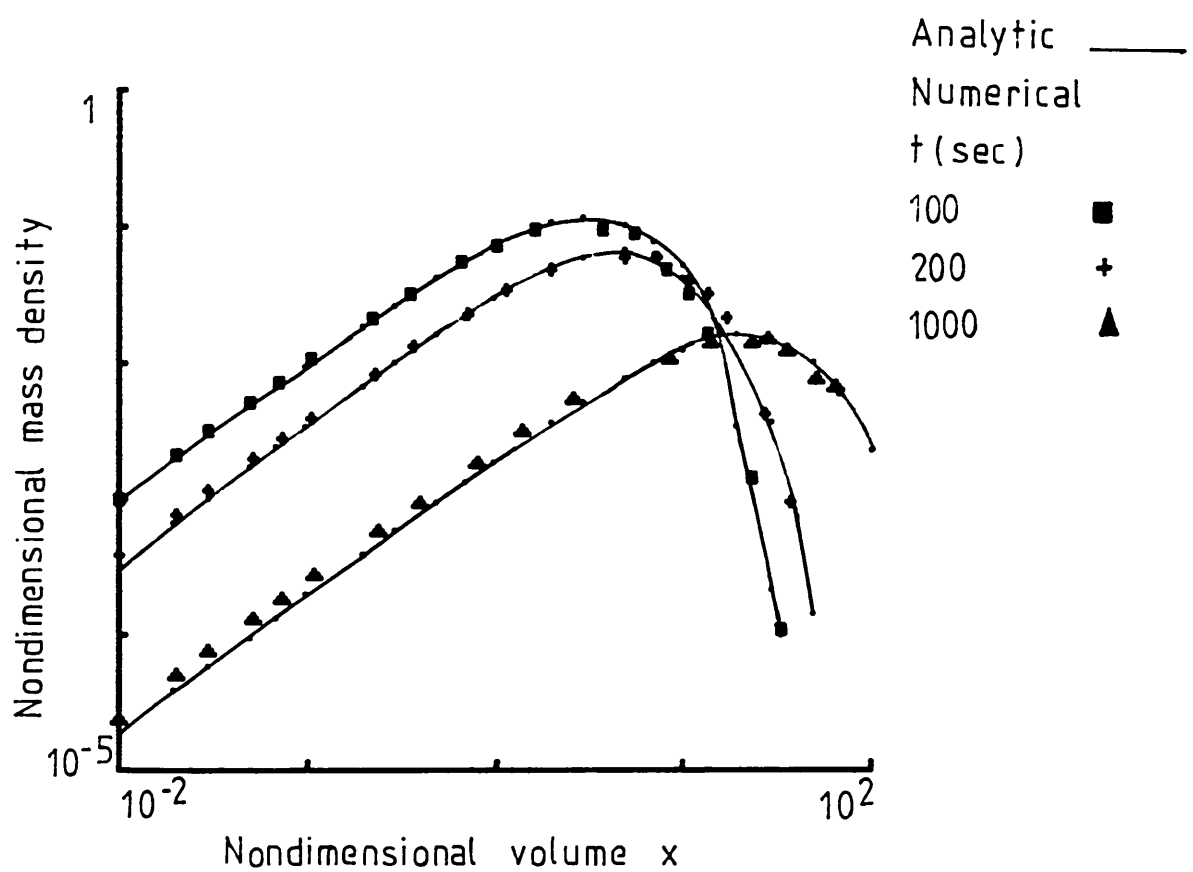


FIGURE 5.5 - The same as Fig. 5.4, but in log scaling, in order to emphasize the behaviour for larger particles.

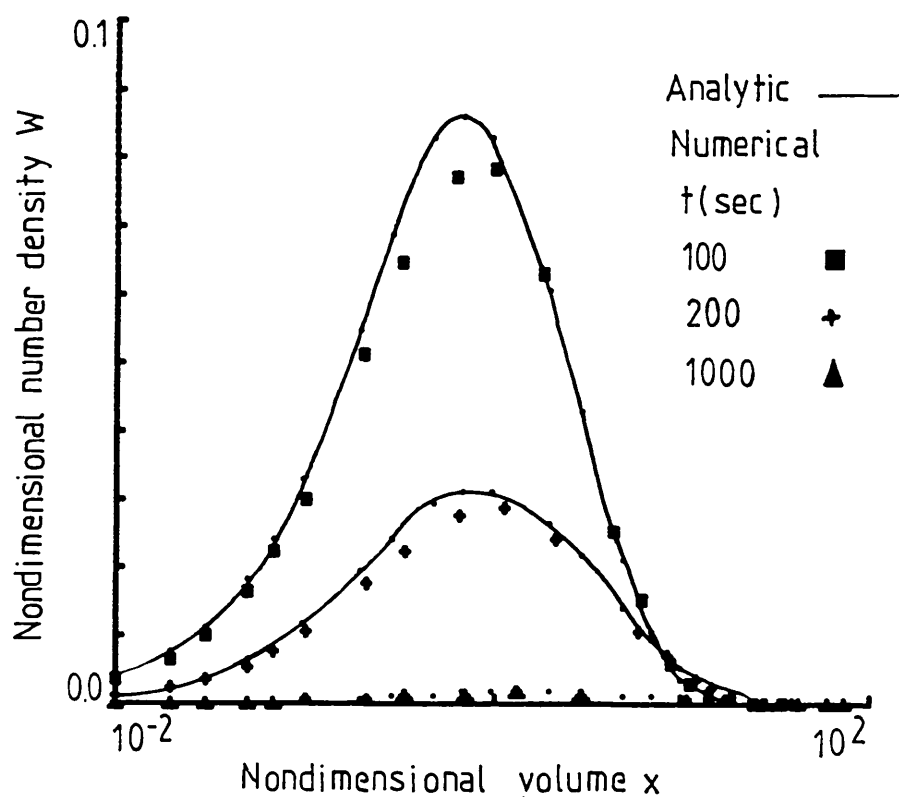


FIGURE 5.6 – Evolution of the nondimensional number density as a function of the volume ratio $x = v/\bar{v}$, with time, for constant kernel and initial condition $s = 1$ in the equation (5.1). Comparison between the analytic solution [1] and the present model.

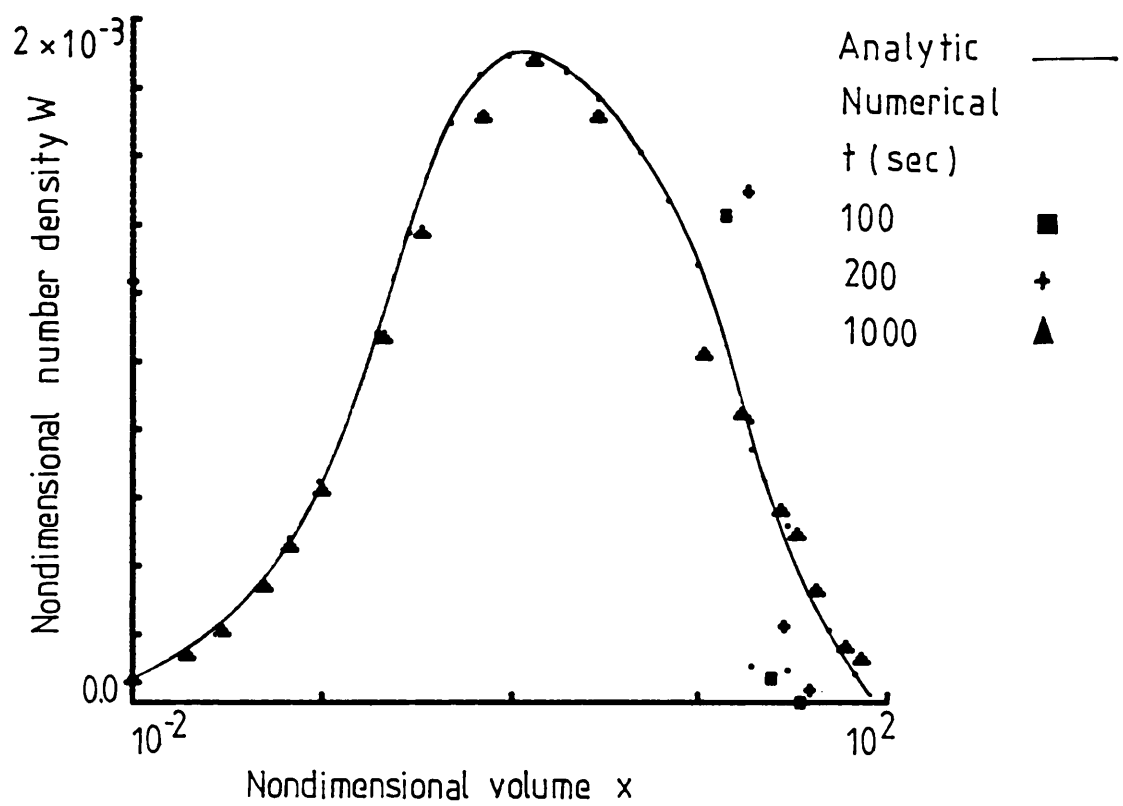


FIGURE 5.7 – Detail of Fig. 5.6, for the time of 1000 seconds.

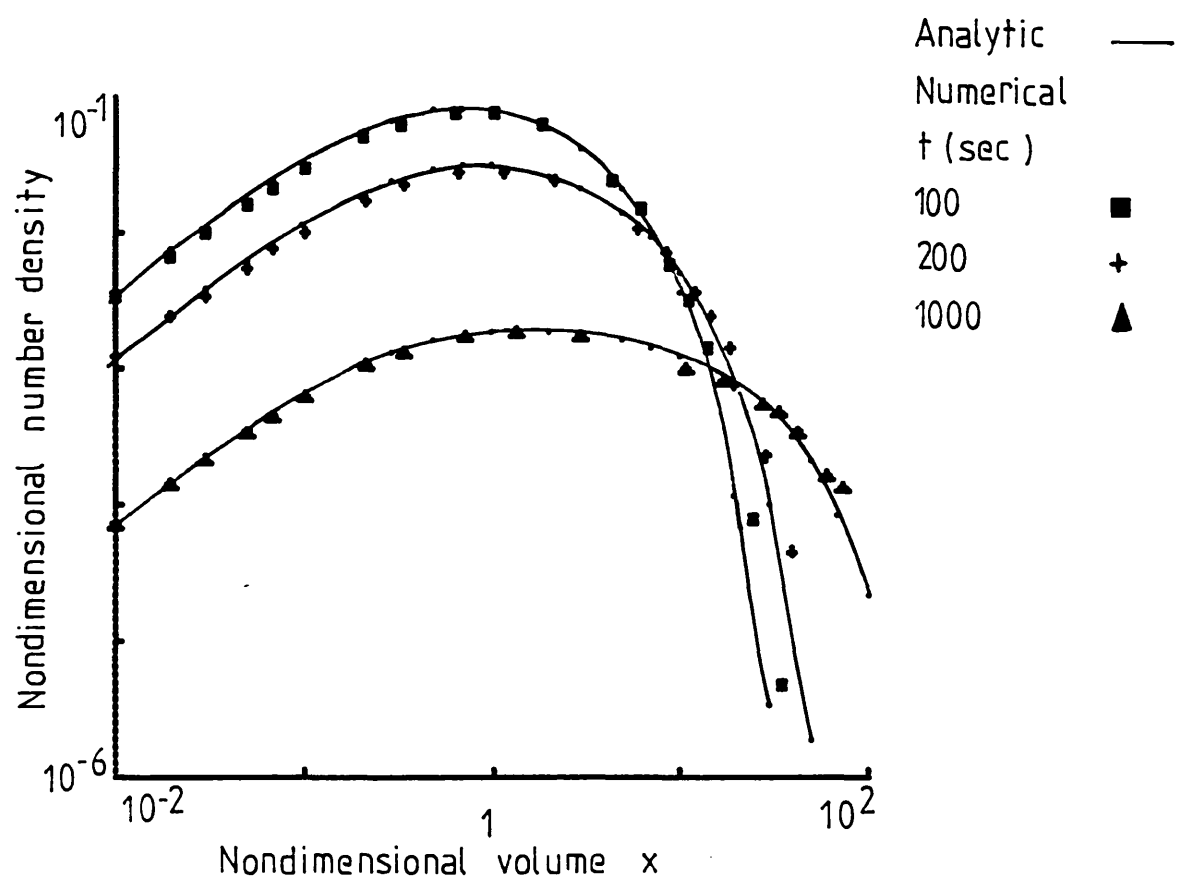


FIGURE 5.8 – The same as Fig. 5.6, but in log scaling, in order to emphasize the behaviour for larger particles.

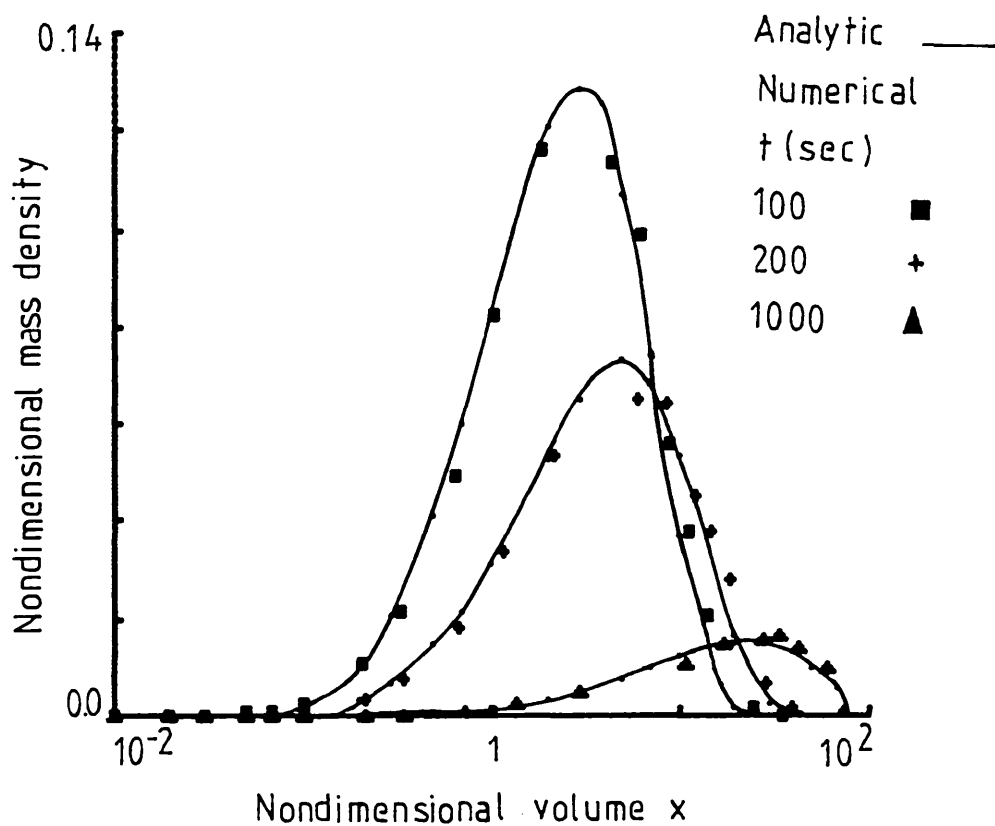


FIGURE 5.9 – Evolution of the nondimensional mass density as a function of the volume ratio $x = v/\bar{v}$, with time, for constant kernel and initial condition $s = 1$ in the equation (5.1). Comparison between the analytic solution [1] and the present model.

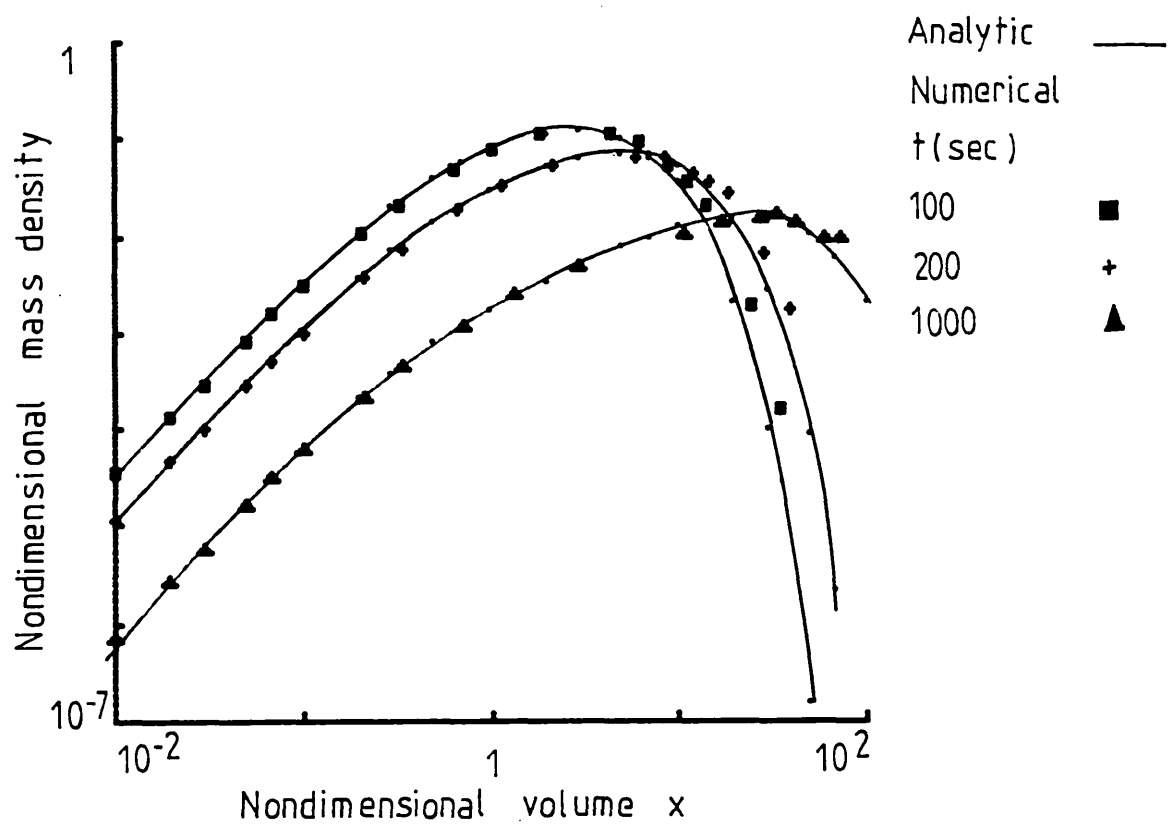


FIGURE 5.10 - The same as Fig. 5.9, but in log scaling, in order to emphasize the behaviour for larger particles.

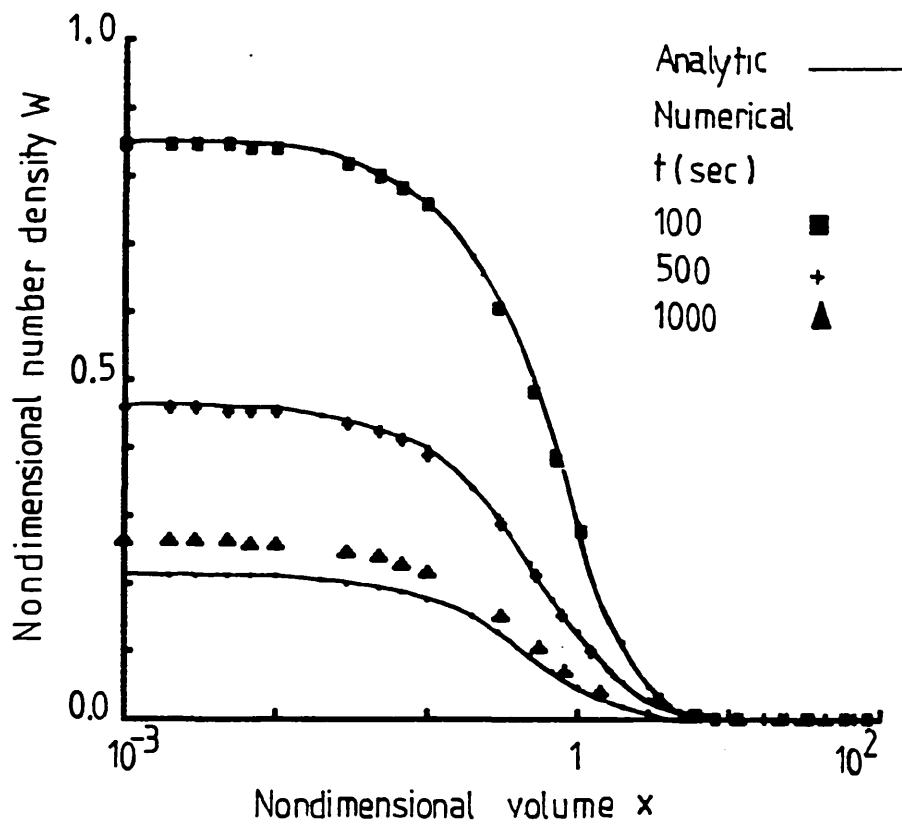


FIGURE 5.11 - Evolution of the nondimensional number density as a function of the volume ratio $x = v/\bar{v}$, with time, for kernel proportional to the sum of the volumes and initial condition $s = 0$ in the equation (5.1). Comparison between the analytic solution [1] and the present model.

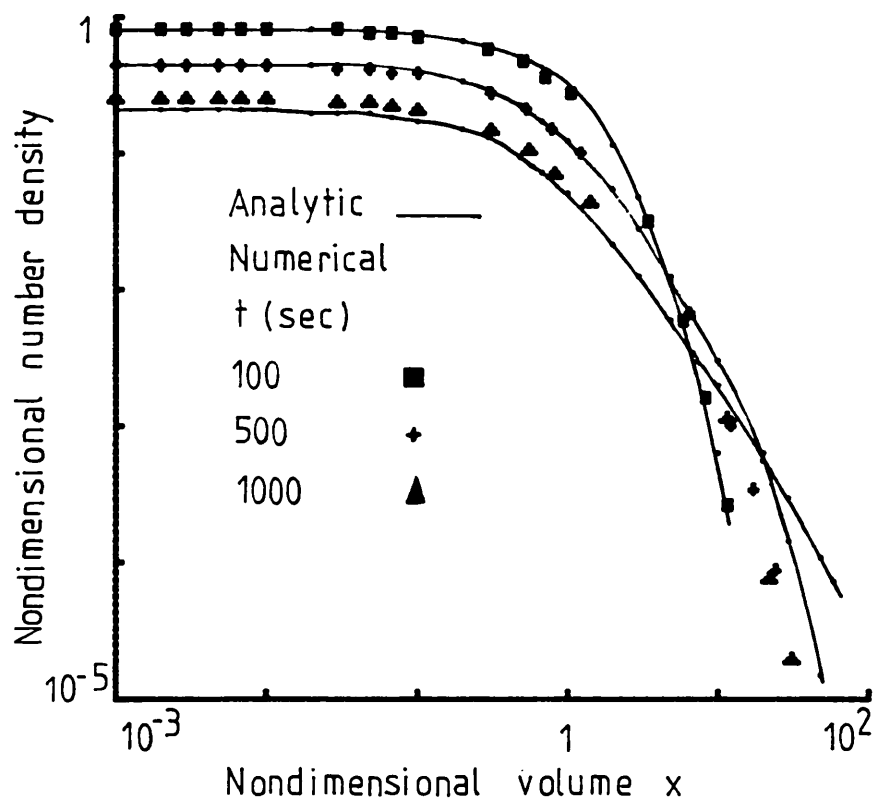


FIGURE 5.12 – The same as Fig. 5.11, but in log scaling, in order to emphasize the behaviour for larger particles.

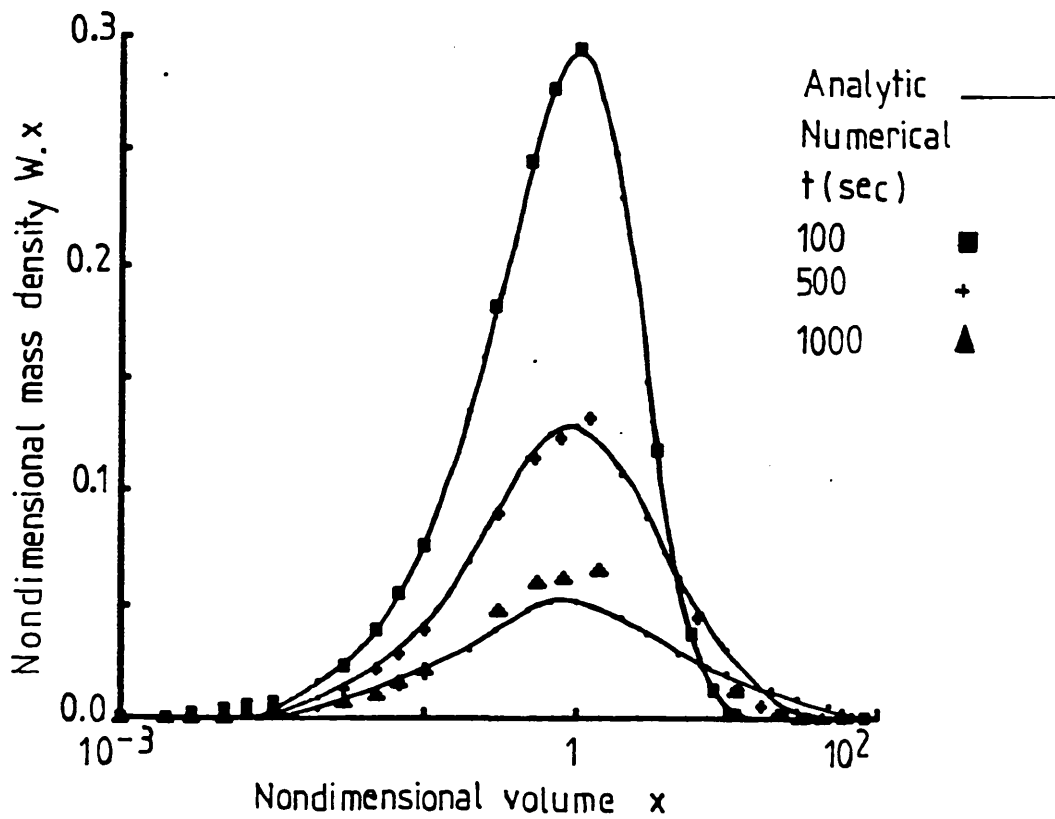


FIGURE 5.13 - Evolution of the nondimensional mass density as a function of the volume ratio $x = v/\bar{v}$, with time, for kernel proportional to the sum of the volumes and initial condition $s = 0$ in the equation (5.1). Comparison between the analytic solution [1] and the present model.

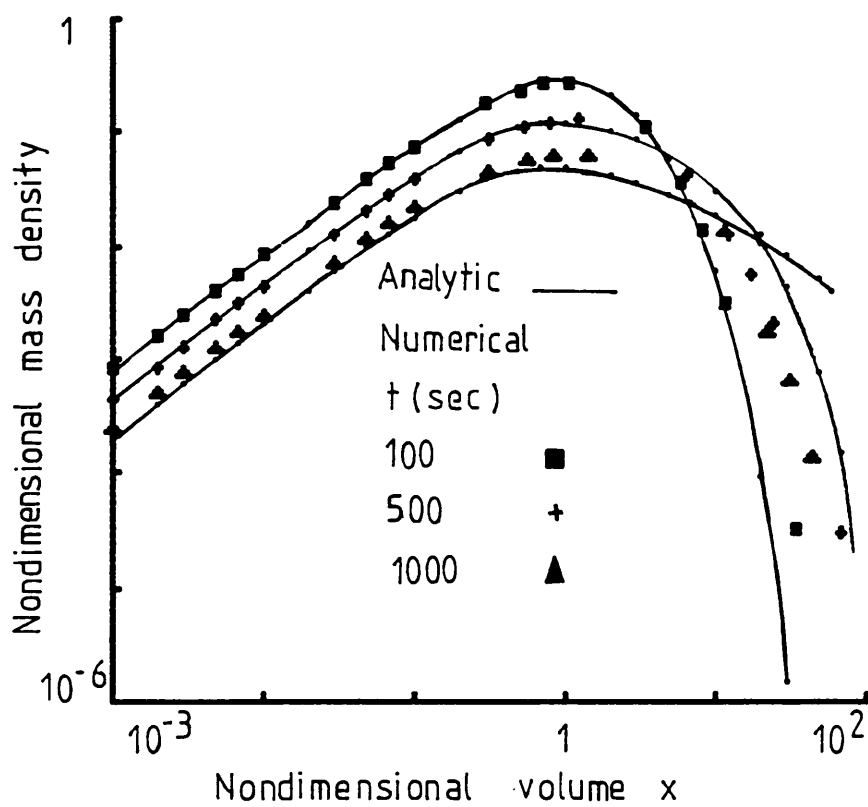


FIGURE 5.14 – The same as Fig. 5.13, but in log scaling, in order to emphasize the behaviour for larger particles.

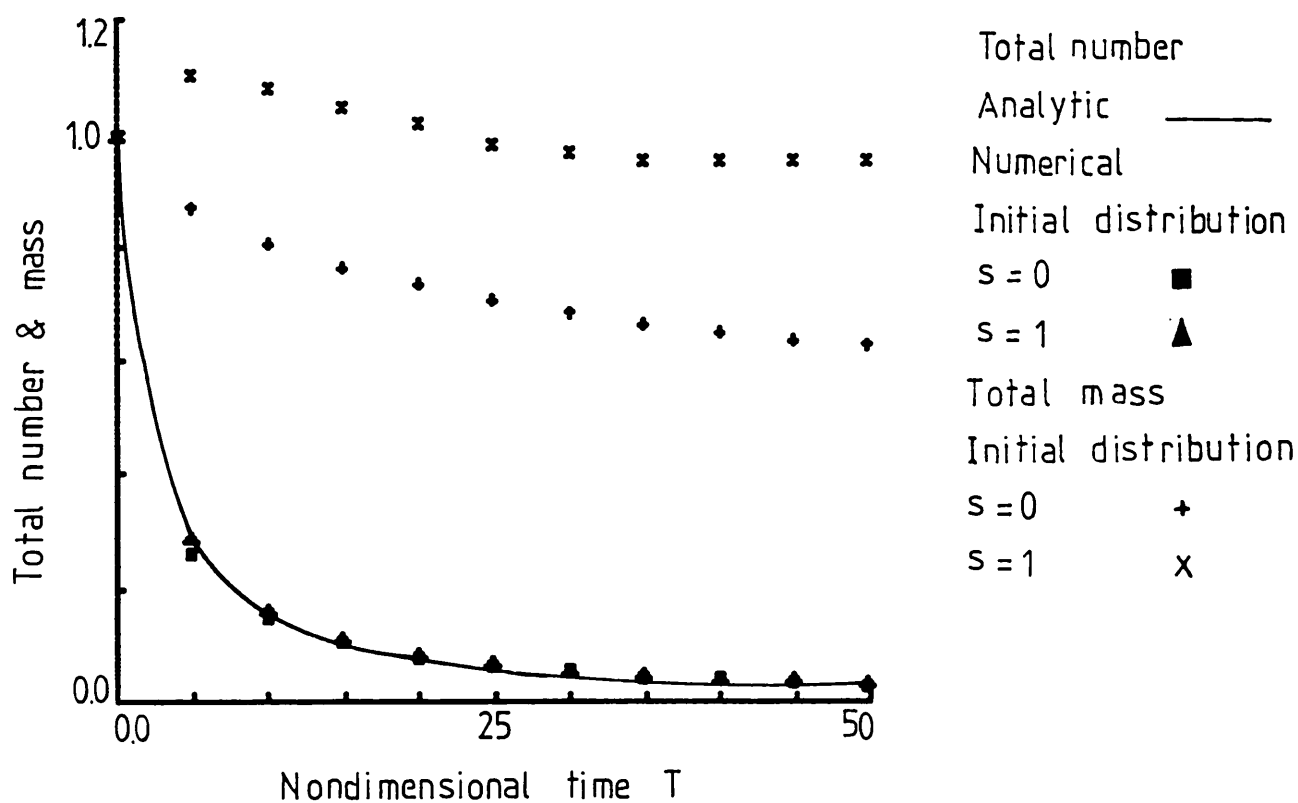


FIGURE 5.15 - Evolution of the nondimensional total number and mass concentration with time, for constant kernel and for both initial conditions, $s = 0$ and $s = 1$ in equation (5.1). Comparison between the analytic solution [1] and the present model.

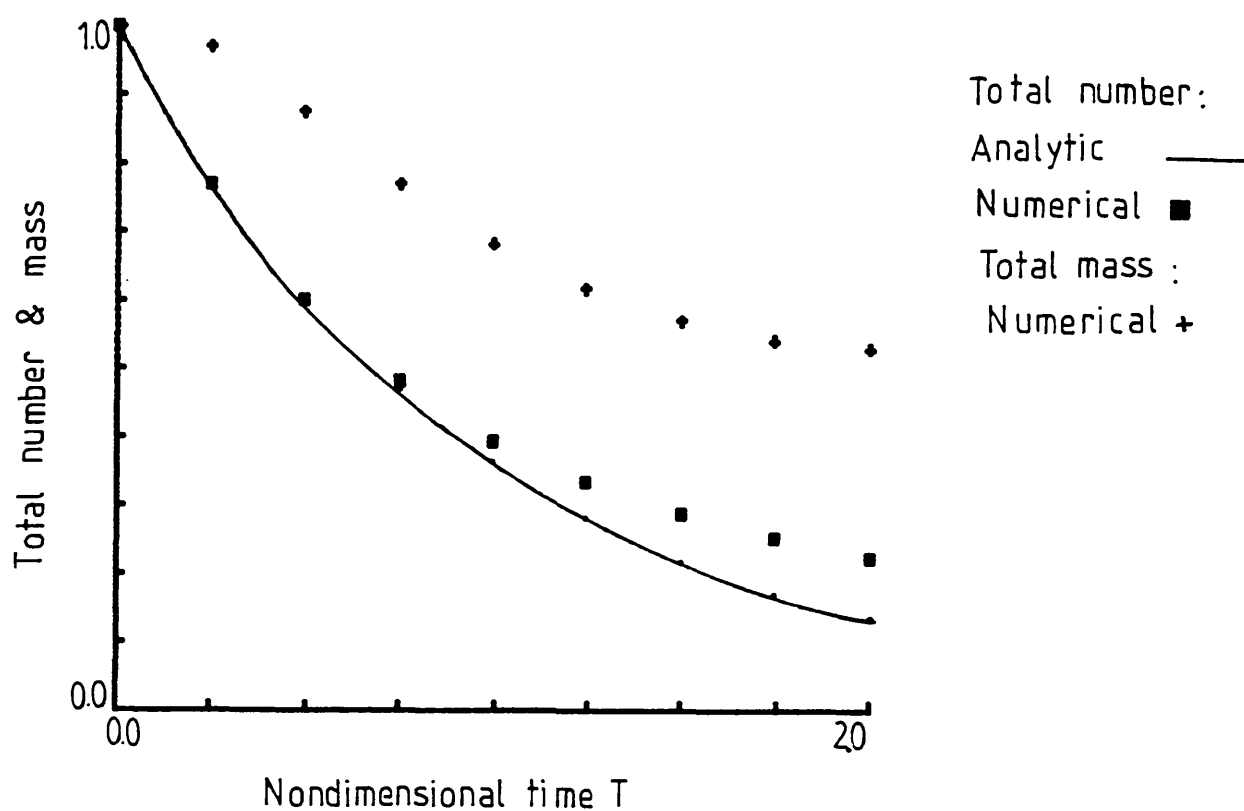


FIGURE 5.16 - Evolution of the nondimensional total number and mass concentration with time, for kernel proportional to the sum of the volumes and for $s = 0$ in equation (5.1). Comparison between the analytic solution [1] and the present model.

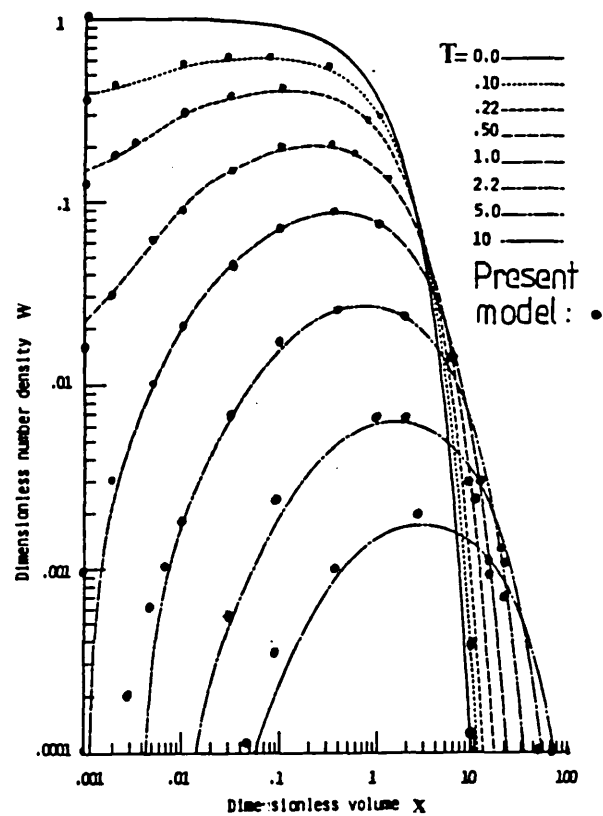


FIGURE 5.17 – Evolution of the nondimensional number density as a function of the volume ratio $x = v/\bar{v}$, for Brownian kernel and exponential initial condition ($s = 0$) with nondimensional time. Comparison between the results by the method in [6] and the present model.

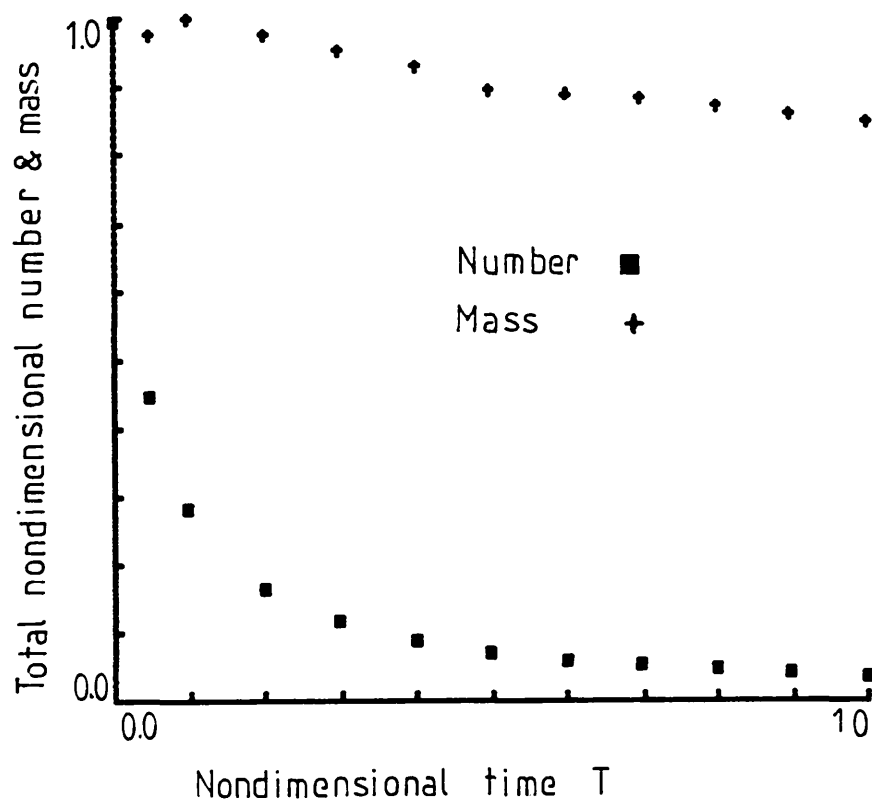


FIGURE 5.18 - Evolution of the nondimensional total number and mass concentration with nondimensional time, for Brownian kernel and $s = 0$.

CHAPTER 6

APPLICATION TO A GAS-PARTICLE FLOW

6.1 INTRODUCTION

Having previously demonstrated by means of the comparisons with test cases that our general model (and numerical formulation) is perfectly capable of dealing with the classic examples of coagulation, we now employ a modified version of it (the flux model), in order to predict the evolution of particles size distribution in a one-dimensional particle-gas flow in a passage, where coagulation is caused by the distinct relative particle velocities induced by the main gas flow - the linear kinetic coagulation.

6.2 THE LINEAR KINETIC COAGULATION AND TWO-PHASE FLOW MODELS

Of all coagulation mechanisms occurring in two-phase flows, the inertial effects, due to either a linear acceleration of the fluid or the curvature of the passage, is one of the least studied. It is frequently neglected, in most instances just to simplify assumptions. However, that particular coagulation mechanism might be of importance in many areas of engineering, such as performance prediction of solid-propellant rocket-motor nozzles, prediction of dry-out in boiler tubes, behaviour of filtration and separation systems, etc.

The solution of particle size and velocity distributions in dense gas-

particle flow is difficult to predict using traditional methods, in which the discrete coagulation equation describes the rate of change of number concentration in each fixed-volume particle size class. Concentration will alter as a result of duct area and velocity changes as well as coagulation. Even the general coagulation equation, such as (2.1), is adequate only for the most simple collision mechanisms in which the mean motion (if any) of the continuous phase does not play a significant role. However, in more complex situations such as in accelerated fluid flows, in which the differing relative velocities developed between fluid and particles are the dominant factor in coagulation, an equation for the change in number concentration of particles of a given volume is not particularly helpful.

On the other hand, usual two-phase flow models, such as those in [1], [2], [3] and [4] for example, preclude coagulation as a matter of principle, since either particles which retain their identity or else a continuum phase are supposed to be immersed in the main phase flow (assumed continuum), and coagulating particles cannot fit into either picture well enough.

Therefore, researchers have resorted to simplified approaches, mainly of phenomenological character. Palatnik and Azhibekov [5] integrated the general coagulation equation (2.1) with pre- and post-corrections at each time step for concentration changes due to varying gas flux. Phillipov and Daskal [6] proposed a new continuous coagulation equation and applied it to one-dimensional high-pressure wet steam flow in nozzles representing turbine blade passages. Their equation gives the rate of change of the particle number flux (number of particles crossing unit area in unit time) with streamwise position and includes the possibility of rebounds

(collisions which do not result in coagulation). They claimed to have solved it using the method of characteristics, employing Normal initial distributions for mass and velocity; there is, however, little information about the solution in their paper. More recently, Williams [7] formulated a one-dimensional space-time model of an aerosol in arbitrary gas stream, and obtained an exact solution for the case when the removal term (additional term to take into account mass-nonconserving mechanisms such as sedimentation), coagulation kernel and velocity in his general equation (borrowed from Friedlander [8]) do not depend on particle size. Brock [9] described the evolution equations, including diffusion and thermophoresis terms, for the aerosol in a laminar coaxial jet, where the coagulation was produced by Brownian motion. The calculation of the coagulation was carried out by using cubic splines for the numerical quadratures and the interpolation evaluations.

6.3 THE FLUX MODEL

We are interested in obtaining a solution for the one-dimensional steady-state case when there are no removal terms, but both the coagulation kernel and the particle velocity do depend on particle volume. In addition, we take into account the variable cross-section of the passage. As there is no established set of equations for two-phase flows dealing with coagulating particles, we develop our equations from first principles, based on the pseudo-Lagrangian approach. Let us consider for a moment that discrete particle classes can be defined, such that each class is given by the initial particle volume, as before. Let us also assume that each class represents a component in a multiphase flow, as does the continuous gas phase. Bearing this in mind, we write the continuity equation for each

component of the mixture as a function of time t and generic point in space $\bar{x}$:

$$\partial c_i(t, \bar{x}) / \partial t + \nabla \cdot (c_i(t, \bar{x}) u_i(t, \bar{x})) = r_i(t, \bar{x}) , \quad (6.1)$$

$$\partial c_g(t, \bar{x}) / \partial t + \nabla \cdot (c_g(t, \bar{x}) u_g(t, \bar{x})) = 0 , \quad (6.2)$$

with

$$c_i(t, \bar{x}) = \rho_p N_i(t, \bar{x}) v_i(t, \bar{x}) , i = 1, \dots, p \quad (6.3)$$

where p is the number of classes, ρ_p is the particle density, assumed constant, c_i and c_g are the particle and gas concentrations (also called partial densities) respectively, that is the mass of species i (or g) per unit of total volume of mixture, N_i is the number concentration of particles belonging to the class i , i.e. the number of i -particles per unit of total volume of mixture, v_i represents their current volume, and r_i is the rate of mass production of i -particles per unit of total volume, by coagulation.

Because we assume no exchange of mass between particles and gas, we can express the total particle concentration as (functions of t and $\bar{x}$)

$$c_p = \sum_i c_i = \rho_p \sum_i N_i v_i , \quad (6.4)$$

and, since coagulation preserves mass, the total mass production of particles by coagulation is

$$\sum_i r_i = 0 . \quad (6.5)$$

Therefore, the gas concentration c_g turns out to be

$$c_g = \rho_g (1 - \sum_i N_i v_i) , \quad (6.6)$$

and the total concentration of the mixture is

$$c = c_p + c_g = c_p (1 - \rho_g/\rho_p) + \rho_g . \quad (6.7)$$

Here, we can notice the difference between the mass concentrations c_i , c_g , and the material densities ρ_p , ρ_g . Even assuming the latter as constants, from (6.7) we realize that the only way for the mixture to be incompressible is when $\rho_g = \rho_p$, i.e. the particles are neutrally buoyant. Although that is hardly our case, from (6.6) we conclude that if the volume

occupied by the particles is much smaller than the total volume of the mixture, then $c_g \equiv \rho_g$ and the gas phase can be considered as incompressible.

The particle mass fraction w_i , i.e. the mass of i -particles per unit mass of mixture, is written as

$$w_i = c_i / c \quad . \quad (6.8)$$

Consequently, from (6.4) and (6.7) the total particle mass fraction is

$$w_p = \sum_i c_i / (\sum_i c_i (1 - \rho_g / \rho_p) + \rho_g) \quad . \quad (6.9)$$

Now, assuming steady state and integrating (6.1) in the volume element $dV = A(z) dz$, where $A(z)$ represents the cross-section at the streamwise position z , we write

$$\int \nabla \cdot (\rho_p N_i v_i u_i) dV = \int r_i dV \quad . \quad (6.10)$$

After applying the Green's (or divergence) theorem [10] and assuming that all quantities are uniform along $A(z)$, we obtain

$$\rho_p (N_i(z + dz) v_i(z + dz) u_i(z + dz) A(z + dz) - \\ N_i(z) v_i(z) u_i(z) A(z)) = r_i(z) A(z) dz ,$$

or

$$dF_i(z)/dz = r_i A(z) , \quad (6.11)$$

and, similarly,

$$dF_g(z)/dz = 0 , \quad (6.12)$$

where $F_i = \rho_p N_i v_i u_i A(z)$ and $F_g = c_g u_g A(z)$ are the mass rate of i -particles and gas respectively, that is the mass of i -particles (or gas) that cross the section $A(z)$ per unit time.

From (6.12) we conclude that F_g is constant (as expected) or

$$c_g u_g A(z) = c_{g_o} U_o A_o , \quad (6.13)$$

where c_{g_0} is the initial gas mass concentration, U_0 is the initial gas velocity, and A_0 is the initial cross-section of the passage.

Let us define N_0 as the initial total particle number concentration as before, and $\bar{v}$ the initial mass average volume, such that, considering the particles initially in equilibrium with the gas,

$$N_0 \bar{v} = \sum_i N_i(0) v_i(0) . \quad (6.14)$$

Now, using (6.14) and (6.9) we obtain, after some simplification, that

$$N_0 \bar{v} = w_{p_0} (\rho_g/\rho_p) / \{1 - w_{p_0} (1 - \rho_g/\rho_p)\} , \quad (6.15)$$

where w_{p_0} is the initial particle mass fraction (possibly given). From (6.15), we realize that, even for relatively large w_{p_0} , $N_0 \bar{v}$ is still small. Summarizing, we say that either $\rho_g = \rho_p$ and the mixture is incompressible ($c = \rho_g$), or $(\rho_g/\rho_p) \ll 1$ and the gas phase is incompressible ($c_g \equiv \rho_g$). For example, for saturated steam at 30 bars, $\rho_g/\rho_p = 0.02$ [11]. Choosing $w_{p_0} = 0.1, 0.5$ and 0.9 , $N_0 \bar{v}$ turns out to be equal to 0.0022, 0.02 and 0.15, respectively.

Note that if ρ_g is not constant then

$$\rho_g(z) u_g(z) A(z) = \rho_g(0) U_0 A_0 , \quad (6.18)$$

and we need a thermodynamic relationship to determine ρ_g .

Before going any further, we allow the number of classes to go to infinity and work from now on with the continuous version of the previous equations. Therefore, if we employ the same reasoning as before, we arrive at the expression

$$\partial m^*(v_0, z) / \partial z = r^*(v_0, z) A(z) , \quad (6.19)$$

where $m^*(v_0, z) = \rho_p \int_{v_0}^{v_0 + dv_0} f^*(v_0, z) v u^*(v_0, z) A(z) dv_0$ is the mass rate density of particles whose initial volume was between v_0 and $v_0 + dv_0$, $f^*(v_0, z)$ and $u^*(v_0, z)$ is the corresponding number density and velocity. Observe that the equation (6.19) is not the same as

$$\partial m(v, z) / \partial z = r(v, z) A(z) , \quad (6.20)$$

where $m(v, z) = \rho_p \int_v^{v+dv} f(v, z) v u(v, z) A(z) dv$ is the mass rate density of particles whose volume is between v and $v+dv$. In this case, we can write for the rate of mass production of particles whose volume is $(v, v + dv)$:

$$r(v, t) = \rho_p v \left\{ - \int_0^\infty K(v, r; u(v, z), u(r, z)) f(v, z) f(r, z) dr + \right. \\ \left. + 1/2 \int_0^v K(v-r, r; u(v-r, z), u(r, z)) f(v-r, z) f(r, z) dz \right\} , \quad (6.21)$$

where $K(x,y;u(x),u(y))$ is the coagulation kernel depending on volumes and velocities of the particle pair, such as the hydrodynamical (or geometric) kernel we defined in Chapter 2, with unity collection efficiency:

$$K(x,y;u(x),u(y)) = \pi/4 (x^{1/3} + y^{1/3})^2 |u(x) - u(y)| (3/(4\pi))^{2/3}.$$

We already know that

$$\partial m^*(v_o, z)/\partial z = \partial m(v, z)/\partial z + (\partial m/\partial v) \partial v(v_o, z)/\partial z, \quad (6.22)$$

or

$$\partial m^*(v_o, z)/\partial z = \partial m(v, z)/\partial z + \rho_p (q(v, z) + v \partial q(v, z)/\partial v) \partial v(v_o, z)/\partial z, \quad (6.23)$$

where we defined $q(v, z) = f(v, z) u(v, z) A(z)$, the number rate density, and analogously, $q^*(v_o, z) = f^*(v_o, z) u^*(v_o, z) A(z)$. Thus using (6.19) and (6.20), (6.23) becomes

$$r^*(v_0, z) A(z) = r(v, z) A(z) + \rho_p (q(v, z) + v \partial q(v, z) / \partial v) (\partial v(v_0, z) / \partial z) , \quad (6.24)$$

resulting in

$$\rho_p \partial q^*(v_0, z) / \partial z = r(v, z) A(z) + \rho_p (\partial q(v, z) / \partial v) (\partial v(v_0, z) / \partial z) ,$$

or else, substituting (6.21) and $q(v, z)$

$$\begin{aligned} \partial q^*(v_0, z) / \partial z = 1/A(z) \{ & - \int_0^\infty K(v, r; u(v, z), u(r, z)) q(v, z) / u(v, z) \\ & q(r, z) / u(r, z) dr + \\ & 1/2 \int_0^v K(v-r, r; u(v-r, z), u(r, z)) q(v-r, z) / u(v-r, z) \\ & q(r, z) / u(r, z) dr \} + \\ & \partial q(v, z) / \partial v \partial v(v_0, z) / \partial z . \end{aligned} \quad (6.25)$$

Now, we assume as before that the volume increase for one particle of volume $v(v_0, z)$ is given by the collision-coagulation with all smaller particles than v . Therefore, we write that

$$\partial v(v_0, z)/\partial z = 1/A(z) \int_0^v K(v, r; u(v, z), u(r, z)) q(r, z)/u(r, z) r dr , \quad (6.26)$$

our rule for the volume increase.

The particle velocities are yet to be determined. In order to accomplish this we consider the exchange of momentum among the particles. Let us discuss first the case of discrete classes. From the balance of momentum, where, due to the difficulty of evaluating the proper expression, the momentum produced by coagulation is given approximately, but not very correctly, by $r_i \bar{u}_i$, we write

$$\partial c_i \bar{u}_i / \partial t + \nabla \cdot (c_i \bar{u}_i \bar{u}_i) = c_i \bar{D}_i + r_i \bar{u}_i , \quad (6.27)$$

where $\bar{u}_i$ is the vector velocity of the i -particles, $\bar{D}_i$ is the aerodynamic drag force on each i -particle, acting in the same direction as the relative velocity, and $\bar{u}_i \bar{u}_i$ is the dyadic product tensor [12]. It is clear from (6.27) that the local rate of momentum is given by the net flux of momentum in and out of the control volume, by the external forces and by the momentum produced by coagulation ($r_i \bar{u}_i$). We suppose also that there is no other external forces other than the drag per unit mass, and pressure gradients (if any) do not act on the drops.

In one-dimensional steady-state flow, (6.27) becomes

$$d(c_i u_i^2)/dz = c_i D_i + r_i u_i , \quad (6.28)$$

or, integrating on $dV = A(z) dz$, as before

$$d(c_i u_i^2 A(z))/dz = c_i D_i A(z) + r_i u_i A(z) . \quad (6.29)$$

Expanding terms and using the continuity equation (6.11) we get

$$du_i/dz = D_i/u_i . \quad (6.30)$$

Now, taking the limit to infinite classes gives us

$$\partial u(v,z)/\partial z = D(v,z)/u(v,z) . \quad (6.31)$$

In terms of v_o and z , we know that

$$\partial u^*(v_o,z)/\partial z = \partial u(v,z)/\partial z + (\partial u/\partial v) (\partial v(v_o,z)/\partial z) , \quad (6.32)$$

analogously to the expression (6.22), and therefore

$$\partial u^*(v_o, z)/\partial z = D(v, z)/u(v, z) + (\partial u/\partial v) (\partial v(v_o, z)/\partial z) . \quad (6.33)$$

As for the aerodynamic drag force $D(v, z)$, we employ a Stokes-like expression corrected for larger particle Reynolds number Re_p :

$$D(v, z) = 18\mu/(\rho_p d^2) (u_g(z) - u(v, z)) f , \quad (6.34)$$

where μ is the gas viscosity, assumed constant, and d is the diameter of a particle whose volume is v .

A good correlation for f (for Re_p up to 1000) is [13]:

$$f = 1 + 0.15 Re_p^{0.687} , \quad (6.35)$$

with

$$Re_p = \rho_g d/\mu |u_g(z) - u(v, z)| , \quad (6.36)$$

as the particle Reynolds number.

We have $q^*(v_o, z)$, $u^*(v_o, z)$, $v(v_o, z)$, $u_g(z)$ and $c_g(z)$ as unknowns and the highly nonlinear system of equations (6.6), (6.13),

(6.25), (6.26) and (6.33). If ρ_g is considered as constant, the unknowns could in principle be evaluated.

Let us proceed to the nondimensionalization of the variables. We realize that, because of the mass rate conservation, we can write

$$\int_0^{\infty} q(v,z) v \, dv = N_o \bar{v} U_o A_o , \quad (6.37)$$

that recast into a more convenient form becomes

$$\int_0^{\infty} Q(x,z) x \, dx = 1 , \quad (6.38)$$

where $Q(x,z)$ is defined as

$$Q(x,z) = \bar{v}/(N_o U_o A_o) q(v,z) . \quad (6.39)$$

Also, we define

$$U = u/U_o , \quad (6.40)$$

$$y = z/L , \quad (6.41)$$

$$x = v/\bar{v} = (d/\bar{d})^{1/3} , \quad (6.42)$$

such that we express the important equations into a nondimensionalized form:

$$\begin{aligned} \partial Q^*(x_o, y)/\partial y = B_1 \{ & - \int_0^\infty (x^{1/3} + s^{1/3})^2 |U(x, y) - U(s, y)| \\ & Q(x, y)/U(x, y) Q(s, y)/U(s, y) ds + \\ & 1/2 \int_0^x ((x-s)^{1/3} + s^{1/3})^2 |U(x-s, y) - U(s, y)| \\ & Q(x-s, y)/U(x-s, y) Q(s, y)/U(s, y) ds \} + \\ & (\partial Q/\partial x) (\partial x/\partial y) , \end{aligned} \quad (6.43)$$

$$\begin{aligned} \partial x(x_o, y)/\partial y = B_1 \int_0^x & (x^{1/3} + s^{1/3})^2 |U(x, y) - U(s, y)| \\ & Q(s, y)/U(s, y) s ds , \end{aligned} \quad (6.44)$$

$$\partial U^*(x_o, y)/\partial y = D^*(x, y)/U(x, y) + (\partial U/\partial x) (\partial x/\partial y) , \quad (6.45)$$

$$U_g(y) = A_o/A(y) , \quad (6.46)$$

$$c_g \equiv \rho_g \quad , \quad (6.47)$$

with

$$D^*(x,y) = B_2 (U_g(y) - U(x,y))/x^{2/3} f \quad , \quad (6.48)$$

$$B_1 = \pi/4 N_o \bar{d} L \quad , \quad (6.49)$$

$$B_2 = 18\mu L/(\rho_p \bar{d}^2 U_o) \quad , \quad (6.50)$$

where L represents the length of the passage.

Finally, let us define, as before, the nondimensional number concentration density $W(x,y)$ as

$$W(x,y) = (\bar{v}/N_o) f(v,z) \quad . \quad (6.55)$$

Also, by an earlier definition

$$q(v,z) = f(v,z) u(v,z) A(z) \quad ,$$

which, substituting entities by their nondimensional counterparts, becomes

$$(N_o U_o A_o/\bar{v}) Q = W (N_o/\bar{v}) U_o U A(z) \quad , \quad (6.56)$$

resulting, by eliminating redundant terms, in the expression

$$W(x,y) = Q(x,y)/U(x,y) (A_o/A(y)) \quad . \quad (6.57)$$

Now, as we consider c_g as constant, equation (6.13) becomes

$$A_o/A(y) = U_g \quad ,$$

and consequently

$$W(x,y) = Q(x,y) [U_g(y)/U(x,y)] \quad , \quad (6.58)$$

that is, the larger the particle velocity slip with relation to the gas velocity, the more significant is the distinction between number rate and number concentration.

6.4 THE NUMERICAL SOLUTION

We have used an approach analogous to the one described in Chapter 4, employing osculatory quadratic splines on finite elements for the representation of Q (nondimensional number rate density) and U (nondimensional particle velocity) and interpolations. The quadratures and the space integration schemes are also the same. Differences reside mainly in the number of equations of the system, $3p$ in this case, where p is the number of classes, for Q , U and x , and one equation more for the determination of $U_g(y)$.

6.5 THE CODE

Due both to the characteristics of modularity presented by the Pascal language, and the similarities to the general coagulation case studied in Chapter 4, much of the previous code there developed is maintained. It is interesting to remark that the entire code was written without the necessity of matrices (only one-dimensional vectors), thanks to the use of slicing (extraction of rows and/or columns from matrices) and local copying (redefinition of the same set of working variables along an ordered ensemble). The major changes were confined to the procedures that define and establish the system of equations and the kernel specification. The resulting code is not much larger than the previous one, although it takes

longer to execute (mainly because of the complexity of the kernel), and can be analysed in the Appendix B.

6.6 APPLICATION TO AN IDEALIZED PASSAGE

Ghassemi [14] has produced, by adjusting the coefficients of cubic polynomials, the one-dimensional equivalent cross-section of a typical passage between blades of an experimental high-pressure wet steam turbine. We have used his data, but not his equations. We gave preference to our general-purpose quadratic spline in order to simulate the cross-section as a function of the streamwise position, since with this procedure, we assure that the passage is kept as input data, being otherwise arbitrary. In the Figure 6.1 we reproduce Ghassemi's passage, in which most of Section B and all Section C present a constant cross-section, and in the Table II below, we list the data we have used as a basis for the spline calculations. We remark that attempts employing cubic spline have ended in bad fittings, no doubt due to the knee of the curve.

As for the initial conditions, the upper-limit distribution [15] was thought to be more realistic than other possible alternatives, because this distribution is characterized by a cut-off particle size, above which there the density is strictly zero, representing the largest stable particle under aerodynamic forces, without being torn apart. One particular form of the upper-limit number density function is

$$f(y) = C/(d_m^4 y^4 (1 - y)) \exp\{-[\ln(y/(1-y))]^2\} \quad , \quad (6.51)$$

$y = z/L$	A/A_0
0	1
0.1	0.8737601
0.2	0.6418367
0.3	0.4309371
0.4	0.3625261
0.5	0.3625261
0.6	0.3625261
0.7	0.3625261
0.8	0.3625261
0.9	0.3625261
1.0	0.3625261

TABLE II -
Nondimensional cross-
section A/A_0 , at
selected nondimensional
streamwise positions
along Ghassemi's
passage [14]

where C is a normalization constant, d_m is the cut-off particle diameter and $y = d/d_m$.

Equation (6.51), however, is not in a very convenient form for our purposes. In the Appendix A we show that we can recast (6.51) in terms of the average volume $\bar{v}$, and normalized such that the total mass rate is unity. The final expression for the nondimensional initial number rate density is

$$Q_0(x) = 1/(3 A^2 y^6 (1 - y)) \exp\{-[\ln(y/(1-y))]^2\} , \quad (6.52)$$

with

$$x = v/\bar{v} = A y^3 , \quad (6.53)$$

$$A = v_{\text{m}}/\bar{v} = 1 + 3e^{1/4} + 3e + e^{9/4} . \quad (6.54)$$

It should be noticed that by using (6.52), we avoid having to recalculate the distribution every time the maximum particle size is changed, making (6.52) extremely convenient even for other researchers.

6.7 RESULTS

We have chosen some initial data to be representative of a high-pressure wet steam turbine: an initial pressure of 30 bars, saturated vapour properties, the length of the passage of 4.635 cm, an initial gas velocity of 70 m/s (initially in equilibrium with all particles), maximum particle size for the initial distribution of 20 μm , a total particle mass fraction of 10%. With the help of equation (6.15), we obtain for the initial number concentration N_0 a value of order of 10^{13} particles per cubic meter.

All variables are dimensionless, unless stated otherwise. The number rate (Fig. 6.2) and mass rate (Fig. 6.3) densities, for both 10 and 20 classes of particles, and the gas velocity (Fig. 6.4) are depicted as functions of the streamwise position along the passage discussed earlier. Also represented is the particle velocity distribution as a function of volume (Figure 6.5) and diameter (Figures 6.6 and 6.7). Figure 6.8 shows the number concentration density, in terms of particle volume, while both the total number and mass rates are pictured in Figure 6.9. Finally, Figures 6.10 and 6.11 represent the behaviour for larger particles of the number rate and number concentration densities respectively.

6.8 DISCUSSION

We have assumed all particles initially in equilibrium with the gas, and made this fact our basis for nondimensionalization, just for the purpose of assuring that nondimensional number (concentration) densities could be used as initial conditions for the flux model. In the Fig. 6.4 such an equilibrium is represented by the horizontal axis. Owing to the changes in the cross-section of the passage (Fig. 6.1), the gas velocity rises sharply up to about a third of the passage length, stabilizing afterwards (Fig. 6.5). The velocity, relative to the gas, adopted by a class of particles, depends on its volume (or diameter), because the relaxation distance, which furnishes an idea about the ability of the particle to react to changes in the gas velocity, is given by the inverse of the inertia parameter B_2 in the equation (6.50), hence it is proportional to the square of diameter. It can be seen (Fig. 6.6) that particle diameters smaller than $\bar{d}$ imply very small relative velocities. In our case, that corresponds to diameters less than $7 \mu\text{m}$. On the side of the larger particles, much larger relative

velocities can be found. Significantly, there is very little coagulation among the smaller particles, attested by the almost vertical broken line in Fig. 6.6. Those particles, however, are collected by the larger ones, making them bigger, as shown by the broken line in Fig. 6.7. It is interesting to notice, by the way, that Figs. 6.6 and 6.7 (or even Fig. 6.5) represent actual examples of the scheme in the Figure 3.1. Coagulation between the larger particles does not seem to be very important (little difference in the relative velocities). Since even one coalescence between two large particles implies an enormous increase in mass (or volume), their number is bound to be small and collisions among them infrequent. Therefore, the system of particles divides itself into two natural groups of particles - projectiles (the smaller) and targets (the larger) - in such a way, that there is little point in discussing coalescence (and coalescence efficiency, for that matter) among particles belonging to the same group. In fact, we developed, prior to the work described in this Chapter, a two-class (projectiles and targets) model for coagulation in gas-particle flow. This provided useful experience of flux models and the appropriate choice of variables, but clearly could not represent real size distributions.

Figure 6.9 shows that, with the chosen conditions, a reasonable amount of coagulation can be expected. Unfortunately, there is no analytic data to compare with, although the excellent agreement in number rate density for 10 and 20 classes (Fig. 6.2), confirmed by the coincidence of values of total number rate for both number of classes (Fig. 6.9), demonstrates that the flux model is keeping the consistency of results previously shown by the static model (Chapter 3). The total mass rate, however, is not conserving throughout (Fig. 6.9), making us suspect added inaccuracies in

the spline representation of number rate and velocities. It should be recalled that the total mass rate is evaluated by integrating the product of number rate and volume, so that inaccuracies are, in some sense, added.

Changes in number rate, representative of coagulation, are, according to (6.43), proportional to N_0 , which in turn is a function of the particle mass-fraction (wetness fraction, for wet steam) through equation (6.15). $N_0 \bar{v}$ is proportional to the density ratio ρ_g/ρ_p . Therefore, for low pressures $N_0 \bar{v}$ is bound to be very small indeed. Any reasonable value for $\bar{v}$ will imply a small N_0 , and, consequently, very little coagulation (if any). For high pressures, decreasing the particle-mass fraction should produce a similar effect. For instance, let us suppose wet steam, pressure of 0.1 bar, 10% wetness fraction and average diameter $\bar{d}$ of $0.4 \mu\text{m}$. That data gives us a very reasonable N_0 of order of 10^{15} droplets/ m^3 . However, for the same initial velocity, the ratio between the low- and high-pressure inertia parameter B_2 is about 150, Knudsen number effects included [11]. For this reason, no attempt has been made to run the model for low-pressure wet steam (e.g. to examine the extent of any coagulation in the non-equilibrium flow downstream of a shock wave).

In common with most works, we have assumed collection (collision and coalescence) efficiency of unity. The importance of this parameter can be assessed as follows. Let suppose a constant collision efficiency of 30% (and unity coalescence efficiency). From the main equations (6.43) and (6.44), we notice that a constant collision efficiency is equivalent to a direct reduction in N_0 . In our case, that would correspond to a particle-mass fraction of 3.2%, i.e. 2/3 of the particle mass is unavailable for coagulation. According to analytical-empirical data by Davis [16], the maximum collision efficiency for a $30 \mu\text{m}$ water droplet in air is 50%,

corresponding to a pair 30–15 μm , while the maximum for 20 μm is 10%. In this sense, our results are certainly overestimating the rate of coagulation. Nevertheless, with very little change in the present equations, we would be able to take into account the collision efficiency, just by introducing into the kernel definition an efficiency function of the pair of particles. As for the coalescence efficiency, it is not that simple. Because a collision does not always result in coalescence, breakup integral terms must be included in the equations, inside which there are breakup kernels, whose importance has made them subject of research by many authors, from Ryley [17], studying large drop instability after coalescence in turbines, to Beard [18], developing an energy model to predict instability. Unfortunately, we feel that this absorbing theme is out of the scope of the present work.

6.9 CONCLUSION

The application of the pseudo-Lagrangian flux model to a steady state flow through a one-dimensional equivalent of a high-pressure wet steam turbine passage, assuming an upper-limit distribution as an initial condition, has produced results that, for 10 and 20 classes of particles, have shown encouraging consistency, although there are no analytic or other numerical data to compare with. In addition, we have concluded that in this velocity-related coagulation, only the largely unequally sized pairs of particles are relevant for coalescence.

In the following Chapter, we assess the whole work, discuss some consequences and applications, and propose possible developments.

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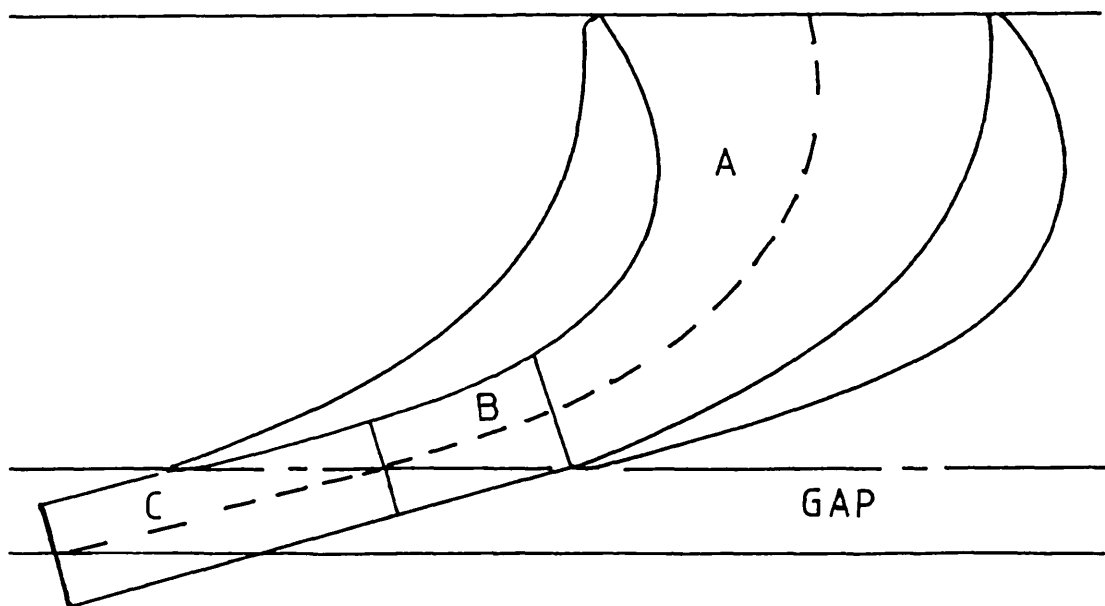


FIGURE 6.1 - Diagram (not to scale) representing the steam turbine blade passage, whose one-dimensional equivalent cross-section [14] has been used as input data for the flux model.

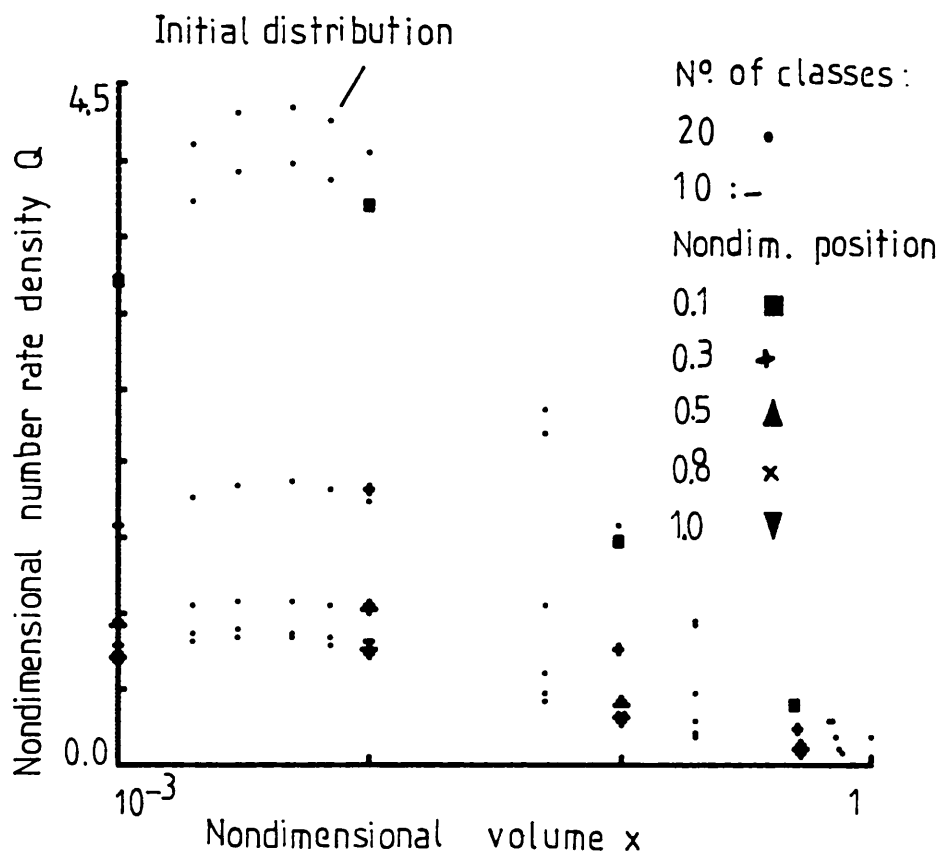


FIGURE 6.2 - Evolution of the nondimensional number rate density Q as a function of $x = v/\bar{v}$, with the nondimensional streamwise position along the passage [14] $y = z/L$, for the geometric kernel, and upper-limit density as initial condition. Comparison between the results for 10 and 20 classes of particles.

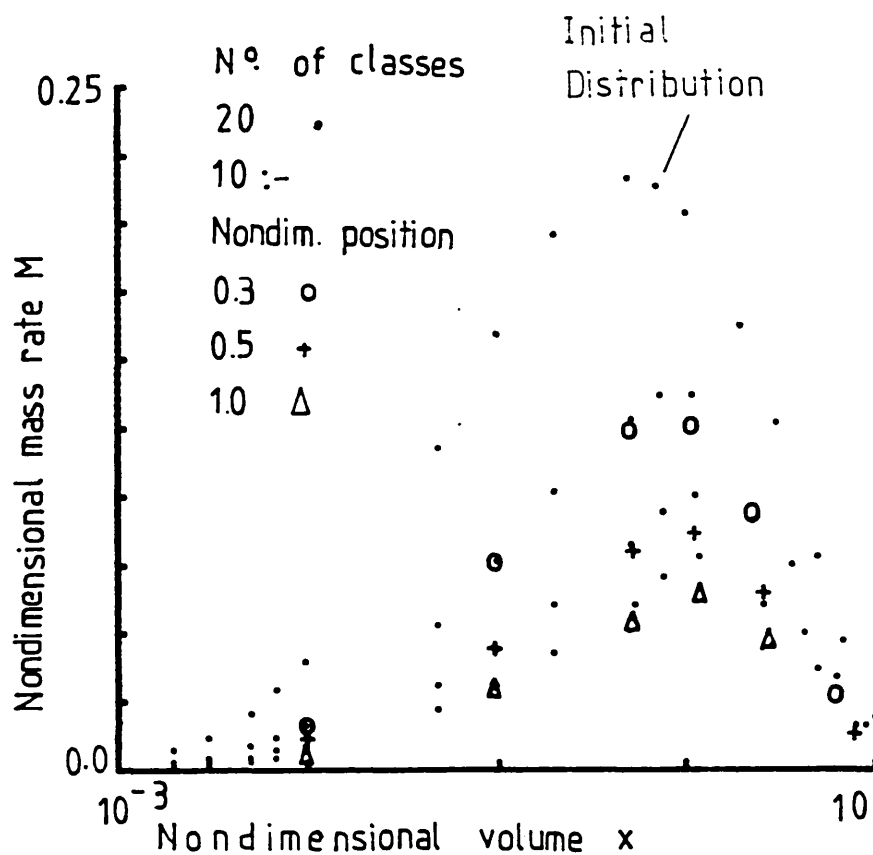


FIGURE 6.3 - Evolution of the nondimensional mass rate density M as a function of $x = v/\bar{v}$, with the nondimensional streamwise position along the passage [14] $y = z/L$, for the geometric kernel, and upper-limit density as initial condition. Comparison between the results for 10 and 20 classes of particles.

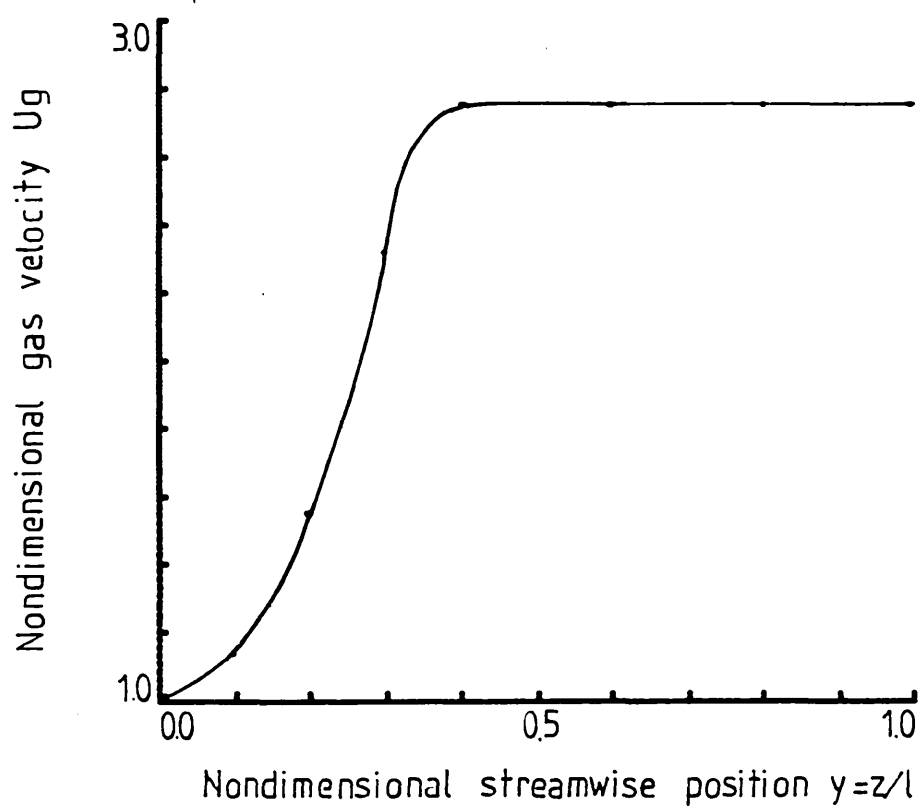


FIGURE 6.4 – Nondimensional gas velocity U_g as a function of the cross-section ratio A/A_0 at the nondimensional streamwise position y along the passage [14].

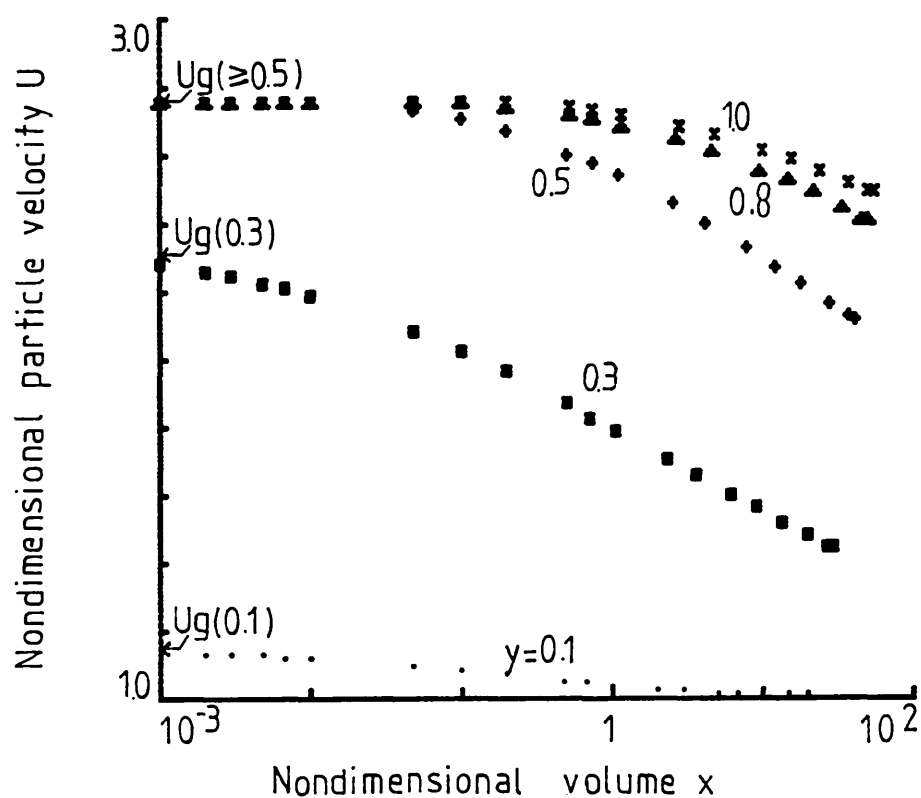


FIGURE 6.5 - Evolution of the nondimensional particle velocity distribution U as function of $x = v/\bar{v}$, with the nondimensional streamwise position along the passage [14] $y = z/L$, for the geometric kernel, and upper-limit density as initial condition.

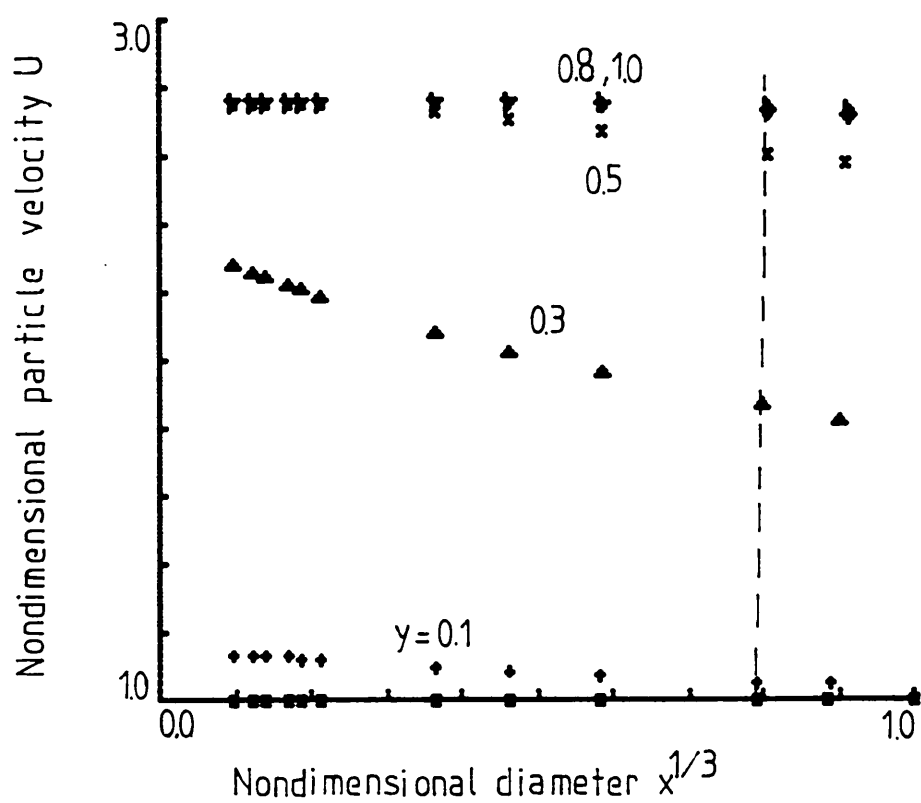


FIGURE 6.6 – The same as Fig. 6.5, but as a function of the linearly scaled nondimensional diameter $x^{1/3}$, which assumes values from 0 to 1.

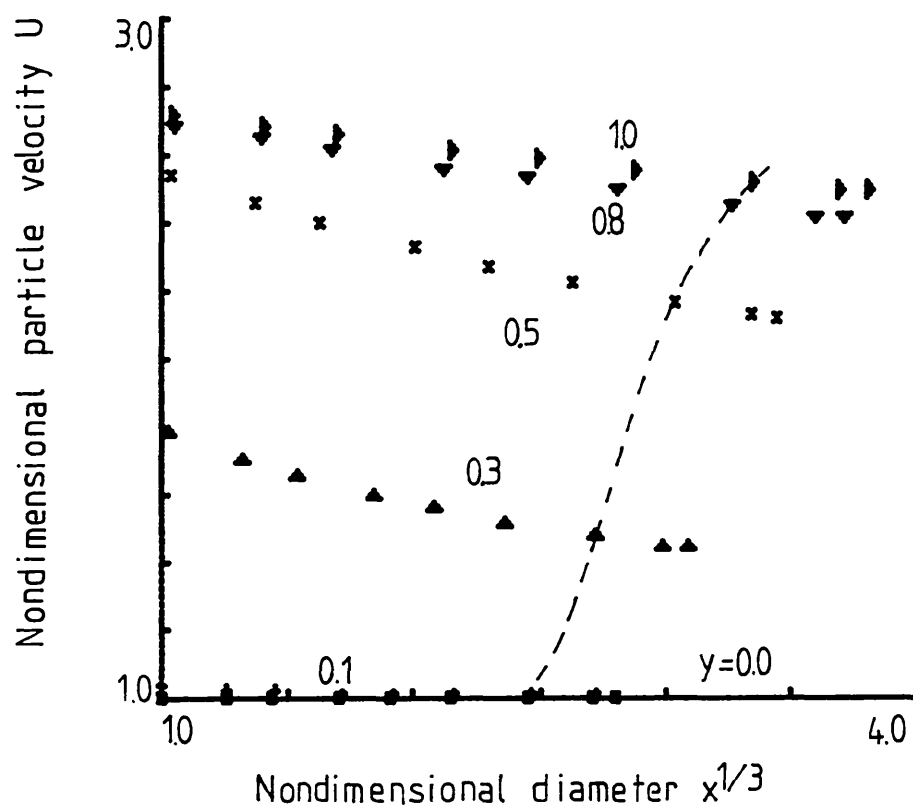


FIGURE 6.7 – The same as Fig. 6.5, but as a function of the linearly scaled nondimensional diameter x , which assumes values from 1 to 4.

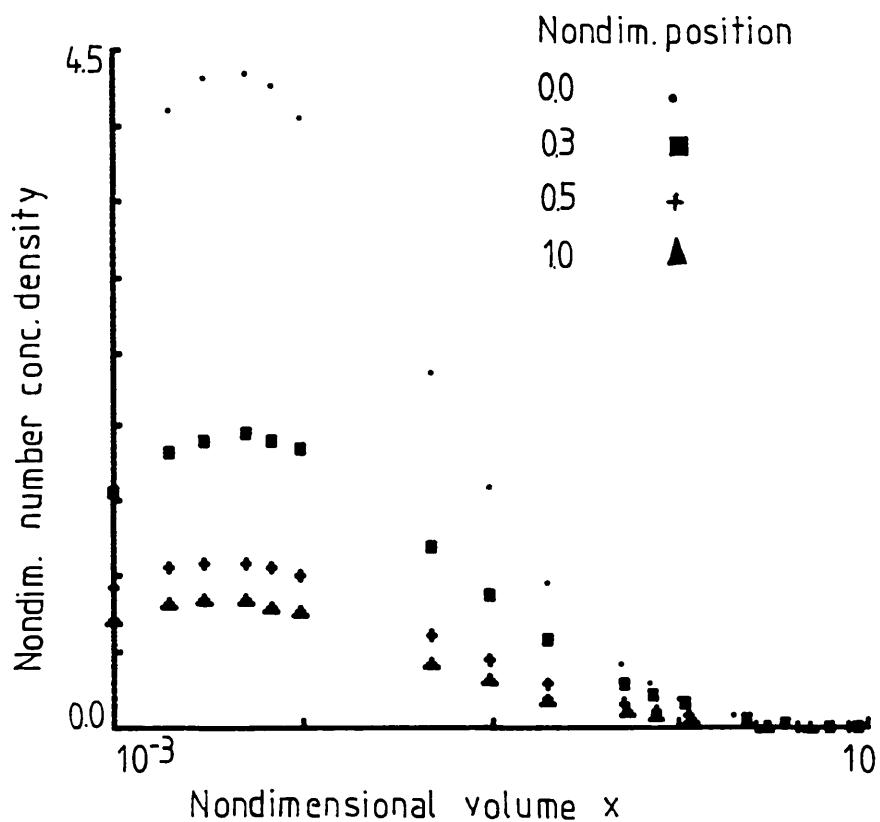


FIGURE 6.8 - Evolution of the nondimensional number concentration density W as a function of $x = v/\bar{v}$, with the nondimensional streamwise position along the passage [14] $y = z/L$, for the geometric kernel, and upper-limit density as initial condition.

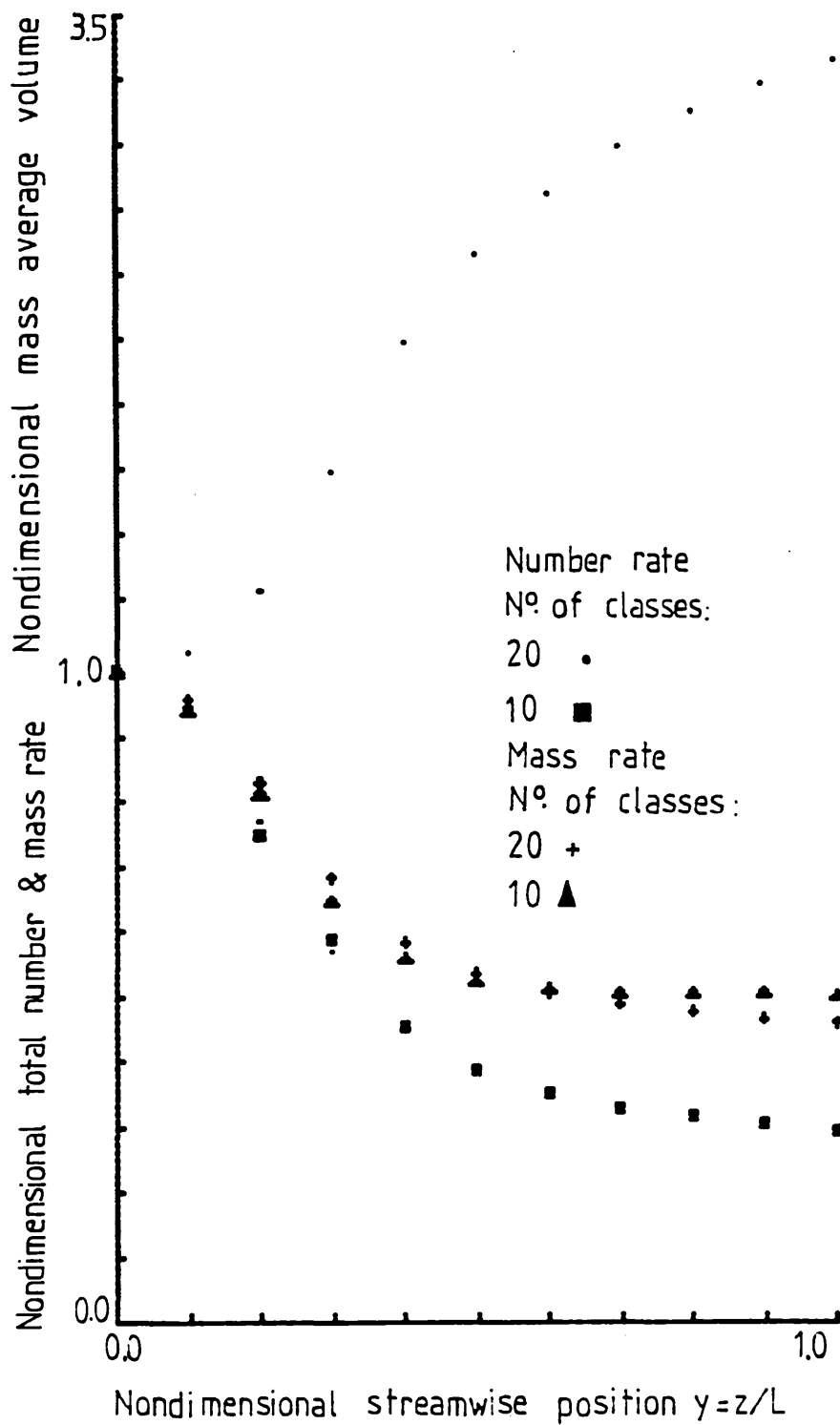


FIGURE 6.9 - Evolution of the nondimensional total number, mass rate and average volume along the nondimensional streamwise position $y = z/L$.

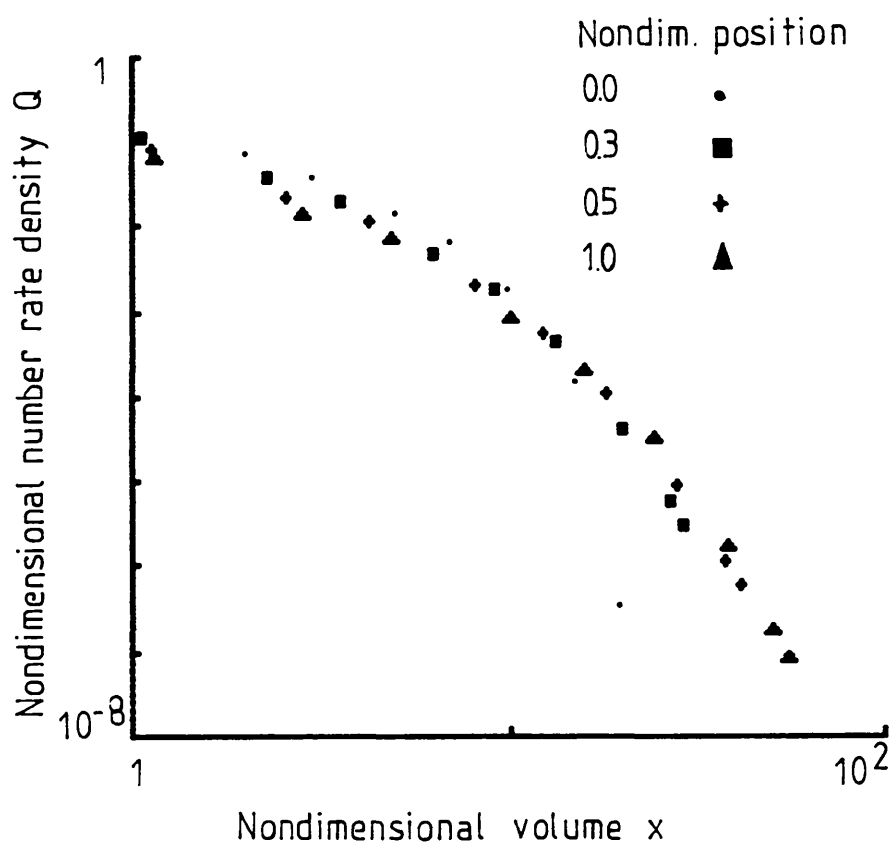


FIGURE 6.10 – The same as Fig. 6.1, but in log scaling in order to emphasize the behaviour for larger particles.

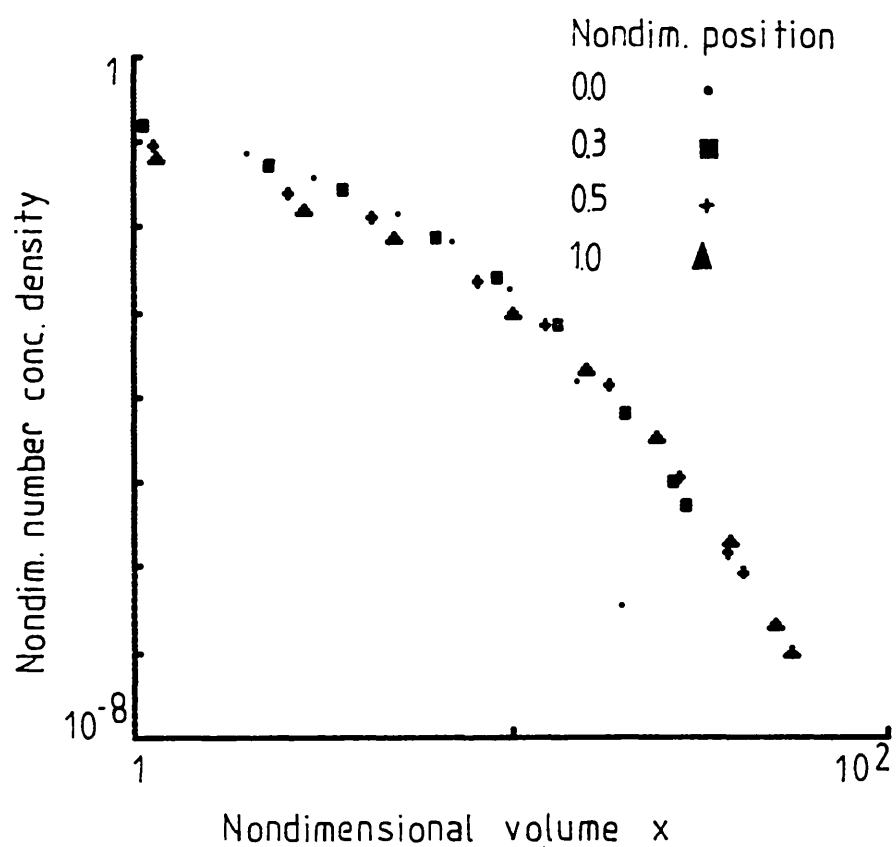


FIGURE 6.11 - The same as Fig. 6.8, but in log scaling in order to emphasize the behaviour for larger particles.

CHAPTER 7

GENERAL CONCLUSIONS AND RECOMENDATIONS FOR FUTURE WORK

7.1 ASSESMENT OF THE WORK

The aim of the present work has been to study inertia-related coagulation in particle-gas flows. Considering that a Lagrangian model for coagulation was better posed than Eulerian ones to deal with particle velocities, we were forced to develop our own general continuous pseudo-Lagrangian model since an earlier model by Sternin (see Chapter 2) has never been properly demonstrated. We have chosen a continuous formulation not only because the validity of the classic deterministic coagulation equation is conditioned to the large number of particles involved, but also because the coarse-graining process, necessary for the discrete version, makes the definition and allocation of mass in classes a rather arbitrary operation (Chapter 2). We have shown that it was possible to recover Sternin's model from ours, if certain terms were simply neglected. After obtaining a highly nonlinear partial integrodifferential system of equations (Chapter 3), our next natural step was to develop a numerical solution for it, analytic solutions ruled out due to the complexity of the equations and generality of the kernels. Therefore, we proposed a (nonoptimal) collocation method using splines in finite elements. We tried cubic splines at first, but soon found out that this kind of spline tend to oscillate around sharp corners, unless special provisions were made against it, such as controlling the

behaviour of the first derivatives using a Sobolev Norm. Thus, we decided on a very special spline - the quadratic osculatory, based on Bernstein polynomials, with special derivative properties. As for the time integration, we realized that coagulation was usually very fast at the beginning, slowing down afterwards, and, in consequence, developed a truncation-error controlled interval-adjusting scheme, based on the Runge-Kutta-Fehlberg integration procedure (Chapter 4). To test the model, we selected some classic analytic solutions and kernels and a comparison with another numerical method specially developed for Brownian coagulation and we found a good, and in the case of Brownian kernel, an outstanding agreement (Chapter 5). However favourable the comparisons, we were still unable to tackle gas-particle flows. Since there has not been available any consolidated theory for two-phase flow with coagulation, we developed from first principles what we called a flux model, a spatially one-dimensional set of equations, which included simple particle dynamics based on Stokes' drag, with corrections for larger values of Re_p . Finally, we applied the flux model to a one-dimensional flow along a high-pressure wet steam turbine blade passage, extracted from the literature. We have obtained highly consistent results for 10 and 20 classes of particles, suggesting a reduction in number flow rate by a factor of 3 on the basis of unit collision and coalescence efficiency, and showing the process to be dominated by collisions between droplet groups of widely-differing diameter. However, mass rate did not conserve as it should, revealing that the flux model was presenting some significant inaccuracies (Chapter 6).

7.2 THE CODES FOR THE MODELS

For reasons of cleanliness, modularity, better programming techniques and

data structures, we employed standard Pascal in order to write the computer programs, suitable for microcomputers, for both models. Thanks to special techniques, only one-dimensional vectors were defined throughout, in such a way that, besides modularity, we have achieved compactness and parallelism. Owing to that modularity and to the similarity of the systems of equations between both models, they share most of the code (Appendix B). Finally, we add that, for the present work, most of the output data was plotted in form of curves by employing our own graphics program (in Basic) and screen-dumped to a printer.

7.3 THE FLUX MODEL AND EXPERIMENTAL WORK

The results, for the case of the one-dimensional passage, considered in Chapter 6, have shown a significant amount of coagulation. It can be noticed also that even after the stabilization of the gas velocity (by the last two-thirds of the passage) the particles, due to their inertia, are still far from equilibrium, meaning that, even if coagulation is not considered, nonequilibrium two phase flow models such as ours, might become essential for a realistic representation of the phenomena involved. In order to test those models, experiments that are capable of not only measuring particle concentration, but also particle velocity must be designed. Although optically based techniques for measurement of particle size distribution have been available for some time, it is only recently that researchers have become interested in the simultaneous determination of particle velocities and concentration. One of those techniques is based on the comparison of phases of multiple Doppler signals from detectors located at different positions in space [1], and another, on a two-colour visibility technique [2], although both would probably be unsuitable for

the high concentrations necessary to obtain significant coagulation, since at those levels of concentration, secondary effects, such as multiple scattering, might invalidate the outcome.

7.4 APPLICATIONS OF THE FLUX MODEL AND FUTURE WORK

In its present one-dimensional form, the flux model could be useful for predictions of particle coagulation in solid-fuel rocket nozzles [3], venturis for measurements in two-phase flows [4] and for scrubbers [5] used in gas cleaning, in combustors [6], turbines [7] and pneumatic conveyors [8], for instance, although within highly idealized representations of reality. Nevertheless, it is not difficult to devise extensions to the basic model: a two-dimensional model, incorporating function of position, angle of collision and centrifugal forces, to predict inertial coagulation and spatial inhomogeneities in curved passages, or a model incorporating collection efficiency, breakup terms, evaporation and condensation, to nominate just some of the possibilities. Besides that, the numerical method could perhaps be improved, by employing cubic (instead of quadratic) Bernstein polynomials, and sped up, by introducing a better search procedure, necessary for the interpolations. We can even foresee a much-improved flux model as part of a larger package capable of dealing with nonequilibrium two-phase flows, with or without coagulation.

7.5 REFERENCES

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A P P E N D I X A

A GENERALIZED NONDIMENSIONAL UPPER-LIMIT DENSITY FUNCTION

One particular form of the so-called Upper-Limit density function is the following:

$$f(d) = K d_m / [d^4 (d_m - d)] \exp\{-[\ln(d/(d_m - d))]^2\} , \quad (A.1)$$

where $f(d) dd$ represents the number of particles whose diameter is between d and $d + dd$, d_m is the cut-off diameter, above which the density is strictly zero, and K is a normalization constant.

Let us define

$$y = d/d_m = (v/v_m)^{1/3} , \quad (A.2)$$

and, conveniently

$$(1 - y)/y = e^z , \quad (A.3)$$

where v is the volume of a particle whose diameter is d .

Substituting (A.2) and (A.3) into (A.1) we get

$$f(y) = K/[d_m^4 y^4 (1 - y)] e^{-z^2} . \quad (A.4)$$

The total particle volume concentration is

$$V = \pi/6 \int_0^{d_m} d^3 f(d) dd = \pi/6 \int_0^1 d_m y^3 f(y) dy . \quad (A.5)$$

Substituting (A.4) into (A.5):

$$V = \pi K/6 \int_0^1 1/(y (1 - y)) e^{-z^2} dy . \quad (A.6)$$

In order to determine K as a function of V , we need to solve the integral.

The definition (A.3) has the properties

a) if $y \rightarrow 0$ then $z \rightarrow \infty$,

b) if $y \rightarrow 1$ then $z \rightarrow -\infty$,

$$c) -dy/y^2 = e^z dz . \quad (A.7)$$

Substituting (A.7) into (A.6), we write

$$V = \pi K/6 \int_{-\infty}^{\infty} e^{-z^2} dz . \quad (A.8)$$

But, from any Table of integrals (e.g. Mathematical Handbook, M. R. Spiegel, McGraw-Hill, 1968):

$$\int_{-\infty}^{\infty} e^{-(ax^2 + bx + c)} dx = \sqrt{\pi/a} e^{(b^2 - 4ac)/4a} . \quad (A.9)$$

Consequently

$$V = \pi/6 K \sqrt{\pi} . \quad (A.10)$$

Now, the total particle number concentration N_0 is given by

$$N_0 = \int_0^{d_m} f(d) dd = \int_0^1 d_m f(y) dy , \quad (A.11)$$

or, using (A.3) and (A.4):

$$N_O = K/d_m^3 \int_0^1 1/(y^4 (1 - y)) e^{-z^2} dy , \quad (A.12)$$

that is the same as

$$N_O = K/d_m^3 \int_{-\infty}^{\infty} (1 + e^z)^3 e^{-z^2} dz , \quad (A.13)$$

resulting in

$$N_O = K/d_m^3 \sqrt{\pi} A , \quad (A.15)$$

with

$$A = 1 + 3e^{1/4} + 3e + e^{9/4} . \quad (A.16)$$

Using (A.15) and (A.10), we find the all important relationship between the average volume $\bar{v}$ and the cut-off diameter d_m (or v_m):

$$\bar{v} = \pi/6 (d_m^3/A) = v_m/A , \quad (A.17)$$

and, additionally

$$x = A y^3 . \quad (A.18)$$

Now, according to our well-known (from Chapters 4 and 6) nondimensionalization principles

$$W(x) = (\bar{v}/N_o) f^*(v) . \quad (A.19)$$

We do not know $f^*(v)$ (the particle number density in terms of particle volume) yet, although we can write

$$N_o = \int_0^{v_m} f^*(v) dv = \int_0^{d_m} f(d) dd = \int_0^1 (3 \pi/6) d^2 f^*(d) dd . \quad (A.20)$$

Therefore

$$f^*(v) = 6/(3\pi) f(d)/d^2 , \quad (A.21)$$

or, substituting (A.4) into (A.21)

$$f^*(y) = (K/d_m^4) 6/(3\pi d_m^2) 1/(y^6 (1 - y)) e^{-z^2} . \quad (A.22)$$

We finally rewrite (A.19), with the help of (A.15), (A.17), (A.18) and (A.22):

$$W(x) = 1/(3\sqrt{\pi}A^2) 1/(y^6 (1 - y)) \exp\{-[\ln(y/(1 - y))]^2\} , \quad (A.24)$$

with

$$x = A y^3 .$$

It should be noticed that equation (A.24), along with (A.18), is a completely general nondimensional Upper-Limit density function that needs to be evaluated just once, regardless of the values of d_m , $\bar{v}$, N_o , etc. In addition, once d_m is given, $\bar{v}$ can be determined by means of the equation (A.17).

A P P E N D I X B

THE CODE FOR THE FLUX MODEL

B.1 TABLE OF FUNCTIONS

F	Function of gas and particle velocities and streamwise position: real.
FINDPOS	Finds the index corresponding to the interval adequate for interpolation: integer.
GASVEL	Gas velocity, as a function of the cross section at the current streamwise position: real.
INTEGRAL	Trapezoidal quadrature: real.
INTEGRAL2	Returns the integral over several intervals: real.
KERNEL	Defines the kernel as a function of the volumes and velocities: real.
POSITION	Returns the value interpolated by means of the spline: real.
POWER	Any real power of x, for real x: real.
PRINT	Returns true if the current streamwise position is a correct one for printout: boolean.

SIMPSON Three-point Simpson quadrature: real.

B.2 TABLE OF PROCEDURES

ENTERDATA Procedure composed of:

- READPART;
- Particle mass fraction (wetness fraction, for wet steam) and ratio of specific volume of particle material to that of gas.

READPART Procedure for the input of:

- Total number of classes of particles;
- Nondimensional volume, number concentration, and initial velocity for each class of particles;
- Maximum nondimensional streamwise distance, interval for printout, and maximum integration step.

ENTERTABLE Procedure for input of the nondimensional values of the cross-section as a function of the nondimensional streamwise position.

WRITEDATA Outputs data from ENTERDATA to the output file and screen.

WRITETABLE Outputs data from ENTERTABLE to the output file and screen.

ZRELATION The main procedure: Produces some variable initialization, updates the streamwise position, and controls most of the other procedures and functions.

DERIV Evaluates the derivatives for SPLINE.

SPLINE Evaluates the parameters necessary for the spline calculation.

UPDATEFD	Creates one vector composed of number rate, volume and velocity, for use of RUNGKFEL. After manipulation by RUNGKFEL, recovers an updated value for number rate, volume and velocity, ready for integration by INTEGRAL2, in order to determine the total number and mass rate.
PRINTOUT	Outputs, if authorized by PRINT, results to an output file and screen.
H	Generates blanks for printout.
RUNGKFEL	Controls the Runge-Kutta-Fehlberg scheme, with auto-adjusting integration step, and the six evaluations of KEVAL and GASVEL. Outputs the resulting vector to UPDATEFD, if the current position corresponds to the updated one, furnished by ZRELATION.
KEVAL	Buffer for NUMVOL.
NUMVOL	Controls the evaluation of derivatives, splines, interpolations and kernels, for the functions that define the system of equations in terms of number rate, volume and velocity.

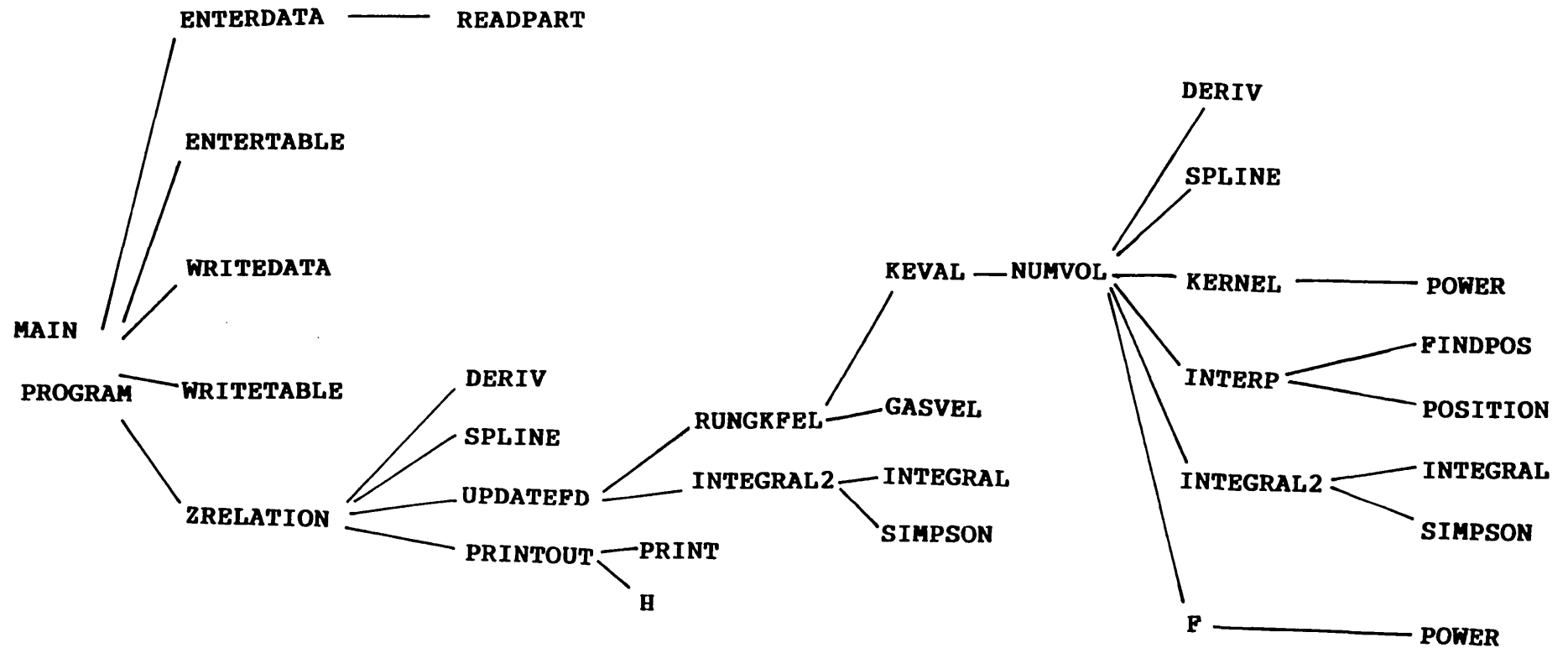


FIGURE B.1 - The map of procedure and function calls for the program PARTVEL (flux model).

B.3 PROGRAM PARTVEL(INPUT,OUTPUT)(* 10/12/87 *)

CONST AVDIAM=7.08495E-6;
L=4.6350E-2;

(* GAS PROPERTIES *)

VISCG=1.8E-5;
ROP=1E3;
U0=70;

PI=3.141592;
LN10=2.30258;
MAXPART=30;
TRIPLPART=90;
MAXPOINT=30;

TYPE PARTDIST=RECORD
NRATE,VOLUME,VELOC:REAL
END;

POINTNUM=1..MAXPOINT;

SPACETIME=RECORD
ZPRINT,ZFINAL,INTVAL:REAL
END;

PROP=RECORD
PMF,RVOL:REAL
END;

NPARTICL=ARRAY[1..MAXPART] OF PARTDIST;

CLASSNUM=1..MAXPART;

NPOINT=ARRAY[1..MAXPOINT] OF REAL;

SETDATA=RECORD
NUMBER:CLASSNUM;
PARTICLE:NPARTICL;

```

        SETUP:SPACETIME;
        MIXPROP:PROP
    END;

    SETTABLE=RECORD
        MAXX,MAXY:CLASSNUM;
        XDIAM,YDIAM:NPOINT;
    END;

    FOUR=1..4;

    NAME=STRING[13];

VAR    INFILE,OUTFILE,TABFILE1,TABFILE2:TEXT;

        INFILNAME,OUTFILNAME,TABNAME1,TABNAME2:NAME;

        DATA:SETDATA;

        TABLE,LIST:SETTABLE;

    (*.....*)

    FUNCTION CUBE(X:REAL):REAL;
    BEGIN
        CUBE:=SQR(X)*X;
    END;(* CUBE *)

    (*.....*)

    FUNCTION POWER(X:REAL;Y:REAL):REAL;
    BEGIN
        IF X<=0 THEN POWER:=0
        ELSE
            POWER:=EXP(Y*LN(X))
        END;(* POWER *)

    (*.....*)

    PROCEDURE DERIV(M:CLASSNUM;

```

```

        X,Y:NPOINT;
        VAR SLOPE:NPOINT);
VAR    I:INTEGER;
        S:NPOINT;

BEGIN
    FOR I:=2 TO M DO
        S[I]:=(Y[I]-Y[I-1])/(X[I]-X[I-1]);

    IF M>2 THEN
        BEGIN
            FOR I:=2 TO M-1 DO
                BEGIN
                    IF S[I]*S[I+1]<=0 THEN
                        SLOPE[I]:=0
                    ELSE
                        SLOPE[I]:=2*S[I]*S[I+1]/(S[I]+S[I+1]);
                END;(* FOR *)

            IF S[M-1]*S[M]<0 THEN
                SLOPE[M]:=2*S[M]
            ELSE
                SLOPE[M]:=2*S[M]-SLOPE[M-1];

            IF S[2]*S[3]<0 THEN
                SLOPE[1]:=2*S[2]
            ELSE
                SLOPE[1]:=2*S[2]-SLOPE[2];

            END(* IF M>2 *)
        ELSE
            BEGIN
                SLOPE[1]:=S[2];
                SLOPE[2]:=S[2];
            END;(* ELSE *)

        END;(* DERIV *)

    (*.....*)

```

```

PROCEDURE SPLINE(X1,X2,Y1,Y2,SLOPE1,SLOPE2:REAL;
                VAR P1,P2,P3,XINT:REAL);
VAR    TINT,TINT1,DLTX:REAL;

BEGIN
    DLTX:=ABS(X2-X1);
    TINT:=0.5;

    IF SLOPE1<>SLOPE2 THEN
        BEGIN
            TINT1:=((Y2-Y1)/DLTX-SLOPE2)/(SLOPE1-SLOPE2);
            IF (TINT1>0) AND (TINT1<1) THEN
                IF (TINT1<0.25) OR (TINT1>0.75) THEN
                    TINT:=TINT1;
            END;(* SLOPE1<>SLOPE2 *)

            XINT:=TINT*DLTX+X1;

            P1:=DLTX*SLOPE1*TINT/2+Y1;

            P2:=DLTX*SLOPE2*(TINT-1)/2+Y2;

            P3:=P1+TINT*(P2-P1);

        END;(* SPLINE *)

        (*.....*)

    FUNCTION INTEGRAL(X1,X2,F1,F2:REAL):REAL;
    BEGIN
        INTEGRAL:=(X2-X1)/2*(F1+F2);
    END;(* INTEGRAL *)

    (*.....*)

    FUNCTION SIMPSON(X1,X2,X3,F1,F2,F3:REAL):REAL;
    VAR    T:REAL;
    BEGIN
        T:=(X2-X1)/(X3-X1);

```

```

        SIMPSON:=(X3-X1)*((X3*T-1)*F1/T+F2/(T*(1-T))+(2-3*T)*F3/(1-T))/6;
END;(* SIMPSON *)

```

```

(*.....*)

```

```

FUNCTION POSITION(F1,P1,P3,T:REAL):REAL;
VAR      DLTT:REAL;

```

```

BEGIN

```

```

        POSITION:=F1+T*(2*(P1-F1)+T*(F1-2*P1+P3));

```

```

END;(* POSITION *)

```

```

(*.....*)

```

```

FUNCTION FINDPOS(N:CLASSNUM;VAR X:NPOINT;
                XGIVEN:REAL):CLASSNUM;

```

```

VAR      J:INTEGER;
        FOUND:BOOLEAN;

```

```

BEGIN

```

```

        J:=0;
        REPEAT

```

```

            J:=J+1;
            FOUND:=XGIVEN<=X[J];

```

```

        UNTIL
            FOUND OR (J=N);

```

```

        FINDPOS:=J;

```

```

        IF NOT FOUND THEN
            WRITE( 'NOT FOUND ' );

```

```

END;(* FINDPOS *)

```

```

(*.....*)

```

```

FUNCTION INTERP(M:CLASSNUM; X,F,PN1,PN2,PN3,XN:NPOINT;
                XGIVEN:REAL):REAL;

```

```

VAR    PS:CLASSNUM;
        T:REAL;
BEGIN
    PS:=FINDPOS(M,X,XGIVEN);

    IF XGIVEN<XN[PS-1] THEN
    BEGIN
        T:=(XGIVEN-X[PS-1])/(XN[PS-1]-X[PS-1]);

        INTERP:=POSITION(F[PS-1],PN1[PS-1],PN3[PS-1],T);

    END
    ELSE
    BEGIN
        T:=(XGIVEN-XN[PS-1])/(X[PS]-XN[PS-1]);

        INTERP:=POSITION(PN3[PS-1],PN2[PS-1],F[PS],T);

    END;

```

```

END;(* POSITION *)

```

```

(*.....*)

```

```

FUNCTION GASVEL(Q:CLASSNUM;XZ,S,PZ1,PZ2,PZ3,XINTZ:NPOINT;
                ZGIVEN:REAL):REAL;

```

```

VAR    TPZ:REAL;

```

```

BEGIN

```

```

    TPZ:=INTERP(Q,XZ,S,PZ1,PZ2,PZ3,XINTZ,ZGIVEN);

```

```

    GASVEL:=1/TPZ;

```

```

END;(* GASVEL *)

```

```

(*.....*)

```

```

FUNCTION KERNEL(X,Y,UX,UY:REAL):REAL;

```

```

BEGIN

```

```

    IF (X<>0) AND (Y<>0) AND (UX<>0) AND (UY<>0) THEN

```

```

        KERNEL:=SQR(POWER(X,1/3)+POWER(Y,1/3))*ABS(UY-UX)/(UX*UY)

```

```

    ELSE

```

```

                                KERNEL:=0;
END; (* KERNEL *)

(*.....*)

PROCEDURE ZRELATION(DATA:SETDATA;TABLE:SETTABLE);

TYPE    VOVELRATE=ARRAY[1..TRIPLPART] OF REAL;

VAR      NINP,NINT:INTEGER;
          INTV,Z,IZ,VG,REALCON,CURRATE,MASSRATE,COEF1,COEF2,COEF3:REAL;
          INRATE,INMASRATE:REAL;
          S:CLASSNUM;
          ERR:VOVELRATE;
          SLOPEZ,PZ1,PZ2,PZ3,XINTZ,INIX,LNINIX:NPOINT;

          FIRSTPASS,SUCCESS:BOOLEAN;

(*.....*)

FUNCTION F(COEF1,COEF2,R,V,VG:REAL):REAL;
VAR      D,REY:REAL;

BEGIN
  IF R>0 THEN
    D:=POWER(R,1/3)
  ELSE
    D:=0;

  REY:=COEF2*D*ABS(VG-V);

  IF (V<>0) AND (D<>0) THEN
    IF REY>0 THEN
      F:=COEF1/(D*D*V)*(1+0.15*POWER(REY,0.687))*(VG-V)
    ELSE
      F:=COEF1/(D*D*V)*(VG-V)
    ELSE
      F:=0;
END; (* F *)

```

```

(*.....*)

FUNCTION INTEGRAL2(B:INTEGER;X,F:NPOINT):REAL;
VAR    J,K,W:INTEGER;
        QUAD:REAL;
        ENDEVEN:BOOLEAN;

BEGIN
    QUAD:=0;
    ENDEVEN:=B MOD 2=0;

    IF ENDEVEN THEN
    BEGIN
        QUAD:=INTEGRAL(X[B-1],X[B],F[B-1],F[B]);
        K:=TRUNC(B/2)-1;
    END
    ELSE
        K:=TRUNC((B-1)/2);

    FOR J:=1 TO K DO
    BEGIN
        W:=2*J-1;
        QUAD:=QUAD+SIMPSON(X[W],X[W+1],X[W+2],
            F[W],F[W+1],F[W+2]);
    END;(* FOR J *)

    INTEGRAL2:=QUAD;
END;(* INTEGRAL2 *)

(*.....*)

PROCEDURE NUMVOL(M:CLASSNUM;
    Z,VG:REAL;
    INIX:NPOINT;
    VAR Y:VOVELRATE;
    VAR G:VOVELRATE);

```

```

VAR    R,V,T,PN1,PN2,PN3,XN:NPOINT;
        SLOPEV,SLOPER,SLOPEX,PV1,PV2,PV3,XV:NPOINT;
        T1,T2,T3,T4:NPOINT;
        I,J,S:INTEGER;
        DLTR,TPS,TPV,SUM1,SUM2,SUM3,SUM4:REAL;
        NOINTERP:BOOLEAN;

BEGIN
    FOR I:=1 TO M DO
    BEGIN
        V[I]:=Y[2*M+I];
        R[I]:=Y[M+I];
        T[I]:=Y[I];
    END; (* FOR I *)

    DERIV(M,INIX,R,SLOPEX);

    DERIV(M,R,T,SLOPER);

    DERIV(M,R,V,SLOPEV);

    FOR J:=1 TO M-1 DO
    BEGIN
        SPLINE(R[J],R[J+1],T[J],T[J+1],

                SLOPER[J],SLOPER[J+1],PN1[J],PN2[J],PN3[J],XN[J]);

        SPLINE(R[J],R[J+1],V[J],V[J+1],
                SLOPEV[J],SLOPEV[J+1],PV1[J],PV2[J],PV3[J],XV[J]);

    END; (* FOR J *)

    FOR I:=1 TO M DO
    BEGIN
        SUM1:=0;SUM2:=0;SUM3:=0;SUM4:=0;

        FOR J:=1 TO M DO
        BEGIN
            T1[J]:=0;T2[J]:=0;T3[J]:=0;T4[J]:=0;

```

```

IF (J<>I) THEN
    T1[J]:=KERNEL(R[I],R[J],V[I],V[J])*T[J]*SLOPEX[J];

IF (J<I) THEN
BEGIN
    T2[J]:=T1[J]*R[J];

    T4[J]:=(V[J]-V[I])*T2[J];

    DLTR:=R[I]-R[J];

    NOINTERP:=DLTR>=0.99999*R[I];

    IF NOT NOINTERP THEN
    BEGIN
        IF (DLTR<=R[1]) AND (R[1]<>0) THEN
        BEGIN
            TPS:=DLTR*T[1]/R[1];
            TPV:=V[1]-SLOPEV[1]*(R[1]-DLTR);
        END(* DLTR<=R[1] *)
        ELSE
            IF (DLTR>=R[M]) THEN
            BEGIN
                TPS:=T[M]+SLOPER[M]*(DLTR-R[M]);
                TPV:=V[M]+SLOPEV[M]*(DLTR-R[M]);
            END(* DLTR>=R[M] *)
            ELSE
            BEGIN
                TPS:=INTERP(M,R,T,PN1,
                    PN2,PN3,XN,DLTR);
                TPV:=INTERP(M,R,V,PV1,
                    PV2,PV3,XV,DLTR);
            END(* IF DLTR>R[1] AND <R[M] *)

            T3[J]:=KERNEL(DLTR,R[J],TPV,V[J])*TPS*T[J]*SLOPEX[J];

        END(* INTERP *)
    ELSE
        T3[J]:=T1[J]*T[I];
    
```



```

        UNTIL N=0
END;(* H *)

(*.....*)

PROCEDURE PRINTOUT(VAR OUTFILE:TEXT;S,M,NDELP:POINTNUM;
                   ERR:VOVELRATE;PATICLE:NPARTICL;
                   I,Z,VG,CURRATE,MASSRATE:REAL);

VAR    DIAM:REAL;

BEGIN
    IF PRINT(NDELP,I) THEN
        BEGIN
            IF S=1 THEN
                BEGIN
                    WRITELN(OUTFILE);
                    WRITE(OUTFILE,'Z=',Z:6:3,' NRATE');H(OUTFILE,7);
                    WRITE(OUTFILE,'NERR');H(OUTFILE,6);
                    WRITE(OUTFILE,'NCONC');H(OUTFILE,7);
                    WRITE(OUTFILE,'VELOC');H(OUTFILE,6);
                    WRITE(OUTFILE,'VERR');H(OUTFILE,9);
                    WRITE(OUTFILE,'VRATIO');H(OUTFILE,6);
                    WRITE(OUTFILE,'XERR');H(OUTFILE,6);
                    WRITELN(OUTFILE,'MRATE');
                END;(* S=1 *)
            WITH PARTICLE[S] DO
                BEGIN
                    WRITE(OUTFILE,'P',S:3,NRATE);
                    WRITE(OUTFILE,ERR[S]);
                    WRITE(OUTFILE,NRATE*VG/VELOC);
                    WRITE(OUTFILE,VELOC);
                    WRITE(OUTFILE,ERR[2*M+S]);
                    WRITE(OUTFILE,VOLUME);
                    WRITE(OUTFILE,ERR[M+S]);
                    WRITE(OUTFILE,NRATE*VOLUME);
                    IF S=M THEN
                        BEGIN
                            (*      WRITELN(CURRATE,' ',MASSRATE;      *)

```

```

WRITE(OUTFILE,'  GAS VELOCITY = ',VG);
WRITE(OUTFILE,'  TOTAL NRATE = ',CURRATE);
WRITELN(OUTFILE,'  TOTAL MASSRATE = ',MASSRATE);
WRITELN(OUTFILE);

      END;
END;(* WITH *)

      END;(* IF *)
END;(* PRINTOUT *)

(*.....*)

PROCEDURE KEVAL(M:CLASSNUM;Z,VG:REAL;
               INIX:NPOINT;
               VAR Y:VOVELRATE;VAR K:VOVELRATE);

VAR      G:VOVELRATE;

BEGIN

      NUMVOL(M,Z,VG,INIX,Y,G);

      K:=G;
END;(* KEVAL *)

(*.....*)

PROCEDURE RUNGFEL(M,Q:CLASSNUM;Z,INIV:REAL;VAR VG,LASTINT:REAL;
                 XDIAM,YDIAM,PZ1,PZ2,PZ3,XINTZ,INIX:NPOINT;
                 VAR ERR,Y:VOVELRATE;VAR SUCCESS:BOOLEAN);

CONST      ASSUMEDZERO=1E-20;
           TOL=1E-8;

VAR      J,TM:INTEGER;
           COUNT:INTEGER;
           K1,K2,K3,K4,K5,K6,Y1,Y2:VOVELRATE;
           TOLERR,MAXERR,AVERR,X,MININIV,INIV1,Z1,Z2,ZS,VGS,VG2:REAL;
           STATE:(STEPPING,REACHED,INTSMALL);

```

```

SHORTRANGE:BOOLEAN;

BEGIN
  TM=3*M;
  X:=0;
  STATE:=STEPPING;
  SHORTRANGE:=FALSE;
  MININTV:=INTV/1024;
  INTV1:=INTV;
  TOLERR:=TOL*SQR(INTV1);

  COUNT:=1;

  Y1:=1;
  Z1:=Z;

  REPEAT
    MAXERR:=0;
    AVERR:=0;

    KEVAL(M,Z1,VG,INIX,Y1,K1);

    FOR J:=1 TO TM DO
      Y2[J]:=Y1[J]+INTV*K1[J]/4;

    Z2:=Z1+INTV/4;
    VG2:=GASVEL(Q,XDIAM,YDIAM,PZ1,PZ2,PZ3,XINTZ,Z2);
    KEVAL(M,Z2,VG2,INIX,Y2,K2);

    FOR J:=1 TO TM DO
      Y2[J]:=Y1[J]+INTV*(3*K1[J]+9*K2[J])/32;

    Z2:=Z1+3*INTV/8;
    VG2:=GASVEL(Q,XDIAM,YDIAM,PZ1,PZ2,PZ3,XINTZ,Z2);
    KEVAL(M,Z2,VG2,INIX,Y2,K3);

    FOR J:=1 TO TM DO
      Y2[J]:=Y1[J]+INTV*(1932*K1[J]-7200*K2[J]+7296*K3[J])/2197;

```

```

Z2:=Z1+12*INTV/13;
VG2:=GASVEL(Q,XDIAM,YDIAM,PZ1,PZ2,PZ3,XINTZ,Z2);
KEVAL(M,Z2,VG2,INIX,Y2,K4);

FOR J:=1 TO TM DO
    Y2[J]:=Y1[J]+INTV*(439*K1[J]/216-8*K2[J]+3680*K3[J]/513-
        845*K4[J]/4104);

ZS:=Z1+INTV;
VGS:=GASVEL(Q,XDIAM,YDIAM,PZ1,PZ2,PZ3,XINTZ,ZS);
KEVAL(M,ZS,VGS,INIX,Y2,K5);

FOR J:=1 TO TM DO
    Y2[J]:=Y1[J]+INTV*(-8*K1[J]/27+2*K2[J]-3544*K3[J]/2565+
        1859*K4[J]/4104-11*K5[J]/40);

Z2:=Z1+INTV/2;
VG2:=GASVEL(Q,XDIAM,YDIAM,PZ1,PZ2,PZ3,XINTZ,Z2);
KEVAL(M,Z2,VG2,INIX,Y2,K6);

FOR J:=1 TO TM DO
    BEGIN
        ERR[J]:=INTV*ABS(K1[J]/360-128*K3[J]/4275-
            2197*K4[J]/75240+
            K5[J]/50+2*K6[J]/55);

        Y2[J]:=Y1[J]+INTV*(25*K1[J]/216+1408*K3[J]/2565+
            2197*K4[J]/4104-K5[J]/5);

        IF Y2[J]<>0 M THEN
            ERR[J]:=ERR[J]/Y2[J];

        IF (ERR[J]<0) OR (ERR[J]>=1E2) THEN
            ERR[J]:=9.99999E+09;

        IF ERR[J]>MAXERR THEN
            MAXERR:=ERR[J];

        AVERR:=AVERR+ERR[J];
    
```

```

END;(* FOR J *)

AVERR:=AVERR/TM;
WRITELN(OUTPUT,COUNT,' ',INTV,AVERR,MAXERR,X,' ',VG);
WRITELN(OUTFILE,COUNT,' ',INTV,AVERR,MAXERR,X,' ',VG);

IF AVERR>TOLERR/SQR(INTV) THEN
BEGIN
    INTV:=INTV/2;
    IF INTV<MININTV THEN
        STATE:=INTSMALL

END
ELSE
BEGIN
    X:=X+INTV/INTV1;
    Y1:=Y2;
    Z1:=ZS;
    VG:=VGS;

    IF ABS(1-X)<=ASSUMEDZERO THEN
        STATE:=REACHED
    ELSE
    BEGIN
        IF AVERR<=TOLERR/(32*SQR(INTV)) THEN
            INTV:=2*INTV;

        SHORTRANGE:=INTV>(1-X)*INTV1;

        IF SHORTRANGE THEN
        BEGIN
            LASTINT:=INTV;
            INTV:=(1-X)*INTV1;
        END;(* IF SHORTRANGE *)
    END;(* ELSE *)
END;(* ELSE *)

COUNT:=COUNT+1;

UNTIL
STATE<>STEPPING;

```

```

        IF NOT SHORTRANGE THEN
            LASTINT:=INTV;

        SUCCESS:=STATE=REACHED;

        WRITELN(OUTPUT);WRITELN(OUTFILE);

        IF SUCCESS THEN
            Y:=Y2;
END;(* RUNGKFEL *)

(*.....*)
PROCEDURE UPDATEFD(M,N:CLASSNUM;INTV,Z:REAL;
                  XDIAM,YDIAM,PZ1,PZ2,PZ3,XINTZ,INIX,LNINIX:NPOINT;
                  VAR ERR:VOVELRATE;VAR PARTICLE:NPARTICL;
                  VAR VG,INRATE,INMASRATE,CURRATE,MASSRATE:REAL;
                  VAR FIRSTPASS,SUCCESS:BOOLEAN);

VAR    W:VOVELRATE;
        S:INTEGER;
        P1,P2,P3,XINT:REAL;
        R,T,Q,SLOPE,SLOPEM,SLOPEX:NPOINT;

BEGIN
    FOR S:=1 TO M DO
        WITH PARTICLE[S] DO
            BEGIN
                W[S]:=NRATE;
                W[M+S]:=VOLUME;
                W[2*M+S]:=VELOC;
            END;(* WITH *)
            IF NOT FIRSTPASS THEN
                RUNGKFEL(M,N,Z,INTV,VG,INTV,XDIAM,YDIAM,
                        PZ1,PZ2,PZ3,XINTZ,INIX,ERR,W,SUCCESS);

            IF SUCCESS THEN
                BEGIN
                    FOR S:=1 TO M DO
                        WITH PARTICLE[S] DO
                            BEGIN

```

```

        NRATE:=W[S];
        VOLUME:=W[M+S];
        VELOC:=W[2*M+S];
        R[S]:=VOLUME;
    END;(* WITH *)

    DERIV(M,INIX,R,SLOPEX);

    FOR S:=1 TO M DO

    BEGIN
        T[S]:=W[S]*SLOPEX[S];
        Q[S]:=T[S]*W[M+S];
    END;(* FOR S *)

    CURRATE:=INTEGRAL2(M,INIX,T);

    MASSRATE:=INTEGRAL2(M,INIX,Q);

    IF FIRSTPASS THEN
    BEGIN
        INRATE:=CURRATE;
        INMASRATE:=MASSRATE;

        WRITELN(OUTPUT,INRATE);
        WRITELN(OUTPUT,INMASRATE);
    END;(* FIRTPASS *)

    CURRATE:=CURRATE/INRATE;
    MASSRATE:=MASSRATE/INMASRATE;

    END(* IF SUCCESS *)
    ELSE
        WRITELN(OUTPUT,'UNSUCCESSFUL INTEGRATION');
    END;(* UPDATEFD *)

    (*.....*)

    BEGIN
        WITH TABLE DO

```

```

BEGIN
  DERIV(MAXX,XDIAM,YDIAM,SLOPEZ);

  FOR S:=1 TO MAXX-1 DO
    BEGIN
      SPLINE(XDIAM[S],XDIAM[S+1],YDIAM[S],YDIAM[S+1],
        SLOPEZ[S],SLOPEZ[S+1],PZ1[S],PZ2[S],PZ3[S],XINTZ[S]);

      END;(* FOR S *)
    END;(* WITH TABLE *)

  WITH DATA DO
    BEGIN
      REALCON:=6*MIXPROP.PMF*MIXPROP.RVOL/((1-MIXPROP.PMF)*
        PI*CUBE(AVDIAM));
      WRITELN(OUTPUT,REALCON);

      COEF1:=18*VISCG*L/(ROP*SQR(AVDIAM)*U0);
      COEF2:=MIXPROP.RVOL*ROP*AVDIAM/VISCG*J0/2;
      COEF3:=PI*SQR(AVDIAM)*REALCON*L/4;

      WITH SETUP DO
        BEGIN
          NINT:=TRUNC(ZFINAL/INTVAL);
          NINP:=TRUNC(ZPRINT/INTVAL);
          INTV:=INTVAL;
        END;(* WITH *)

      VG:=1;

      FOR S:=1 TO NUMBER DO
        BEGIN
          INIX[S]:=PARTICLE[S].VOLUME;
          LNINIX[S]:=LN(INIX[S]);
          ERR[S]:=0;
          ERR[NUMBER+S]:=0;
          ERR[2*NUMBER+S]:=0;
        END;(* FOR *)

      Z:=0; IZ:=0;

```

```

SUCCESS:=IZ=0;
FIRSTPASS:=TRUE;

WHILE (IZ<NINT) AND SUCCESS DO
BEGIN
    WITH TABLE DO
        UPDATEFD(NUMBER,MAXX,INTV,Z,XDIAM,YDIAM,
            PZ1,PZ2,PZ3,XINTZ,INIX,LNINIX,ERR,PARTICLE,VG,INRATE,
            INMASRATE,CURRATE,MASSRATE,FIRSTPASS,SUCCESS);

        IF NOT FIRSTPASS THEN
        BEGIN
            IZ:=IZ+1;
            Z:=Z+INTV;

        END;(* NOT FIRSTPASS *)

        IF SUCCESS THEN
            FOR S:=1 TO NUMBER DO
            BEGIN
                PRINTOUT(OUFILE,S,NUMBER,NINP,ERR,PARTICLE,
                    IZ,Z,VG,CURRATE,MASSRATE);

                PRINTOUT(OUTPUT,S,NUMBER,NINP,ERR,PARTICLE,
                    IZ,Z,VG,CURRATE,MASSRATE);

            END;(* FOR S *)

            FIRSTPASS:=FALSE;

        END;(* WHILE Z<=ZFINAL *)

    END;(* WITH DATA *)
END;(* ZRELATION *)

(*.....*)

PROCEDURE READPART(VAR INFILE:TEXT;K:INTEGER;VAR PARTICLE:NPARTICL);
VAR    S:INTEGER;
BEGIN

```

```

    FOR S:=1 TO K DO
    BEGIN
        WITH PARTICLE[S] DO
        BEGIN
            READLN(INFILE,VOLUME,NRATE,VELOC);
        END;(* WITH *)
    END;(* FOR *)
END;(* READPART *)

(*.....*)

PROCEDURE ENTERDATA(VAR INFILE:TEXT;VAR INFILNAME,OUTFILNAME:NAME;VAR DATA:SETDATA);
BEGIN

    WRITELN('ENTER FILE NAME FOR INPUT');
    READLN(INFILNAME);WRITELN;
    RESET(INFILE,INFILNAME);
    WITH DATA DO
    BEGIN
        WRITELN('ENTER FILE NAME FOR OUTPUT');
        READLN(OUTFILNAME);
        WRITELN('ENTER NUMBER OF CLASSES OF PARTICLES');
        READLN(INFILE,NUMBER);

        READPART(INFILE,NUMBER,PARTICLE);

        WITH SETUP DO
            READLN(INFILE,ZFINAL,ZPRINT,INTVAL);WRITELN;

            WRITE('ENTER PARTICLE MASS FRACTION ');
            WRITELN('AND SPECIFIC VOLUME RATIO: ');
            WITH MIXPROP DO
                READLN(INFILE,PMF,RVOL);WRITELN;

            END;(* WITH DATA *)
    END;(* ENTERDATA *)

    (*.....*)

PROCEDURE ENTERTABLE(VAR INFILE:TEXT;VAR INFILNAME,OUTFILNAME:NAME;VAR TABLE:SETTABLE);

```

```

VAR I,J:INTEGER;
BEGIN
    WRITELN;
    WRITELN('ENTER FILE NAME FOR TABLE INPUT');
    READLN(INFILENAME)WRITELN;
    RESET(INFILE,INFILENAME);
    WITH TABLE DO
    BEGIN
        READLN(INFILE,MAXX,MAXY);WRITELN;

        IF MAXY<>0 THEN
        BEGIN
            FOR I:=1 TO MAXX DO
            BEGIN
                READLN(INFILE,XDIAM[I]);
                FOR J:=I TO MAXY DO
                BEGIN
                    READLN(INFILE,YDIAM[J]);
                END;(* FOR J *)
            END;(* FOR I *)

            READLN(INFILE);
        END;(* MAXY<>0 *)
        ELSE
        IF MAXY=0 THEN
        BEGIN
            FOR I:1 TO MAXX DO
                READLN(INFILE,XDIAM[I],YDIAM[I]);

            END;(* MAXY=0 *)
        END;(* WITH TABLE *)
    END;(* ENTERTABLE *)

    (*.....*)
    PROCEDURE WRITEDATA(VAR OUTFILE:VAR DATA:SETDATA);
    VAR
        S:INTEGER;
    BEGIN
        WRITELN(OUTFILE);

```

```

WRITELN(OUTFILE,INFILNAME);WRITELN(OUTFILE);
WITH DATA DO
BEGIN

    WRITELN(OUTFILE,NUMBER:13);

    FOR S:=1 TO NUMBER DO
        WITH PARTICLE[S] DO
            WRITELN(OUTFILE,VOLUME:13,NRATE:13,VELOC:13);

        WRITELN;

    WITH SETUP DO
        WRITELN(OUTFILE,ZFINAL:13,ZPRINT:13,INTVAL:13);
    WRITELN;

    WITH MIXPROP DO
        WRITELN(OUTFILE,PMF:13,RVOL:13);

    END;(* WITH DATA *)
END;(* WRITEDATA *)

(*.....*)

PROCEDURE WRITETABLE(VAR OUTFILE:TEXT;TABNAME:NAME;VAR TABLE:SETTABLE);
VAR    I,J:INTEGER;
BEGIN
    WRITELN(OUTFILE);
    WRITELN(OUTFILE,TABNAME);WRITELN(OUTFILE);
    WITH TABLE DO
    BEGIN

        WRITELN(OUTFILE,MAXX:13,MAXY:13);

        IF MAXY<>0 THEN
        BEGIN

            FOR I=1 TO MAXX DO

```

```

        WRITELN(OUTFILE,XDIAM[I]:13);
        FOR J:=I TO MAXY DO
            WRITELN(OUTFILE,YDIAM[J]:13);
        END;(* FOR I *)
    END(* MAXY<>0 *)
    ELSE
        IF MAXY=0 THEN
            BEGIN
                FOR I:=1 TO MAXX DO
                    WRITELN(OUTFILE,XDIAM[I]:13,YDIAM[I]:13);
                END+(* MAXY=0 *)
            END;(* WITH TABLE *)
        END+(* WRITETABLE *)

        (*.....*)

    BEGIN(* MAIN PROGRAM *)

        ENTERDATA(INFILE,INFILENAME,OUTFILENAME,DATA);

        ENTERTABLE(TABFILE2,TABNAME2,OUTFILENAME,LIST);

        REWRITE(OUTFILE,OUTFILENAME);

        WRITEDATA(OUTFILE,DATA);WRITEDATA(OUTPUT,DATA);
        WRITETABLE(OUTFILE,TABNAME2,LIST);WRITETABLE(OUTPUT,TABNAME2,LIST);

        WRITELN(OUTFILE);WRITELN;
        WRITELN(OUTFILE,OUTFILENAME);WRITELN(OUTFILENAME);

        ZRELATION(DATA,LIST);

        CLOSE(OUTFILE,LOCK);

    END.(* PROGRAM *)

    (*.....*)

```