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**Prediction of Colloidal Suspension Stability
for SiC/Si_3N_4 and $FeAl/Al_2O_3$ Fiber Systems
Using Material and System Parameters**

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Prediction of Colloidal Suspension Stability for SiC/Si_3N_4 and $FeAl/Al_2O_3$ Fiber Systems Using Material and System Parameters.

By

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ABSTRACT

Prediction of Colloidal Suspension Stability for SiC/Si_3N_4 and $FeAl/Al_2O_3$ Fiber Systems Using Material and System Parameters.

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In this investigation a method to predict the stability of multicomponent colloidal suspensions at different pH values from system and material data such as particle size, volume fraction, electrolyte concentration, zeta potential verses pH, and Hamaker constant data was developed from an existing method. A computer program was written and used for a SiC/Si_3N_4 powder system. The predictions of stability ranges were found to be within a half a pH unit of actual stability ranges as found from sedimentation results, but was dependent upon accurate zeta potential data. The dependency of the program on temperature variations, relative component volume fraction variations, and the accuracy of the input Hamaker constants was examined. For a $FeAl/Al_2O_3$ fiber composite, the method the predicted ideal processing conditions when the components were mixed at pH 5 followed by an increase to pH 8, which would prevent differential separation of the components.

DEDICATION

To my Mom and Dad
without whom, for me, none of this would have been possible.

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INTRODUCTION

Advanced ceramic materials are currently being used in an increasing number of different fields. Areas in which ceramics are presently found include electronics, dentistry, automotive engines, industrial tooling, and biological prostheses. Within these different fields ceramics are being used in a wider variety of applications. In electronics, for example, ceramic uses vary from electrical insulation to chip carriers and substrates to piezoelectrics to superconductors.

The vast majority of ceramic materials are made by the processing of raw material powders into a green body and subsequent heat treatment of the green body, which causes the elimination of pores, densification, and microstructural development. Uniformity in the green compact is very important since it governs the microstructures of the final sintered body, and the microstructure of the final body determine the resulting properties of the body, such as mechanical strength and various electrical and magnetic properties. Problems with advanced ceramics arise from difficulties in the ability to repeatedly process ceramics with identical microstructures and properties. The formation of non-uniform ceramics is caused by inhomogeneities which are the result of unsuccessfully making a uniform green body. Agglomerates are one of the main causes of inhomogeneities since they tend to cause the formation of a non-uniform green body containing an uneven distribution of pores and a change in the pore size distribution due to resulting larger pores. The preparation of well dispersed, stable suspensions help alleviate the problems caused by agglomeration and lead to the formation of a uniform green body and consequently result in better sintered bodies. It therefore becomes important to increase control of the processing in order to reduce microstructural defects and to maximize reliability.

Processing of ceramics can be divided into three areas. First is powder formation, then dispersion of the powder, and finally powder packing during drying and compaction. The dispersion of the powder consists of two elements: dispersion of the powder into a suspension and the stability of the suspension. While ideally it is desirable to have a disperse, stable suspension in order to improve the final microstructure by removing agglomerates, new processing methods contain steps which call for switching from stable suspensions to unstable coagulated suspensions containing large loosely bound agglomerates and switching back to a stable suspension. Coagulated suspensions with loosely bound agglomerates prevent segregation of the different system components and make it possible to remove excess salts and surfactants by washing. Due to the marked importance of preparing stable suspensions and the combined use of stable and unstable suspensions, the prediction of the stability of ceramic suspensions would be an important tool to aid in the control of processing advanced ceramics.

Pioneering work in this area was done in the 1940's and is known as DLVO theory. This theory describes the total interaction energy between particles in a single component suspension. From this information some insight into the stability behavior of the suspension can be inferred. However, with the increasing use of multi-component systems due to the addition of reinforcements and of processing additives (e.g. sintering aids, stabilizers, composites, etc.), it is necessary to develop a theory for the prediction of the stability of multi-component systems. While work has been done to develop theories to predict the stability behavior of two-component systems, the majority of the application and experimental verification of these theories has been done by colloid chemists with little work done with advanced ceramic systems. This demonstrates the need for further research in this area of ceramics.

The following work will investigate the stability behavior of multi-component ceramic systems. The prediction of their stability will be examined by inputing system and material data (such as pH, electrolyte concentration, particle size, Hamaker constant, and zeta potential) into a computer program which uses a method that is an adaptation of a method originally developed by Healy, Hogg, and Fuerstenau from the pioneering DLVO theory, while experimental investigations will examine their actual stability states.

LITERATURE REVIEW

The vast majority of ceramic materials are made by the processing of raw material powders into a green body, followed by subsequent heat treatment of the green body which causes the elimination of pores, densification, and microstructural developments (1). Uniformity in the green body is very important since it governs the microstructures of the final sintered body (2, 3), which in turn determines the resulting properties of the body, such as mechanical strength, and various electrical and magnetic properties (4-6). The formation of non-uniform ceramics is caused by inhomogeneities which are mainly the result of the formation of agglomerates of particles in the ceramic suspension(8, 9). New processing methods use temporary aggregation of the suspension in order to prevent segregation of the system components between processing steps(9-11). The prediction of the state of aggregation would therefore be an important tool in the control of processing advanced ceramics.

The knowledge gained in predicting the stability of ceramic suspensions may be readily applied to a wide variety of other applications where similar colloid theory is being applied. Such applications include selective flocculation in waste treatment (12-15), biological/medical studies of blood coagulation (16) and cholesterol stability (17), paint stability (18) and retention (19), and deposition and adhesion of material coatings (20-22).

To understand colloidal suspension stability, it is first important to elaborate on what is a colloidal suspension. The first important characteristic of a colloidal suspension is the size of the particles. For the case of a ceramic colloidal suspension, which is a lyophobic solid in a liquid, the size of the solid particles should be large enough so that they are not considered to be in solution with the liquid and small enough so that they are affected by collisions with the liquid (23). There is no absolute size range for colloidal particles (23, 24); however, a range of 1 nm to 1 μm is often regarded as the typical range for a colloidal suspension (15, 23, 24). Because of the small size of particles in a colloidal suspension another important characteristic of these suspensions is that the particles, because of their small size, have a large surface area when compared to their volume (23, 25).

Another important characteristic of colloidal particles is that when the particles are put in the suspending liquid they develop a surface charge. There are several different ways in which this charge is developed which all depend on the specific chemistry and thermodynamics of the system (the system includes the particle surface, the liquid, and any electrolytes that may be present in the liquid). One mechanism for surface charge generation is the creation of crystal lattice defects through the replacement of ions in the crystal lattice structure of the particle by ions of lower charge (25). This type of charge generation mechanism is seen most often in clay minerals where ions in the crystal lattice structure with a valence of three are substituted for by ions from the liquid with a valence of two causing a net charge on the surface (25).

If the colloidal particles have an ionic crystal structure then one mechanism for surface charge generation is the unequal dissociation and adsorption of oppositely charged ions from the particle surface (25, 26). This unequal dissociation and adsorption of surface ions results in a slight imbalance in the number of crystal cations (positively charged ions) and anions (negatively charged ions) which causes the development of a net positive or negative charge on the surface (25). The classic example of this is given in most colloid texts (15, 18, 25, 27, 28). This example is AgI which has Ag^+ and I^- ions which dissociate from the surface in equal numbers according to equilibrium conditions determined by the solubility product (25). However, the iodine ions are preferentially adsorbed back onto the surface (compared to the silver ions) which results in the net surface charge.

Another mechanism for surface charge generation is the dissociation of ionic surface groups or the interaction of ionic surface groups with H^+ and OH^- ions in water (25, 26). Hunter (25) notes that it is sometimes quite difficult to discern between the two because their net results are the same. For oxide particles in water the surfaces are hydroxylated and these hydroxyl groups can then undergo further ionization (29). An example of this is given by James and Parks for alumina (29):

$$\begin{gathered} Al + AlO + H_2O \rightleftharpoons 2AlOH \\ AlOH \rightleftharpoons AlO^- + H^+ \\ H^+ + AlOH \rightleftharpoons AlOH_2^+ \end{gathered}$$

where: Al = aluminum (III) ion on the surface
AlO = oxide ion bound to surface Al ion
AlOH = hydroxylated group
AlO^- = ionized hydroxyl group
$AlOH_2^+$ = ionized hydroxyl group.

In a general form after hydroxylation this can be written as (25):

$$\begin{gathered} MOH \rightleftharpoons MO^- + H^+ \\ MOH + OH^- \rightleftharpoons MO^- + H_2O. \end{gathered}$$

Extensive investigations and modeling have been done to describe this type of surface charge generation and charge generation from the dissociation of ionic surface groups (29-32).

It is important to point out what a potential determining ion is. A potential determining ion is an ion which helps determine the potential of a particle surface or as in the previous discussion helps generate charge on the particle surface. For the example mentioned earlier of AgI particles, Ag^+ is a potential determining ion (28). For particles with surface charge generation resulting from the interaction of ionic surface groups with H^+ and OH^- ions as was the case for alumina, the potential determining ions are H^+ and OH^-. In this case adding more H^+ and OH^- through the addition of an acid or base will change the concentration of potential determining ions which will change the degree of interaction of the potential determining ions with the ionic surface groups and consequently will change the charge on the particle surface. Similarly, changing the concentration of any potential determining ion will result in a net change of surface charge.

As a consequence of the characteristics described previously the interface between the solid particles and the liquid medium becomes tremendously important in the behavior of colloidal suspensions. This is why physical chemistry of surfaces and interfaces has become such an integral part of colloid chemistry.

From a physical standpoint, particles in a colloidal suspension are in continual motion due to a variety of different types of motion. Particle movement in the medium is caused by collisions of the particles with the molecules of the medium, gravitational forces, and convection forces (23, 33). Movement caused by particle collisions with the suspending medium is termed Brownian motion (23). This motion is completely random with millions of changes in direction per second (34). As the particle size increases, compared to the size of the molecules of the liquid, the effects of Brownian motion are reduced (15). Gravitation movement is seen as sedimentation as the particles are slowly forced by gravity to 'fall' through the liquid medium. This gravitational movement is increased as the particle size is increased. Thermal movement is caused by convective forces resulting from thermal gradients through the liquid medium and rapidly decreases as particle size is increased. The net result of these different types of motion is that the particles in the suspension are in continual motion and will approach one another for collision. Collision, however, depends upon the forces interacting between colloidal particles.

Forces which are acting on approaching colloid particles are van der Waals forces, steric forces and repulsion forces which are the result of the electrical charges on particle surfaces. Steric forces are forces caused by co-polymers which are added to a colloidal suspension and which are adsorbed on the surfaces of particles (15). The work of this thesis will be for suspensions which do not contain co-polymers so that steric repulsion forces will not be considered hereafter. Van der Waals forces are caused by three different types of attraction. The first type is called a Keesom interaction and is where a dipole molecule orients and attracts another dipole molecule. Another type is called a Debye interaction and is where a dipole molecule induces a dipole in a polarizable molecule and attracts it. The third type is called a London force and is where a fluctuation in a molecules' electron distribution results in an instantaneous dipole which causes a dipole in another molecule and so attracts this other molecule (35).

London forces are dominant in suspensions unless the materials are highly polar(15). Hamaker (36-38) calculated the force due to van der Waals attraction which results from London forces by using a simple pair-wise addition of atomic forces with the potential decreasing as the inverse of the sixth power of separation distance (39). Casimer and Polder (40-42) showed that for larger separations there was a retarding effect which made the potential decrease as the inverse of the seventh power of separation distance (33). This retarding effect results because, at larger separations, by the time the electric field from one dipole reaches and causes a dipole in another molecule; the electron distribution of the first molecule will have already changed (39). J. T. G. Overbeek notes, however, that for most colloidal suspensions retardation effects are not important (33). Van der Waals attraction without retardation for two different interacting particles of radius, a_1 and a_2, separated by a distance, H, can be represented by an expression derived by Hamaker (38):

$$V_A = -\frac{A}{12}\left[\frac{y}{x^2+xy+x}+\frac{y}{x^2+xy+x+y}+2\log\frac{x^2+xy+x}{x^2+xy+x+y}\right] \qquad [1]$$

where: A = Hamaker constant
$x = H/(a_1 + a_2)$
$y = a_1 / a_2$.

The Hamaker constant, A, must be calculated in order to evaluate the force of attraction due to van der Waals forces. There are two methods for calculating the Hamaker constant. The first is a microscopic method which was developed by Hamaker. This method integrates over all pairs of atoms in order to get a total energy for the macroscopic body (43), but uses molecular constants for evaluation which are difficult to ascertain. The second method is a macroscopic method and was developed by Lifshitz (44, 45). This method uses macroscopic properties such as refractive index and dielectric constants in calculating the Hamaker constant. J. Gregory shows the following expression derived using the Lifshitz method (46):

$$A=0.230h\nu_v\frac{(\epsilon_o-1)^2}{(\epsilon_o+1)^{3/2}(\epsilon_o+2)^{1/2}} \qquad [2]$$

where: ε_0 = limiting dielectric constant
$\varepsilon_0 = n_o^2$
n_o = limiting refractive index in visible region

h = Plank's constant
v_v = characteristic dispersion frequency.

Bleier simplifies this expression to (47):

$$A_i(kT) = 113.7\frac{(\epsilon_i-1)^2}{(\epsilon_i+1)^{3/2}(\epsilon_i+2)^{1/2}}. \qquad [3]$$

The previous calculation determines the Hamaker constant for particles in a vacuum. Particle interactions in a medium are less than in vacuum due to the molecules of the medium being between the two interacting particles. To account for this an effective Hamaker constant is used. For two identical particles in a medium (15):

$$A_{eff}=(a_i^{1/2}-A_m^{1/2})^2 \qquad [4]$$

where: A_{eff} = the effective Hamaker constant
A_i = Hamaker constant of particle i in vacuum
A_m = Hamaker constant of medium in vacuum.

For two different particles in a medium (15):

$$A_{eff}=(A_i^{1/2}-A_m^{1/2})(A_j^{1/2}-A_m^{1/2}). \qquad [5]$$

As stated previously, the repulsive forces in a colloidal suspension are due to electrical charge on the particle surfaces which is generated by the various methods described earlier. What transpires is that the charged particle surfaces attracts ions in the liquid to the particle surface. These attracted ions can be from the liquid medium itself or from electrolytes in the medium. For a water medium, ions from the medium itself would be hydrogen and hydroxide ions since water dissociates into these two ions. The concentration of each of these ions is determined by the pH which is defined as the negative of the log of the hydrogen ion concentration. For example, at a pH of 7 the concentration of $[H^+]$ and $[OH^-]$ is 10^{-7} M and for a pH of 4 the concentration of $[H^+]$ and $[OH^-]$ is 10^{-4} M and 10^{-10} M, respectively.

Electrolytes are materials which when added to the suspension which will go into solution with the liquid and are generally added in concentrations ranging from 10^{-2} M to 10^{-5} M. Common examples of electrolytes are potassium hydroxide (KOH), sodium chloride (NaCl), calcium carbonate ($CaCO_3$), and magnesium chloride ($MgCl_2$). KOH, NaCl and $CaCO_3$ are called mono-valent electrolytes because when they go into solution each molecule forms the same number of cations as anions, while $MgCl_2$ is called a di-valent electrolyte since one molecule will form an unequal number of cations compared to anions upon going into solution. KOH and NaCl are called monatomic electrolytes since both of the ions formed in solution ions have a valency of one, while $CaCO_3$ is not a monatomic electrolyte since the ions formed upon solution have valencies of two.

As shown previously, the concentration of H^+ and OH^- ions changes fairly dramatically with pH. Electrolytes are added in order to overwhelm this effect and to keep a constant concentration of ions. An illustration of the reason for this can be found in the following example, for water at a pH of 7 with an electrolyte concentration of 10^{-3} M the electrolyte ions are more dominant than the water since the concentration of ions in the water is 10^{-7} M which means that the electrolyte ion concentration is 4 orders of magnitude greater. Now if the pH in this example is changed to 4 then the H^+ ion concentration will change to 10^{-4} M which is still an order of magnitude less than the electrolyte concentration.

Another important point about electrolytes is the concept of indifferent electrolytes as opposed to potential determining ions. As mentioned earlier, potential determining ions are specifically adsorbed (chemisorption) by the surface and result in surface charge generation. Indifferent ions, on the other hand, are not specifically adsorbed on the particle and result in no net surface charge generation. The adsorption of indifferent ions is merely attraction due to the charge of the ions and the charge of the particle surfaces (physisorption).

The particle surface attracts ions of opposite charge which are initially physically adsorbed to the surface. These ions are termed counter-ions since they are of opposite charge to the surface and counter the charge of the surface. The concentration of counter-ions is very high close to the surface, but their concentration decreases as the distance from the surface is increased until the concentration is eventually the same as the concentration of the ions in the bulk liquid (15). The opposite is true for ions with the same charge as the surface. These ions are called co-ions and their concentration is very high at the surface, but increases as the distance from the surface is increased until the concentration eventually becomes the same as that in the bulk liquid (15). The distance where co-ions and counter-ions reach their bulk concentration is of the order of tens of nanometers (25).

Figure 1 illustrates this phenomenon. Figure 1a shows the particle surface as the vertical line with a positive surface charge shown to the left. To the right of the surface are the ions which have been attracted to the surface. The reason that the particle surface is shown is shown as having no curvature is due to the extremely small size of the ions (on the order of a few tenths of a nanometer or less) compared to the amount of particle surface area (on the order of 10^5 square nanometers for a 0.1 micron particle (28)) which makes it such that as far as the ions are concerned, the particle surface is a big flat plate.

Figure 1b shows how the concentration of ions changes with distance away from the particle surface as previously explained. The distance $1/\kappa$ shown in the figure is known as

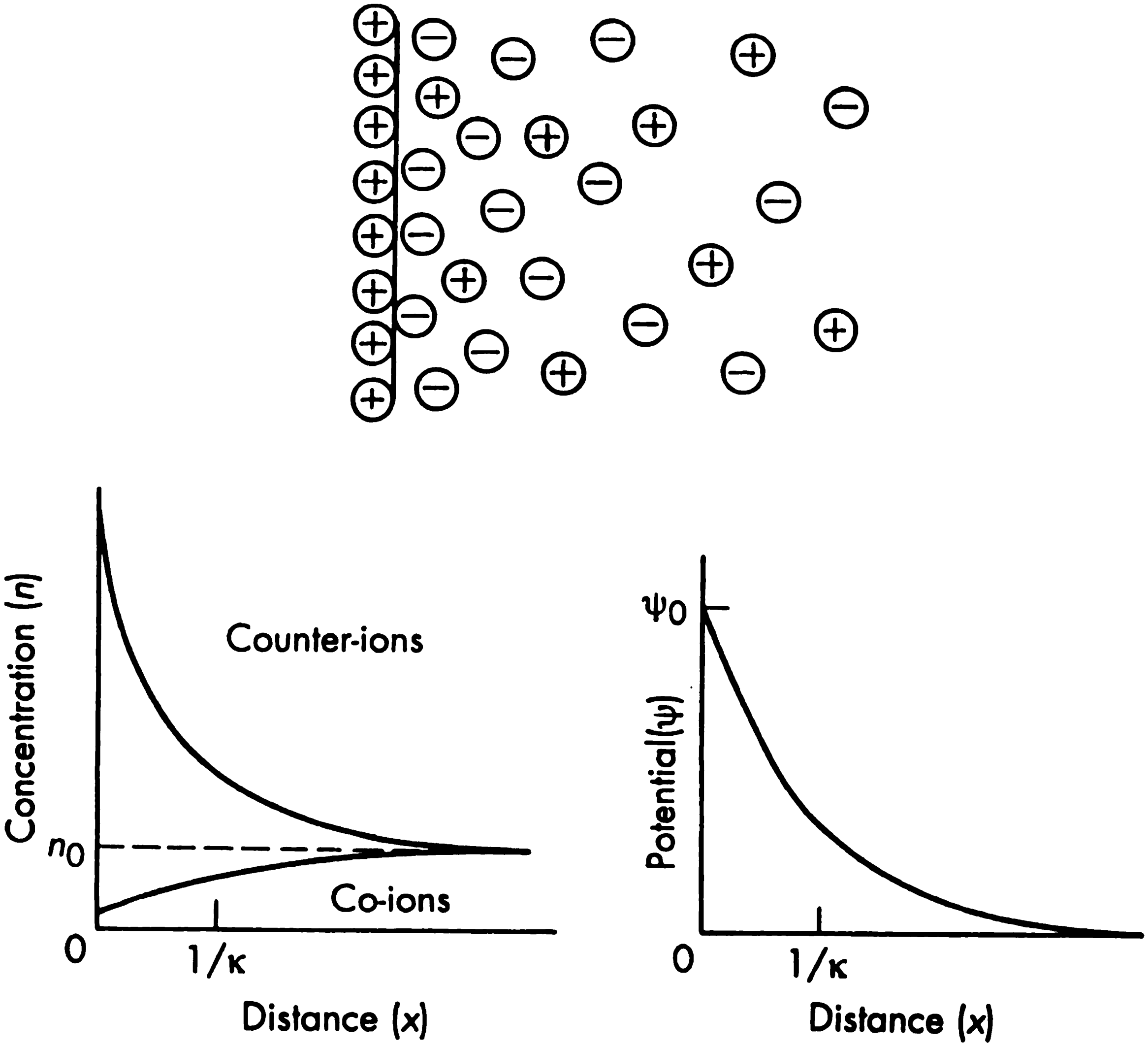


Figure 1 Illustration of a) the attraction of counter-ions to the surface of particles and the effects of distance from the surface on b) ion concentration and c) potential (taken from (15)).

the Debye length. The Debye length is used to characterize the size of the layer of adsorbed ions. The quantity κ is known as the Debye-Hückel parameter and is a function of concentration of ions in the bulk, the valency of those ions, and the temperature. An exact function for the Debye-Hückel parameter will be derived in more detail later. Figure 1c shows how the potential changes with distance away from the particle surface. The figure shows how the potential begins at ψ_0 due to the charge on the surface and decreases in magnitude as distance is increased due to the countering of the surface charge by the adsorbed counter-ions.

If an electrolyte is added to the medium of a colloidal suspension the concentration of the electrolyte in the medium is usually in the range of 10^{-5} to 10^{-2} M. As the concentration of ions in the liquid is increased through electrolyte addition, the distance from the particle surface to where the ion concentration reach its bulk value is decreased (23, 25), which as will seen later reduces the amount of interparticle repulsion. Adding an electrolyte which has ions with a valency of more than one (e.g. di-valent and tri-valent ions) will also cause a decrease in the distance from the particle surface where ion concentrations reach bulk values (23), which is why monatomic electrolytes are most often used.

Gouy and Chapman (48, 49) described this phenomenon of ion adsorption to charged particle surfaces by saying that particles in a medium have a double layer of charge which consists of two distinct layers of ions around the particle. The first layer is the compact inner layer of adsorbed counter-ions, which is often termed the Stern layer after O. Stern who later developed a model describing this layer in more detail (50). The second layer is a diffuse layer of both counter-ions and co-ions with a distribution which depends on electrical considerations and random thermal motion (15). Gouy and Chapman modeled this layer (48, 49). Their model assumes that the particle surfaces are flat (with respect to the ions) and uniformly charged, that the ions can be considered to be point charges from a symmetric electrolyte of charge z, that the distribution of the point charges is a Boltzmann distribution, and that the only influence of the medium is through the dielectric constant which does not vary in the liquid (15).

Figure 2 shows this phenomenon. Figure 2a shows the particle surface as the vertical line with positive surface charge to the left. The dotted vertical line closest to the surface is the Stern plane which is the outer boundary of the compact inner layer of adsorbed counter-ions (the Stern layer). The bumpy curved line which is the next furthest out from the particle surface is known as the surface of shear. This is the surface where if the particle itself

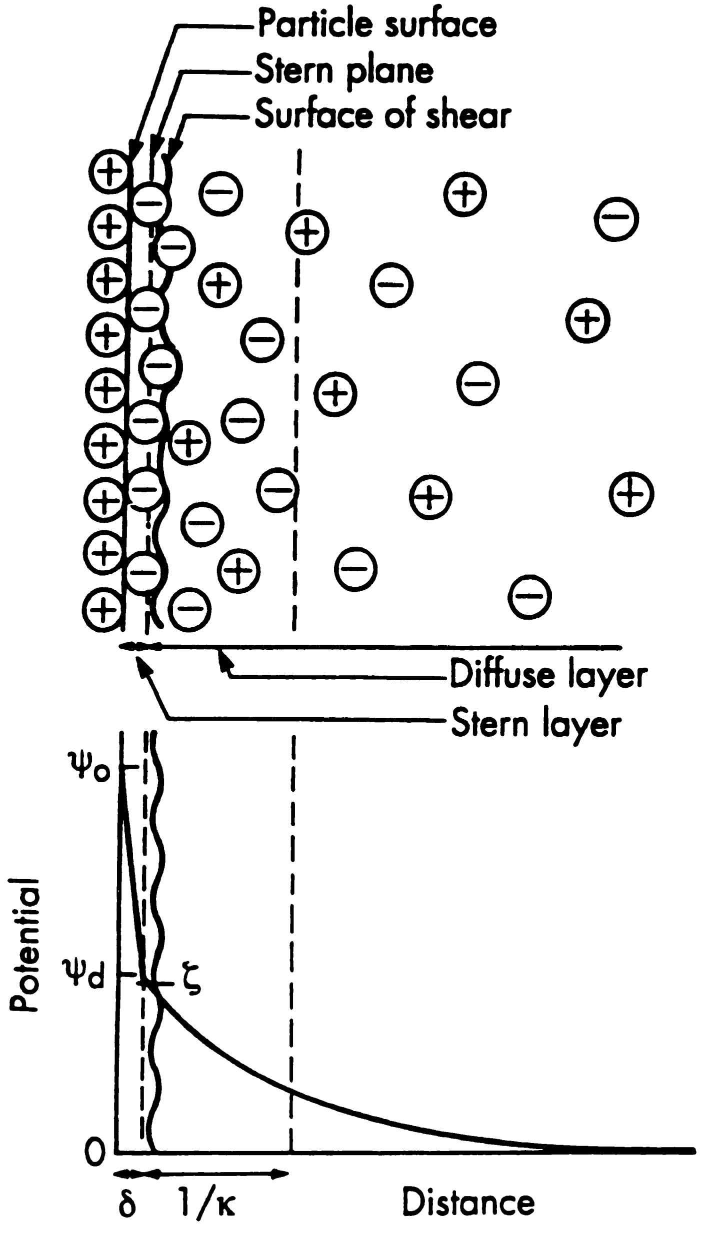


Figure 2 Illustration of a) the double layer surrounding a colloidal particle and b) the change of potential with distance from the particle surface (taken from (15)).

moves the ions inside this surface of shear move with the particle as if they were a part of the surface and those outside the surface of shear do not.

Figure 2b shows the potential as a function of distance from the surface. The potential begins with a value of ψ_o at the surface. The potential then decreases quickly to the value ψ_d at a distance of δ which corresponds to the edge of the Stern layer. The potential decreases as a result of the specifically adsorbed counter-ions which counter the charge at the surface. The potential then decreases gradually in the second, diffuse layer also due to the counter-ions in this layer. The potential at the surface of shear is shown in Figure 2b to be equal to a value ζ and is commonly referred to as the zeta potential. The zeta potential will be discussed in more detail later, especially with respect to ways of measuring the zeta potential and the difference (if any) between ζ and ψ_d. The Debye length, $1/\kappa$, shown in Figure 2b is often called the double layer thickness, even though it is actually only an indication of the actual size of the double layer and not an absolute thickness (28).

The repulsive force upon particle interaction results from the energy of interaction of each particles' double layer as they begin to overlap. Consequently, the repulsive force is a function of the magnitude of the charge generated on the particle surface and the size of the double layer around the particle (25). An expression of this interaction energy is extremely difficult to obtain. Derivations for an expression usually use the Poisson equation to describe the flow of the electric field in a dielectric medium and the Boltzmann equation to describe the charge distribution in the diffuse layer (51-63). Specific derivations of repulsive double layer interactions will be discussed extensively later.

Several interesting characteristics of colloidal particles with an electrical double layer are grouped together as electrokinetic phenomena. Generally, electrokinetics is the combination of particle electrical effects and particle motion (28). An important classical example of electrokinetics is electrophoresis in which motion of the particle in suspension is caused by the application of an external electric field (25). Actually in electrophoresis when the charged particle moves it takes with it some adsorbed ions(namely those inside the plane of shear) and this movement is relative to the medium which does not move (15). The velocity at which the particle moves is directly proportional to the magnitude of the applied electric field (25) and the constant of proportionality is called the electrophoretic mobility, μ_e (25). Microelectrophoresis is the experimental technique of using optical microscopy to visibly see the particle motion and measure its net velocity for a given electric field (15) in order to find the mobility, μ_e.

As referred to earlier, the plane of shear separates the layer of ions which moves with the particle and the layer of ions which remains stationary with the liquid. The potential at this plane of shear is called the zeta potential, ζ, and is determined by using the electrophoretic mobility. For particle suspensions where the particle radius is much larger than the size of its double layer (i.e. such that $r/\kappa^{-1} >> 1$), the equation to calculate the zeta potential is known as the Helmholtz-Smoluchowski equation (25):

$$\zeta = \frac{\mu_e \eta}{\epsilon_o \epsilon_r} \qquad [6]$$

where: ε_o = permitivity in a vacuum
ε_r = relative permitivity
η = viscosity of liquid medium.

The Helmholtz-Smoluchowski equation is generally valid for aqueous suspensions. For particle suspensions where the particle radius is much less than the double layer thickness (i.e. such that $r/\kappa^{-1} << 1$), the equation to calculate the zeta potential is known as the Hückel equation (15):

$$\zeta = \frac{1.5 \mu_E \eta}{\epsilon_o \epsilon_r}. \qquad [7]$$

The Hückel equation is generally valid for non-aqueous suspensions with low conductivity (15).

The potential at the plane of shear is often assumed to be equal to the potential at the outer edge of the stern layer (15, 64). Lyklema (64) reports in his investigations that within experimental error the zeta potential equals the potential at the Stern layer.

Other examples of electrokinetic phenomena are electroacoustic phenomena and are described in detail by O' Brien and Oja (65-67). The first of the two electrokinetic phenomena results from the application of an alternating pressure field in a colloidal suspension in the form of an acoustic wave. As a result of the density difference between the particles and the liquid there is a relative motion between the particles and the liquid. An alternating dipole is formed at the frequency of the acoustic wave as a result of the relative displacement of the particles and the oppositely charged particles in the double layer caused by the relative motion. The formation of this alternating dipole is termed the Ultrasonic Vibration Potential (UVP), and is measured as voltage per amplitude velocity of the acoustic wave applied.

The other electroacoustic phenomena results from the application of an alternating electric field to a colloidal suspension. An acoustic wave is generated by the particles as they move back and forth in the electric field due to their charge and a density difference between the particles and the liquid. The formation of this acoustic wave is termed the Electrokinetic Sonic Amplitude (ESA) and is measured as pressure amplitude per unit electric field applied.

The dynamic mobility can be found for both these electroacoustic phenomena by using equations derived by O' Brien (65, 66):

$$\mu_d(\omega) = \frac{ESA(\omega)}{\phi \Delta \rho c} \qquad [8]$$

and

$$\mu_d(\omega) = \frac{UVP(\omega)}{\phi \Delta \rho c} K^* \qquad [9]$$

where: μ_d = dynamic mobility
ω = angular frequency
Φ = volume fracture of particles
$\Delta\rho$ = density difference of particles and liquid
c = velocity of sound in suspension
ESA = pressure amplitude per unit electric field
UVP = voltage per amplitude velocity of wave
K^* = high frequency conductivity correction.

The zeta potential can be calculated using the mobility as in electrophoresis with the addition of a correction for the inertia of the particle in an alternating field since this reduces the velocity amplitude of particle motion. The equation to calculate the zeta potential was derived by O' Brien using the Helmholtz-Smoluchowski equation (65, 66):

$$\zeta = \frac{\mu_d \eta}{\epsilon_o \epsilon_r} |G(\alpha)^{-1}| \qquad [10]$$

$$|G(\alpha)^{-1}| = \sqrt{X^2 + Y^2} \qquad [11]$$

$$X=\frac{1+2A^3B}{9(2A^2+2a+1)} \qquad [12]$$

$$Y=\frac{2A^2B(1+A)}{9(2A^2+2A+1)} \qquad [13]$$

$$A=\sqrt{\frac{\alpha}{2}} \qquad [14]$$

$$B=(3+2\frac{\Delta\rho}{\rho}) \qquad [15]$$

$$\alpha=\frac{\omega a^2\rho}{\nu}. \qquad [16]$$

where: a = particle radius.

The stability of a colloidal suspension refers to whether or not particles come together in clusters called agglomerates or whether particles stay as individual particles (25). Suspensions which are from agglomerates are said to have coagulated and are unstable. Suspensions which do not form agglomerates are said to be stable. It should be noted that contrary to popular usage in the literature the term flocculation refers to the formation of loose agglomerates formed as the result of polymers adsorbed onto particle surfaces and not just from normal coagulation (25). Therefore, in this thesis the term coagulation will be used to describe agglomeration and not flocculation since as mentioned before all suspension considered for this thesis will not contain polymers.

Colloidal suspensions, as Hunter points out (25), are thermodynamically metastable. This means that a stable suspension is only stable in a kinetic sense and that coagulation is a rate process. The study of colloidal stability predictions should therefore be more a study of the rate of these processes than the thermodynamics of them (33).

Pioneering work in describing particle interactions of single component colloid systems was done by Derjaguin, Landau, Verwey, Overbeek (51, 52). The compilation of their work is known as DLVO theory. DLVO theory describes the energy of interaction for identical particles in an electrolyte solution. In DLVO theory, the particles are treated as having a double layer of ions which surround them as described previously by Gouy and Chapman (48, 49). This double layer, as described earlier, consists of a diffuse layer in which ions are treated as point charges which can be described by a Boltzmann distribution, and a rigidly held inner layer of essentially adsorbed ions.

The interaction energy between two particles is described as a sum of the potential energy of attraction and repulsion energies:

$$V_t = V_A + V_R \qquad [17]$$

where: V_T = total energy
V_A = attractive energy
V_R = repulsive energy.

The attraction energy is due to van der Waals attraction and is described by equations derived for two equal spheres by Hamaker (38):

$$V_A = -\left(\frac{Aa}{12H}\right) \qquad [18]$$

where: H = interparticle separation distance
a = particle radius
A = Hamaker constant (from Equation [4]).

The repulsive energy during particle interaction is caused by the overlapping of particles' double layers. This repulsive interaction is described by the Poisson-Boltzmann equation:

$$\nabla^2\psi = -\frac{1}{\epsilon_o\epsilon_r}\sum_i n_i^o z_i e \exp\left(-\frac{z_i e\psi}{kT}\right) \qquad [19]$$

where: ∇^2 is the Laplacian operator
ψ = particle surface potential
ε_o = permitivity in a vacuum
ε_o = 8.854E-12 (C^2/J m)
ε_r = relative permitivity
n_i = number of ions of type i
z_i = valence of ion i
e = electron charge
e = 1.602E-19 (C)
k = Boltzmann's constant
k = 1.381E-23 (J/K)
T = temperature (K).

This equation is the combination of the Poisson equation which describes the flow of the electric field in a dielectric medium as detailed by Hunter (25):

$$\nabla^2\psi = -\frac{\rho}{\epsilon_o\epsilon_r} \qquad [20]$$

where:ρ = density of charges

and the Boltzmann equation which described the distribution of charges in the diffuse double layer:

$$n_i = n_i^o\exp(-\frac{\omega_i}{kT}) \qquad [21]$$

where:n_i = number of ions of type i at the distance from the surface where the potential is ψ
n_{io} = number of ions type i in the bulk
ω_i = work to bring ions from the bulk medium to this distance.

As an approximation ω_i is assumed to be:

$$\omega_i = z_ie\psi \qquad [22]$$

so that the density of charges becomes

$$\rho = \sum_i n_i^oz_ie = \sum_i n_i^o\exp(-\frac{z_ie\psi}{kt}) \qquad [23]$$

which in combination with the Poisson equation results in the Poisson-Boltzmann equation [19] shown previously.

In DLVO to get an expression for the energy of repulsion the Poisson-Boltzmann equation was solved using the Debye-Hückel approximation. The Debye-Hückel approximation assumes that (28):

$$|ze\psi| < kT$$

or:

solving this for ψ *at*
room temperature (25°C)
$\psi < 25.7 mV$. [24]

This allows for the following simplification if only the first term of the series expansion is taken (15):

$$\exp\left(\frac{ze\psi}{kT}\right) \approx 1+\frac{ze\psi}{kT}. \qquad [25]$$

So that the Poisson-Boltzmann equation becomes:

$$\nabla^2\psi = -\frac{1}{\epsilon_o\epsilon_r}\left[\sum_i n_i^o z_i e - \sum_i \frac{z_i^2 e^2 n_i^o \psi}{kT}\right]. \qquad [26]$$

Due to the need for electroneutrality in the bulk medium the sum of the charges must equal zero, so (25):

$$\sum_i z_i e n_i = 0. \qquad [27]$$

The Poisson-Boltzmann equation then simplifies to:

$$\nabla^2\psi = \frac{1}{\epsilon_o\epsilon_r}\left[\sum_i \frac{z_i^2 e^2 n_i^o}{kT}\right]\psi \qquad [28]$$

or:

$$\nabla^2\psi = \kappa^2\psi \qquad [29]$$

where: κ=Debye-Hückel parameter

$$\kappa=\sqrt{\frac{e^2\sum n_i^o z_i^2}{kT}}. \qquad [30]$$

The linear form of this equation becomes (28):

$$\frac{d^2\psi}{dx^2}=\kappa^2\psi. \qquad [31]$$

The linear form of this equation is then solved in DLVO with the boundary conditions that (28):

$$\psi \to \psi_o \; as \; x \to 0$$
$$and \qquad [32]$$
$$\psi \to 0 \; as \; x \to \infty$$

where: x = distance from the surface.

The solution of which is (28):

$$\psi = \psi_o \exp(-\kappa x). \qquad [33]$$

The repulsion for identical spheres was then found by Derjaguin (68, 69) to be:

$$V_R = 2\epsilon_o \epsilon_R \psi^2 \ln[1 + \exp(-\kappa H_o)] \qquad [34]$$

where: H_o = shortest distance between particle surfaces.

Now the total potential energy interaction as a function of interparticle distance can be calculated (and subsequently graphed) in the DLVO method by using Equation [34] and [18] to solve Equation [17] as a function of varying distance of particle separation, H. The graph of total potential energy versus particle separation is used to indicate the stability of a single component system and a maximum potential energy of 20 kT is often noted to indicate that a suspension will be stable (25). However, this does not indicate the stability for multicomponent systems and does not address the kinetic aspect of stability at all.

Empirically, colloid experimentalists have noted that colloid suspensions which have room temperature zeta potential values above 25.7 mV generally will be stable (70). One way in which this empirical relationship would be used would be for a system where H^+ and OH^- ions are potential determining ions and the zeta potential would be measured over a range of pHs. Since changes in pH will change the concentration of potential determining ions, the magnitude of the surface charge generated will change and so the magnitude of the zeta potential will change. Measurements of these changes in the potential will indicate the change in the repulsive force of particle interaction. The empirical theory then implies that if for any pH the zeta potential is greater than 25.7 mV then the suspension will be stable at that point. Again, however, this does not indicate stability for multicomponent systems and does not address the kinetic aspect of stability. A solution of the interparticle potentials for multicomponent systems is therefore needed together with a means of incorporating the kinetic aspect of stability.

For the case of nonidentical particles with varied potential, an exact solution of the Poisson-Boltzmann equation is extremely difficult or impossible (71). Consequently, approximate solutions of the Poisson-Boltzmann equation must be made for nonidentical particles. One of the first solutions for nonidentical particles was in the mid 1950's by Derjaguin (54) who extended DLVO theory to systems with nonidentical particles. Other extensions of the DLVO theory to systems with nonidentical particles were made by Bierman (61) and by Devereux and de Bruyn (55).

These solutions, however required extensive numerical or graphical iterations making them extremely difficult to apply to actual systems (53).

In the mid 1960's, Hogg, Healy, and Fuerstenau built upon DLVO theory to develop a quantitative kinetic stability theory for nonidentical particles which was more easily applied to actual systems (53). Their solution was for systems in which the particle potentials remain constant. Their theory has come to be known as HHF theory. HHF theory uses the same approach to describe the total potential energy of interaction as DLVO theory, but uses an expanded attraction and repulsion force equations in order to take into account the differences between the two different particle types. The attraction force equation then becomes:

$$V_A = -\frac{A a_1 a_2}{6(a_1+a_2)H} \qquad [35]$$

where: H = interparticle distance
A = Hamaker constant (from Equation [5])
a_i = radius of particle of type i.

In developing an equation to describe the repulsive energy of interaction, the linear form of the Debye-Hückel form of the Poisson-Boltzmann equation (Equation [31]) is used just as in DLVO. In the development of the HHF theory, though, Hogg, et al. show that the approximation is good for ψ_1 and ψ_2 values of less than 50 to 60 mV as opposed to the less than 25 mV that is assumed in DLVO.

To solve Equation [31] in HHF the two different types of particles are treated as two plates separated by a distance, 2d, with the boundary conditions:

$$\psi = \psi_{o_1} \text{ as } x \to 0$$

$$\text{and}$$

$$\psi \to \psi_{o_2} \text{ as } x \to 2d.$$

The solution then becomes:

$$\psi = \psi_{o_1} \cosh(\kappa x) + \left(\frac{\psi_{o_2} - \psi_{o_1} \cosh(2\kappa d)}{\sinh(2\kappa d)}\right). \qquad [36]$$

The energy of repulsion for HHF was then found using Derjaguin's method (68, 69), as in DLVO:

$$V_R = \epsilon_o \epsilon_R \pi \left(\frac{a_1 a_2}{(a_1 + a_2)}\right) (\psi^2{}_{o_1} + \psi^2{}_{o_2}) * \qquad [37]$$
$$\left[\frac{2\psi_{o_1}\psi_{o_2}}{\psi^2{}_{o_1} + \psi_{o_2}} \ln\left(\frac{1+\exp(-\kappa H)}{1-\exp(-\kappa H)}\right) + \ln(1-\exp(-2\kappa H))\right].$$

The total potential energy as a function of interparticle distance for two nonidentical spherical particles is calculated by using Equation [35] and [37] to solve Equation [16] as a function of varying separation distance, H.

In order to better describe the effects of mutual agglomeration and to develop a quantitative theory for the overall kinetic stability of the system of nonidentical particles, Hogg et al. (53) develop a variable, W_t, which is similar to an equation by Fuchs (72):

$$W_t = [\frac{n^2}{W_{11}} + \frac{(1-n)^2}{W_{22}} + \frac{2n(1-n)}{W_{12}}]^{-1} \qquad [38]$$

where: n = overall proportion of particle type 1
n^2 = probability type 1 particles will encounter each other
(1-n) = overall proportion of particle type 2 in the system.

The factor, W_t, is a factor by which rapid coagulation, as described by von Smoluchowski (73, 74), is slowed due to a potential barrier to coagulation caused by the repulsive potential energy of particle interactions (33, 34). This factor is called the stability ratio and is essentially the ratio of particle collisions to collisions resulting in coagulation (25). For identical particles with radius, a, and a distance of separation, r, (measured from particle center to particle center) Fuchs showed the stability ratio to be (34):

$$W = 2a\int_{2a}^{\infty} \exp(\frac{V}{kt}) \frac{dr}{r^2}. \qquad [39]$$

For two nonidentical particles of radius, a_i and a_j, the stability ratio becomes:

$$W_{ij} = (a_i + a_j) \int_{a_i+a_j}^{\infty} \exp(\frac{V}{kt}) \frac{dr}{r^2}. \qquad [40]$$

As previously stated the HHF solution of repulsive interparticle potential was for systems in which particle potentials remain constant, Wiese and Healy later derived a similar solution with the same form as the constant potential form for systems with particle charges which remain constant (56):

$$V_R=\epsilon_0\epsilon_R\pi\left(\frac{a_1a_2}{a_1+a_2}\right)\left(\psi^2_{o_1}+\psi^2_{o_2}\right)*\left[\frac{2\psi_{o_1}\psi_{o_2}}{\psi^2_{o_1}+\psi^2_{o_2}}\ln\left(\frac{1+\exp(-\kappa H)}{1-\exp(-\kappa H)}\right)-\ln(1-\exp(-2\kappa))\right]. \quad [41]$$

Kar, Chander and Mika used an approach similar to the one used by Hogg, et al. and developed a solution for systems in which one of the components has constant charge and the other one has constant potential (75). Barouch and Matijević have done work with various others (57-60) to develop an extremely complex quantitative theory to describe the interaction potential for nonidentical particles that uses an approximate solution of the Poisson-Boltzmann equation in its two dimensional form by assuming constant potential.

In their work Barouch and Matijević (59) compare the results of their solution for the interaction potential with that of Hogg, Healy and Fuerstenau (53). The authors say that the two models agree fairly well for unlike particles with potentials of opposite sign and similar magnitudes, but claim that for particles with the same sign and different magnitudes the HHF equation overestimates the interparticle repulsion. However, the model developed by Barouch, Matijević et al. is extremely complex mathematically and its solution is quite complicated involving intricate use of various algorithms as the authors acknowledge (60).

With all of these different models of the repulsive interaction for unlike particles the HHF method, though, still remains as the only quantitative theory for the overall stability of a system of nonidentical particles. This overall method is therefore best suited for use in prediction of suspension stability. Another advantage of this method is that various different adjustments can be made within the model to help improve the fit of the method's stability prediction. One of the first adjustments which could be made would be to use zeta potential data for the particle potential, ψ, instead of using point of zero charge data to calculate a surface potential, as was done originally by Hogg, et al (53). This would be an improvement since calculation of the surface charge from point of zero charge data requires use of a model for surface charge generation which requires considerable knowledge of ion groups present on the particle surface and how these groups react with the medium to generate charge Zeta potential, on the other hand, is simply an experimental measurement which requires little knowledge about the particle, other than particle size and density (67), has recently become a more common measurement technique and has recently become a much easier measurement than in the past

(67, 70). Other adjustments which could be made would be alternate expressions for attraction and repulsion potential as well as alternate methods for calculating the Hamaker constant.

EXPERIMENTAL PROCEDURE

A model was used to predict the stability of suspensions over a given pH range which was an adaptation of a method originally developed by Hogg, Healy and Fuerstenau (53). The adaptation included several changes or adjustments to the original method. The first of these was the use of zeta potential vs. pH data for the potential, ψ, instead of using a surface potential calculated at the given pH, a calculation which relies on models for surface charge generation and point of zero charge data. Another change or adjustment was the use of an effective Hamaker constant (Equation [5]) instead of just using an in vacuo Hamaker constant. This allows the effect of the medium to be taken into account in reducing interparticle attraction. Along with this is the addition of the Lifshitz method for calculating Hamaker constants (Equation [3]) since a method for their calculation was not addressed by the original theory.

Another change was the use of an expanded expression for the potential of interparticle attraction (Equation [1]) instead of the equation used in the original method (Equation [35]) which is a simplification of Equation [1] which assumes small particle separation. For the potential of interparticle repulsion the original HHF equation (Equation [37]) was used although, the constant charge solution of Wiese and Healy (Equation [41]) (56) was used in some cases.

The repulsion equation was not changed for several reasons. The first reason was that the equation was reported to be accurate in many cases (59). The second was that use of this constant potential equation made substitution of a constant charge solution (namely that of Wiese and Healy) quite simple due to the almost identical nature of the two equations. Another reason was that other solutions for interparticle repulsion which are reported to be more accurate (59), require very elaborate calculation schemes which would have required much more calculation time than needed with the HHF equation. The final reason was that even if the equation proved unsatisfactory it could easily be substituted for in later versions of this adapted method.

The equation for total overall kinetic stability (Equation [38]) and the equation for the stability factor (Equation [40]) were used as in the original method. However, instead of using the overall relative proportion of particles of type 1 in the system, n, as a system input as in the original method, a relationship was derived which related the relative volume fraction of particle of type 1 to type 2 and the particle radii to the overall number proportion, n. This derivation which can be found in appendix A allowed use of the relative volume fraction of components as an input. This was an improvement since, from an experimental viewpoint, volume fraction is a much more realistic and useful quantity than number fraction.

With the adapted method described, the total overall kinetic stability at a certain pH was calculated by solving Equation [38]. For the equation n was found by using input values for particle radii and relative component volume fraction to solve Equation [A11] and was W_{ij} found by solving Equation [40]. The solution of Equation [40] was found by using particle radii, the input temperature and total interparticle potential vs. separation distance to integrate from a minimum separation distance (a_i+a_j) to an infinite separation distance. The interparticle potential was found using the solutions for the attractive potential described by Equation [1] and the repulsive interaction potential described by Equation [37] (or Equation [41]) to solve Equation [16] for different separation distances. Solving Equation [1] required particle radii input data and effective Hamaker constants which were found by solving Equation [5] using input Hamaker constants. The input Hamaker constants were either calculated values found by using dielectric constant data to solve Equation [3] or were values found in the literature. Solving Equation [37] (or

Equation [41]) required use of input particle radii and zeta potential versus pH data along with the Debye-Hückel parameter. The value for this parameter is calculated by using the input bulk monatomic ion concentration and temperature data to solve Equation [30] All electrolytes, acids and bases are assumed to be monatomic with this method, but this assumption could be eliminated in future versions.

The input data necessary for using this method were in vacuo Hamaker constants, particle radii, relative component volume fraction, concentration of monatomic electrolyte, temperature, zeta potential data as a function of pH, and finally the pH range where stability calculations were performed. A computer program was necessary to perform these calculations since, to calculate the total overall stability ratio at just one pH, it would be necessary to calculate the stability ratio, W_{ij}, for each of the three different types of particle interactions (i.e. W_{11}, W_{12}, W_{22}). Theoretically, this would require integration to infinity and evaluation of the attractive and repulsive interactions to infinity. This would have to be repeated for each pH.

The computer program was written in Fortran code for use on a PC. The program code was edited using Personal Editor (version 4.21) and was compiled using Microsoft Fortran Compiler (version 5.00.03). The program consisted of a main program and ten separate subroutines. Computer flow diagrams can be found in Figures 3 though 11 and list files of the code can be found in appendix B. The program was run from a DOS operating system batch file which allowed the program to run many times successively with different input data without requiring the operator to wait for one program run to end in order to input new data as normal program lasted anywhere from 30 minutes to 2 hours.

The program starts with the main program, STABILITY PREDICTION. The input data is read into the program from a file by the subroutine FDATA INPUT. The subroutine CALCZP calculates the total overall stability ratio at each pH using zeta potential data. Subroutine WKO finds the stability ratio for each of the possible interaction types and at each pH writes the interparticle potential vs. separation distance data for each of the different interactions to an ASCII data file. The subroutine WC actually calculates the stability ratio for a given interaction and returns the value to subroutine WKO. Integrating to infinity was accomplished by integrating in interval steps to avoid integrating infinity. When integration passed a minimum limit of integration,it was allowed to stop before infinity if the area added by a certain interval steps of integration was smaller than a specified tolerance. This decreased program time with the introduction of minimal error. The actual integration was done using Simpson's rule in subroutine SI. The values for

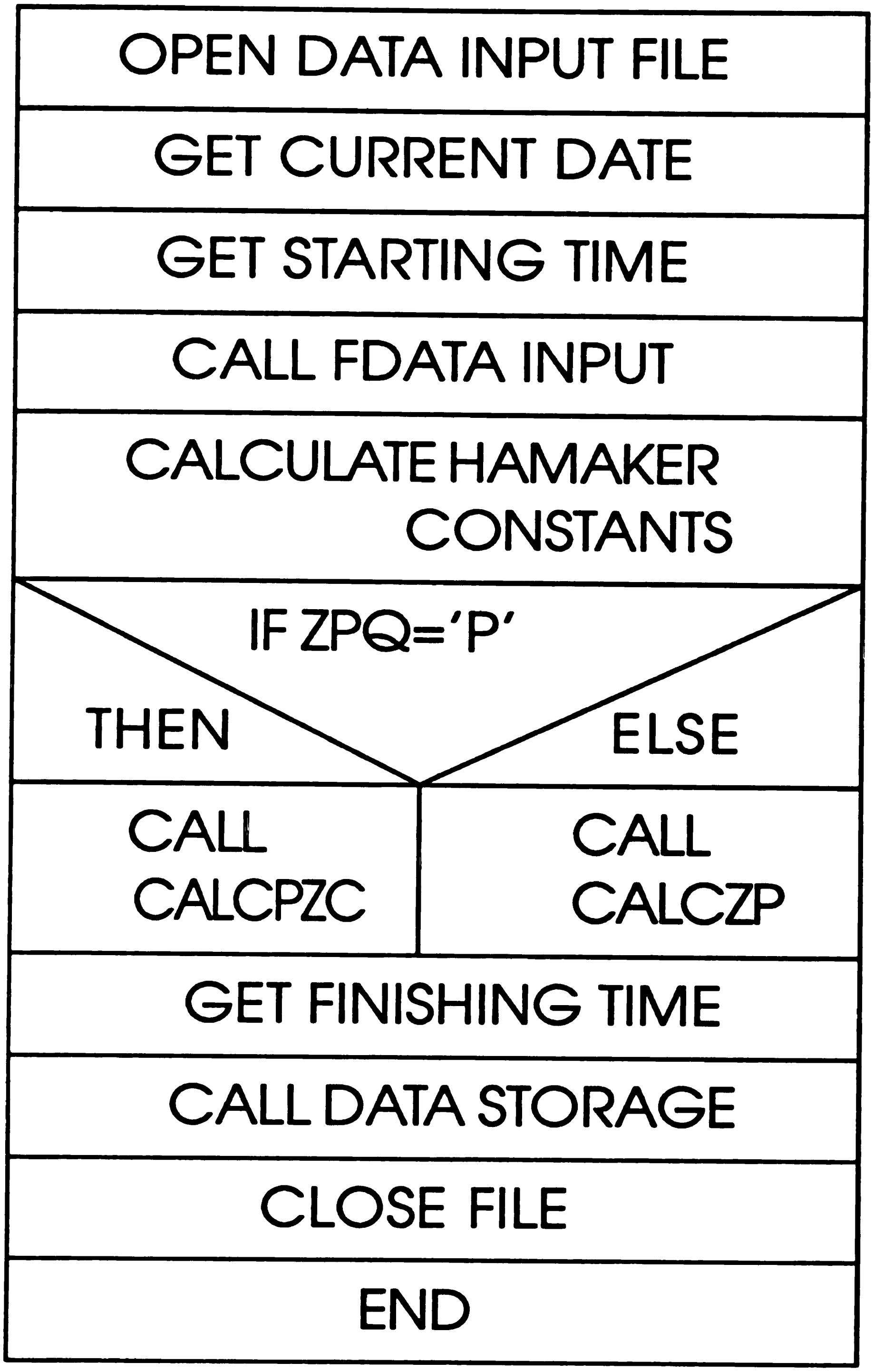
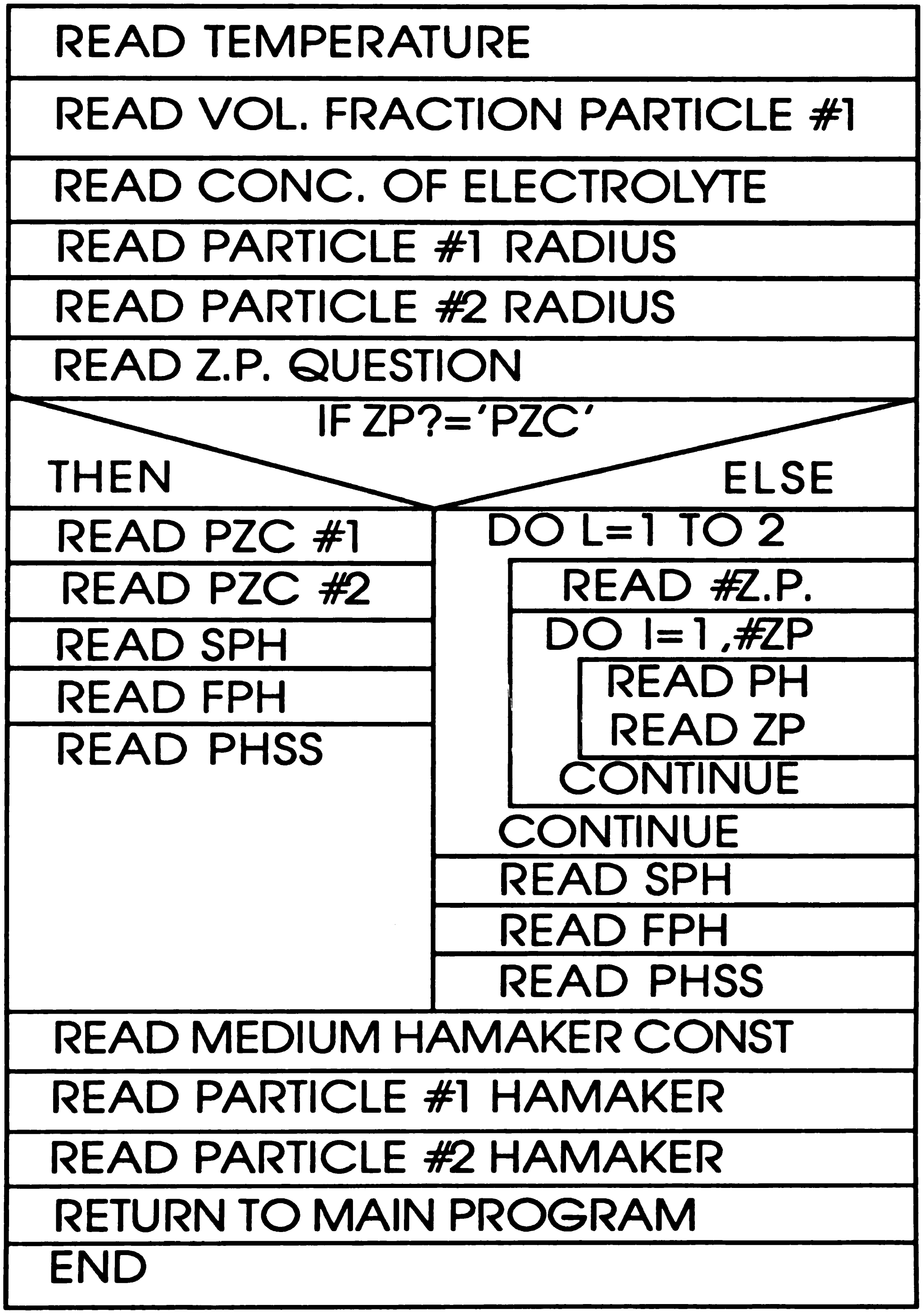
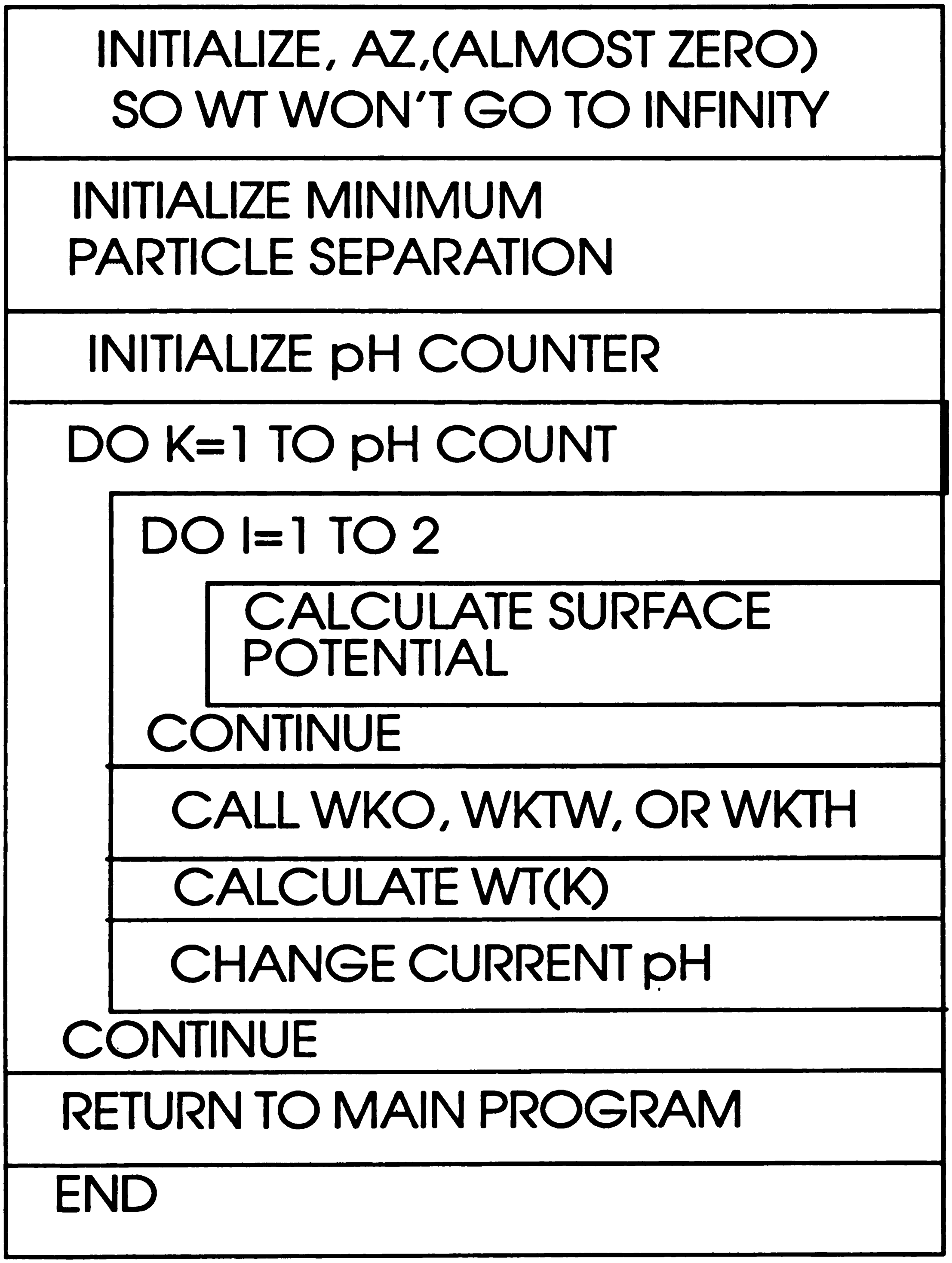


Figure 3 Computer flow diagram for main program STABILITY PREDICTION.



```
READ TEMPERATURE
READ VOL. FRACTION PARTICLE #1
READ CONC. OF ELECTROLYTE
READ PARTICLE #1 RADIUS
READ PARTICLE #2 RADIUS
READ Z.P. QUESTION
IF ZP?='PZC'
THEN
    READ PZC #1
    READ PZC #2
    READ SPH
    READ FPH
    READ PHSS
ELSE
    DO L=1 TO 2
        READ #Z.P.
        DO I=1,#ZP
            READ PH
            READ ZP
        CONTINUE
    CONTINUE
    READ SPH
    READ FPH
    READ PHSS
READ MEDIUM HAMAKER CONST
READ PARTICLE #1 HAMAKER
READ PARTICLE #2 HAMAKER
RETURN TO MAIN PROGRAM
END
```

Figure 4 Computer flow diagram for subroutine FDATA INPUT.



```
INITIALIZE, AZ,(ALMOST ZERO)
SO WT WON'T GO TO INFINITY
INITIALIZE MINIMUM
PARTICLE SEPARATION
INITIALIZE pH COUNTER
DO K=1 TO pH COUNT
    DO I=1 TO 2
        CALCULATE SURFACE
        POTENTIAL
    CONTINUE
    CALL WKO, WKTW, OR WKTH
    CALCULATE WT(K)
    CHANGE CURRENT pH
CONTINUE
RETURN TO MAIN PROGRAM
END
```

Figure 5 Computer flow diagram for subroutine CALCPZC.

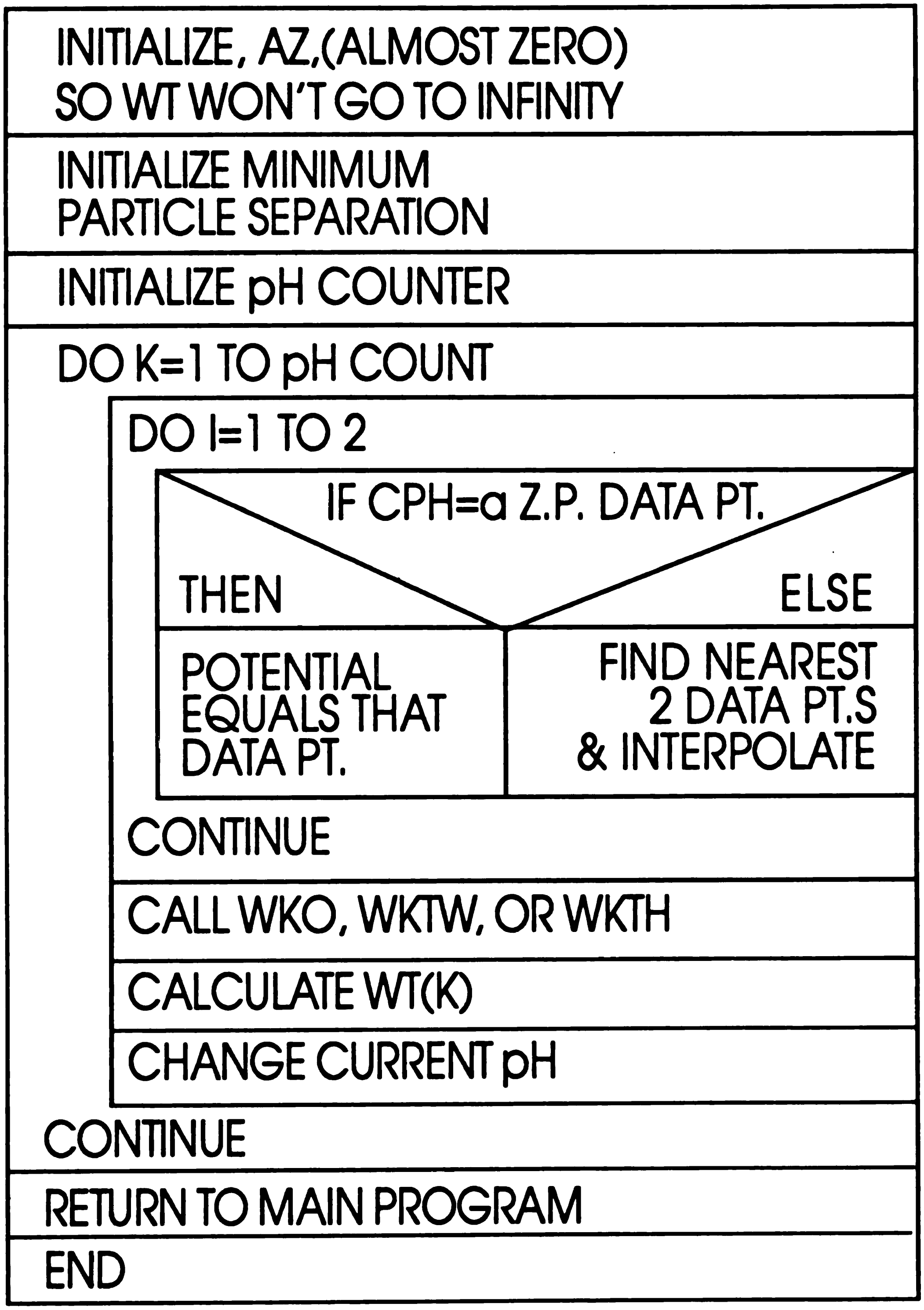


Figure 6 Computer flow diagram for subroutine CALCZP.

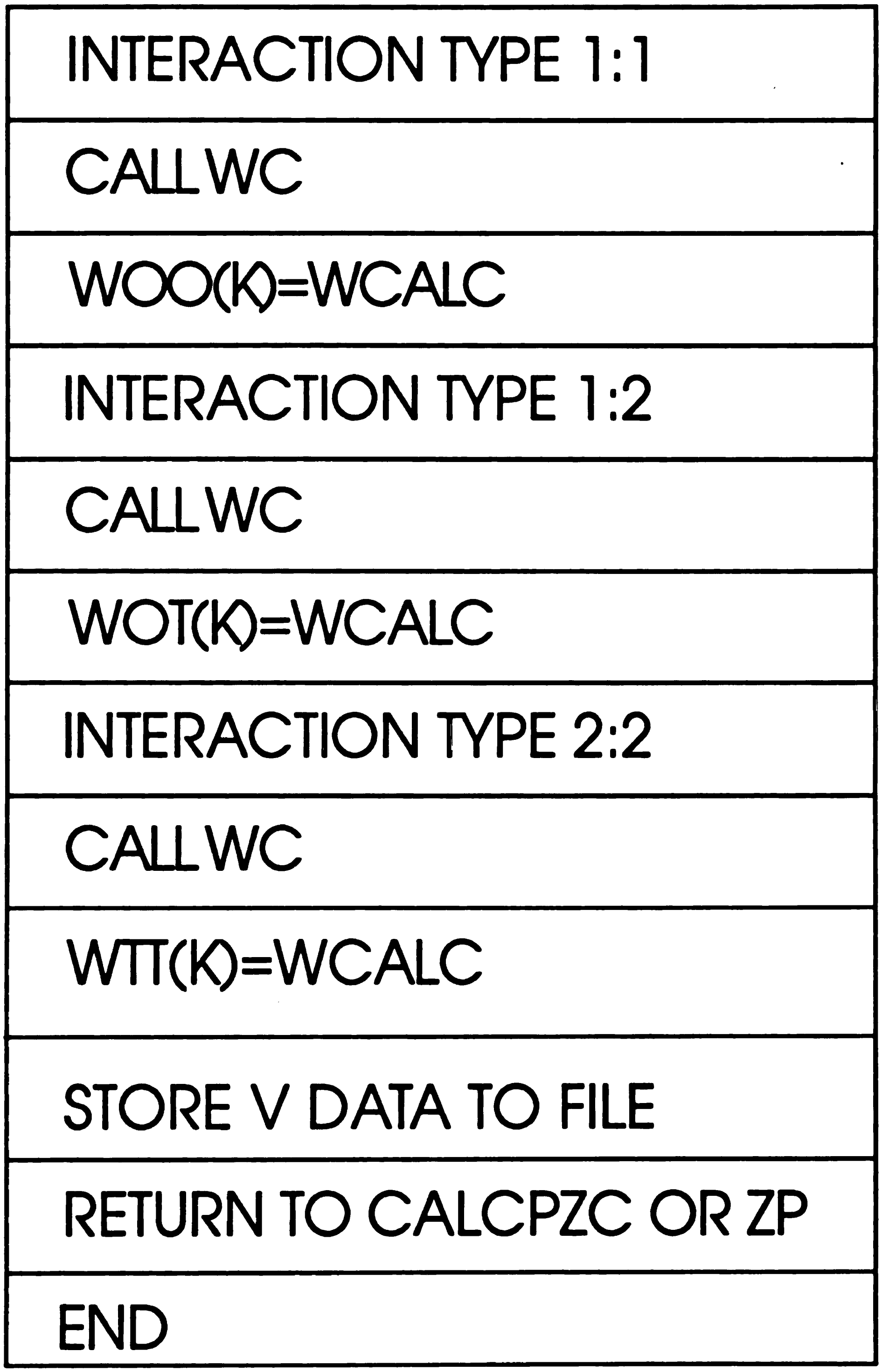


Figure 7 Computer flow diagram for subroutine WKO.

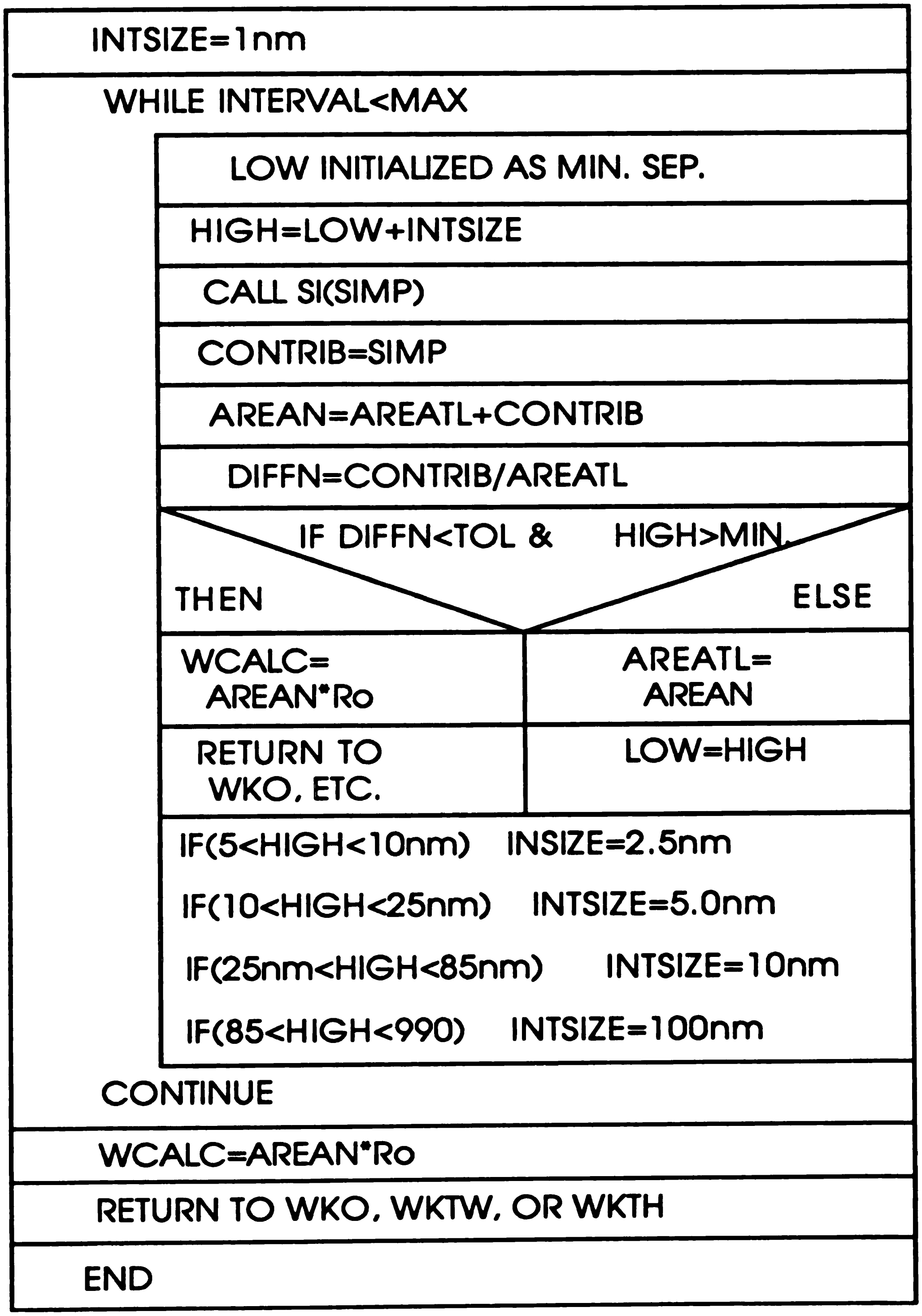
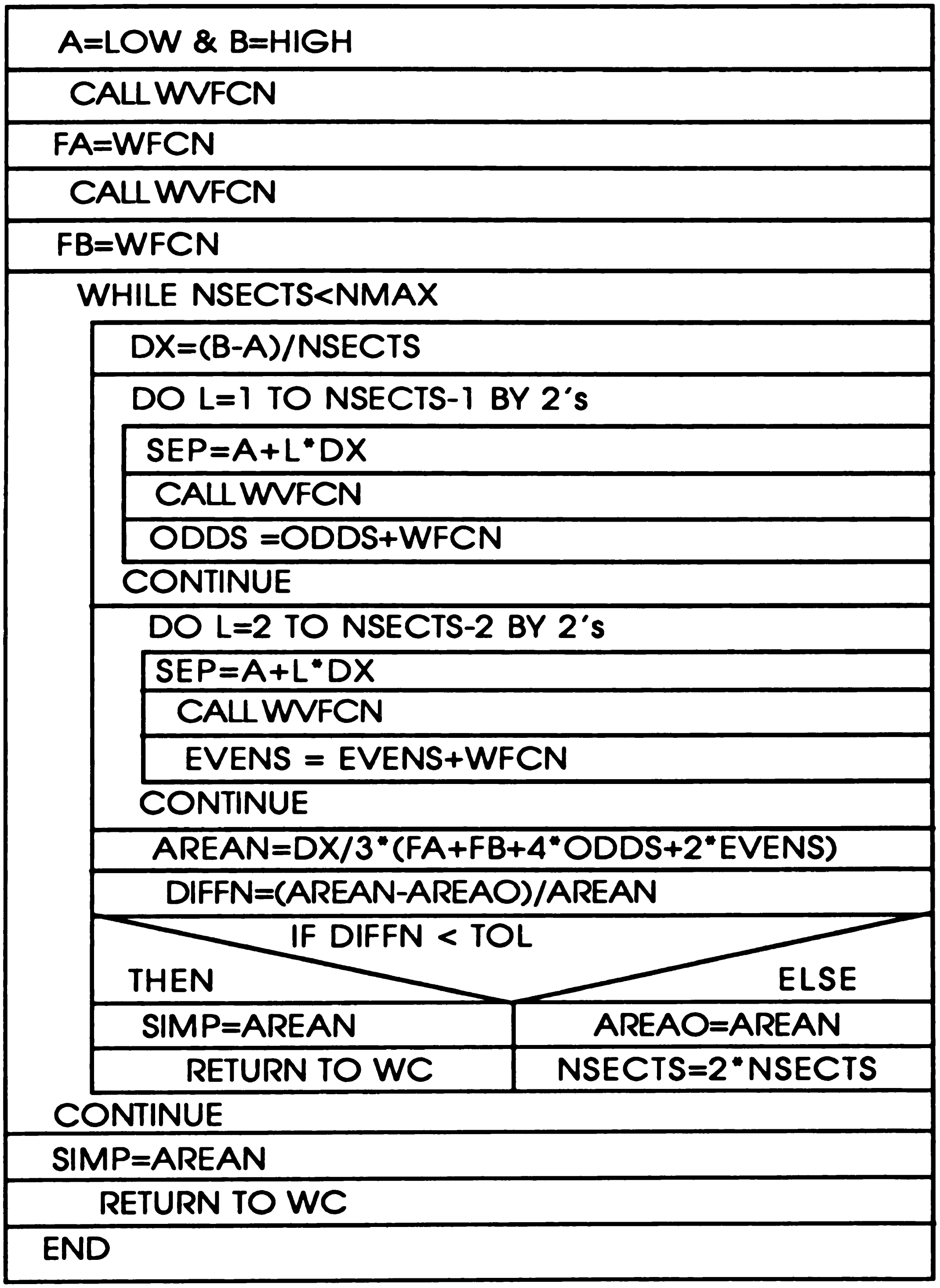


Figure 8 Computer flow diagram for subroutine WC.



```
A=LOW & B=HIGH
CALL WVFCN
FA=WFCN
CALL WVFCN
FB=WFCN
WHILE NSECTS<NMAX
    DX=(B-A)/NSECTS
    DO L=1 TO NSECTS-1 BY 2's
        SEP=A+L*DX
        CALL WVFCN
        ODDS =ODDS+WFCN
    CONTINUE
    DO L=2 TO NSECTS-2 BY 2's
        SEP=A+L*DX
        CALL WVFCN
        EVENS = EVENS+WFCN
    CONTINUE
    AREAN=DX/3*(FA+FB+4*ODDS+2*EVENS)
    DIFFN=(AREAN-AREAO)/AREAN
    IF DIFFN < TOL
    THEN
        SIMP=AREAN
        RETURN TO WC
    ELSE
        AREAO=AREAN
        NSECTS=2*NSECTS
CONTINUE
SIMP=AREAN
RETURN TO WC
END
```

Figure 9 Computer flow diagram for subroutine SI.

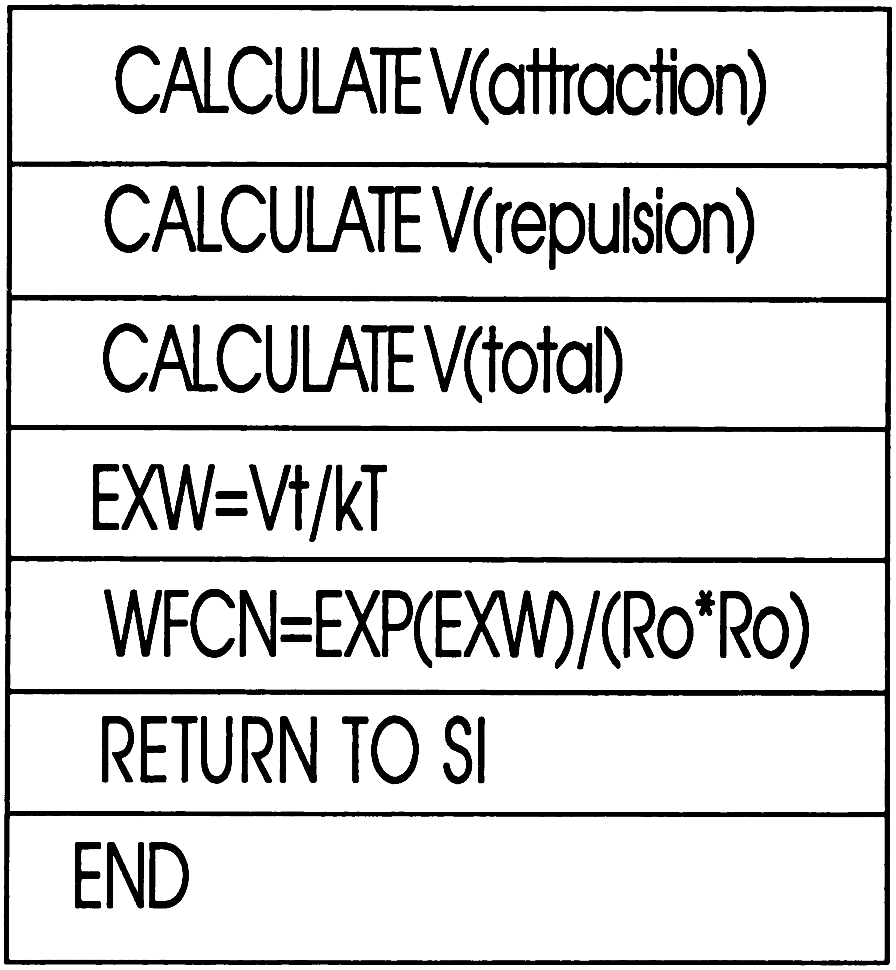


Figure 10 Computer flow diagram for subroutine WVFCN.

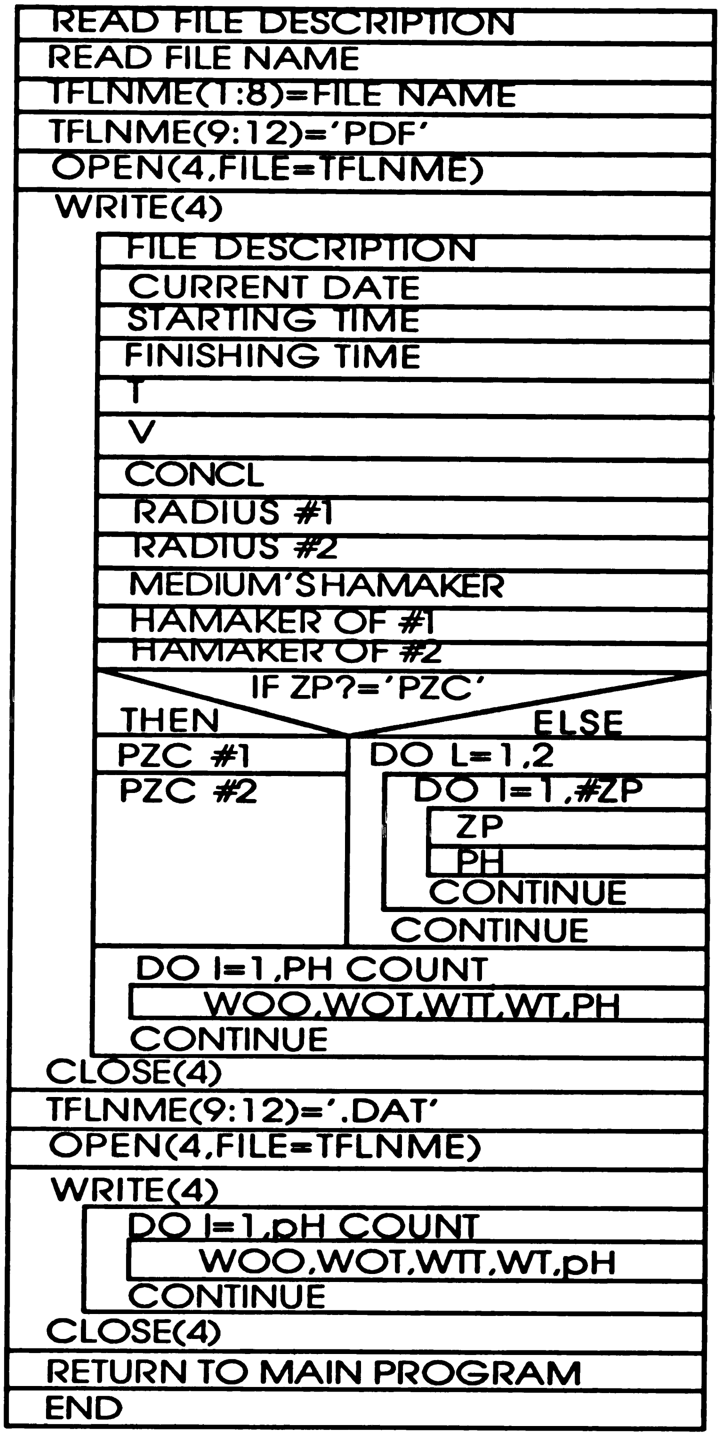


Figure 11 Computer flow diagram for subroutine DATA STORAGE.

the evaluation of the integral were calculated by the subroutine WVFCN.

Much care in writing the program was taken since values for the variables used in the program often approached zero or infinity leading to fatal math overflow errors and premature termination of the program. Checks and corrections for values which were becoming too large or small in magnitude were written into most of the subroutines.Once all the calculations were made the data was then stored in ASCII data files by subroutine DATA STORAGE. This ASCII data was later imported into a plotting program, Harvard Graphics (version 3.0), in order to plot the data. This allowed for more flexibility for the final graphical form of the data than if the data were plotted directly in the Fortran program itself.

Systems for which the program was applied were the SiC powder/Si_3N_4 powder system and the FeAl powder/Al_2O_3 fiber system. Extensive work was done with the SiC/Si_3N_4 system since much was known about the colloidal and surface characteristics of the system due extensive investigations of this system by Crimp (76, 77). For this system there were three different SiC powders used, all of which were α-SiC and manufactured by Lonza Inc. The three types used were LS-5, UF-10 and UF-15 for which the manufacturer reported 50% cumulative mass percent of particles with diameters finer than 5.5, 1.8, and 0.8 microns, respectively. The Si_3N_4 used was an α-Si_3N_4 manufactured by UBE. The type used was SN-E10 which the manufacture reports has an average particle diameter of 0.5 microns.

This system was suspended in deionized water which had a variable indifferent electrolyte concentration of 10^{-2} M, 10^{-3} M and 10^{-5} M. The indifferent electrolyte used was KNO_3 and the bulk of the work was carried out with an electrolyte concentration of 10^{-3} M. The pH was varied for this system by the addition of HNO_3 and KOH. The systems were dispersed using an ultrasonic probe which would eliminate previous particle agglomeration.

The zeta potential data used in this investigation was of two different types. The first was microelectrophoresis zeta potential data previously collected by Crimp (70) using a PEN-KEM SYSTEM 3000 automated electrokinetics analyzer. These data were collected for the SN-E10 Si_3N_4 and the UF-10 SiC at all three different electrolyte concentrations mentioned above. These data is shown in Figures 12 and 13. The data shown in Figure 13 stop at pH 5 since the zeta potential values level off (70) at this point. A logarithmic regression was done in order to extend this data to higher pHs using the standard logarithmic regression program of a HP-11C calculator and is shown in Figure 14. The other type of data used was Electrokinetic Sonic Amplitude (ESA) zeta potential data collected in this investigation using a Matec ESA-8000 system.ESA zeta

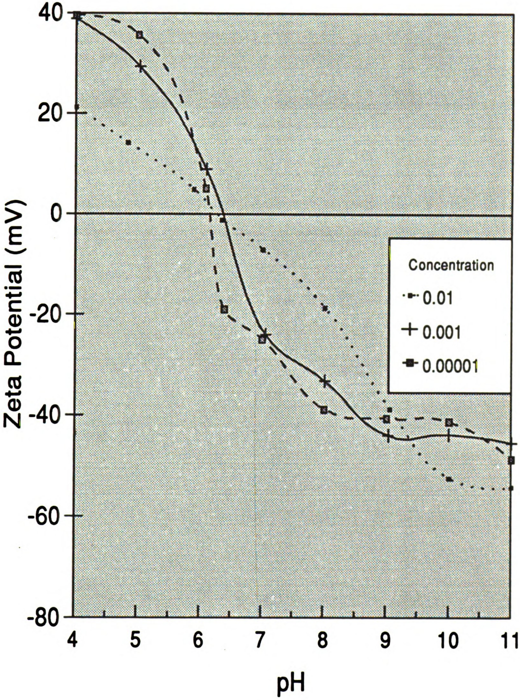


Figure 12 Electrophoretic zeta potential measurents for SN-E10 Si_3N_4 at varing electrolyte concentrations (M).

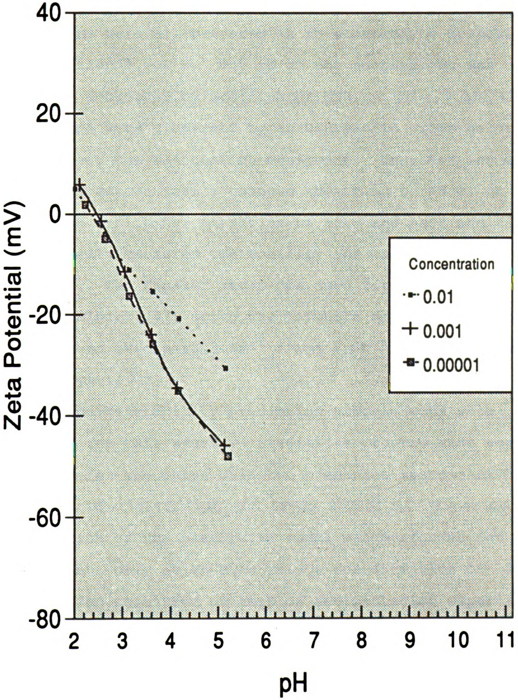


Figure 13 Electrophoretic zeta potential measurents for UF-10 SiC at varing electrolyte concentrations (M).

potential measurements were performed on all of the different types of SiC powders and on the Si_3N_4 powder. The suspensions were all prepared in an electrolyte solution of concentration 0.001 M. The pH of the suspensions was initially decreased by addition of HNO_3 to pH 4.0 and the suspensions were dispersed by an ultrasonic probe before loading into the ESA testing equipment. Once testing began, the system automatically changed the pH up to pH 11 or back down to pH 4 with the titration of acid and base and also automatically measured the mobility and calculated the zeta potential. The Hamaker constants used for this system were found by Bleier (47) using the Lifshitz method. The values reported and used were $3.0E^{-19}$ J and $1.6E^{-19}$ J for SiC and Si_3N_4, respectively.

Extensive stability prediction program runs were performed for this system. Predictive program runs were performed for the three main two component systems of LS-5 SiC/Si_3N_4, UF-10 SiC/Si_3N_4 and UF-15 SiC/Si_3N_4. Experimental verification of the predictive model was performed for these systems, but only at an electrolyte concentration of 10^{-3} M. Verification consisted of sets of sedimentation experiments. Sedimentation experiments were performed for single component suspensions of each of the four powder types as well as for suspension of each of the three main two component systems listed above which were done with equal relative volume for each of the components. One more two

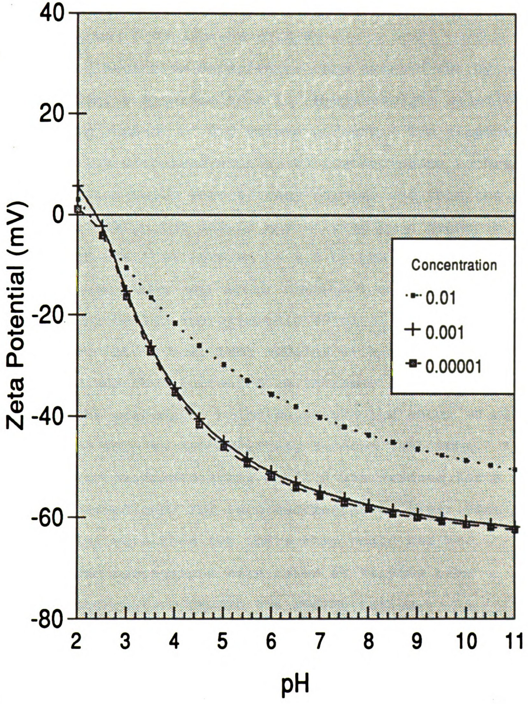


Figure 14 Electrophoretic zeta potential measurents for UF-10 SiC at varing electrolyte concentrations (M) with regression analysis.

component sedimentation experiment was performed for the UF-10 SiC/Si_3N_4 system in which the relative volume fraction of SiC to Si_3N_4 was 0.75 instead of 0.5.

The sedimentation experiments were carried out by making a 500ml suspension in a 10^{-3} M electrolyte solution with a solid content of 0.5 volume percent. The suspensions were initially dispersed with an ultrasonic probe to break up agglomerates which were already formed, and then the pH was measured while the sample was stirred by a magnetic stir bar. The pH was then lowered to 4.0 by the addition of HNO_3. The suspension was again dispersed with the ultrasonic probe and approximately 40 ml of the suspension being poured into a test tube labeled with the appropriate pH. The pH was then increased in increments of half of a pH unit with the suspension being sonicated and about 40 ml being poured into an appropriately labeled test tube. This procedure was performed until pH 11.0 was reached for a total of 15 specimens for each sedimentation experiment set. These samples were then set where they would not be disturbed and photographs were taken at varying time intervals in order to record the sedimentation.

The other system of FeAl/Al_2O_3 fiber was investigated in only a preliminary manner in order to predict the ideal pH for processing at which the individual components would be stable, but at which heterocoagulation occurs (i.e. where the powder and fiber are attracted to each other, but not to themselves). The FeAl powder used was AMDRY FeAl and was manufactured by Alloy Metals, Inc. The as received powder had a particle size range of 177 microns down to tenths of microns. The powder was sedimented down to a size range of 10 microns to tenths of microns through the efforts of Jeff Bajt and Chris Suydam. The average particle diameter was determined to be 7 microns, and a SEM micrograph of this sedimented powder can be seen in Figure 15. The Al_2O_3 fiber was manufactured by DuPont and is a continuous, pure alumina fiber of type Fiber FP. The average fiber diameter was reported by the manufacturer to be 25 to 30 microns which was confirmed by SEM observations. The fibers were chopped up and ground to smaller lengths with mortar and pestle. A SEM micrograph of the chopped fiber can be seen in Figure 16.

This system was also suspended using a KNO_3 electrolyte solution in deionized water and pH changes were made with HNO_3 and KOH as with the previous system, but only a KNO_3 concentration of 10^{-3} M was used. The zeta potential data used for this system was collected in this investigation using the Matec ESA-8000 system. The Hamaker constant for the alumina fiber was calculated from refractive index data (78) using the Lifshitz method (Equation [3]) and found to be $1.1E^{-19}$ J. Since no refractive index or dielectric constant data could be found for the FeAl, the Hamaker constant used was a value for metals given by Shaw (15) to

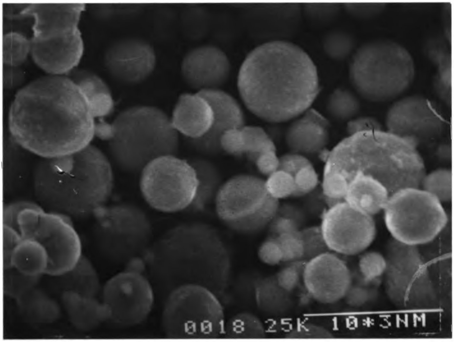


Figure 15 SEM micrograph of sedimented FeAl powder.

Figure 16 SEM micrograph of chopped Al_2O_3 fiber.

be 2.2E^{-19} J.

Three different predictive program runs were performed for the FeAl/Al_2O_3 fiber system. The first was performed using the particle size data mentioned earlier (i.e. particle diameters of 7 microns and 30 microns for the FeAl and alumina fiber, respectively). The other two predictive runs used increasing FeAl particle size to see if larger FeAL particle sizes would also be possible to get the ideal processing conditions of individual component stability coupled with heterocoagulation.

RESULTS

The results for the acoustophoresis (ESA) measurement data for LS-5 SiC, UF-10 SiC, UF-15 SiC and the SN-E10 Si_3N_4 can be seen in Figures 17, 18 19, and 20, respectively. Predictive program runs were performed for the three main two component systems of LS-5 SiC/Si_3N_4, UF-10 SiC/Si_3N_4, and UF-15 SiC/Si_3N_4. The first of these experimental runs was performed using the constant potential repulsive equation and electrophoretic zeta potential data at a concentration of 10^{-3} M. The results of this data run are shown in Figure 21. Another of these experimental runs was performed using the constant potential repulsive equation along with ESA zeta potential data at a concentration of 10^{-3} M. The results of these data run are shown in Figure 22. The constant charge form of the repulsive potential equation was used along with electrophoretic data for an electrolyte concentration 10^{-3} M for the third run for these systems. These results are shown in Figure 23. The interparticle potential vs. interparticle separation distance for each pH of the first data run(i.e. Figure 21) is plotted in Figure 24. A fourth program run was performed which used the constant potential form for the repulsive potential equation

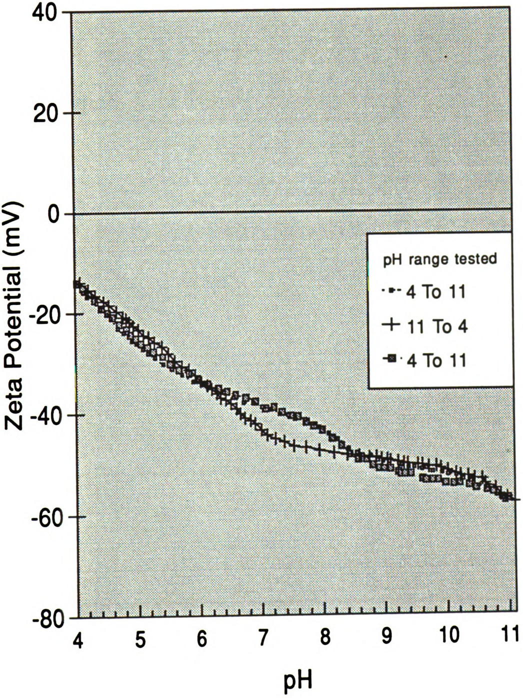


Figure 17 ESA zeta potential measurements for LS-5 SiC at an electrolyte concentration of 10^{-3} M KNO_3.

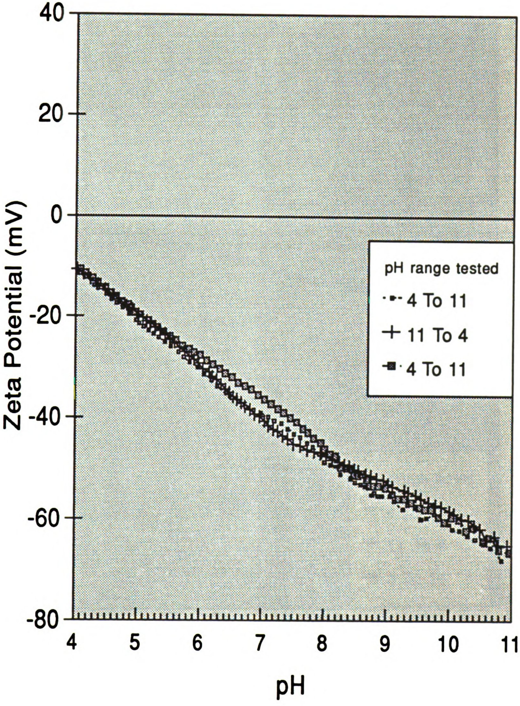


Figure 18 ESA zeta potential measurements for UF-10 SiC at an electrolyte concentration of 10^{-3} M KNO_3.

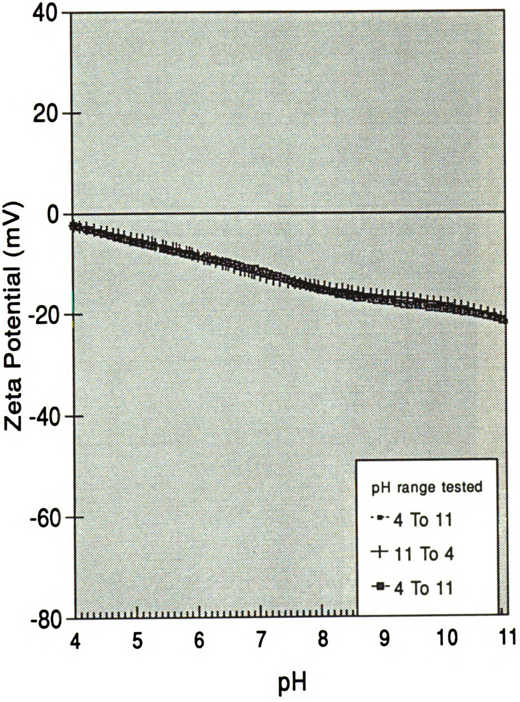


Figure 19 ESA zeta potential measurements for UF-15 SiC at an electrolyte concentration of 10^{-3} M KNO_3.

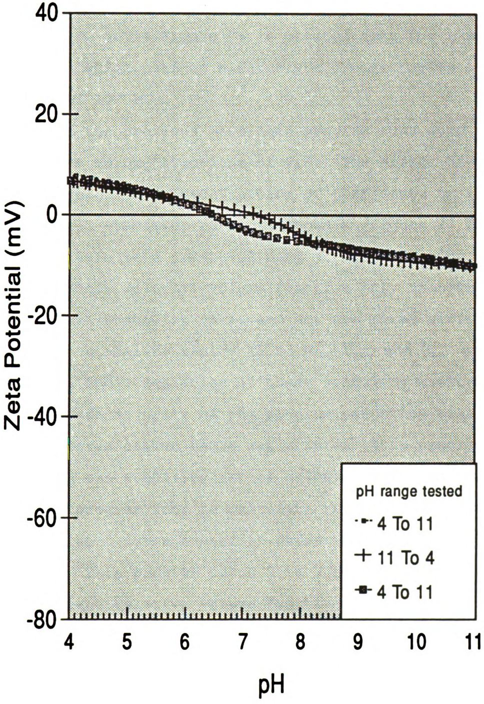
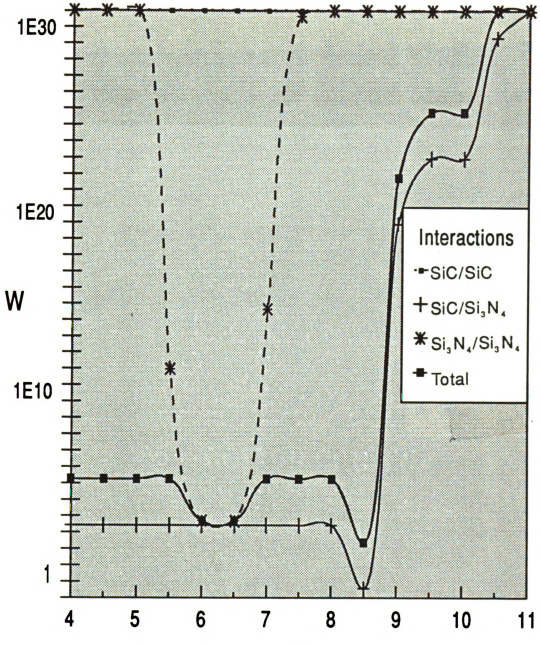


Figure 20 ESA zeta potential measurements for SN-E10 Si_3N_4 at an electrolyte concentration of 10^{-3} M KNO_3.

and used electrophoresis zeta potential data for an electrolyte concentration of 10^{-2} M. This data is plotted in Figure 25, while Figure 26 is plotted data for a similar program run which uses an electrolyte concentration of 10^{-5} M instead of 10^{-2} M.

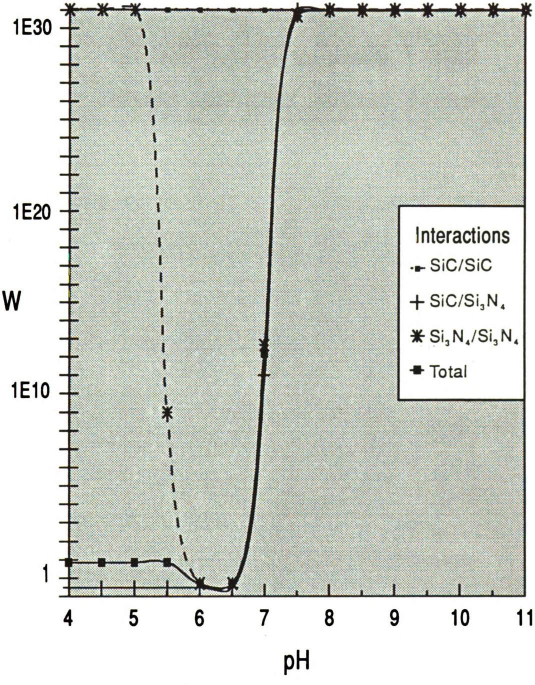
All of the previous mentioned program runs were done for relative volume fractions of 0.5. The effect of different relative volume fraction of components on the total overall stability ratio is shown in Figure 27 for electrophoresis zeta potential data at concentration of 0.001 M. Since relative volume fraction only changes the total overall stability ratio and not the three different interaction stability ratios (i.e. W_{11}, W_{12}, and W_{22}) and since it is the calculation of these stability ratios which takes the vast majority of the program execution time another program called VARYN was written. This program simply uses the stability ratios calculated in the Stability Prediction program runs to calculate the total overall stability ratio for a number of different relative volume fractions. This program takes 2 to 3 seconds to execute five different relative volume fractions as opposed to the Stability Prediction program which takes from 30 minutes to 2 hours per different volume fraction.

Predictive program runs were also performed to see the sensitivity of the programs to variations of the input data. The first of these program runs varied the temperature for



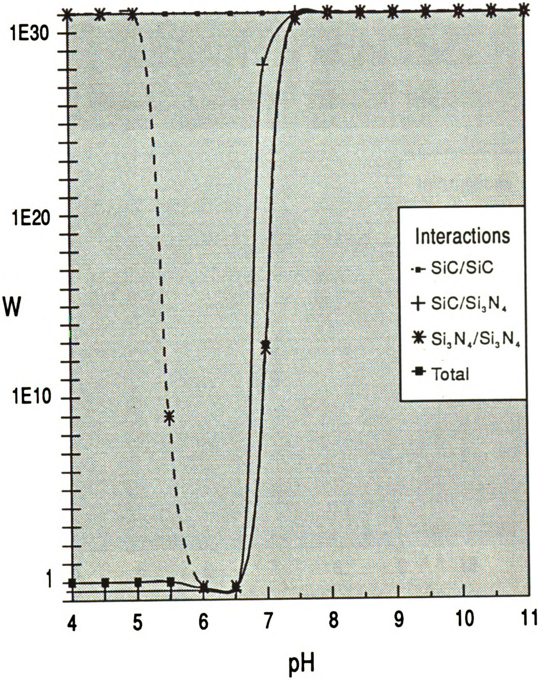
(a)

Figure 21 Stability ratio data from the predictive program using the constant potential repulsive equation and electrophoretic zeta potential for a) LS-5 SiC/SN-E10 Si_3N_4, b) UF-10 SiC/SN-E10 Si_3N_4, and c) UF-15 SiC/SN-E10 Si_3N_4 where: temperature is 25 °C, volume fraction of components is 0.5 and electrolyte concentration is 10^{-3} M KNO_3.



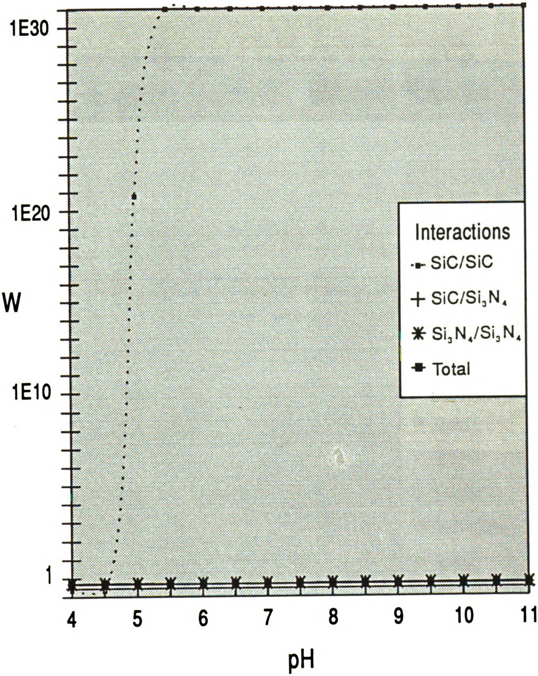
(b)

Figure 21 cont.



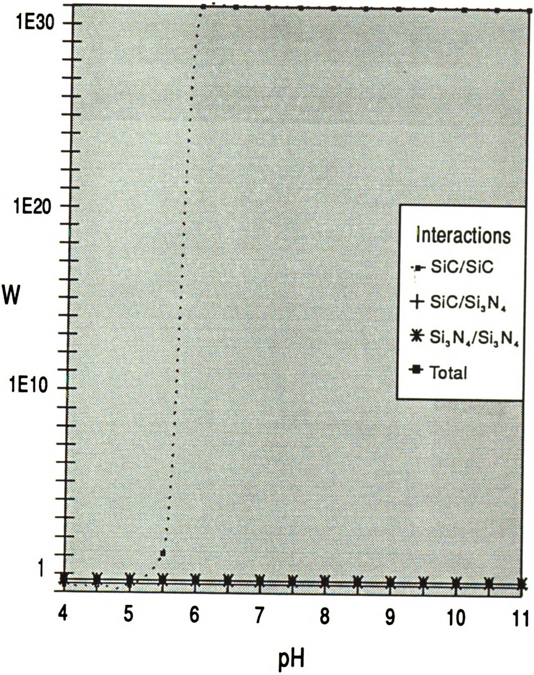
(c)

Figure 21 Cont.



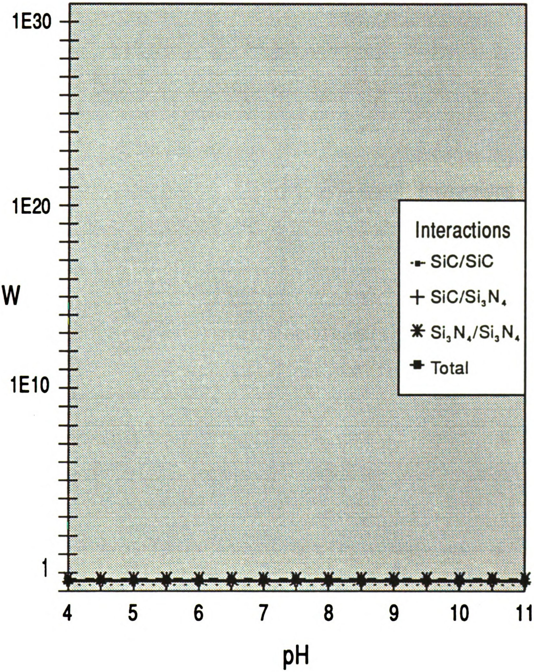
(a)

Figure 22 Stability ratio data from the predictive program using the constant potential repulsive equation and ESA zeta potential for a) LS-5 SiC/SN-E10 Si_3N_4, b) UF-10 SiC/SN-E10 Si_3N_4, and c) UF-15 SiC/SN-E10 Si_3N_4 where: temperature is 25 °C, volume fraction of components is 0.5 and electrolyte concentration is 10^{-3} M KNO_3.



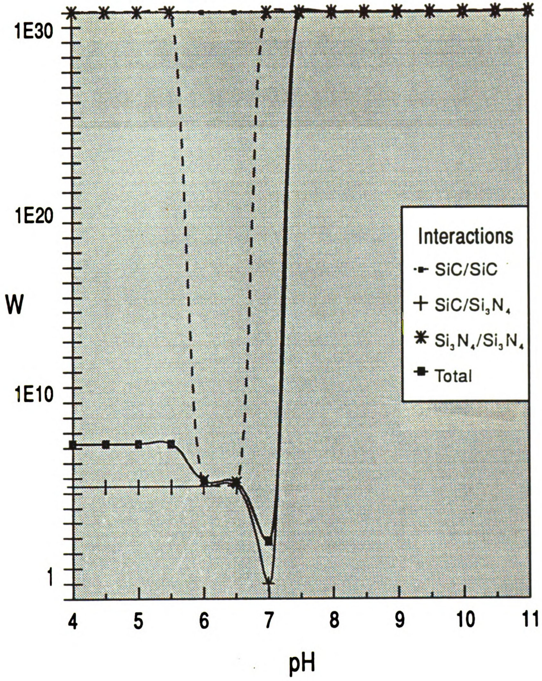
(b)

Figure 22 Cont.



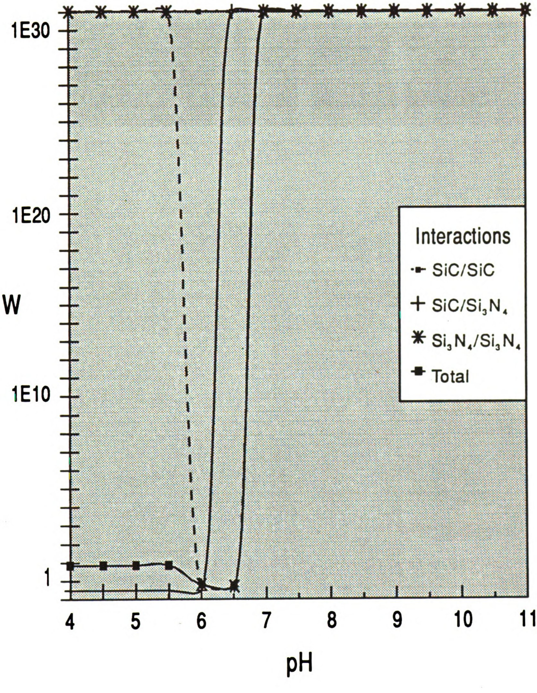
(c)

Figure 22 cont.



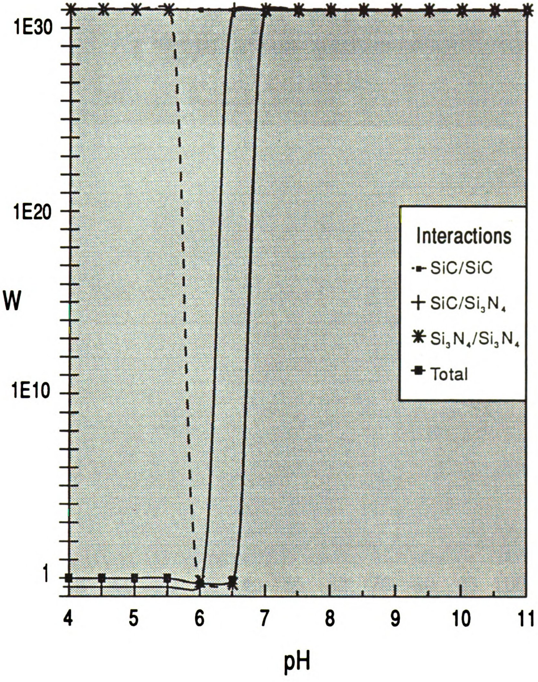
(a)

Figure 23 Stability ratio data from the predictive program using the constant charge repulsive equation and ESA zeta potential for a) LS-5 SiC/SN-E10 Si_3N_4, b) UF-10 SiC/SN-E10 Si_3N_4, and c) UF-15 SiC/SN-E10 Si_3N_4 where: temperature is 25 °C, volume fraction of components is 0.5 and electrolyte concentration is 10^{-3} M KNO_3.



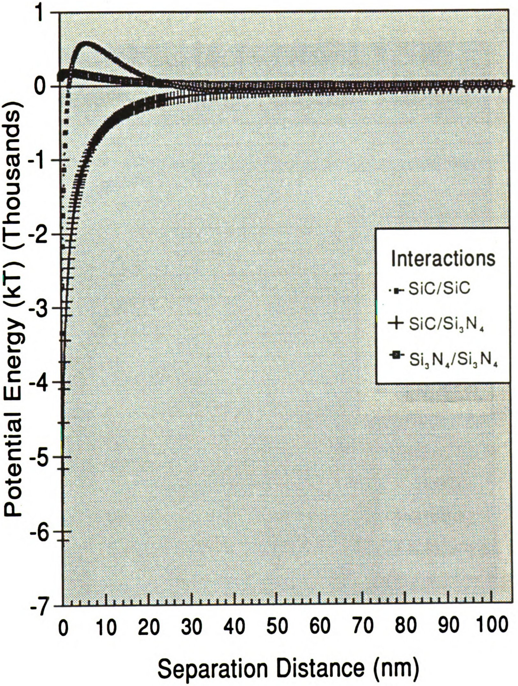
(b)

Figure 23 Cont.



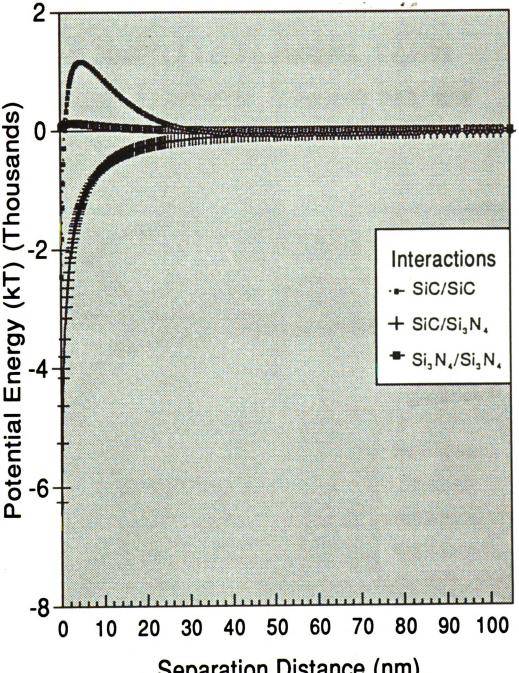
(C)

Figure 23 Cont.



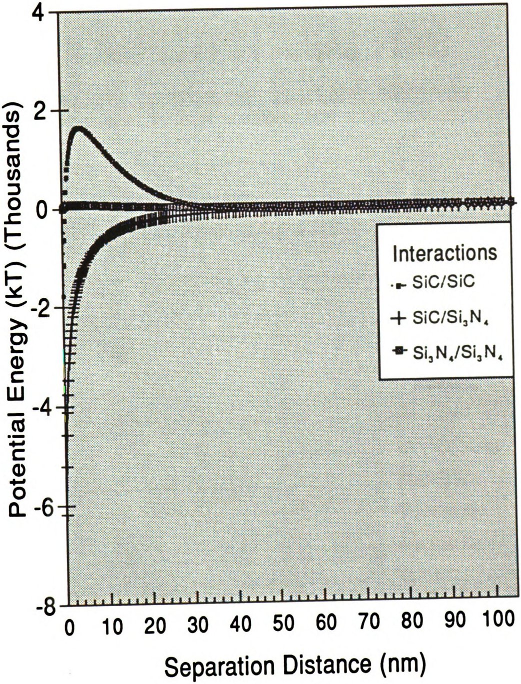
(a) pH=4.0

Figure 24 Interaction potential data from the predictive program using the constant potential repulsive equation and electrophoretic zeta potential for LS-5 SiC/SN-E10 Si_3N_4 where: temperature is 25°C, volume fraction of components is 0.5 and electrolyte concentration is 10^{-3} M.



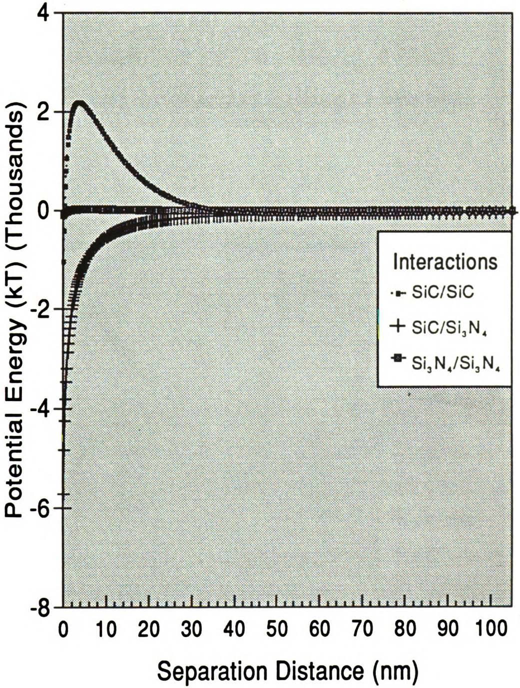
(b) pH= 4.5

Figure 24 Cont.



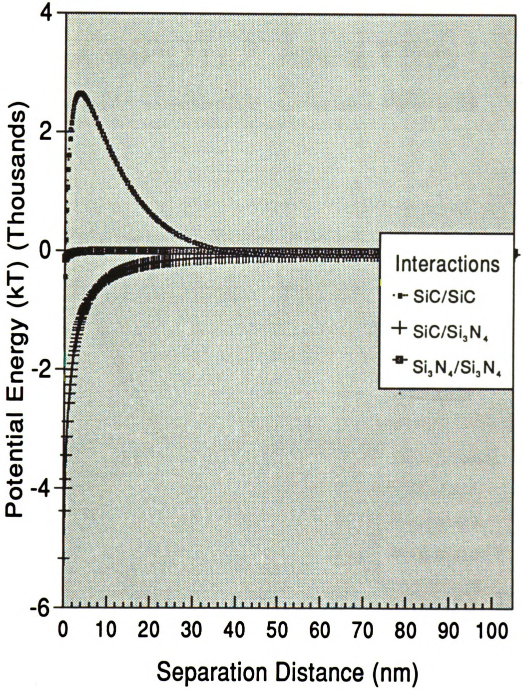
(c) pH= 5.0

Figure 24 Cont.



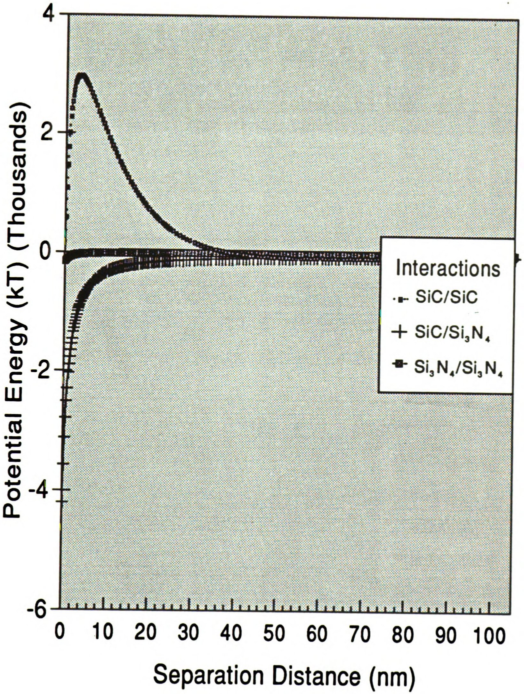
(d) pH= 5.5

Figure 24 Cont.



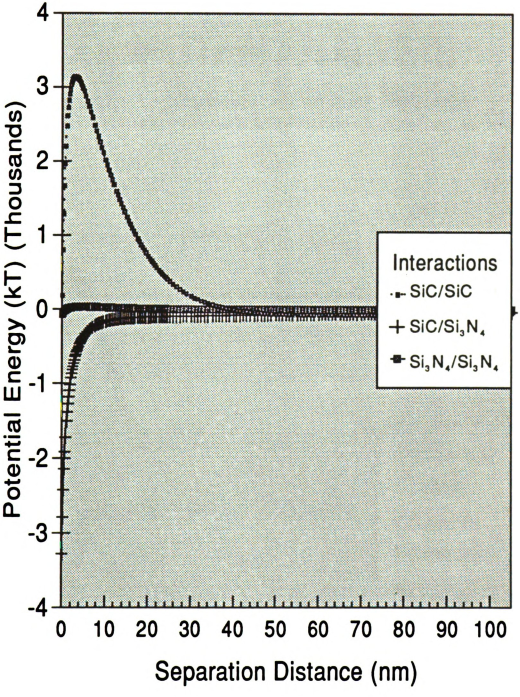
(e) pH= 6.0

Figure 24 Cont.



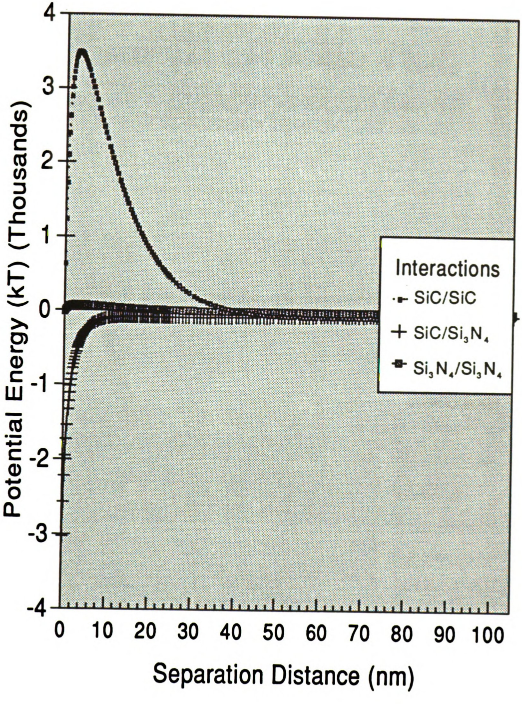
(f) pH= 6.5

Figure 24 Cont.



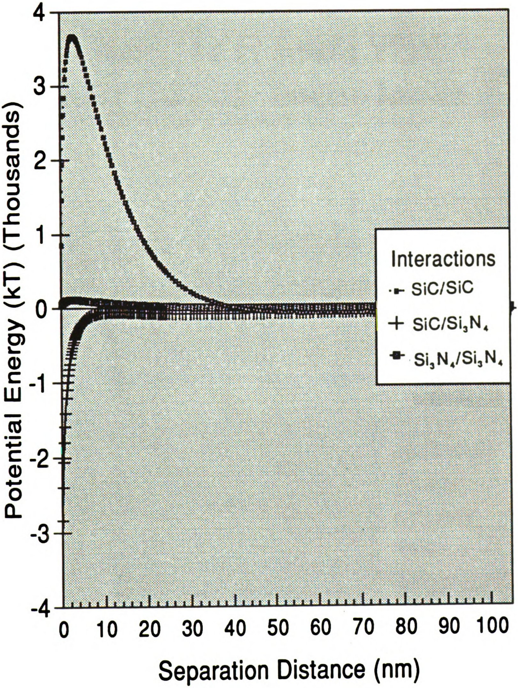
(g) pH= 7.0

Figure 24 Cont.



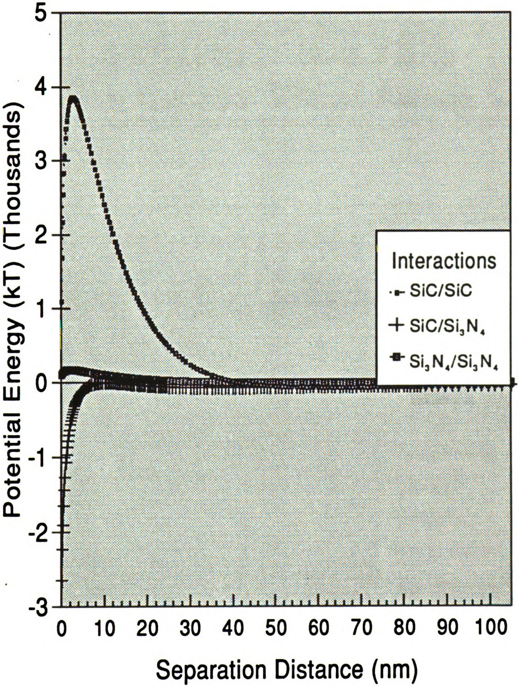
(h) pH= 7.5

Figure 24 Cont.



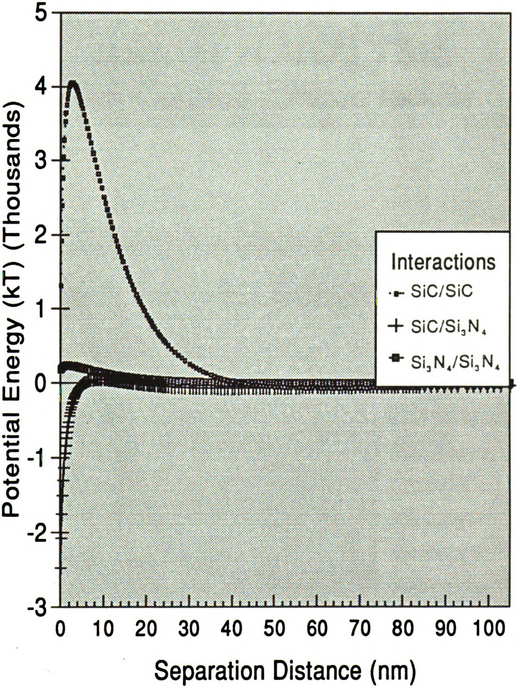
(i) pH= 8.0

Figure 24 Cont.



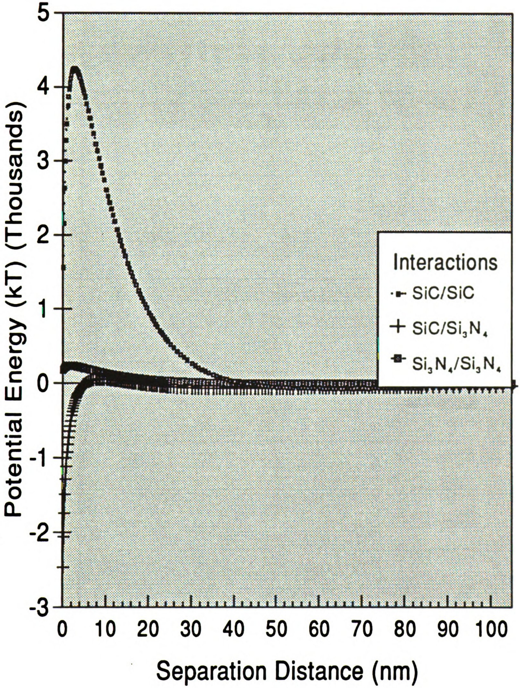
(j) pH= 8.5

Figure 24 Cont.



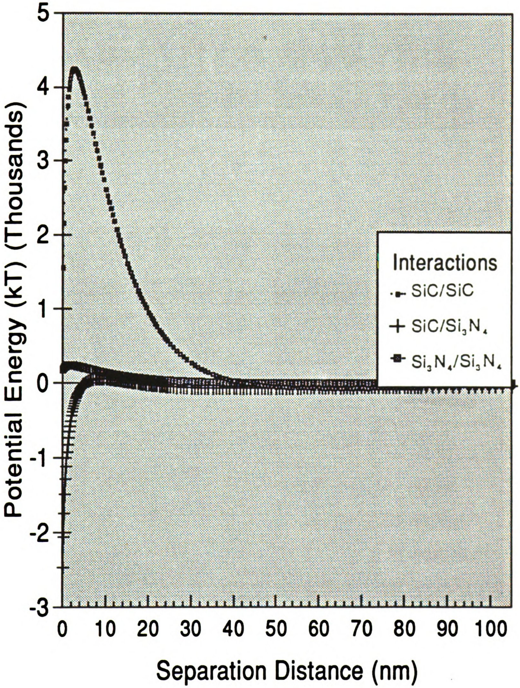
(k) pH= 9.5

Figure 24 Cont.



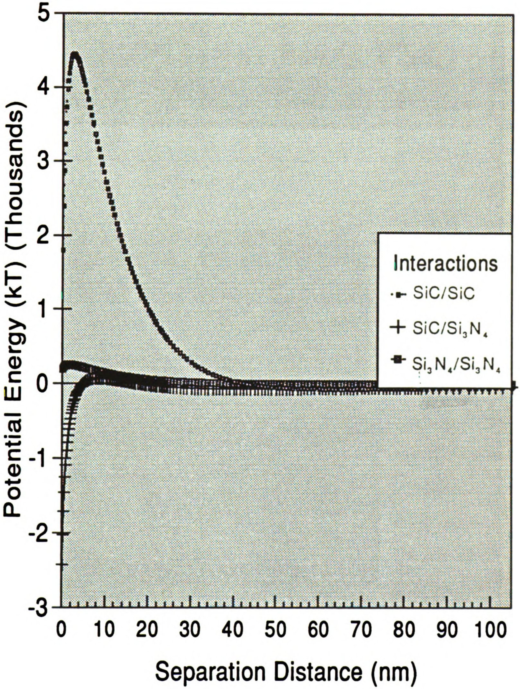
(l) pH= 9.5

Figure 24 Cont.



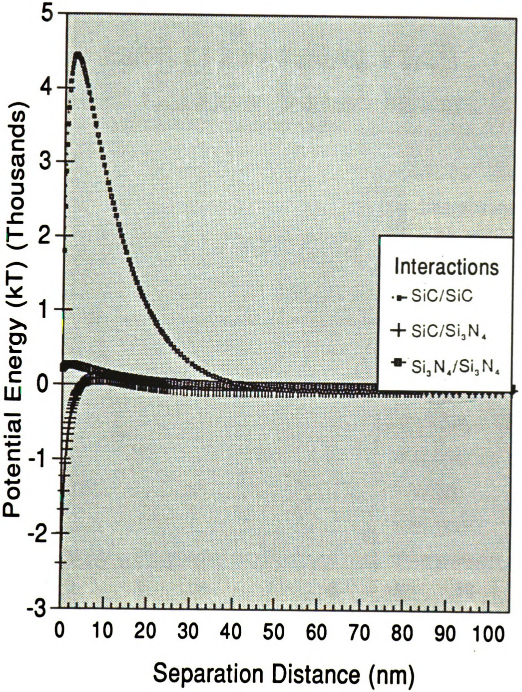
(m) pH= 10.0

Figure 24 Cont.



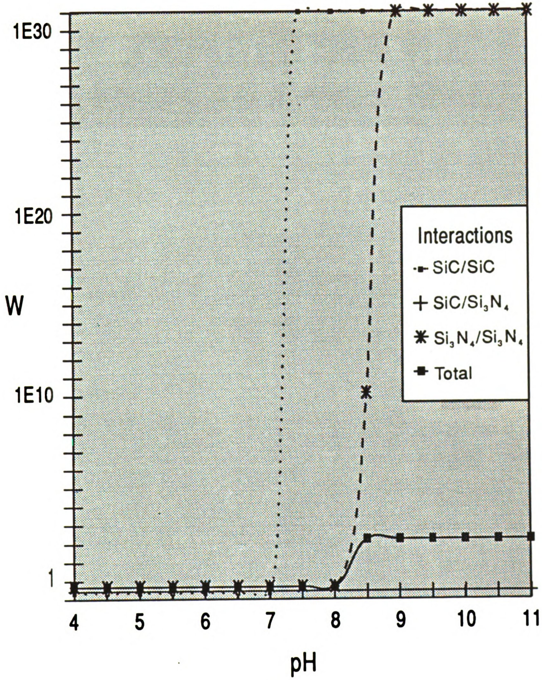
(n) pH= 10.5

Figure 24 Cont.



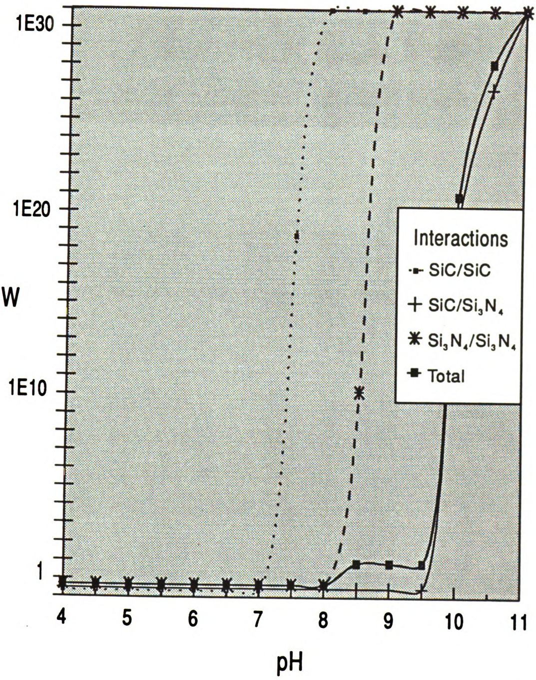
(o) pH = 11.0

Figure 24 cont.



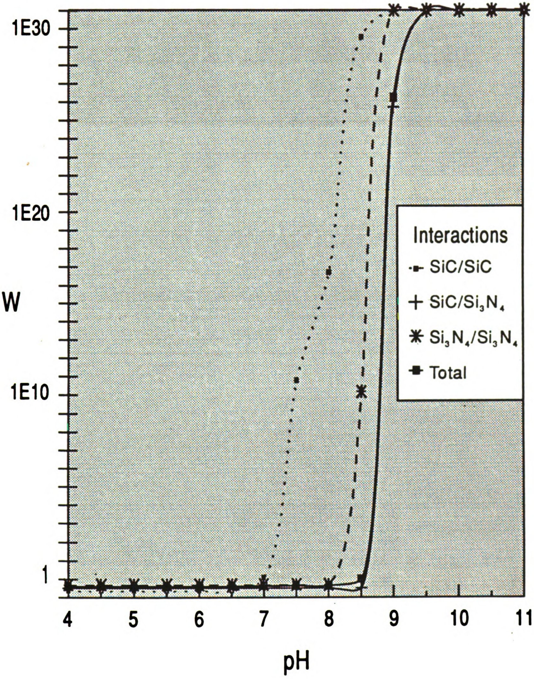
(a)

Figure 25 Stability ratio data from the predictive program using the constant potential repulsive equation and electrophoretic zeta potential for a) LS-5 SiC/SN-E10 Si_3N_4, b) UF-10 SiC/SN-E10 Si_3N_4, and c) UF-15 SiC/SN-E10 Si_3N_4 where: temperature is 25 °C, volume fraction of components is 0.5 and electrolyte concentration is 10^{-2} M.



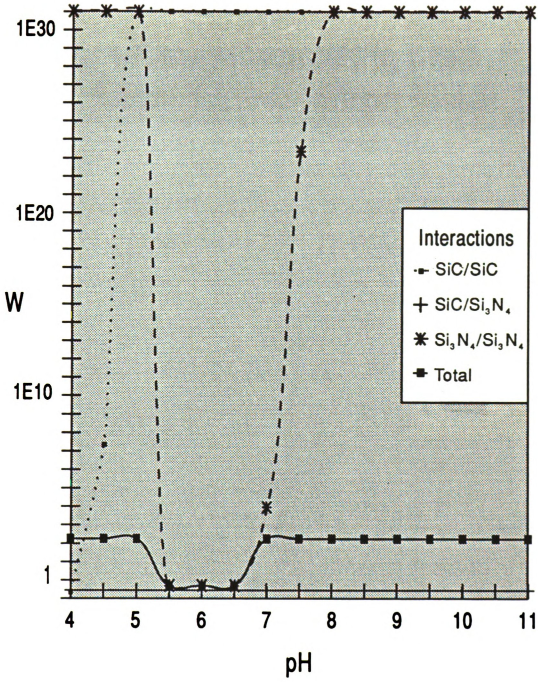
(b)

Figure 25 Cont.



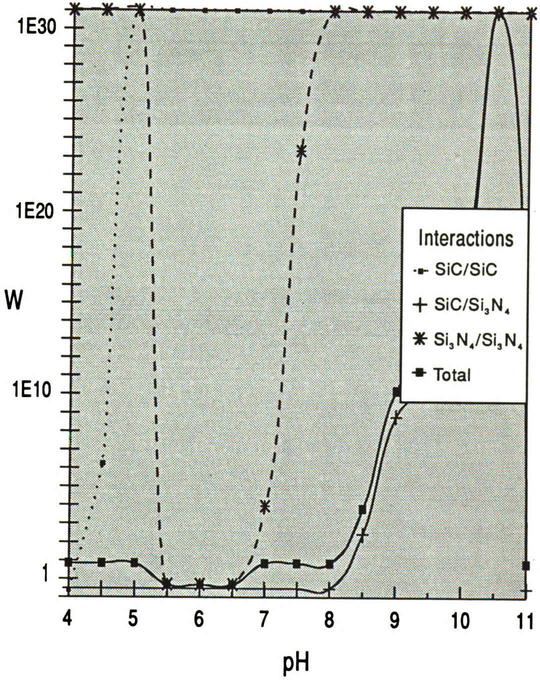
(c)

Figure 25 Cont.



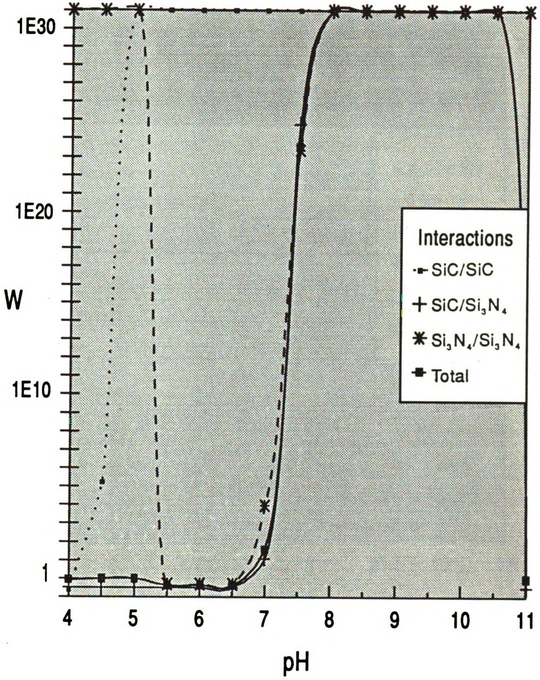
(a)

Figure 26 Stability ratio data from the predictive program using the constant potential repulsive equation and electrophoretic zeta potential for a) LS-5 SiC/SN-E10 Si_3N_4, b) UF-10 SiC/SN-E10 Si_3N_4, and c) UF-15 SiC/SN-E10 Si_3N_4 where: temperature is 25 °C, volume fraction of components is 0.5 and electrolyte concentration is 10^{-5} M.



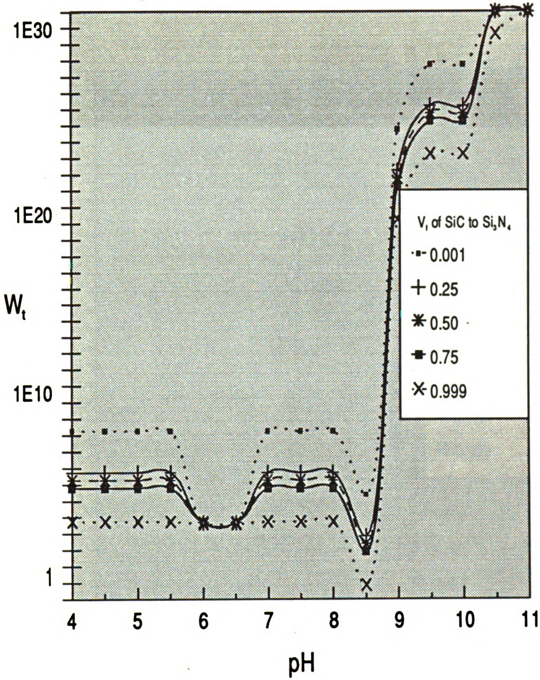
(b)

Figure 26 Cont.



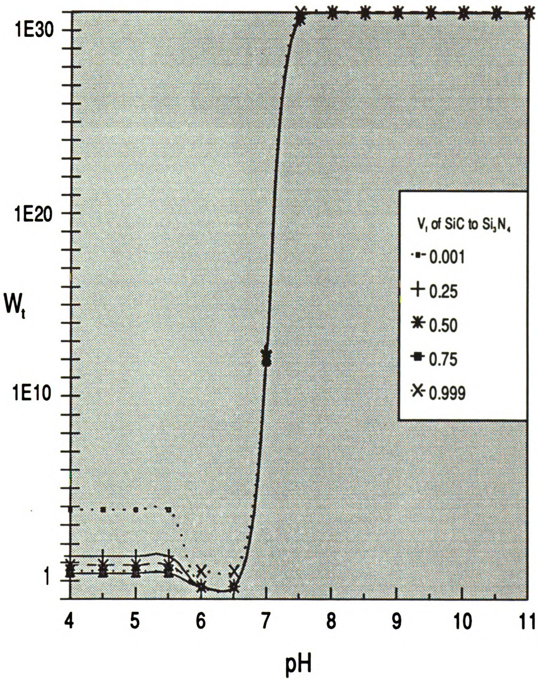
(c)

Figure 26 Cont.



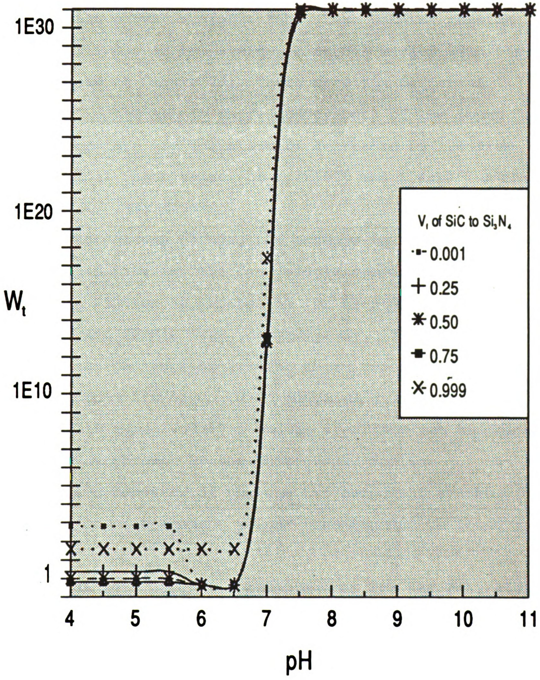
(a)

Figure 27 Total stability ratio data from the program VARYN using data from the predictive program which used the constant potential repulsive equation and electrophoretic zeta potential for a) LS-5 SiC/ SN-E10 Si_3N_4, b) UF-10 SiC/SN-E10 Si_3N_4, and c) UF-15 SiC/SN-E10 Si_3N_4 where: temperature is 25 °C, volume fraction of components is varied and electrolyte concentration is 10^{-3} M.



(b)

Figure 27 Cont.



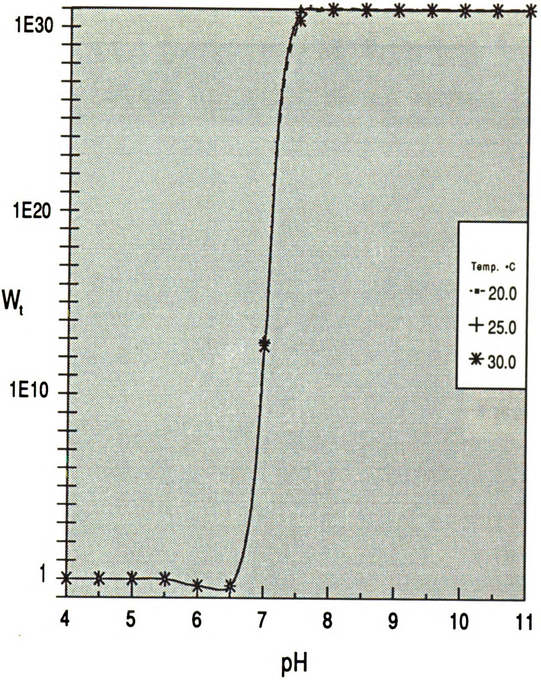
(c)

Figure 27 Cont.

the system with variations from room temperature of plus or minus 5 °C being shown in Figure 28a) and larger temperature changes being shown in Figure 28b). The Hamaker constant was another input of the system which was varied with the results shown in Figure 29. There were six different variations in the values where one or both of the input Hamaker constants was increased or decreased by 10% from their original input values of 3.0×10^{-19} and 1.6×10^{-19} J for SiC and Si_3N_4, respectively.

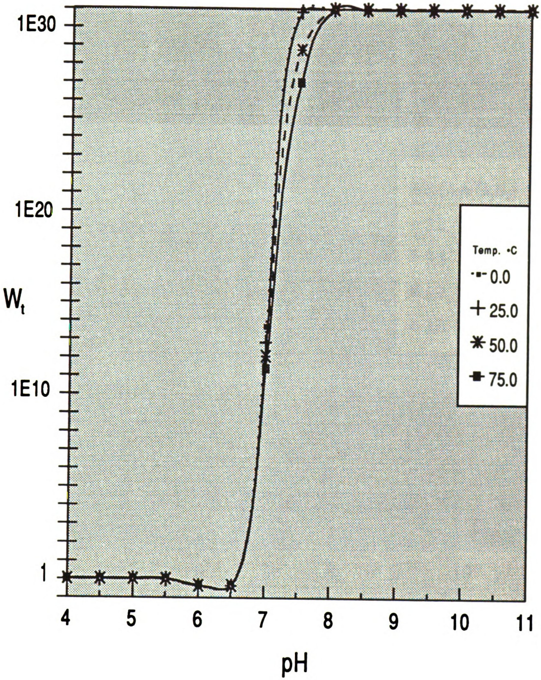
The photographs showing the changes in sedimentation as a function of time for the four single component systems can be found in Figures 30 through 33 for LS-5 SiC, UF-10 SiC, UF-15 SiC, and SN-E10 Si_3N_4, respectively. The sedimentation photographs for the three two component systems of LS-5 SiC/Si_3N_4, UF-10 SiC/Si_3N_4 , and UF-15 SiC/Si_3N_4 with equal relative volume fractions can be found in Figures 34 through 36 and photographs for the sedimentation behavior of the one two component system with unequal relative component volume fraction can be found in Figure 37.

The ESA zeta potential measurements for the FeAl/Al_2O_3 fiber system in an electrolyte solution of concentration equal to 10^{-3} M are shown in Figures 38 and 39. These data was used along with the constant potential solution for the repulsive interaction potential in stability prediction runs for the system. This data generated in these prediction



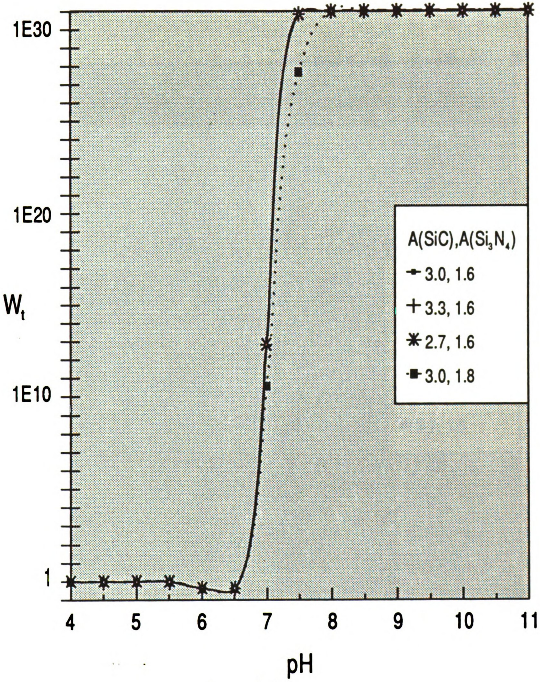
(a)

Figure 28 Stability ratio data from the predictive program using the constant potential repulsive equation and electrophoretic zeta potential for UF-15 SiC/SN-E10 Si_3N_4 where: temperature is a) 20, 25, and 30 °C and b) 0, 25, 50, 75 °C volume fraction of components is 0.5 and electrolyte concentration is 10^{-3} M.



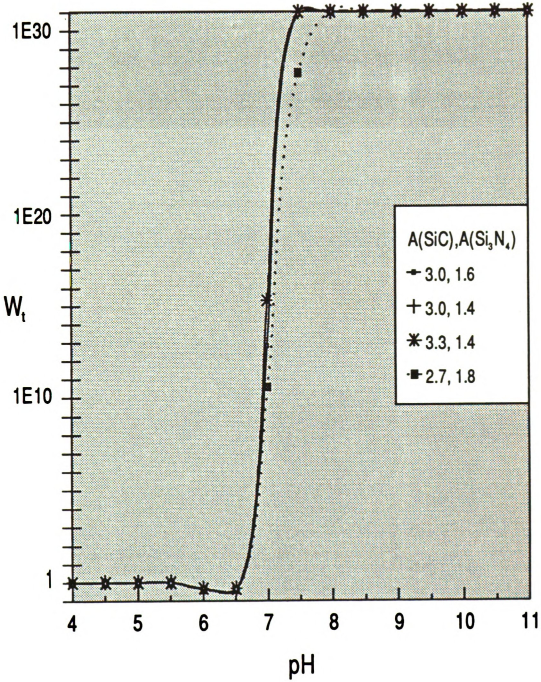
(b)

Figure 28 Cont.



(a)

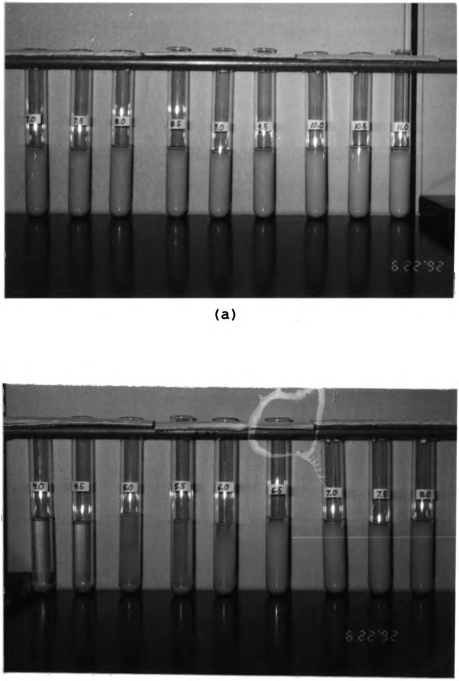
Figure 29 Stability ratio data from the predictive program using the constant potential repulsive equation and electrophoretic zeta potential for UF-15 SiC/SN-E10 Si_3N_4 where: temperature is 25 °C volume fraction of components is 0.5, the electrolyte concentration is 10^{-3} M, and the Hamaker constants in units of 10^{-19} J are varied by +/- 10% to the values noted in a) and b).



(b)

Figure 29 Cont.

runs are plotted in Figure 40.



(a)

(b)

Figure 30 Sedimentation samples for a single component suspension of LS-5 SiC with an electrolyte concentration of 10^{-3} M KNO_3 after sedimentation for a) 21 hours, b) 21 hours, c) 21 hours, d) 73 hours, and e) 73 hours.

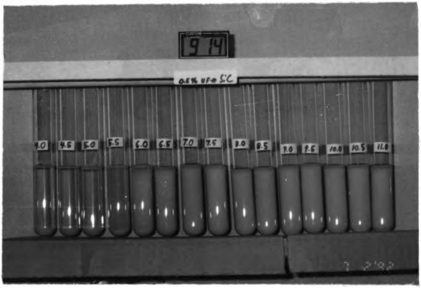
(c)

(d)

Figure 30 Cont.

(e)

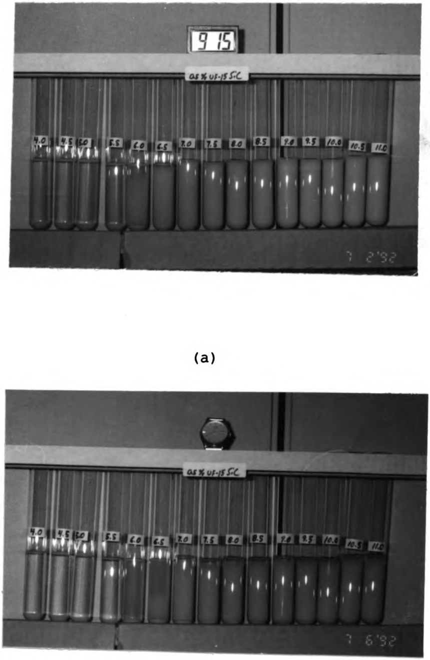
Figure 30 Cont.



(a)

(b)

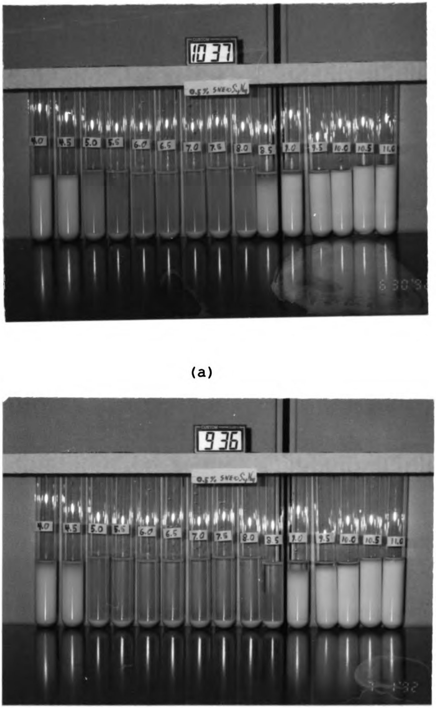
Figure 31 Sedimentation samples for a single component suspension of UF-10 SiC with an electrolyte concentration of 10^{-3} M KNO_3 after sedimentation for a) 21 hours, and b) 119 hours.



(a)

(b)

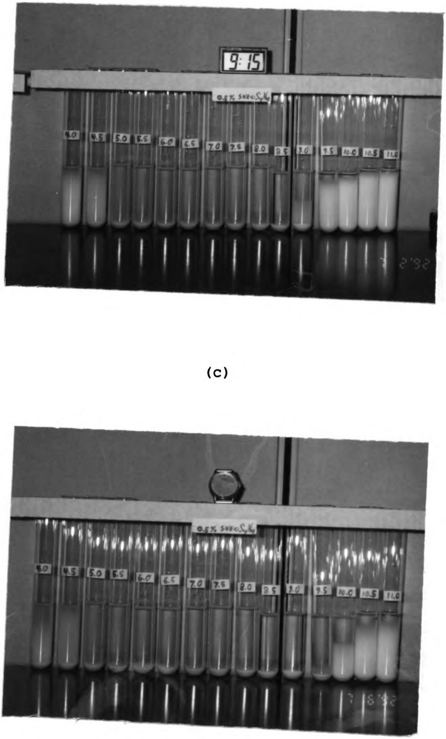
Figure 32 Sedimentation samples for a single component suspension of UF-15 SiC with an electrolyte concentration of 10^{-3} M after sedimentation for a) 20 hours, and b) 118 hours.



(a)

(b)

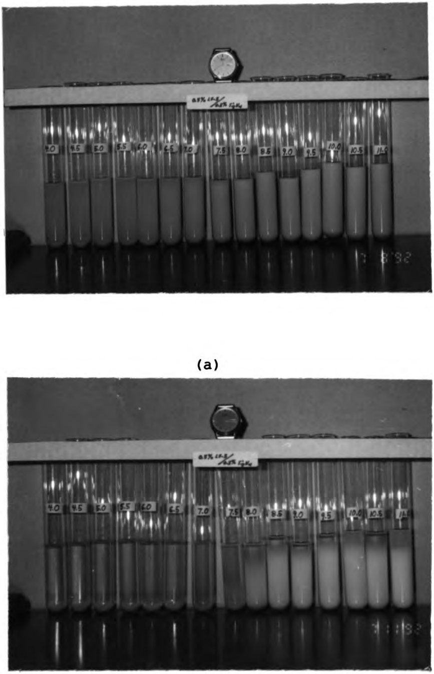
Figure 33 Sedimentation samples for a single component suspension of SN-E10 Si_3N_4 with an electrolyte concentration of 10^{-3} M KNO_3 after sedimentation for a) 1.5 hours, b) 24 hours, c) 48 hours and d) 146 hours.



(c)

d)

Figure 33 Cont.



(a)

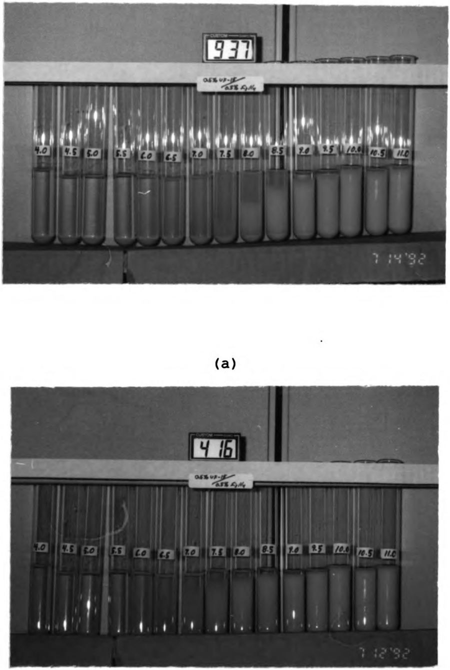
(b)

Figure 34 Sedimentation samples for a two component suspension of 0.5 relative volume fraction of LS-5 SiC and SN-E10 Si_3N_4 with an electrolyte concentration of 10^{-3} M KNO_3 after sedimentation for a) 0 hours, and b) 72 hours.

(a)

(b)

Figure 35 Sedimentation samples for a two component suspension of 0.5 relative volume fraction of UF-10 SiC and SN-E10 Si_3N_4 with an electrolyte concentration of 10^{-3} M KNO_3 after sedimentation for a) 29 hours, and b) 70 hours.

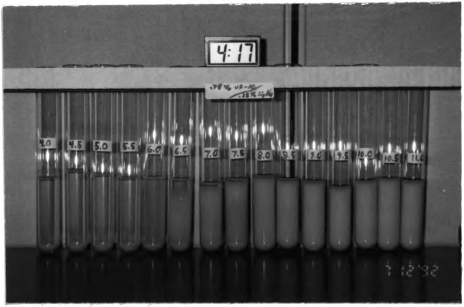


(a)

(b)

Figure 36 Sedimentation samples for a two component suspension of 0.5 relative volume fraction of UF-15 SiC and SN-E10 Si_3N_4 with an electrolyte concentration of 10^{-3} M KNO_3 after sedimentation for a) 23 hours, and b) 64 hours.

(a)



(b)

Figure 37 Sedimentation samples for a two component suspension of 0.75 relative volume fraction of UF-10 SiC and SN-E10 Si_3N_4 with an electrolyte concentration of 10^{-3} M KNO_3 after sedimentation for a) 22 hours, and b) 63 hours.

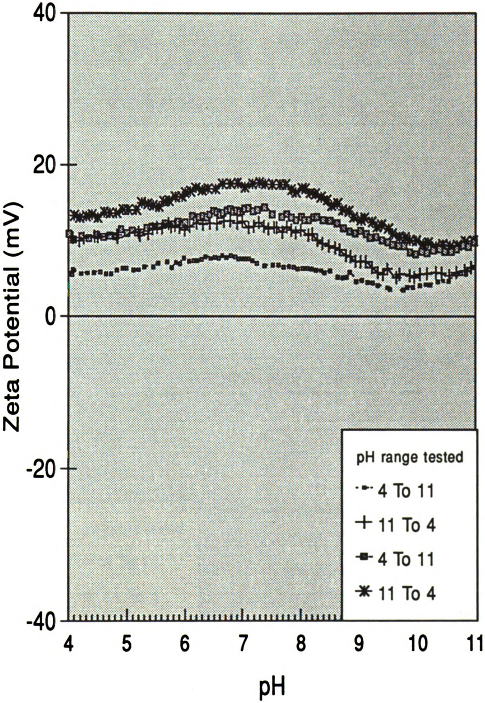


Figure 38 ESA zeta potential measurements for FeAl powder at an electrolyte concentration of 10^{-3} M KNO_3.

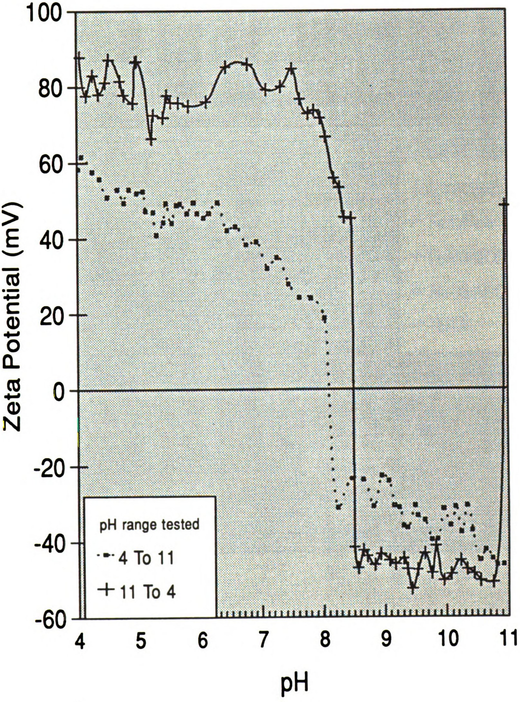
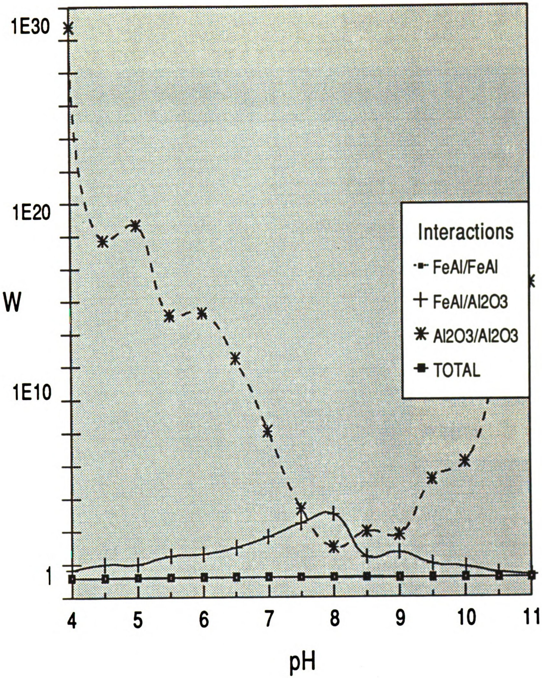
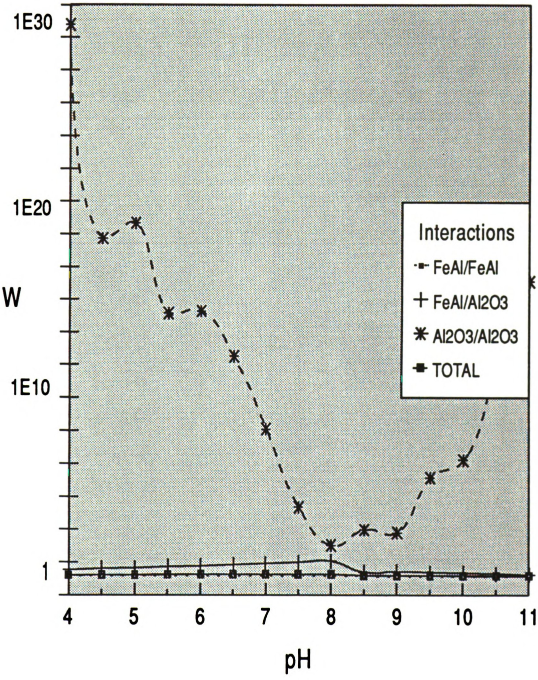


Figure 39 ESA zeta potential measurements for Al_2O_3 fiber at an electrolyte concentration of 10^{-3} M KNO_3.



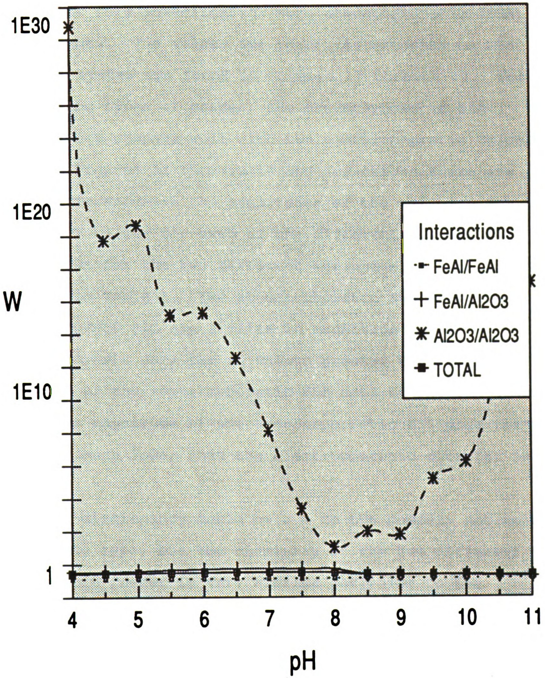
(a)

Figure 40 Stability ratio data from the predictive program using the constant potential repulsive equation and ESA zeta potential for FeAl and Al_2O_3 radii of a) 3.5 and 15.0 microns, b) 7.5 and 15.0 microns, and c) 12.5 and 15.0 microns respectively, where: temperature is 25 °C, volume fraction of components is 0.5 and electrolyte concentration is 10^{-3} M KNO_3.



(b)

Figure 40 Cont.



(c)

Figure 40 Cont.

DISCUSSION

The zeta potential data measured in the experimental portion of this investigation were acoustophoretic (ESA) measurements. The values for these measurements on the SiC/Si_3N_4 system are found in Figures 17 through 20. For some of the types of powder, the acoustophoretic ESA measurements compare well with the electrophoretic values shown in Figures 12 through 14 and for others there are major differences in the magnitudes of the values. A summary of values for each of the different powders at several pHs for the two different measurement techniques can be found in Table 1. The acoustophoretic ESA data for the LS-5 and UF-10 SiC are similar in magnitude to the electrophoresis data for pH values greater than 5, while the magnitude of the acoustophoretic ESA data at lower pHs are less. The magnitude of the acoustophoretic ESA data for UF-15 SiC is much lower than the electrophoretic data for the UF-10 SiC.

This discrepancy could be due to the powders not being of the same type, but the chemistry of the two different types of SiC powder is very similar according to the manufacturer and so surface charge generation and zeta potential values would be expected to be similar. Examination of the Si_3N_4 acoustophoretic ESA data shows a similar behavior, with the magnitude of the acoustophoretic

Table 1 Zeta potential values at several pHs from acoustophoresis (ESA) and electrophoresis measurements.

pH Values	ESA LS-5	ESA UF-10	ESA UF-10	ESA SN-E10	Electrophoresis UF-10	Electrophoresis SN-E10
4	-10	-14	-2.2	8.0	-34	44
5	-20	-26	-5.5	5.7	-44	29.4
7	-39	-38	-11	-3.5	-54	-24
8.5	-52	-47	-16	-5.8	-58	-38
10	-61	-52	-19	-7.8	-60	-43

ESA zeta potential data being much lower in magnitude than the values of the electrophoresis data for the same type of Si_3N_4 powder. Both the UF-15 SiC and Si_3N_4 powder are of a similar small size range. A similar discrepancy between measured acoustophoretic ESA data and electrophoresis data was discussed by James, Hunter, and O' Brien (79) in testing several different types of alumina powders and UBE SN-E10 Si_3N_4. For Si_3N_4, these authors showed that if an effective radius was used for the average particle size to calculate the zeta potential with the acoustophoretic ESA technique, the results were found to approximately match the electrophoresis data. The reason was found in Equations [10] through [16]. Equation [10] calculated the zeta potential once the dynamic mobility was found using the measured ESA amplitude to solve Equation [8]. The term $G(\alpha)$ was the inertial contribution to the dynamic mobility which was dependent upon both the frequency of the acoustic wave and the particle size and was found by solving Equations [11] through [16]. Generally, $G(\alpha)$ was an inverse function of the particle radius. If the radius was underestimated, the inertial contribution $G(\alpha)$ was overestimated, resulting in an underestimation of the zeta potential. James et al. showed calculations where the reported particle size was half of the true particle size, resulting in a $G(\alpha)$ 1.75 times higher. This indicates that the zeta potential will be reported as 1.75 times smaller in magnitude than it should be.

Part of the problem in finding the correct particle size to calculate the acoustophoretic ESA zeta potential was that each method used will give different average particle sizes. For example for Si_3N_4, the manufacturer reports an average particle radius of 0.25 µm, Crimp reports a BET equivalent spherical radius of 0.06 µm (76), James et al. (79) report a particle analyzer mass average radius of 0.275 µm and a light scattering radius of 0.55 µm. James et al. found the best results using photon correlation spectroscopy (PCS). A major factor responsible for the difference in the particle radius and need for use of an effective radius, was agglomeration of particles into larger sized particles during ESA testing (71). As will be discussed later and can be seen in Figures 30 through 32, SiC agglomerates at low pH values. These were the pH values where the acoustophoretic ESA measurements were slightly lower than the electrophoresis values for LS-5 and UF-10 SiC. This agglomeration and the need for an effective particle radius would explain this behavior. Electrophoresis does not "see" the need for an effective particle radius for two reasons. The electrophoresis measurements are carried out at much lower particle volume percents of solids to liquids in the suspension and the electrophoresis values do not require particle size in the calculation of the zeta potential.

Figure 21 is the first of the graphs of stability vs.

pH from data produced by the predictive program for the SiC/Si_3N_4 system. Figure 21(a) is the predictive data found using the constant potential repulsion equation along with electrophoresis data for the LS-5 SiC/Si_3N_4 system with equal relative component volume fraction in an electrolyte concentration of 10^{-3} M at room temperature (25°C). Figure 21(b) and (c) are for the same system conditions, but are for UF-10 SiC/Si_3N_4 and UF-15 SiC/Si_3N_4, respectively. For all of the stability vs. pH plots, the maximum value plotted for the stability ratio is 10^{31} due to limitations of the available graphics software. Four different curves were plotted on each graph. The curves represent the different types of interactions which are possible for the system. SiC/SiC, SiC/Si_3N_4, and Si_3N_4/Si_3N_4 represent the interactions of SiC particles with themselves (W_{11}), SiC particles with Si_3N_4 particles(W_{12}), and Si_3N_4 particles with themselves (W_{22}), respectively. The curve for the total interaction represents the total overall particle interaction (W_t).

The SiC/SiC curves in Figures 21(a), (b), and (c) are horizontal lines at a value of W equal to 10^{31}. This means that the SiC particles are predicted to be stable with respect to themselves at all pH values from a pH of 4 to 11. the Si_3N_4/Si_3N_4 curves for these plots begins at stability values of 10^{31} at pH 4 to 5, decreasing to lower values for pH 5.5 to 7, and increases to the maximum for pH 7.5 and above. The prediction is then that Si_3N_4 is stable at low pH values and high pH values, but is unstable for intermediate pH values with respect to itself.

The SiC/Si_3N_4 curves differ in the three plots of Figure 21. In Figure 21(a) the curve is constant at stability values of about 10^3 from pH 4 to 8, decreases to a value of less than 1 at pH 8.5, and then increases to values above 10^{19}. This means that the method predicts SiC and Si_3N_4 particles will be attracted to one another to form agglomerates for pH less than 9 and so instability is predicted in this range. For pH 9 to 10 it is unclear if the stability ratio is large enough to predict stability or partial stability (i.e. where the particles will be stable but only for smaller time periods). The actual stability ratio values which delineate stability from instability or partial stability will have to be determined by application to a real system. For Figures 21(b) and (c), the SiC/Si_3N_4 curves are very similar with instability predicted for pH less than 7, partial stability for pH 7, and stability for pH values greater than pH 7. For the three curves plotted in Figure 21 the total stability is predicted to follow closely each of the SiC/Si_3N_4 interaction curves with only small shifts in stability values. This would indicate total system instability below pH 9, partial stability from 9 to 10 and stability above pH 10 for the LS-5 SiC/Si_3N_4 system and instability below pH 7 with stability above pH 7 for both the UF-10 and UF-15/Si_3N_4 systems. Figure 22 contains plots of computer predicted stability for the same three systems except that the ESA zeta potential data was used instead of the electrophoretic data. All three of the plots predict complete instability of the SiC/Si_3N_4, Si_3N_4/Si_3N_4, and total interactions at all pH values. This is due to the smaller magnitudes reported for the Si_3N_4 ESA zeta potential data compared to the electrophoresis. Figures 22 (a) and (b) predict instability for the SiC/SiC interactions at low pH values and stability at higher pH values, while Figure 22 (c) predicts instability at all pH values (again this is due to the lower ESA zeta potential values).

Figure 23 contains plots of computer predicted stability for the same systems as Figure 21, but uses the constant charge repulsion equation instead of the constant potential equation. Figure 23 (a) predicts SiC/SiC interaction stability for all pH values and Si_3N_4/Si_3N_4 stability for pH below 6 and above 6.5. The SiC/Si_3N_4 and total interactions are predicted to be unstable below pH 7. Figures 23 (b) and (c) are almost identical predicting SiC/SiC interaction stability for all pH values and Si_3N_4/Si_3N_4 stability for pH below 6 and above 6.5. The SiC/Si_3N_4 and total interactions are predicted to be stable below pH 6.5.

Figure 24 (a) through (o) are plots of the potential energy of interaction versus particle separation distance for each of the 15 pH values for which data was calculated for the LS-5 SiC/Si_3N_4 system with equal relative component volume fraction in an electrolyte of concentration 10^{-3} at room temperature (corresponds to stability data in Figure 21 (a)). In the figures the higher the maximum repulsive peak, the larger the barrier to agglomeration, the higher the corresponding stability ratio will be in Figure 21 (a). An example of this can be seen for the Si_3N_4/Si_3N_4 interaction. Figure 24 (f) shows the potential energy at pH 6.5 for this interaction. This curve is the middle curve of the three and is shown as barely reaching a positive potential value and corresponds to a low stability value in Figure 21 (a). Figure 24 (j) shows the potential energy at pH 8.5 for this interaction. This curve is the middle curve of the three and is shown as reaching a positive potential peak of approximately 100 kT or so and corresponds to a stability value in Figure 21 (a) which indicates stability.

These figures illustrate an advantage of the stability prediction theory used in this investigation over methods which simply look at the interparticle potential curves. Instead of using one figure (e.g. Figure 21 (a)) to predict the system stability over a pH range, as in this theory, it would be necessary to look at a plot of potential verses separation for each pH in the pH range (e.g. the 15 plots in Figure 24) in order to use the interaction energy versus separation to predict stability.

The plots in Figure 25 are for data from the predictive program using the constant potential repulsion equation and electrophoresis data for the three main two-component systems with equal relative volume fraction as in Figure 21, but with an electrolyte concentration of 10^{-2} M. The curves predict instability for SiC/SiC interactions at pH below 7.5 and below 8.5 or 9 for Si_3N_4/Si_3N_4 interactions. For the SiC/Si_3N_4 and total interactions instability is predicted for all pH values for the LS-5 SiC/Si_3N_4 system and for pH below 10 and 9 for the UF-10 and UF-15 SiC/Si_3N_4 systems, respectively.

The plots in Figure 26 are the same as in Figure 25, but with an electrolyte concentration of 10^{-5} M. For each of the three systems shown, stability is predicted for the SiC/SiC interaction for pH above 5 and for the Si_3N_4 interaction stability is predicted for pH below 5.5 or above 7.5. The SiC/Si_3N_4 and total interactions are different for each of the three systems. For the LS-5 SiC/Si_3N_4 system, the method predicts instability at all pHs. For the UF-10 SiC/Si_3N_4 system, instability is predicted for all pHs below 10.5, while for the UF-15 SiC/Si_3N_4 system, instability is predicted for all pHs below 8. The method predicts changes in stability behavior with changes in the electrolyte concentration. This is expected since variations in electrolyte concentration will change the size of the repulsive double layer as was discussed earlier. An increase in electrolyte concentration reduces the double layer size since the ion concentration reaches the bulk value in a shorter distance from the particle surface. Increasing the electrolyte concentration from 10^{-3} M to 10^{-2} M reduced the predicted stability behavior which is seen by comparing the plots of Figure 21 and Figure 25.

The effect of variations in the relative volume fraction of components on the total overall stability is shown in Figure 27. The conditions chosen to show the variation were for systems in which there was the largest difference between the stability behavior for SiC and Si_3N_4. Therefore, the largest changes in the total stability should be seen for these systems. All three systems show that for these conditions the method does not predict much change in the total overall stability of each system for different relative volume fractions.

The effect of temperature on the total overall stability is shown in Figure 28. Figure 28 (a) shows the total overall stability for room temperature and room temperature +/- 5°C. This figure shows that stability is predicted to barely change for the temperature range of normal laboratory temperature fluctuations. Figure 28 (b) shows the total overall stability for much larger temperature changes. Even the large variations in temperature show little change in predicted stability except at pH 7 where the stability might change from complete stability to partial stability for a temperature increase of

50°C. A plot of the log of the stability ratio versus pH shows all curves as being almost identical except for the 0°C curve which is shifted to the left of the other curves by about a half a pH unit. This indicates that processing in an ice bath or similar low temperature environment, would allow for stability at a half a pH lower than if the processing was done at room temperature. This could be an important processing aid for systems in which components are soluble at high pH or have surface groups which are unstable at high pH as is the case for Si_3N_4 (70).

Figure 29 shows the effect on the predicted stability from variations in the input Hamaker constants of plus or minus 10% for SiC and/or Si_3N_4. This was done because the values for the Hamaker constants vary depending on the method (i.e. microscopic method Equation [2] or macroscopic method of Equation [3]) used to calculate them. Figure 29 little change in the overall stability predicted even for variations as large as a 10% increase in one and a 10% decrease in the other input Hamaker constant. This means that the predictions are not strongly sensitive to the accuracy of the Hamaker constants input.

To verify the stability predictions, sedimentation experiments were performed. With the small size and similar appearance of all the powders upon dispersion, it was not possible to identify any heterocoagulation between SiC and Si_3N_4. For future investigations the heterocoagulation

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predictions could be examined using SEM or TEM studies. In the current investigation, single component sedimentation experiments were performed along with the two component systems tested so that the each of the SiC/SiC and Si_3N_4/Si_3N_4 interactions could be known experimentally along with the total overall stability for the two component systems. The sedimentation of each of these single and two component systems at varying time intervals can be seen in Figures 30 through 37.

The reason sedimentation experiments indicate the agglomeration state and stability for a system results from the fact that as agglomerates form, the sizes of these agglomerates are larger than the single particle. The more agglomeration that takes place larger the agglomerates become. The larger a particle or agglomerate becomes the more gravity affects it and the quicker it falls. Factors which indicate the degree of agglomeration are sedimentation rate, sedimentation height and whether the liquid above the sedimentation level is clear or cloudy (80). If the sedimentation height is small, the system is strongly coagulated. Larger sedimentation heights with clear liquid above the sedimentation show a partially stable suspension and suspensions which remain cloudy above any sedimentation height show stable suspensions (70).

Figure 30 shows the sedimentation behavior for LS-5 SiC by itself. At a time of 21 hours, the suspension is unstable below pH 5.5, partially stable at pH 6.0, and stable for all higher pH values. At 73 hours, the same stability is shown. Figure 31 shows the stability of UF-10 SiC. At 21 hours the UF-10 is unstable for pH values less than 6 and stable for values of 6 or greater. After 119 hours, the UF-10 is unstable for pH less than 6, is partially stable for pH 6 and 6.5, and stable for higher pHs. Figure 32 shows the stability for UF-15 SiC. At 20 hours, the UF-15 is unstable for pHs less than 6, partially stable for pH 6, and stable for values of greater than 6. After 118 hours, the UF-15 is unstable for pH 6 or less, is partially stable for pH 6.5, and stable for higher pH values. Figure 33 shows the stability for SN-E10 Si_3N_4. At 24 hours, the SN-E10 is stable for pH less than 5, unstable for pH 5 to 8, partially stable for pH 8.5, and stable for values greater than 8.5. At 48 hours, the SN-E10 is stable for pH less than 5, unstable for a pH 5 to 8.5, partially stable for pH 9 and 9.5, and stable for values greater than 9.5. At 146 hours, the SN-E10 is stable for pH less than 5, unstable for a pH 5 to 9, partially stable for pH 9.5 and 10, and stable for values greater than 10.0.

For the two component systems of LS-5 SiC/Si_3N_4 in equal volume fractions Figure 34 shows the total stability. At 72 hours, the system is unstable for pH less than 7.5, partially stable for pH 7.5 and 8, and stable for pH greater than 8. For the UF-10 SiC/Si_3N_4 in equal volume fractions,

Figure 35 shows the total stability. At 29 hours, the system is unstable for pH less than 7, partially stable for pH 7, and stable for pH greater than 7. At 70 hours, the system is unstable for pH less than 7, partially stable for pH 7 to 8.5, and stable for pH greater than 8.5. For the UF-15 SiC/Si_3N_4 in equal volume fractions, Figure 36 shows the total stability. At 23 hours, the system is unstable for pH less than 7, partially stable for pH 7 to 8, and stable for pH greater than 8. At 64 hours, the system is unstable for pH less than 7, partially stable for pH 7 to 8.5, and stable for pH greater than 8.5. For the 0.75 v% UF-10 SiC/0.25 v% Si_3N_4 Figure 37 shows the total stability. At 22 hours, the system is unstable for pH less than 6, partially stable for pH 6 and 6.5, and stable for pH greater than 7. At 63 hours, the system is unstable for pH less than 6.5, partially stable for pH 6.5 to 7.5, and stable for pH greater than 7.5.

The prediction for LS-5 and UF-10 SiC using the acoustophoretic ESA data and the constant potential repulsion equation predicts the change from partial stability to stability to occur for pH 5 to 5.5 and 5.5 to 6, respectively. The single component sedimentation experiments for these powders at 21 hours show this transition to be at 5.5 to 6 for both of the powder types. The prediction for the Si_3N_4 using the acoustophoretic ESA data and the constant potential equation predicts stability for pH less than 5.5 and greater than 7. The single component sedimentation experiment for Si_3N_4 shows stability of less than 5 and greater than 8.5. This prediction is close for the lower pH range, but while the program did predict the second stability range, it was not very close as to where this range began.

For the total overall stability of the LS-5 SiC/Si_3N_4 system with the constant potential repulsion equation and zeta potential data used for prediction, a stability prediction determines the suspension to be unstable below pH 9 and partially stable at 9 to 10 and stable for pH above 10. The sedimentation results after 72 hours for this system indicate a stable suspension below 8.5 and stable at 8.5 and above. For the total overall stability of the UF-10 SiC/Si_3N_4 system with the constant potential repulsion equation and zeta potential data used for prediction, a stability prediction determines the suspension to be unstable below pH 7 and partially stable at 7 and stable for pH above 7. The sedimentation results after 29 hours for this system indicate a stable suspension below 7 and stable at 7.5 and above.

Some of the results can be seen as quite encouraging, but with the acoustophoretic ESA data not being correct for Si_3N_4 or UF-15 SiC, much of the accuracy of the predictions is decreased. This points out how necessary accurate zeta potential measurements are. For future work with the program, acoustophoretic ESA zeta potential data need to be taken using an effective particle radius.

The FeAl zeta potential curves are shown in Figure 38. The zeta potential data curves are relatively flat over the pH range. Shaw (15) shows a zeta potential curve for latex particles which is also fairly flat over the pH range. The flatness of the curve indicates one of two things. Either hydrogen and hydroxyl ions are not the potential determining ions for FeAl or there are competing charge generation mechanisms. The charge generation mechanism is unknown, but could be a variety of different mechanisms such as various corrosion reactions or hydroxylation reactions. This points to another advantage of this prediction method. From a purely processing standpoint, a prediction of the stability for this system can be made with accurate zeta potential data without knowing the charge mechanisms, although from a scientific standpoint the it would be desirable to know the charge mechanisms.

The ESA zeta potential data for the alumina fibers are shown in Figure 39. The magnitude of the values are similar to values reported by James et al. (79) for alumina powder and an i.e.p. that is similar to that shown by James et al. (79). However, the shapes of the curves differ. This is probably due to the authors taking approximately ten data points and then drawing a best fit curve through them. The data scatter of the ESA zeta potential data is probably due to the large distribution of fiber lengths as can be seen in the SEM photograph in Figure 61. To improve the acoustophoretic ESA data, a better method for shortening the fibers is needed.

The stability prediction curves in Figure 40 show complete instability of FeAl. Observation of the FeAl suspensions made in this investigation show this not to be true. This poor prediction is due to the use of an inaccurate average particle radius in calculating the ESA zeta potential. An improved method for finding an effective particle radius is needed. If it is assumed that correct particle size would shift the stability up, it would follow that the FeAl would be stable for all pH values, although there might be instability above a pH of 9 where the acoustophoretic ESA curve dips slightly.

The stability for alumina is predicted to be stable for pH under 6.5 to 7 or above 10.5 or 11. The FeAl/alumina interaction is shown to be stable for the whole pH range, but if the FeAl stability curve were shifted up, the FeAl/alumina curve would be also. The curve is at a maximum at pH 7 and drops off for higher and lower values of pH. The ideal pH for processing this composite system would be where the FeAl/FeAl and alumina/alumina interactions would be stable, but the FeAl/alumina interaction would be unstable so that the matrix and fiber are attracted to each other. This would occur at pH 5 or 6. If after initial mixing of the composite at pH 5 to allow for a uniform distribution of FeAl and alumina fibers the pH was increased to 8, in order to induce total coagulation of the system, so differential settling of the composite components could be reduced or eliminated.

CONCLUSIONS

Due to the importance of using both stable and agglomerated suspensions in ceramic processing along with the increasing use of ceramic processing for multicomponent and composite systems, a method for predicting the stability of multicomponent colloidal suspensions at different pH values was developed from a method originated by Hogg, Healy, and Fuerstenau (53). A computer program was written to perform the calculations required in using this method. Material and system data such as particle radii, relative volume fraction of components, monatomic electrolyte concentration, Hamaker constants, and zeta potential versus pH measurements were input into the computer program. The stability ratio versus pH data was output by the program into ASCII files for plotting using graphics software.

The SiC/Si_3N_4 system was investigated in detail using both electrophoresis and electroacoustic zeta potential data. The method was used to make general predictions to be compared with actual stability experiments, and to show the effect of relative volume fraction of components, temperature and the accuracy of the Hamaker values on the predicted stability. The regions of stability predicted by the method were found to be within a half a pH in some instances. However, the predictions were found to be strongly dependent upon the accuracy of the electroacoustic zeta potential measurement data. Problems with these data were discovered and found to be the result of the particle size data which were used to calculate the electroacoustic zeta potential from the measured dynamic mobilities. Contrary to what was intuitively expected, the predicted total overall stability was found to be only slightly changed for different relative volume fractions of components. This was also shown for actual stability in the sedimentation results for a SiC/Si_3N_4 system with 0.75 relative volume fraction of SiC. The prediction method was shown not to be dependent on the precision of the Hamaker constant values used for stability calculations nor upon the system temperature.

The stability prediction method was also applied to a FeAl/Al_2O_3 fiber composite system. The method was used to determine the pH where the processing conditions would be ideal. The ideal composite processing would have the fiber coated by the matrix while having the fiber and the matrix stable enough to form a uniform distribution of fiber within the matrix. This would occur at the pH where the fiber and matrix were attracted to each other and agglomerated together while the fiber and the matrix were individually stable with respect to themselves. The method predicted that the ideal pH where this would occur would be 5 and that a subsequent increase to pH 8 would then prevent differential settling of the fiber and powder.

In general, future investigations should include: 1) electroacoustic ESA data collected using effective particle radius versus pH data, 2) should use the log of the stability ratio to better indicate stability, 3) should have the heterocoagulation predictions investigated through SEM or TEM studies, and 4) should try to better determine at which values of the stability ratio suspensions become stable. For the FeAl/Al_2O_3 fiber system, future investigations should include 1) the general recommendations listed above, 2) a better method for shortening the fibers for the electroacoustic ESA measurements, and 3) determination of the surface chemistry of FeAl.

APPEDIX A

Derivation relating n to particle radii and relative component volume fraction.

In the HHF method n is the overall number of particles of component 1 in the system. In other words n is the ratio of the total number of type 1 particles to the total number of all particles in the system:

$$n=\frac{TN_1}{TN_1+TN_2}. \qquad [A1]$$

This was deemed as quite impracticle from an experimental viewpoint. In real experimental systems variables which are known include the particle radii (r_1 and r_2) and the relative volume fraction of component 1 ($RVFC_1$):

$$RVFC_1=\frac{TV_1}{TV_1+TV_2}. \qquad [A2]$$

Since the method beibg used assumes spherically shaped particles and the particle radii are known, the volume of an individual particle i is:

$$V_i=\frac{4}{3}\pi r_i^3. \qquad [A3]$$

The total volume of all particles of type i is then:

$$TV_i=TN_iV_i=\frac{4}{3}\pi TN_i r_i^3. \qquad [A4]$$

Equation [A2] for component 1 then becomes:

$$RVFC_1=\frac{TN_1\frac{4}{3}\pi R_1^3}{TN_1\frac{4}{3}\pi r_1^3+TN_2\frac{4}{3}\pi r_2^3}. \qquad [A5]$$

This simplifies to:

$$RVFC_1 = TN_1 \frac{r_1^3}{TN_1 r_1^3 + TN_2 r_2^3}\,. \qquad [A6]$$

Now if Equation [A1] is solved for TN_2, the result is:

$$TN_2 = \frac{TN_1}{n} - TN_1 = TN_1\left(\frac{1}{n} - 1\right). \qquad [A7]$$

Substituting Equation [A7] into [A6] results in:

$$RVFC_1 = \frac{TN_1 r_1^3}{TN_1 r_1^3 + [TN_1(\frac{1}{n} - 1)]\, r_2^3} \qquad [A8]$$

which can be simplified to:

$$RVFC_1 = \frac{TN_1 r_1^3}{TN_1 [r_1^3 + (\frac{1}{n} - 1)\, r_2^3]}\,. \qquad [A9]$$

The equation then becomes:

$$RVFC_1 = \frac{r_1^3}{r_1^3 + (\frac{1}{n} - 1)\, r_2^3}\,. \qquad [A10]$$

Solving this equation for n through simple algebra:

$$n = \frac{1}{\frac{r_1^3 (1 - RVFC_1)}{r_2^3 RVFC_1} + 1}\,. \qquad [A11]$$

APPENDIX B

List files of the computer program STABILITY PREDICTION and its subroutines.

```
Microsoft FORTRAN Optimizing Compiler Version 5.00.03

Line#  Source Line

             PROGRAM STABILITY PREDICTION

       CCCCC REV. 06-22-92

             IMPLICIT NONE
             CHARACTER CODE*6
             CHARACTER ZPQ*1,FLDIR*7
             INTEGER L,NZP1,NZP2
             INTEGER*2 CDATE,STIME,FTIME
             DIMENSION CDATE(3),STIME(4),FTIME(4)
             REAL APR,PHCZI,N,AHP,PHSS,SPH,FPH,PH,AHM,TAH
             REAL ZPPH1,ZPDP1,ZPPH2,ZPDP2,CONCL,TEMP,V
             REAL*8 WOO,WOT,WTT,WT
             DIMENSION PHCZI(2), AHP(2), WT(200), PH(200),
             DIMENSION APR(2)
             DIMENSION ZPPH1(200), ZPDP1(200),
             DIMENSION ZPPH2(200), ZPDP2(200)
             DIMENSION WOO(200),WOT(200),WTT(200),TAH(2:4)

       CCCCC N= OVERALL PROPORTION OF PARTICLES OF COMPONENT
       CCCCC    ONE IN SYSTEM
       CCCCC V= VOLUME PERCENT OF COMPONENT ONE IN SYSTEM
       CCCCC APR= ATOMIC PARTICLE RADIUS (ARRAY VARIABLE)
       CCCCC PHCZI= PH OF ZERO-POINT-OF-CHARGE (ARRAY
       CCCCC        VARIABLE)
       CCCCC AHP= HAMAKER CONSTANT OF PARTICLE (ARRAY
       CCCCC      VARIABLE)(J)
       CCCCC AHM= HAMAKER CONSTANT OF MEDIUM(J)
       CCCCC TAH= TOTAL HAMAKER CONSTANT(J)
       CCCCC TAH(2)=A131
       CCCCC TAH(3)=A132
       CCCCC TAH(4)=A232
       CCCCC TEMP=TEMPERATURE OF SYSTEM (deg. C)
       CCCCC SPH= STARTING PH
       CCCCC FPH FINISHING PH
       CCCCC PHSS= PH STEP SIZE
       CCCCC MSS= MINIMUM STEP SIZE
       CCCCC FLNAME= NAME OF FILE DATA WILL BE STORED IN
       CCCCC FLDIR=NAME OF DIRECTORY DATA FILE IS STORED IN
       CCCCC CICS= CORRECT INPUT CHARACTER STRING
       CCCCC CI= CORRECT INPUT ANSWER VARIABLE
       CCCCC RICS= READ INPUT CHARACTER STRING
       CCCCC WOO,WOT,WTT=INVERSE OF THE PROBABILITY THAT A
       CCCCC             GIVEN PARTICLE
       CCCCC             COLLISION LEADS TO ADHESION
       CCCCC WT=OVERALL STABILITY RATIO
       CCCCC PH=PH COORESPONDING TO AN OVERALL STABILITY
       CCCCC    RATIO VALUE
```

Line# Source Line

```
CCCCC ZPQ=ZETA POTENTIAL QUESTION VARIABLE
CCCCC     ('Z'=ZETA POTENTIAL DATA USED FOR
CCCCC     CALCULATIONS)
CCCCC     ('P'=POINT-OF-ZERO-CHARGE DATA USED FOR
CCCCC     CALCULATIONS)
CCCCC NZP=NUMBER OF ZETA POTENTIAL DATA POINTS
CCCCC ZPDP=ZETA POTENTIAL DATA POINT (ARRAY VARIABLE)
CCCCC ZPPH=COORESPONDING ZETA POTENTIAL PH (ARRAY
CCCCC      VARIABLE)
CCCCC CONCL=CONCENTRATION OF 1-1 ELECTROLYTE IN SYSTEM
CCCCC       (MOLE/L)
CCCCC L=INTERGER USED AS A COUNTER FOR DO LOOPS
CCCCC CDATE=CURRENT DATE
CCCCC STIME=STARTIMG TIME OF RUN
CCCCC FTIME=FINISHING TIME OF RUN

10    OPEN(14,FILE='FLEINPUT.DAT',STATUS='OLD')

CCC----------------------GETTING SYSTEM DATA FROM
C---------------------------FILE----------------------
20    CALL FDATA INPUT (V, APR, PHCZI, AHP, AHM, SPH,
&     FPH, PHSS, ZPQ, NZP1, NZP2,ZPPH1, ZPDP1, ZPPH2,
       ZPDP2, CONCL, FLDIR, TEMP)

CC-----------------------GETTING CURRENT DATE AND
C--------------------------PROGRAM RUN STARTING TIME---
30    CALL GETDAT (CDATE(1),CDATE(2),CDATE(3))
40    CALL GETTIM (STIME(1), STIME(2), STIME(3),
&          STIME(4))

CCC----------------------CALCULATING TOTAL HAMAKER
C---------------------------CONSTANT------------------
50    TAH(2)=(SQRT(AHP(1)) - SQRT(AHM)) *
             (SQRT(AHP(1)) - SQRT(AHM))
60    TAH(3)=(SQRT(AHP(1)) - SQRT(AHM)) *
             (SQRT(AHP(2)) - SQRT(AHM))
70    TAH(4)=(SQRT(AHP(2)) - SQRT(AHM)) *
             (SQRT(AHP(2)) - SQRT(AHM))

CCC----------------------INITIALIZING WT & PH VALUES TO
C---------------------------ZERO----------------------
80    DO 140 L=1,200,1
90       WT(L) = 0.0
100      PH(L) = 0.0
110      WOO(L)=0.0
120      WOT(L)=0.0
130      WTT(L)=0.0
140   CONTINUE

```

```
 Line#  Source Line

    83 CCC---------------------CALCULATING WT & PH VALUES FOR
       C---------------------------SPECIFIED ----------------
    84 C---------------------------PH RANGE & STEP SIZE-----
    85  150   IF (ZPQ.EQ.'P') THEN
    86  160      CALL CALCPZC(V, APR, PHCZI, TAH, SPH, FPH,
     87      & PHSS, WT, PH, CONCL, WOO, WOT, WTT, FLDIR,
             & TEMP)
    88  170   ELSE
    89  180     CALL CALCZP(V, APR, TAH, ZPDP1, ZPPH1, ZPPH2,
    90       & ZPDP2, SPH, FPH, PHSS, WT, PH, CONCL, NZP1,
             & NZP2, WOO, WOT, WTT, FLDIR, TEMP)
    91  190   END IF
    92
    93 CC----------------------GETTING PROGRAM RUN FINISHING
       C--------------------------TIME----------------------
    94  200   CALL GETTIM (FTIME(1), FTIME(2), FTIME(3),
             & FTIME(4))
    95
    96  CCC--------------------STORING INPUT & CALCULATED
        C-----------------------DATA-----------------------
    97  210   CALL DATA STORAGE(N, APR, ZPQ, AHM, AHP, PHCZI,
    98       & NZP1, NZP2, ZPPH1, ZPDP1, ZPPH2, ZPDP2, WT, PH,
    99       & CONCL, WOO, WOT, WTT, CDATE, STIME, FTIME,TEMP)
   100  220   CLOSE(14)
   101
   102 CCC---------------------FORMATTING READ STATEMENTS----
   103  800   FORMAT (A1)
   104
   105  998   STOP
   106  999   END
```

```
main  Local Symbols

Name                          Class   Type        Size   Offset

PH. . . . . . . . . . . . . . local    REAL*4       800    0000
STIME . . . . . . . . . . . . local    INTEGER*2      8    0002
L . . . . . . . . . . . . . . local    INTEGER*4      4    000a
N . . . . . . . . . . . . . . local    REAL*4         4    000e
V . . . . . . . . . . . . . . local    REAL*4         4    0012
AHM . . . . . . . . . . . . . local    REAL*4         4    0016
AHP . . . . . . . . . . . . . local    REAL*4         8    001a
CODE. . . . . . . . . . . . . local    CHAR*6         6    0022
TAH . . . . . . . . . . . . . local    REAL*4        12    0028
FPH . . . . . . . . . . . . . local    REAL*4         4    0034
CDATE . . . . . . . . . . . . local    INTEGER*2      6    0038
APR . . . . . . . . . . . . . local    REAL*4         8    003e
NZP1. . . . . . . . . . . . . local    INTEGER*4      4    0046
```

```
main  Local Symbols

Name                         Class   Type         Size   Offset

NZP2. . . . . . . . . . . . . local   INTEGER*4      4    004a
SPH . . . . . . . . . . . . . local   REAL*4         4    004e
CONCL . . . . . . . . . . . . local   REAL*4         4    0052
FLDIR . . . . . . . . . . . . local   CHAR*7         7    0056
FTIME . . . . . . . . . . . . local   INTEGER*2      8    005e
TEMP. . . . . . . . . . . . . local   REAL*4         4    0066
ZPQ . . . . . . . . . . . . . local   CHAR*1         1    006a
PHSS. . . . . . . . . . . . . local   REAL*4         4    006c
PHCZI . . . . . . . . . . . . local   REAL*4         8    0070
WT. . . . . . . . . . . . . . local   REAL*8      1600    0320
ZPDP1 . . . . . . . . . . . . local   REAL*4       800    0960
ZPDP2 . . . . . . . . . . . . local   REAL*4       800    0c80
ZPPH1 . . . . . . . . . . . . local   REAL*4       800    0fa0
ZPPH2 . . . . . . . . . . . . local   REAL*4       800    12c0
WOO . . . . . . . . . . . . . local   REAL*8      1600    15e0
WOT . . . . . . . . . . . . . local   REAL*8      1600    1c20
WTT . . . . . . . . . . . . . local   REAL*8      1600    2260


Global Symbols

Name                        Class   Type        Size   Offset

CALCPZC . . . . . . . . . . extern  ***          ***      ***
CALCZP. . . . . . . . . . . extern  ***          ***      ***
DATASTORAGE . . . . . . . . extern  ***          ***      ***
FDATAINPUT. . . . . . . . . extern  ***          ***      ***
GETDAT. . . . . . . . . . . extern  ***          ***      ***
GETTIM. . . . . . . . . . . extern  ***          ***      ***
main. . . . . . . . . . . . FSUBRT  ***          ***     0000

Code size = 044b (1099)
Data size = 002b (43)
Bss size  = 0078 (120)

No errors detected
```

Microsoft FORTRAN Optimizing Compiler Version 5.00.03

Line# Source Line

```
      SUBROUTINE FDATA INPUT(N, APR, PHCZI, AHP, AHM,
& SPH, FPH, PHSS, ZPQ, NZP1, NZP2, ZPPH1, ZPDP1, ZPPH2,
& ZPDP2, CONCL, FLDIR, TEMP)
CCCCC REV. 05-03-92

CCC---------------------SUBROUTINE TO READ IN SYSTEM
CC-------------------------DATA FROM A DATA FILE-----

      IMPLICIT NONE
      CHARACTER ZPQ*1,FLDIR*7
      INTEGER I,NZP1,NZP2
      REAL N,APR,PHCZI,AHP,AHM,SPH,FPH,PHSS,TEMP
      REAL ZPDP1,ZPPH1,ZPDP2,ZPPH2,CONCL,SPHL,FPHL
      DIMENSION PHCZI(2),AHP(2),APR(2), ZPDP1(200)
      DIMENSION , ZPPH1(200), ZPPH2(200), ZPDP2(200)

CCCCC MSS=MINIMUM STEP SIZE

10    READ (14,800)TEMP
20    READ (14,805)N
30    READ(14,810)CONCL
40    READ(14,815)APR(1)
50    READ(14,815)APR(2)
60    READ(14,820)ZPQ
70    IF (ZPQ.EQ.'P')THEN
80       READ(14,825)PHCZI(1)
90       READ(14,825)PHCZI(2)
100      READ(14,830)SPH
110      READ(14,830)FPH
120      READ(14,835)PHSS
130   ELSE IF (ZPQ.EQ.'Z') THEN
140        READ(14,840)NZP1
150        DO 180 I=1,NZP1,1
160          READ(14,830)ZPPH1(I)
170          READ(14,845)ZPDP1(I)
180        CONTINUE
190        READ(14,840)NZP2
200        DO 230 I=1,NZP2,1
210          READ(14,830)ZPPH2(I)
220          READ(14,845)ZPDP2(I)
230        CONTINUE

C-----------------------DETERMINING PH RANGE FOR
C---------------------------Z.P. DATA-----------------
240      IF (ZPPH1(1).LE.ZPPH2(1))THEN
250        SPHL=ZPPH2(1)
260      ELSE
270        SPHL=ZPPH1(1)
```

```
Line#  Source Line

   280         END IF
   290         IF (ZPPH1(NZP1).GE.ZPPH2(NZP2))THEN
   300           FPHL=ZPPH2(NZP2)
   310         ELSE
   320           FPHL=ZPPH1(NZP1)
   330         END IF
   340         READ(14,830)SPH
   350         READ(14,830)FPH
   360         READ(14,835)PHSS
   370      END IF
   380      READ(14,850)AHM
   390      READ(14,850)AHP(1)
   400      READ(14,850)AHP(2)
   410      IF (ZPQ.NE.'P'.AND.SPH.LT.SPHL)THEN
   420        SPH=SPHL
   430      ELSE IF (ZPQ.NE.'P'.AND.FPH.GT.FPHL)THEN
   440        FPH=FPHL
   450      END IF
   460      READ(14,855)FLDIR

  CCC----------------------FORMATING READ STATEMENTS----
   800      FORMAT (F4.1)
   805      FORMAT (F4.3)
   810      FORMAT (F7.5)
   815      FORMAT (F7.1)
   820      FORMAT(A1)
   825      FORMAT (F5.2)
   830      FORMAT (F5.2)
   835      FORMAT (F5.3)
   840      FORMAT (I2)
   845      FORMAT (F4.1)
   850      FORMAT (E10.2)
   855      FORMAT (A7)

   998      RETURN
   999      END
```

```
FDATAINPUT  Local Symbols

Name                         Class    Type       Size   Offset

TEMP. . . . . . . . . . . . param                        0006
FLDIR . . . . . . . . . . . param                        000a
CONCL . . . . . . . . . . . param                        000e
ZPDP2 . . . . . . . . . . . param                        0012
ZPPH2 . . . . . . . . . . . param                        0016
ZPDP1 . . . . . . . . . . . param                        001a
ZPPH1 . . . . . . . . . . . param                        001e
```

```
FDATAINPUT  Local Symbols

Name                      Class  Type       Size   Offset
NZP2. . . . . . . . . . . param                      0022
NZP1. . . . . . . . . . . param                      0026
ZPQ . . . . . . . . . . . param                      002a
PHSS. . . . . . . . . . . param                      002e
FPH . . . . . . . . . . . param                      0032
SPH . . . . . . . . . . . param                      0036
AHM . . . . . . . . . . . param                      003a
AHP . . . . . . . . . . . param                      003e
PHCZI . . . . . . . . . . param                      0042
APR . . . . . . . . . . . param                      0046
N . . . . . . . . . . . . param                      004a
I . . . . . . . . . . . . local   INTEGER*4    4     0002
FPHL. . . . . . . . . . . local   REAL*4       4     0006
SPHL. . . . . . . . . . . local   REAL*4       4     000a


Global Symbols

Name                      Class  Type       Size   Offset

FDATAINPUT. . . . . . . . FSUBRT  ***         ***    0000


Code size = 04a1 (1185)
Data size = 00f7 (247)
Bss size  = 000e (14)

No errors detected
```

```
      Microsoft FORTRAN Optimizing Compiler Version 5.00.03

Line#  Source Line

    1         SUBROUTINE CALCPZC (V, APR, PHCZI, TAH, SPH,
    2        & FPH, PHSS, WT, PH, CONCL, WOO, WOT, WTT, FLDIR,
              & TEMP)
    3
    4   CCCCC REV. 06-22-92
    5
    6   CCC---------------------SUBPROGRAM TO CALCULATE
    7   C---------------OVERALL STABILITY RATIO USING
        C---------------POINT-OF-ZERO-CHARGE DATA------------
    8
    9         IMPLICIT NONE
   10         CHARACTER FLDIR*7
   11         INTEGER L,K,ONE,TWO,IPHC,IWIDTH
   12         REAL*8 WT,WOO,WOT,WTT,OOWT,AZ,AZN,AZP
   13         REAL N, APR, PHCZI, SPH, FPH, PHSS, PH, CONCL,
              REAL HOA, HOR, APRC, TEMPK, V, OON
   14         REAL CPH, PSI, RPHC, DELTPH, TAH, KRL, TEMP,
   15         DIMENSION PH(200), WT(200), APR(2), PHCZI(2),
              DIMENSION PSI(2), APRC(2)
   16         DIMENSION WOO(200),WOT(200),WTT(200),TAH(2:4)
   17
   18   CCCCC OOWT=ONE OVER WT
   19   CCCCC CPH=CURRENT PH
   20   CCCCC RPHC=REAL VARIABLE PH COUNTER(FOR DO LOOP)
   21   CCCCC IPHC=INTEGER VARIABLE PH COUNTER(FOR DO LOOP)
   22   CCCCC PSI=SURFACE POTENTIAL CALCULATED FROM
        CCCCC     POINT-OF-ZERO-CHARGE (V)
   23   CCCCC HOA=MINIMUM PARTICLE SEPERATION FOR ATTRACTIVE
        CCCCC     TERMS(M)
   24   CCCCC HOR=MINIMUM SEPERATION FOR REPULSIVE TERMS(M)
   25   CCCCC TEMPK=TEMPERATURE OF SYSTEM IN DEGREES KELVIN
   26   CCCCC IWIDTH=WIDTH OF INTERAGER K (1 DIGIT,2 DIGITS,
        CCCCC        ETC.)
   27   CCCCC DELTPH=CHANGE IN PH FROM FINISHING PH AND
        CCCCC        STARTING PH
   28   CCCCC KRL=REAL VARIABLE REPULSION OF VARIABLE K
   29   CCCCC K=INTEGER VARIABLE USED AS A COUNTER FOR DO LOOP
   30   CCCCC   WHICH CALCULATES OVERALL STABILITY AT EACH
        CCCCC   SPECIFIED PH
   31   CCCCC L=INTEGER USED AS COUNTER FOR VARIOUS DO LOOPS
   32   CCCCC ONE=INTEGER VARIABLE EQUAL TO ONE
   33   CCCCC TWO=INTEGER VARIABLE EQUAL TO TWO
   34   CCCCC AZ=VARIABLE REPRESENTING ALMOST ZERO (1.0E-309)
   35   CCCCC AZP=POSITIVE VALUE OF AZ USED TO PREVENT AN
   36   CCCCC    INVERSE FROM GOING TO INFINITY WHICH CAUSES
   37   CCCCC     A MATH OVERFLOW ERROR RESULTING IN PROGRAM
        CCCCC     TERMINATION
   38   CCCCC AZN=NEGATIVE VALUE OF AZ USED AS AZP IS
```

```
CCCCC APRC=ATOMIC PARTICLE RADIUS CUBED
CCCCC OON=ONE OVER N
CCCCC WKO=SUBROUTINE TO CALCULATE W VALUES IF K IS 1
CCCCC     DIGIT IN LENGTH
CCCCC WKTW=SUBROUTINE CALCULATING W VALUES IF K IS 2
CCCCC      DIGITS LONG
CCCCC WKTH=SUBROUTINE CALCULATING W VALUES IF K IS 3
CCCCC      DIGITS IN LENGTH

10    TEMPK=TEMP+273.2
20    ONE=1
30    TWO=2
CCC---------------------CALCULATING VALUES FOR
C------------------------AZP,AZN--------------------
40    AZ=1.0E-25
50    DO 70 K=1,11,1
60      AZ=AZ/1.0E25
70    CONTINUE
80    AZP=AZ/1.0E9
90    AZN=-1.0*AZP
CC----------------------CONVERTING PH COUNTER TO
C--------------------------INTEGER VARIABLE----------
100   DELTPH = FPH-SPH
110   IF (PHSS.EQ.0.0 .OR. DELTPH.EQ.0.0)THEN
120      IPHC=1
130   ELSE
140      RPHC = (FPH-SPH)/PHSS
150      IPHC = NINT(RPHC)
160      IPHC = IPHC + 1
170   END IF
CC---------------------CALCULATING N FROM V----------
180   APRC(1) = APR(1)**3
190   APRC(2) = APR(2)**3
200   OON = ((APRC(1))-(V*APRC(1)))/(V*APRC(2))
210   OON = OON + 1.00
220   N = 1.00/OON

CC----------------------INITIALIZING CURRENT PH-------
230   CPH = SPH
CC----------------------CALCULATING OVERALL STABILITY
C-------------------------RATIO FOR SPECIFIED PH RANGE
C-------------------------& STEP SIZE----------------
240   DO 530 K=1,IPHC,1
250     KRL=REAL(K)
260     IWIDTH=INT(LOG10(KRL)+1)

C-----------------------CALCULATING POTENTIAL,PSI,FOR
C-------------------------THE TWO DIFFERENT PARTICES
C------------------------FOR CURRENT PH-------------
270      DO 290 L=1,2,1
280        PSI(L)=(8.6205E-5)*(TEMPK)*(2.3026)*
                  (PHCZI(L)-CPH)
```

```
Source Line
290      CONTINUE

C-----------------------SETTING MINIMUM PARTICLE
C--------------------------SURFACE-----------------
C-------------------------SEPERATION FOR VA & VR
C                         CALCULATIONS-------------
300   HOR = 1.0E-10
310   HOA = 0.0

CC----------------------FINDING VARIOUS (INVERSE)
C-------------------------PROBABILITIES OF PARTICLE
C-------------------------COLLISION & ADHESION FOR
C-------------------------COLLISION OF TWO PARTICLES
C------------------------OF TYPE #1----------------
320      IF(IWIDTH.EQ.1)THEN
330       CALL WKO(K, WOO, WOT, WTT, APR, TAH, PSI,
     & CONCL, HOA, HOR, CPH, FLDIR, TEMPK)
340      ELSE IF(IWIDTH.EQ.2)THEN
350       CALL WKTW(K, WOO, WOT, WTT, APR, TAH, PSI,
     & CONCL, HOA, HOR, CPH, FLDIR, TEMPK)
360      ELSE IF(IWIDTH.EQ.3)THEN
370       CALL WKTH(K, WOO, WOT, WTT, APR, TAH, PSI,
     & CONCL, HOA, HOR, CPH, FLDIR, TEMPK)
380      END IF

CC----------------------FINDING THE OVERALL STABILITY
C------------------------RATIO AT CURRENT PH---------

C-----------------------MAKING SURE INVERSES WILL NOT
C---------------------------GO TO INFINITY SO A MATH
C----------------------------OVERFLOW ERROR DOES NOT
C----------------------------RESULT IN PROGRAM
C---------------------------TERMINATION-------------
390      IF(WOO(K).LE.AZP .AND. WOO(K).GE.AZN)THEN
400        WT(K)=WOO(K)
410      ELSE IF(WOT(K).LE.AZP .AND. WOT(K).GE.AZN)
   &             THEN
420        WT(K)=WOT(K)
430      ELSE IF(WTT(K).LE.AZP .AND. WTT(K).GE.AZN)
   &             THEN
440        WT(K)=WTT(K)
C-----------------------ACTUALLY CALCULATING OVERALL
C--------------------------STABILITY----------------
450      ELSE
460        OOWT = (N*N/WOO(K))
470        OOWT=OOWT+((1.0-N)*(1.0-N)/WTT(K))
480        OOWT=OOWT+(2.0*N*(1.0-N)/WOT(K))
490        WT(K)=1.0/OOWT
500      END IF

```

```
 Line#  Source Line

   124  CC----------------------SETTING COORESPONDING PH VALUE
         C--------------------------FOR WT(K)----------------
   125   510       PH(K)=CPH
   126
   127   CC----------------------SETTING NEW CURRENT PH
         C--------------------------VALUE--------------------
   128   520       CPH = CPH + PHSS
   129
   130   530   CONTINUE
   131
   132   CC----------------------RETURNING WT & PH VALUES TO
         C--------------------------MAIN PROGRAM-----CCCCCCCC
   133   998   RETURN
   134   999   END


CALCPZC  Local Symbols

Name                         Class    Type        Size   Offset

TEMP. . . . . . . . . . . . . param                       0006
FLDIR . . . . . . . . . . . . param                       000a
WTT . . . . . . . . . . . . . param                       000e
WOT . . . . . . . . . . . . . param                       0012
WOO . . . . . . . . . . . . . param                       0016
CONCL . . . . . . . . . . . . param                       001a
PH. . . . . . . . . . . . . . param                       001e
WT. . . . . . . . . . . . . . param                       0022
PHSS. . . . . . . . . . . . . param                       0026
FPH . . . . . . . . . . . . . param                       002a
SPH . . . . . . . . . . . . . param                       002e
TAH . . . . . . . . . . . . . param                       0032
PHCZI . . . . . . . . . . . . param                       0036
APR . . . . . . . . . . . . . param                       003a
V . . . . . . . . . . . . . . param                       003e
TEMPK . . . . . . . . . . . . local    REAL*4         4   0000
DELTPH. . . . . . . . . . . . local    REAL*4         4   0004
OOWT. . . . . . . . . . . . . local    REAL*8         8   0008
IWIDTH. . . . . . . . . . . . local    INTEGER*4      4   0010
K . . . . . . . . . . . . . . local    INTEGER*4      4   0014
L . . . . . . . . . . . . . . local    INTEGER*4      4   0018
N . . . . . . . . . . . . . . local    REAL*4         4   001c
HOA . . . . . . . . . . . . . local    REAL*4         4   0020
CPH . . . . . . . . . . . . . local    REAL*4         4   0024
AZ. . . . . . . . . . . . . . local    REAL*8         8   0028
ONE . . . . . . . . . . . . . local    INTEGER*4      4   0030
IPHC. . . . . . . . . . . . . local    INTEGER*4      4   0034
APRC. . . . . . . . . . . . . local    REAL*4         8   0038
KRL . . . . . . . . . . . . . local    REAL*4         4   0040
HOR . . . . . . . . . . . . . local    REAL*4         4   0044
```

```
CALCPZC  Local Symbols

Name                         Class   Type       Size   Offset

AZN . . . . . . . . . . . . . local   REAL*8       8    0048
AZP . . . . . . . . . . . . . local   REAL*8       8    0050
OON . . . . . . . . . . . . . local   REAL*4       4    0058
PSI . . . . . . . . . . . . . local   REAL*4       8    005c
RPHC. . . . . . . . . . . . . local   REAL*4       4    0064
TWO . . . . . . . . . . . . . local   INTEGER*4    4    0068

Global Symbols

Name                         Class   Type       Size   Offset

CALCPZC. . . . . . . . . . . FSUBRT  ***        ***     0000
WKO . . . . . . . . . . . . . extern ***        ***     ***
WKTH. . . . . . . . . . . . . extern ***        ***     ***
WKTW. . . . . . . . . . . . . extern ***        ***     ***

Code size = 082d (2093)
Data size = 003c (60)
Bss size  = 006c (108)

No errors detected
```

Microsoft FORTRAN Optimizing Compiler Version 5.00.03

```
Line#  Source Line

   1         SUBROUTINE CALCZP (V, APR, TAH, ZPDP1, ZPPH1,
   2        & ZPPH2, ZPDP2, SPH, FPH, PHSS, WT, PH, CONCL,
            & NZP1, NZP2, WOO, WOT, WTT, FLDIR, TEMP)
   3
   4   CCCCC REV. 06-22-92
   5
   6   CCC----------------------SUBPROGRAM TO CALCULATE
   7   C--------------------------OVERALL STABILITY RATIO
       C--------------------------USING ZETA POTENTIAL DATA--
   8
   9         IMPLICIT NONE
  10         CHARACTER FLDIR*7
  11         INTEGER ONE,TWQ,IPHC,IWIDTH
  12         REAL N, APR, ZPDP1, ZPPH1, ZPDP2, ZPPH2, SPH,
             REAL FPH, PHSS, PH, TEMP, TEMPK
  13         REAL CPH, RPHC, DELTPH, TAH, KRL, POT, CONCL,
  14         REAL*8 WOO,WOT,WTT,OOWT,WT,AZ,AZP,AZN
  15         DIMENSION PH(200),APR(2),POT(2),TAH(2:4)
  16         DIMENSION WT(200),WOO(200),WOT(200),WTT(200)
  17         DIMENSION ZPDP1(200), ZPPH1(200), ZPDP2(200),
             DIMENSION ZPPH2(200)
  18         INTEGER K,NZP1,NZP2
  19         REAL ZPD,APRC,V,OON
  20         REAL DELTA,HOA,HOR
  21         DIMENSION ZPD(2),APRC(2)
  22         DIMENSION DELTA(2)
  23
  24
  25   CCCCC OOWT=ONE OVER WT
  26   CCCCC W=REAL FCN. USED IN FCN. SUBPROGRAM TO FIND
       CCCCC   WOO,WOT,WTT
  27   CCCCC CPH=CURRENT PH
  28   CCCCC TEMPK=SYSTEM TEMPREATURE IN DEGREES KELVIN
  29   CCCCC DELTA=DISTANCE FROM PARTICLE SURFACE TO STERN
       CCCCC       LAYER(M)
  30   CCCCC RPHC=REAL VARIABLE PH COUNTER(FOR DO LOOP)
  31   CCCCC IPHC=INTEGER VARIABLE PH COUNTER(FOR DO LOOP)
  32  CCCCC POT=ZETA POTENTIAL FOR PARTICLES AT CURRENT PH
  33   CCCCC ZPD=ZETA POTENTIAL DATA AT CPH FOR
       CCCCC     PARTICLE(ARRAY VARIABLE)
  34   CCCCC DELTPH=CHANGE IN PH FROM FINISHING PH TO
       CCCCC        STARTING PH
  35   CCCCC K=INTEGER VARIABLE USED AS COUNTER FOR LOOP TO
  36   CCCCC   CALCULATE STABILITY RATIO FOR EACH SPECIFIED
       CCCCC   PH
  37   CCCCC KRL=REAL REPRESENTATION OF VARIABLE K
  38   CCCCC IWIDTH=WIDTH OF INTEGER K (EX: 1 DIGIT, 2
       CCCCC        DIGITS,ETC.)
```

Line# Source Line

```
CCCCC ONE=INTEGER VARIABLE EQUAL TO ONE
CCCCC TWO=INTEGER VARIABLE EQUAL TO TWO
CCCCC HOA=MINIMUM PARTICLE SEPERATION FOR ATTRACTIVE
CCCCC     TERM (M)
CCCCC HOR=MINIMUM SEPARATION FOR REPULSIVE TERMS (M)
CCCCC AZ=VARIABLE REPRESENTING ALMOST ZERO (1.0E-309)
CCCCC AZP=POSITIVE VALUE OF AZ USED TO PREVENT AN
CCCCC     INVERSE FROM GOING TO INFINITY WHICH WILL
CCCCC     CAUSE A MATH OVERFLOW ERROR RESULTING IN
CCCCC     PROGRAM TERMINATION
CCCCC AZN=NEGATIVE VALUE OF AZ USED AS AZP IS USED
CCCCC WKO=SUBROUTINE TO CALCULATE STABILITY IF K IS
CCCCC     ONE DIGIT WIDE
CCCCC WKTW=SUBROUTINE TO CALCULATE STABILITY IF K IS
CCCCC      TWO DIGITS WIDE
CCCCC WKTH=SUBROUTINE TO CALCULATE STABILITY IF K IS
CCCCC      THREE DIGITS


10    TEMPK=TEMP+273.2
20    DELTA(1)=0.50E-9
30    DELTA(2)=0.50E-9
40    ONE=1
50    TWO=2

CC----------------------CALCULATING VALUES FOR AZP AND
C---------------------------AZN----------------------
60    AZ=1.0E-25
70    DO 90 K=1,11,1
80       AZ=AZ/1.0E25
90    CONTINUE
100   AZP=AZ/1.0E9
110   AZN=-1.0*AZP

CC----------------------CONVERTING PH COUNTER TO
C----------------------------INTEGERVARIABLE---------
120   DELTPH = FPH-SPH
130   IF (PHSS.EQ.0.0 .OR. DELTPH.EQ.0.0) THEN
140    IPHC=1
150   ELSE
160    RPHC = (FPH-SPH)/PHSS
170    IPHC = NINT(RPHC)
180     IPHC = IPHC+1
190   END IF

CC---------------------CALCULATING N FROM V----------
200   APRC(1) = APR(1)**3
210   APRC(2) = APR(2)**3
220   OON = ((APRC(1))-(V*APRC(1)))/(V*APRC(2))
230   OON = OON + 1.00
```

```
Line#  Source Line

 240   N = 1.00/OON

CC----------------------INITIALIZING CURRENT PH-------
 250   CPH = SPH


CC----------------------CALCULATING OVERALL STABILITY
C------------------------RATIO FOR SPECIFIED PH RANGE
C------------------------& STEP SIZE-----------------

 260   DO 550 K=1,IPHC,1
 270     KRL=REAL(K)
 280     IWIDTH=INT(LOG10(KRL)+1)

C----------------------GETTING ZETA POTENTIAL VALUES
C---------------------------FOR SPECIFIED PH VALUES--
 290     CALL INTERP(ZPDP1, ZPPH1, ZPPH2, ZPDP2, CPH,
     & NZP1, NZP2, ZPD)

C----------------------CHANGING UNITS OF V FROM mV---
 300    POT(1)=ZPD(1)*1.0E-3
 310    POT(2)=ZPD(2)*1.0E-3
 320    HOA = DELTA(1)+DELTA(2)
 330    HOR = 1.0E-10

 CC----------------------FINDING VARIOUS (INVERSE)
 C-------------------------PROBABILITIES OF PARTICLE
 C-------------------------COLLISION & ADHESION--------
 340     IF(IWIDTH.EQ.1)THEN
 350      CALL WKO(K, WOO, WOT, WTT, APR, TAH, POT,
     & CONCL, HOA, HOR, CPH, FLDIR, TEMPK)
 360     ELSE IF(IWIDTH.EQ.2)THEN
 370      CALL WKTW(K, WOO, WOT, WTT, APR, TAH, POT,
     & CONCL, HOA, HOR, CPH, FLDIR, TEMPK)
 380     ELSE IF(IWIDTH.EQ.3)THEN
 390       CALL WKTH(K, WOO, WOT, WTT, APR, TAH, POT,
     & CONCL, HOA, HOR, CPH, FLDIR, TEMPK)
 400     END IF

 CC----------------------FINDING THE INVERSE OF THE
 C-------------------------OVERALL STABILITY RATIO AT
 C-------------------------CURRENTPH-----------------

C----------------------ENSURING INVERSES WILL NOT GO
 C-------------------------TO INFINITY, CAUSE A MATH
 C-------------------------OVERFLOW ERROR, AND RESULT
 C-------------------------IN IN PROGRAM TERMINATION--
 410     IF(WOO(K).LE.AZP .AND. WOO(K).GE.AZN)THEN
 420       WT(K)=AZP
430    ELSE IF(WOT(K).LE.AZP .AND. WOT(K).GE.AZN)THEN
```

```
Line#  Source Line

   127  440        WT(K)=AZP
   128  450     ELSE IF(WTT(K).LE.AZP .AND. WTT(K).GE.AZN)THEN
   129  460        WT(K)=AZP
   130  470      ELSE
   131  480       OOWT = (N*N/WOO(K))
   132  490       OOWT = OOWT+((1.0-N)*(1.0-N)/WTT(K))
   133  500       OOWT = OOWT+(2.0*N*(1.0-N)/WOT(K))
   134  510       WT(K)=1.0/OOWT
   135  520      END IF
   136
   137  CC-----------------------SETTING COORESPONDING PH VALUE
        C--------------------------FOR WT(I)-----
   138  530     PH(K)=CPH
   139
   140  CC-----------------------SETTING NEW CURRENT PH VALUE--
   141  540     CPH = CPH + PHSS
   142  550    CONTINUE
   143
   144
   145  CC-----------------------RETURNING WT & PH VALUES TO
        C--------------------------MAINPROGRAM--------------
   146  998    RETURN
   147  999    END


CALCZP  Local Symbols

Name                         Class   Type       Size   Offset

TEMP. . . . . . . . . . . . param                       0006
FLDIR . . . . . . . . . . . param                       000a
WTT . . . . . . . . . . . . param                       000e
WOT . . . . . . . . . . . . param                       0012
WOO . . . . . . . . . . . . param                       0016
NZP2. . . . . . . . . . . . param                       001a
NZP1. . . . . . . . . . . . param                       001e
CONCL . . . . . . . . . . . param                       0022
PH. . . . . . . . . . . . . param                       0026
WT. . . . . . . . . . . . . param                       002a
PHSS. . . . . . . . . . . . param                       002e
FPH . . . . . . . . . . . . param                       0032
SPH . . . . . . . . . . . . param                       0036
ZPDP2 . . . . . . . . . . . param                       003a
ZPPH2 . . . . . . . . . . . param                       003e
ZPPH1 . . . . . . . . . . . param                       0042
ZPDP1 . . . . . . . . . . . param                       0046
TAH . . . . . . . . . . . . param                       004a
APR . . . . . . . . . . . . param                       004e
V . . . . . . . . . . . . . param                       0052
TEMPK . . . . . . . . . . . local   REAL*4        4     0000
```

```
CALCZP  Local Symbols

Name                     Class   Type       Size   Offset

DELTPH. . . . . . . . . . local   REAL*4         4    0004
OOWT. . . . . . . . . . . local   REAL*8         8    0008
IWIDTH. . . . . . . . . . local   INTEGER*4      4    0010
K . . . . . . . . . . . . local   INTEGER*4      4    0014
N . . . . . . . . . . . . local   REAL*4         4    0018
HOA . . . . . . . . . . . local   REAL*4         4    001c
AZ. . . . . . . . . . . . local   REAL*8         8    0020
CPH . . . . . . . . . . . local   REAL*4         4    0028
ONE . . . . . . . . . . . local   INTEGER*4      4    002c
IPHC. . . . . . . . . . . local   INTEGER*4      4    0030
APRC. . . . . . . . . . . local   REAL*4         8    0034
HOR . . . . . . . . . . . local   REAL*4         4    003c
AZN . . . . . . . . . . . local   REAL*8         8    0040
KRL . . . . . . . . . . . local   REAL*4         4    0048
DELTA . . . . . . . . . . local   REAL*4         8    004c
AZP . . . . . . . . . . . local   REAL*8         8    0054
OON . . . . . . . . . . . local   REAL*4         4    005c
RPHC. . . . . . . . . . . local   REAL*4         4    0060
ZPD . . . . . . . . . . . local   REAL*4         8    0064
POT . . . . . . . . . . . local   REAL*4         8    006c
TWO . . . . . . . . . . . local   INTEGER*4      4    0074
```

Line# Source Line

```



      SUBROUTINE INTERP(ZPDP1, ZPPH1, ZPPH2, ZPDP2,
     & CPH, NZP1, NZP2, ZPD)

CCCCC REV. 03-05-92

CCC---------------------SUBPROGRAM TO CALCULATE
C-------------------------OVERALL STABILITY RATIO
C-------------------------USING ZETA POTENTIAL DATA---

      IMPLICIT NONE
      REAL ZPDP1,ZPPH1,ZPPH2,ZPDP2
      REAL CPH
      DIMENSION ZPDP1(200), ZPPH1(200), ZPDP2(200),
      DIMENSION ZPPH2(200)
      INTEGER M,NZP1,NZP2
      REAL ZPD,ZPDN,ZPDD,ZPGT,ZPLT,PHGT,PHLT
      REAL PZPGT,PZPLT,PGTDIF,PLTDIF,CGTDIF,CLTDIF
      REAL PPHGT,PPHLT
      DIMENSION ZPD(2)

CCCCC ZPDN=NUMERATOR TERM USED TO CALCULATE ZPD
CCCCC ZPDD=DENOMENATOR TERM USED TO CALCULATE ZPD
CCCCC PPHGT=PRESENT/PERMANENT PH VALUE GREATER THAN
CCCCC      CPH (i.e.PH PRESENTLY NEAREST TO CPH, BUT
CCCCC       STILL GREATER THAN CPH)
CCCCC PPHGT=PRESENT/PERMANENT PH VALUE LESS THAN CPH
CCCCC       (i.e.PH PRESENTLY NEAREST TO CPH, BUT
CCCCC       STILL LESS THAN CPH)
CCCCC PZPGT=PRESENT/PERMANENT ZETA POTENTIAL VALUE
CCCCC       COORESPONDING TO PPHGT
CCCCC PZPLT=PRESENT/PERMANENT ZETA POTENTIAL VALUE
CCCCC       COORESPONDING TO PPHLT
CCCCC PGTDIF=PRESENT/PERMANENT GREATER THAN DIFFERENCE
CCCCC        BETWEEN PGTPH AND CPH
CCCCC PLTDIF=PRESENT/PERMANENT LESS THAN DIFFERENCE
CCCCC        BETWEEN PLTPH AND CPH
CCCCC CGTDIF=CURRENT(i.e.THIS ITERATION) GREATER THAN
CCCCC        DIFFERENCE BETWEEN CPH AND THE CURRENT
CCCCC       ZPPH VALUE IF IT IS GREATER THAN CPH(THIS
CCCCC        ITERATION)
CCCCC CLTDIF=CURRENT(i.e.THIS ITERATION) LESS THAN
CCCCC        DIFFERENCE BETWEEN CPH AND THE CURRENT
CCCCC        ZPPH VALUE IF IT IS LESS THAN CPH(THIS
CCCCC        ITERATION)
CCCCC PHGT=PH GREATER THAN (CPH AND NEAREST TO IT)
CCCCC PHLT=PH LESS THAN (CPH AND NEAREST TO IT)
CCCCC ZPGT=ZETA POTENTIAL VALUE COORESPONDING TO PHGT
```

```
CCCCC ZPLT=ZETA POTENTIAL VALUE COORESPONDING TO ZPLT
CCCCC M=INTEGER VARIABLE USED AS COUNTER FOR VARIOUS
CCCCC   DO LOOPS


CC----------------------INTERPOLATING Z.P. DATA TO GET
C---------------------------VALUESFOR----------------
C------------------------CURRENT PH (IF NEED BE)-----
10       PLTDIF=20.0
20       PGTDIF=20.0
30       DO 220 M=1,NZP1,1

CC----------------------IF CPH= a ZPPH VALUE:
CC-------------------------RETURNING THAT ZPAS THE
C------------------------DESIRED ZP VALUE------------
40         IF (ZPPH1(M) .EQ. CPH) THEN
50           ZPD(1) = ZPDP1(M)
60           GOTO 300

CC----------------------IF CPH.NE. a ZPPH VALUE:THEN
CC-------------------------MUST INTERPOLATE TO GET A
C-------------------------ZPD FOR THIS CPH-----------
C-----------------------TRYING TO FIND THE NEAREST PH
C------------------------TO CPH THAT IS LESS THAN CPH-
70         ELSE IF (ZPPH1(M) .LT. CPH) THEN
80           CLTDIF = CPH-ZPPH1(M)
90           IF (CLTDIF .LT. PLTDIF) THEN
100         PPHLT = ZPPH1(M)
110         PLTDIF = CLTDIF
120         PZPLT = ZPDP1(M)
130          END IF

C-----------------------TRYING TO FIND THE NEAREST PH
C-------------------------TO CPH THAT IS GREATER THAN
C------------------------CPH------------------------
140        ELSE IF (ZPPH1(M) .GT. CPH) THEN
150          CGTDIF = ZPPH1(M) - CPH
160          IF (CGTDIF .LT. PGTDIF) THEN
170         PPHGT = ZPPH1(M)
180         PGTDIF = CGTDIF
190         PZPGT = ZPDP1(M)
200          END IF
210        END IF
220      CONTINUE

C-----------------------INTERPOLATING WITH NEAREST
C-----------------------VALUES-----------------------
230      PHLT = PPHLT
240      ZPLT = PZPLT
250      PHGT = PPHGT
```

Line# Source Line

```
260      ZPGT = PZPGT
270      ZPDN = ZPLT*(CPH-PHGT) + ZPGT*(PHLT-CPH)
280      ZPDD = PHLT - PHGT
290      ZPD(1) = ZPDN/ZPDD

CC----------------------INTERPOLATING Z.P. DATA TO GET
C-------------------------VALUESFOR----------------
C-----------------------CURRENT PH (IF NEED BE)------
300      PLTDIF=20.0
310      PGTDIF=20.0
320      DO 510 M=1,NZP2,1

CC----------------------IF CPH= a ZPPH VALUE:
CC------------------------RETURNING THAT ZP AS THE
C-------------------------DESIRED ZP VALUE-----------
330        IF (ZPPH2(M) .EQ. CPH) THEN
340          ZPD(2) = ZPDP2(M)
350          GOTO 998

CC----------------------IF CPH.NE. a ZPPH VALUE: THEN
CC------------------------MUST INTERPOLATE TO GET A
C-------------------------ZPD FOR THIS CPH------------
C-----------------------TRYING TO FIND THE NEAREST PH
C------------------------TO CPH THAT IS LESS THAN CPH-
360        ELSE IF (ZPPH2(M) .LT. CPH) THEN
370          CLTDIF = CPH-ZPPH2(M)
380          IF (CLTDIF .LT. PLTDIF) THEN
390         PPHLT = ZPPH2(M)
400         PLTDIF = CLTDIF
410         PZPLT = ZPDP2(M)
420          END IF

C-----------------------TRYING TO FIND THE NEAREST PH
C--------------------------TO CPH THAT IS GREATER THAN
C-------------------------CPH------------------------
430        ELSE IF (ZPPH2(M) .GT. CPH) THEN
440          CGTDIF = ZPPH2(M) - CPH
450          IF (CGTDIF .LT. PGTDIF) THEN
460         PPHGT = ZPPH2(M)
470         PGTDIF = CGTDIF
480         PZPGT = ZPDP2(M)
490          END IF
500        END IF
510      CONTINUE

C----------------------INTERPOLATING WITH NEAREST
C--------------------------VALUES-------------------
520      PHLT = PPHLT
530      ZPLT = PZPLT
540      PHGT = PPHGT
```

```
Line#

 28
 28
 28
 28
 28
 28

 28
 28


INTER

Name

IPD .
NIP2.
NIP1.
CPH .
IPDP
IPPH
IPPH
IPDP
PPHG
PLTD
IPGT
PPHL
IPLT
W .
PIPG
PZPI
CSTD
IPDD
PHGT
CLTD
PHLT
IPDM
PGTI

 Glob

Name

CALC
INTI
WKO
WKTI
WKTI
```

```
 Line#  Source Line

   280  550      ZPGT = PZPGT
   281  560      ZPDN = ZPLT*(CPH-PHGT) + ZPGT*(PHLT-CPH)
   282  570      ZPDD = PHLT - PHGT
   283  580      ZPD(2) = ZPDN/ZPDD
   284
   285  CC----------------------RETURNING WT & PH VALUES TO
        C-------------------------MAIN PROGRAM-----
   286  998   RETURN
   287  999   END


INTERP  Local Symbols

Name                        Class    Type       Size   Offset

ZPD . . . . . . . . . . . . param                        0006
NZP2. . . . . . . . . . . . param                        000a
NZP1. . . . . . . . . . . . param                        000e
CPH . . . . . . . . . . . . param                        0012
ZPDP2 . . . . . . . . . . . param                        0016
ZPPH2 . . . . . . . . . . . param                        001a
ZPPH1 . . . . . . . . . . . param                        001e
ZPDP1 . . . . . . . . . . . param                        0022
PPHGT . . . . . . . . . . . local    REAL*4        4     0078
PLTDIF. . . . . . . . . . . local    REAL*4        4     007c
ZPGT. . . . . . . . . . . . local    REAL*4        4     0080
PPHLT . . . . . . . . . . . local    REAL*4        4     0084
ZPLT. . . . . . . . . . . . local    REAL*4        4     0088
M . . . . . . . . . . . . . local    INTEGER       4     008c
PZPGT . . . . . . . . . . . local    REAL*4        4     0090
PZPLT . . . . . . . . . . . local    REAL*4        4     0094
CGTDIF. . . . . . . . . . . local    REAL*4        4     0098
ZPDD. . . . . . . . . . . . local    REAL*4        4     009c
PHGT. . . . . . . . . . . . local    REAL*4        4     00a0
CLTDIF. . . . . . . . . . . local    REAL*4        4     00a4
PHLT. . . . . . . . . . . . local    REAL*4        4     00a8
ZPDN. . . . . . . . . . . . local    REAL*4        4     00ac
PGTDIF. . . . . . . . . . . local    REAL*4        4     00b0

Global Symbols

Name                        Class    Type       Size   Offset

CALCZP. . . . . . . . . . . FSUBRT   ***         ***    0000
INTERP. . . . . . . . . . . FSUBRT   ***         ***    079e
WKO . . . . . . . . . . . . extern   ***         ***     ***
WKTH. . . . . . . . . . . . extern   ***         ***     ***
WKTW. . . . . . . . . . . . extern   ***         ***     ***
```

```
Code  size = 0ec7 (3783)
Data  size = 0044 (68)
Bss size  = 00b4 (180)

No errors detected
```

```
Line#  Source Line

      SUBROUTINE WKO(K, WOO, WOT, WTT, APR, TAH,
     & PSI, CONCL, HOA, HOR, CPH, FLDIR, TEMPK)

CCCC  REV. 05-04-92

      IMPLICIT NONE
      CHARACTER FLNME*28,FLDIR*7
      INTEGER ONE,TWO,K,POS,KI,L
      REAL APR,TAH,PSI,CONCL,HOA,HOR,CPH,X,TEMPK
      REAL*8 WOO,WOT,WTT,WCALC,VOO,VOT,VTT
      DIMENSION X(250), VOO(250), VOT(250),
      DIMENSION VTT(250), TAH(2:4), APR(2), PSI(2)
      DIMENSION WOO(200), WOT(200), WTT(200)

CCCCC ONE=INTEGER VARIABLE EQUAL TO 1
CCCCC TWO=INTEGER VARIABLE EQUAL TO 2
CCCCC WCALC=CALCULATED W VALUE FROM SUBROUTINE WC
CCCCC KI=INTEGER VARIABLE REPRESENTATION OF K USED
CCCCC    TO MAKE A CHARACTER VARIABLE REPRESENTATION
CCCCC    OF K FOR FILENAME
CCCCC X=SEPARATION DISTANCE (ARRAY) (M)
CCCCC VOO,VOT,VTT=POTENTIAL FOR A GIVEN PARTICLE
CCCCC             INTERACTION AT COORESPONDING
CCCCC             SEPERATION DISTANCE X (ARRAY)

10    ONE=1
20    TWO=2
30    KI=K

CC----------------------FINDING VARIOUS (INVERSE)
C-------------------------PROBABILITIES OF PARTICLE
C-------------------------COLLISION & ADHESION------

C-----------------------FOR COLLISION OF TWO
C--------------------------PARTICLES OF TYPE #1-----
40    FLNME(1:14)='C:\JK\LL\DATA\'
50    FLNME(15:21)=FLDIR
60    FLNME(22:22)='\'
70    FLNME(23:23)='V'
80    FLNME(24:24)=CHAR(MOD(KI,10)+ICHAR('0'))
90   FLNME(25:28)='.DAT'
100   CALL WC(WCALC, APR, TAH, PSI, ONE, ONE, CONCL,
     & HOA, HOR, CPH, VOO,VOT,VTT, X, FLDIR, TEMPK)
110   WOO(K)=WCALC

```

Line# Source Line

```
 C-----------------------FOR COLLISION OF PARTICLES 1
C------------------------& 2------------------------
 120   CALL WC(WCALC, APR, TAH, PSI, ONE, TWO, CONCL,
      & HOA, HOR, CPH, VOO,VOT,VTT, X, FLDIR, TEMPK)
 130   WOT(K)=WCALC

 C-----------------------FOR COLLISION OF TWO
 C-------------------------PARTICLES OF TYPE #2-----
 140   CALL WC(WCALC, APR, TAH, PSI, TWO, TWO, CONCL,
      & HOA, HOR, CPH, VOO,VOT,VTT, X, FLDIR, TEMPK)
 150   WTT(K)=WCALC

 CC----------------------WRITING V DATA TO FILE-----
 160   OPEN(15,FILE=FLNME,STATUS='NEW')
 170   WRITE(15,*)'CPH,APR(1),APR(2)'
 180   WRITE(15,*)CPH,APR(1),APR(2)
 190   WRITE(15,*)'PSI(1),PSI(2),CONCL,TAH'
 200   WRITE(15,*)PSI(1),PSI(2),CONCL,TAH
 210   WRITE(15,900)
 220   WRITE(15,910)
 230   DO 300 L=1,240,1
 240     IF(X(L).NE.0.0)THEN
 250       WRITE(15,920)X(L),VOO(L),VOT(L),VTT(L)
 260     END IF
 270   CONTINUE
 280   CLOSE(15)

 CCC---------------------FORMAT STATEMENTS-----------
 900   FORMAT (5X,'SEP',12X,'V11',12X,
      & 1X,'V12',12X,
      & 1X,'V22')
 910   FORMAT (5X,'---',12X,'---',12X,
      & 1X,'---',12X,
      & 1X,'---')
 920   FORMAT (1X,E12.4,1X,',',1X,E12.4,1X,',',
      & 1X,E12.4,1X,',',
      & 1X,E12.4,1X)

 998   RETURN
 999   END

```

```
WKTW  Local Symbols

Name                         Class    Type         Size   Offset

TEMPK . . . . . . . . . . .  param                         0006
FLDIR . . . . . . . . . . .  param                         000a
CPH . . . . . . . . . . . .  param                         000e
HOR . . . . . . . . . . . .  param                         0012
HOA . . . . . . . . . . . .  param                         0016
CONCL . . . . . . . . . . .  param                         001a
PSI . . . . . . . . . . . .  param                         001e
TAH . . . . . . . . . . . .  param                         0022
APR . . . . . . . . . . . .  param                         0026
WTT . . . . . . . . . . . .  param                         002a
WOT . . . . . . . . . . . .  param                         002e
WOO . . . . . . . . . . . .  param                         0032
K . . . . . . . . . . . . .  param                         0036
X . . . . . . . . . . . . .  local    REAL*4       1000    0000
L . . . . . . . . . . . . .  local    INTEGER*4       4    0002
KI. . . . . . . . . . . . .  local    INTEGER*4       4    0006
ONE . . . . . . . . . . . .  local    INTEGER*4       4    000a
WCALC . . . . . . . . . . .  local    REAL*8          8    000e
POS . . . . . . . . . . . .  local    INTEGER*4       4    0016
FLNME . . . . . . . . . . .  local    CHAR*29        29    001a
TWO . . . . . . . . . . . .  local    INTEGER*4       4    0038
VOO . . . . . . . . . . . .  local    REAL*8       2000    03e8
VOT . . . . . . . . . . . .  local    REAL*8       2000    0bb8
VTT . . . . . . . . . . . .  local    REAL*8       2000    1388


Global Symbols

Name                         Class    Type         Size   Offset

WC. . . . . . . . . . . . .  extern   ***           ***     ***
WKTW. . . . . . . . . . . .  FSUBRT   ***           ***    0000

Code size = 045e (1118)
Data size = 0089 (137)
Bss size  = 003c (60)

No errors detected
```

Microsoft FORTRAN Optimizing Compiler Version 5.00.03

Line# Source Line

```
      SUBROUTINE WKTW(K, WOO, WOT, WTT, APR, TAH,
     & PSI, CONCL, HOA, HOR, CPH, FLDIR, TEMPK)

CCCC  REV. 05-04-92

      IMPLICIT NONE
      CHARACTER FLNME*29,FLDIR*7
      INTEGER ONE,TWO,K,POS,KI,L
      REAL APR,TAH,PSI,CONCL,HOA,HOR,CPH,X,TEMPK
      REAL*8 WOO,WOT,WTT,WCALC,VOO,VOT,VTT
      DIMENSION X(250), VOO(250), VOT(250),
      DIMENSION VTT(250), TAH(2:4), APR(2), PSI(2)
      DIMENSION WOO(200), WOT(200), WTT(200)

CCCCC ONE=INTEGER VARIABLE EQUAL TO 1
CCCCC TWO=INTEGER VARIABLE EQUAL TO 2
CCCCC WCALC=CALCULATED W VALUE FROM SUBROUTINE WC
CCCCC KI=INTEGER VARIABLE REPRESENTATION OF K USED
CCCCC    TO MAKE A CHARACTER VARIABLE REPRESENTATION
CCCCC    OF K FOR FILENAME
CCCCC X=SEPARATION DISTANCE (ARRAY) (M)
CCCCC VOO,VOT,VTT=POTENTIAL FOR A GIVEN PARTICLE
CCCCC             INTERACTION AT COORESPONDING
CCCCC             SEPERATION DISTANCE X (ARRAY)

10    ONE=1
20    TWO=2
30    KI=K

CC----------------------FINDING VARIOUS (INVERSE)
C-------------------------PROBABILITIES OF PARTICLE
C-------------------------COLLISION & ADHESION------

C-----------------------FOR COLLISION OF TWO
C--------------------------PARTICLES OF TYPE #1-----
40    FLNME(1:14)='C:\JK\LL\DATA\'
50    FLNME(15:21)=FLDIR
60    FLNME(22:22)='\'
70    FLNME(23:23)='V'
80    DO 110 POS=25,24,-1
90       FLNME(POS:POS)=CHAR(MOD(KI,10)+ICHAR('0'))
100      KI=KI/10
110   CONTINUE
120   FLNME(26:29)='.DAT'
130   CALL WC(WCALC, APR, TAH, PSI, ONE, ONE, CONCL,
     & HOA, HOR, CPH, VOO,VOT,VTT, X, FLDIR, TEMPK)
140   WOO(K)=WCALC

```

Line# Source Line

```
 C-----------------------FOR COLLISION OF PARTICLES 1
C------------------------& 2------------------------
 150   CALL WC(WCALC, APR, TAH, PSI, ONE, TWO, CONCL,
      & HOA, HOR, CPH, VOO,VOT,VTT, X, FLDIR, TEMPK)
 160   WOT(K)=WCALC

 C-----------------------FOR COLLISION OF TWO
 C-------------------------PARTICLES OF TYPE #2-----
 170   CALL WC(WCALC, APR, TAH, PSI, TWO, TWO, CONCL,
      & HOA, HOR, CPH, VOO,VOT,VTT, X, FLDIR, TEMPK)
 180   WTT(K)=WCALC

 CC---------------------WRITING V DATA TO FILE-----
 190   OPEN(15,FILE=FLNME,STATUS='NEW')
 200   WRITE(15,*)'CPH,APR(1),APR(2)'
 210   WRITE(15,*)CPH,APR(1),APR(2)
 220   WRITE(15,*)'PSI(1),PSI(2),CONCL,TAH'
 230   WRITE(15,*)PSI(1),PSI(2),CONCL,TAH
 240   WRITE(15,900)
 250   WRITE(15,910)
 260   DO 300 L=1,240,1
 270     IF(X(L).NE.0.0)THEN
 280       WRITE(15,920)X(L),VOO(L),VOT(L),VTT(L)
 290     END IF
 300   CONTINUE
 310   CLOSE(15)

 CCC---------------------FORMAT STATEMENTS-----------
 900   FORMAT (5X,'SEP',12X,'V11',12X,
      & 1X,'V12',12X,
      & 1X,'V22')
 910   FORMAT (5X,'---',12X,'---',12X,
      & 1X,'---',12X,
      & 1X,'---')
 920   FORMAT (1X,E12.4,1X,',',1X,E12.4,1X,',',
      & 1X,E12.4,1X,',',
      & 1X,E12.4,1X)

 998   RETURN
 999   END
```

```
WKTW  Local Symbols

Name                      Class   Type       Size   Offset

TEMPK . . . . . . . . . . param                      0006
FLDIR . . . . . . . . . . param                      000a
CPH . . . . . . . . . . . param                      000e
HOR . . . . . . . . . . . param                      0012
HOA . . . . . . . . . . . param                      0016
CONCL . . . . . . . . . . param                      001a
PSI . . . . . . . . . . . param                      001e
TAH . . . . . . . . . . . param                      0022
APR . . . . . . . . . . . param                      0026
WTT . . . . . . . . . . . param                      002a
WOT . . . . . . . . . . . param                      002e
WOO . . . . . . . . . . . param                      0032
K . . . . . . . . . . . . param                      0036
X . . . . . . . . . . . . local   REAL*4     1000    0000
L . . . . . . . . . . . . local   INTEGER*4     4    0002
KI. . . . . . . . . . . . local   INTEGER*4     4    0006
ONE . . . . . . . . . . . local   INTEGER*4     4    000a
WCALC . . . . . . . . . . local   REAL*8        8    000e
POS . . . . . . . . . . . local   INTEGER*4     4    0016
FLNME . . . . . . . . . . local   CHAR*29      29    001a
TWO . . . . . . . . . . . local   INTEGER*4     4    0038
VOO . . . . . . . . . . . local   REAL*8     2000    03e8
VOT . . . . . . . . . . . local   REAL*8     2000    0bb8
VTT . . . . . . . . . . . local   REAL*8     2000    1388


Global Symbols

Name                      Class   Type       Size   Offset

WC. . . . . . . . . . . . extern  ***         ***     ***
WKTW. . . . . . . . . . . FSUBRT  ***         ***    0000

Code size = 045e (1118)
Data size = 0089 (137)
Bss size  = 003c (60)

No errors detected
```

Microsoft FORTRAN Optimizing Compiler Version 5.00.03

Line# Source Line

```
       SUBROUTINE WKTH(K, WOO, WOT, WTT, APR, TAH,
      & PSI, CONCL, HOA, HOR, CPH, FLDIR, TEMPK)

 CCCC  REV. 05-04-92

       IMPLICIT NONE
       CHARACTER FLNME*30,FLDIR*7
       INTEGER ONE,TWO,K,POS,KI,L
       REAL APR,TAH,PSI,CONCL,HOA,HOR,CPH,X,TEMPK
       REAL*8 WOO,WOT,WTT,WCALC,VOO,VOT,VTT
       DIMENSION VOO(250), VOT(250), VTT(250), X(250)
       DIMENSION TAH(2:4), APR(2), PSI(2)
       DIMENSION WOO(200), WOT(200), WTT(200)

 CCCCC ONE=INTEGER VARIABLE EQUAL TO 1
 CCCCC TWO=INTEGER VARIABLE EQUAL TO 2
 CCCCC WCALC=CALCULATED W VALUE FROM SUBROUTINE WC
 CCCCC KI=INTEGER VARIABLE REPRESENTATION OF K USED
 CCCCC    TO MAKE A CHARACTER VARIABLE REPRESENTATION
CCCCC    OF K FOR FILENAME
 CCCCC X=SEPARATION DISTANCE (ARRAY) (M)
 CCCCC VOO,VOT,VTT=POTENTIAL FOR A GIVEN PARTICLE
 CCCCC             INTERACTION AT COORESPONDING
 CCCCC             SEPERATION DISTANCE X (ARRAY)


 10    ONE=1
 20    TWO=2
 30    KI=K

 CC-----------------------FINDING VARIOUS (INVERSE)
 C-------------------------PROBABILITIES OF PARTICLE
 C-------------------------COLLISION & ADHESION------

 C-----------------------FOR COLLISION OF TWO
 C-------------------------PARTICLES OF TYPE #1------
 40    FLNME(1:14)='C:\JK\LL\DATA\'
 50    FLNME(15:21)=FLDIR
 60    FLNME(22:22)='V'
 70    FLNME(23:23)='\'
 80    DO 110 POS=26,24,-1
 90       FLNME(POS:POS)=CHAR(MOD(KI,10)+ICHAR('0'))
 100      KI=KI/10
 110   CONTINUE
 120   FLNME(27:30)='.DAT'
 130   CALL WC(WCALC, APR, TAH, PSI, ONE, ONE, CONCL,
      & HOA, HOR, CPH, VOO,VOT,VTT, X, FLDIR, TEMPK)
 140   WOO(K)=WCALC
```

Line# Source Line

```

C-----------------------FOR COLLISION OF PARTICLES 1
C------------------------& 2------------------------
150   CALL WC(WCALC, APR, TAH, PSI, ONE, TWO, CONCL,
     & HOA, HOR, CPH, VOO,VOT,VTT, X, FLDIR,TEMPK)
160   WOT(K)=WCALC

C-----------------------FOR COLLISION OF TWO
C------------------------PARTICLES OF TYPE #2-------
170   CALL WC(WCALC, APR, TAH, PSI, TWO, TWO, CONCL,
     & HOA, HOR, CPH, VOO,VOT,VTT, X, FLDIR, TEMPK)
180   WTT(K)=WCALC

CC----------------------WRITING V DATA TO FILE------
190    OPEN(15,FILE=FLNME,STATUS='NEW')
200   WRITE(15,*)'CPH,APR(1),APR(2)'
210   WRITE(15,*)CPH,APR(1),APR(2)
220   WRITE(15,*)'PSI(1),PSI(2),CONCL,TAH'
230   WRITE(15,*)PSI(1),PSI(2),CONCL,TAH
240   WRITE(15,900)
250   WRITE(15,910)
260   DO 300 L=1,240,1
270     IF(X(L).NE.0.0)THEN
280       WRITE(15,920)X(L),VOO(L),VOT(L),VTT(L)
290     END IF
300   CONTINUE
310   CLOSE(15)

CCC---------------------FORMAT STATEMENTS----------
900   FORMAT (5X,'SEP',12X,'V11',12X,
     & 1X,'V12',12X,
     & 1X,'V22')
910   FORMAT (5X,'---',12X,'---',12X,
     & 1X,'---',12X,
     & 1X,'---')
920   FORMAT (1X,E12.4,1X,',',1X,E12.4,1X,',',
     & 1X,E12.4,1X,',',
     & 1X,E12.4,1X)

998   RETURN
999   END
```

```
WKTH  Local Symbols

Name                          Class   Type         Size   Offset

TEMPK . . . . . . . . . . . . param                        0006
FLDIR . . . . . . . . . . . . param                        000a
CPH . . . . . . . . . . . . . param                        000e
HOR . . . . . . . . . . . . . param                        0012
HOA . . . . . . . . . . . . . param                        0016
CONCL . . . . . . . . . . . . param                        001a
PSI . . . . . . . . . . . . . param                        001e
TAH . . . . . . . . . . . . . param                        0022
APR . . . . . . . . . . . . . param                        0026
WTT . . . . . . . . . . . . . param                        002a
WOT . . . . . . . . . . . . . param                        002e
WOO . . . . . . . . . . . . . param                        0032
K . . . . . . . . . . . . . . param                        0036
X . . . . . . . . . . . . . . local   REAL*4       1000    0000
L . . . . . . . . . . . . . . local   INTEGER*4       4    0002
KI. . . . . . . . . . . . . . local   INTEGER*4       4    0006
ONE . . . . . . . . . . . . . local   INTEGER*4       4    000a
WCALC . . . . . . . . . . . . local   REAL*8          8    000e
POS . . . . . . . . . . . . . local   INTEGER*4       4    0016
FLNME . . . . . . . . . . . . local   CHAR*30        30    001a
TWO . . . . . . . . . . . . . local   INTEGER*4       4    0038
VOO . . . . . . . . . . . . . local   REAL*8       2000    03e8
VOT . . . . . . . . . . . . . local   REAL*8       2000    0bb8
VTT . . . . . . . . . . . . . local   REAL*8       2000    1388


Global Symbols

Name                          Class   Type         Size   Offset

WC. . . . . . . . . . . . . . extern  ***           ***     ***
WKTH. . . . . . . . . . . . . FSUBRT  ***           ***    0000

Code size = 045e (1118)
Data size = 0089 (137)
Bss size  = 003c (60)

No errors detected
```

```
Microsoft FORTRAN Optimizing Compiler Version 5.00.03

Line#  Source Line

      SUBROUTINE WC(WCALC, APR, TAH, PSI, I, J,
     & CONCL, HOA, HOR, CPH, VOO, VOT, VTT, X,
     & FLDIR, TEMPK)

CCCCC REV. 05-04-92

CCC-----------SUBPROGRAM TO INTEGRATE FROM
CCC-------------MINIMUM PARTICLE SEPARATION TO AN
CCC-------------INFINITE SEPARATION IN SEGMENTS SO
CCC-------------THAT WHEN AN AREA OF A SEGMENT ADDS
CCC-------------A SMALL ENOUGH AMOUNT TO THE TOTAL
CCC-------------AREA OF ALL THE SEGMENTS SO FAR THEN
CCC-------------CAN STOP INTEGRATING BEFORE GET TO
CCC-------------INFINITY---------------------------

      IMPLICIT NONE
      CHARACTER FLDIR*7
      INTEGER I,J,XN
      REAL*8 AREAN,CONTRIB,DIFFN,SIMP,AREATL,TOL
      REAL*8 CONTMX,SUMARG,SUMMAX,SUMMIN,OOAT,SOC
      REAL HIGH,LOW,HIMAX,HIMIN,APR,TAH,PSI,CONCL
      REAL HOA,HOR,ROR,CPH,INTSIZE,LOWEST,X,TEMPK
      REAL*8 WCALC,VOO,VOT,VTT
      DIMENSION APR(2),PSI(2),TAH(2:4)
      DIMENSION X(250),VOO(250),VOT(250),VTT(250)


CCCCC XN=COUNTER FOR TRACKING POSITION IN ARRAYS IN
CCCCC    SUBROUTINE SI FOR ENTIRE INTERVAL OF
CCCCC    INTEGRAL
CCCCC I=FIRST PARTICLE TYPE OF INTERACTION
CCCCC J=OTHER PARTICLE TYPE OF INTERACTION
CCCCC HIGH=HIGH VALUE OF LIMITS OF INTEGRATION OF
CCCCC      CURRENT SEGMENT
CCCCC LOW=LOW VALUE OF LIMITS OF INTEGRATION OF
CCCCC     CURRENT SEGMENT
CCCCC INTSIZE=INTERVAL SIZE FOR EACH SEGMENT
CCCCC LOWEST=LOWEST VALUE OF LOW VALUE OF LIMITS OF
CCCCC        INTEGRATION
CCCCC       =MINIMUM SEPARATION DISTANCE
CCCCC TOL=TOLERANCE FOR A DIFFERENCE IN TOTAL AREA
CCCCC     UPON ADDITION OF AREA OF CURRENT SEGMENT
CCCCC     AT WHICH MAY RETURN A VALUE FOR COMPLETE
CCCCC     INTERVAL IF PASSED MIMIN
CCCCC HIMIN=MINIMUM VALUE OF INTEGRATION LIMITS
CCCCC       BEFORE A VALUE FOR COMPLETE INTEGRAL MAY
CCCCC       BE RETURNED IF TOLERENCE IS MET
CCCCC HIMAX=MAXIMUM VALUE OF INTEGRATION LIMITS AT
```

Line# Source Line

```
  CCCCC       WHICH TIME THE PRESENT VALUE FOR THE
  CCCCC       COMPLETE INTEGRAL WILL BE RETURNED EVEN
  CCCCC       IF TOLERENCE HAS NOT BEEN MET SO THAT
  CCCCC       THE PROGRAM DOES NOT RUN FOREVER OR
  CCCCC       CAUSE A MATH OVERFLOW ERROR AND PROGRAM
  CCCCC       TERMINATION
  CCCCC SUMMAX=MAXIMUM POSITVE VALUE FOR A REAL
  CCCCC        VARIABLE BEFORE A MATH OVERFLOW ERROR
  CCCCC        OCCURS AND CAUSES PROGRAM TERMINATION
  CCCCC SUMMARG=ARGUMENT USED TO CALCULATE SUMMAX
  CCCCC SUMMIN=MINIMUM POSITVE VALUE FOR A REAL
  CCCCC        VARIABLE BEFORE A MATHOVERFLOW ERROR
  CCCCC        OCCURS AND CAUSES PROGRAM TERMINATION
  CCCCC SIMP=VALUE OF SEGMENT INTEGRAL CALCULATED BY
  CCCCC      SUBROUTINE SI
  CCCCC CONTRIB=CONTRIBUTION BY AREA OF CURRENT SGMENT
 CCCCC         TO TOTAL AREA
  CCCCC CONTMX=MAXIMUM CONTRIBUTION TO TOTAL AREA
  CCCCC        BEFORE A MATH OVERFLOW ERROR CAUSES
  CCCCC        PROGRAM TERMINATION
  CCCCC AREATL=TOTAL AREA OF ALL PREVIOUS SEGMENTS OF
CCCCC        INTEGRAL
  CCCCC AREAN=NEW AREA WITH ADDITION OF CURRENT
  CCCCC       SEGMENT AREA TO AREATL
  CCCCC DIFFN=DIFFERENCE IN AREA CONTRIBUTED TO TOTAL
  CCCCC       AREA WITH TOTAL AREA
  CCCCC OOAT=ONE OVER AREA TOTAL
  CCCCC SOC=SUMMAX OVER CONTRIB


  CC----------------------SETTING VARIOUS INITIAL
  C---------------------------VALUES------------------
  05    XN=1
  10    SUMARG=663.0
  15    SUMMAX=EXP(SUMARG)
  20    SUMMAX=SUMMAX*1.0E+20
  25    SUMMIN=1.0/SUMMAX
  30    HIMIN=100.0E-9
  35    TOL=1.0E-5
  40    HIMAX=APR(I)+APR(J)+HOA
  45    HIGH=HOR
  50    LOWEST=HOR
  55    INTSIZE=1.0E-9

  C-----------------------SENDING PROGRAM PROGRESS
  C-------------------------MESSAGE TO SCREEN---------
  60    WRITE(*,900)FLDIR,CPH,I,J

  CC----------------------BEGIN ITERATION LOOP--------
  65    IF (HIGH.LT.HIMAX) THEN
```

Line# Source Line

```
70       LOW=HIGH
75       HIGH=LOW+INTSIZE

CC----------------------CALCULATING AREA OF CURRENT
C-------------------------SEGMENT-------------------
80       CALL SI(SIMP, LOW, HIGH, APR, TAH, PSI, I,
     &           J, CONCL, HOA, CPH, VOO,VOT,VTT, X,
     &           XN, TEMPK)
85       CONTRIB=SIMP

CC----------------------CALCULATING VARIABLES TO
C-------------------------PREVENT MATH OVERFLOW
C-------------------------ERRORS AND PROGRAM
C-------------------------TERMINATION---------------
90       CONTMX=SUMMAX-AREATL
95       IF (CONTRIB.GE.1.0)THEN
100        SOC=SUMMAX/CONTRIB
105        IF (AREATL.LT.SUMMIN)THEN
110          OOAT=SUMMAX
115        ELSE
120          OOAT=1.0/AREATL
125        END IF
130      ELSE
135        SOC=1.0
140        OOAT=0.0
145      END IF

CC----------------------CALCULATING AREAN AND
C--------------------------PREVENTING MATH OVERFLOW
C--------------------------ERRORS AND PROGRAM
C--------------------------TERMINATION--------------
150      IF (LOW.EQ.LOWEST)THEN
155        AREAN=CONTRIB
160        AREATL=AREAN*2
165      ELSE IF (CONTRIB.GE.CONTMX)THEN
170        AREAN=SUMMAX
175      ELSE
180        AREAN=AREATL+CONTRIB
185      END IF

CC----------------------CALCULATING DIFFN AND
C--------------------------PREVENTING MATH OVERFLOW
C--------------------------ERRORS AND PROGRAM
C--------------------------TERMINATION--------------
190      IF (AREATL.EQ.0.0)THEN
195          DIFFN=0.0
200      ELSE IF (AREAN.EQ.SUMMAX) THEN
205          DIFFN=0.0
210      ELSE IF (OOAT .GE. SOC)THEN
215          DIFFN=0.0
```

```
Line#  Source Line

220      ELSE
225        DIFFN=(ABS((AREATL-AREAN)/AREATL))
230      END IF

CC----------------------RETURNING AREA VALUE IF
C-------------------------DIFFERANCE BETWEEN
C-------------------------SUCCESSIVE ITERATIONS IS
C-------------------------WITHIN TOLERENCE AND
C-------------------------SEPERATION IS MORE THAN
C-------------------------MINIMUM-------------------
235      IF (DIFFN.LT.TOL .AND. HIGH.GE.HIMIN) THEN
240        ROR=HOA+((APR(I)+APR(J))/1.0E+9)
245        WCALC=ROR*AREAN
250        RETURN
C----------------------RESETTING AREATL IF NOT------
255      ELSE
260        AREATL=AREAN
265        IF (AREATL.LT.SUMMIN)AREATL=SUMMIN
270      END IF

CC----------------------RETURNING AREA VALUE SINCE
C-------------------------UPPER INTEGRATION LIMIT IS
C-------------------------TOO LARGE-----------------
275   ELSE IF(HIGH.GE.HIMAX)THEN
280      WRITE(*,*)' '
285      WRITE(*,*)'WHILE INTEGRATING INTERACTION'
290      WRITE(*,*)'BETWEEN PARTICLES',I,J
295      WRITE(*,*)'UPPER INTEGRATION LIMIT',
     &               'EXCEEDED', HIMAX,'nm'
300      ROR=HOA+((APR(I)+APR(J))/1.0E+9)
305      WCALC=AREAN*ROR
310      RETURN
315   END IF

CC----------------------SINCE DIFFERENCE IS NOT
C-------------------------WITHIN TOLERANCE THEN
C-------------------------PREPARE FOR ANOTHER
C-------------------------ITERATION-----------------

C-----------------------INCREASING INTSIZE AS
C-------------------------SEPARATION INCREASES------
320   IF(HIGH.GT.5.0E-9 .AND. HIGH.LE.25.0E-9) THEN
325      INTSIZE=2.5E-9
330   ELSE IF(HIGH.GT.25.0E-9 .AND.
     &                   HIGH.LE.85.0E-9) THEN
335      INTSIZE=5.0E-9
340   ELSE IF(HIGH.GT.85.0E-9 .AND.
     &                   HIGH.LE.170.0E-9) THEN
345      INTSIZE=10.0E-9
350   ELSE IF(HIGH.GT.170.0E-9 .AND.
```

```
 Line#  Source Line

             &                  HIGH.LE.500.0E-9) THEN
   161  355      INTSIZE=100.0E-9
   162  360   ELSE IF(HIGH.GT.500.0E-9) THEN
   163  365      INTSIZE=1000.0E-9
   164  370   END IF
   165  375   GOTO 65
   166
   167  CCC---------------------MESSAGE REPORTING CURRENT
   168  CC-----------------------FILE, CURRENT INTERACTIONS
   169  CC-----------------------BEING CALCULATED AND THAT
        CC-----------------------THE COMPUTER IS RUNNING A
        CC-----------------------LONG PROGRAM-------------
   170  900   FORMAT(/,/,/,/,/,/,/,/,11X, 58('C')/,
   171       & 11X,'C',4X,'This computer is currently',
             & 26X,'C'/,
   172       & 11X,'C',4X,'running a program',35X,'C'/,
   173       & 11X,'C',4X,'which has many lengthy',30X,'C'/,
   174       & 11X,'C',4X,'calculations.',39X,'C'/,
   175       & 11X,'C',56X,'C'/,
   176       & 11X,'C',4X,'PLEASE DO NOT INTERUPT THE',
             & 'PROGRAM!!',16X,'C'/,
   177       & 11X,'C',56X,'C'/,
   178       & 11X,'C',4X,'If there is a problem',
             & 'contact',23X,'C'/,
   179       & 11X,'C',4X,5X,'Brett Wilson: Office',
             & 'A234',22X,'C'/,
   180       & 11X,'C',56X,'C'/,
   181       & 11X,58('C')/,
   182       & 11X,'C',28X,A7,21X,'C'/,
   183       & 11X,'C',28X,'CURRENT PH: ',F5.2,11X,'C'/,
   184       & 11X,'C',28X,'INTERACTIONS BETWEEN: ',
             & I1,',',I1,3X,'C'/,
   185       & 11X,58('C'),/,/,/,/,/,/,/)
   186
   187
   188
   189
   190  CCC---------------------RETURNING TO CACLUL
        CC-----------------------SUBPROGRAM---------------
   191  999   END


WC  Local Symbols

Name                         Class   Type       Size   Offset

TEMPK . . . . . . . . . . . param                        0006
FLDIR . . . . . . . . . . . param                        000a
X . . . . . . . . . . . . . param                        000e
VTT . . . . . . . . . . . . param                        0012
```

```
WC  Local Symbols

Name                      Class   Type       Size   Offset

VOT . . . . . . . . . . . param                      0016
VOO . . . . . . . . . . . param                      001a
CPH . . . . . . . . . . . param                      001e
HOR . . . . . . . . . . . param                      0022
HOA . . . . . . . . . . . param                      0026
CONCL . . . . . . . . . . param                      002a
J . . . . . . . . . . . . param                      002e
I . . . . . . . . . . . . param                      0032
PSI . . . . . . . . . . . param                      0036
TAH . . . . . . . . . . . param                      003a
APR . . . . . . . . . . . param                      003e
WCALC . . . . . . . . . . param                      0042
SUMARG. . . . . . . . . . local   REAL*8        8    0002
CONTRIB . . . . . . . . . local   REAL*8        8    000a
SUMMIN. . . . . . . . . . local   REAL*8        8    0012
CONTMX. . . . . . . . . . local   REAL*8        8    001a
SUMMAX. . . . . . . . . . local   REAL*8        8    0022
LOWEST. . . . . . . . . . local   REAL*4        4    002a
HIGH. . . . . . . . . . . local   REAL*4        4    002e
SOC . . . . . . . . . . . local   REAL*8        8    0032
INTSIZE . . . . . . . . . local   REAL*4        4    003a
XN. . . . . . . . . . . . local   INTEGER*4     4    003e
DIFFN . . . . . . . . . . local   REAL*8        8    0042
AREAN . . . . . . . . . . local   REAL*8        8    004a
TOL . . . . . . . . . . . local   REAL*8        8    0052
LOW . . . . . . . . . . . local   REAL*4        4    005a
ROR . . . . . . . . . . . local   REAL*4        4    005e
OOAT. . . . . . . . . . . local   REAL*8        8    0062
HIMIN . . . . . . . . . . local   REAL*4        4    006a
HIMAX . . . . . . . . . . local   REAL*4        4    006e
AREATL. . . . . . . . . . local   REAL*8        8    0072
SIMP. . . . . . . . . . . local   REAL*8        8    007a


Global Symbols

Name                      Class   Type       Size   Offset

SI. . . . . . . . . . . . extern  ***         ***     ***
WC. . . . . . . . . . . . FSUBRT  ***         ***    0000


Code size = 0643 (1603)
Data size = 00dd (221)
Bss size  = 0082 (130)
No errors detected
```

```
     Microsoft FORTRAN Optimizing Compiler Version 5.00.03

Line#  Source Line

   1          SUBROUTINE SI(SIMP, A, B, APR, TAH, PSI, I, J,
   2         & CONCL, HOA, CPH, VOO,VOT,VTT, X, XN, TEMPK)
   3
   4   CCCCC REV. 05-04-92
   5
   6   CCC----------SUBPROGRAM TO INTEGRATE A GIVEN SEGMENT
   7   C---------------OF AN INTEGRAL USING SIMPSON'S RULE-
   8
   9          IMPLICIT NONE
  10          INTEGER I,J,L,NSECTS,NMAX,XN,VN
  11          REAL A, B, DX, APR, TAH, PSI, HOA, SEP, CPH,
              REAL CONCL, X, XV, TEMPK
  12          REAL*8 ODDS,EVENS,DIFFT,FA,FB,AREAO,CONTMX
  13          REAL*8 AREAN,DIFFN,VFCN,WFCN,SUMARG,SUMMAX
  14          REAL*8 SIMP,V,VOO,VOT,VTT
  15          DIMENSION APR(2),PSI(2),X(250)
              DIMENSION VOO(250),VOT(250),VTT(250)
  16          DIMENSION V(140),XV(140),TAH(2:4)
  17
  18   CCCCC NSECTS=NUMBER OF SECTIONS INTERVALL TO BE
       CCCCC        DIVIDED INTO
  19   CCCCC DIFFT=TOLERABLE DIFFERANCE BETWEEN SUCCESSIVE
       CCCCC       ITERATIONS
  20   CCCCC NMAX=MAXIMUM NUMBER OF SECTIONS TO BE TAKEN
  21   CCCCC A=LOWER LIMIT OF INTEGRATION
  22   CCCCC B=UPPER LIMIT OF INTEGRATION
  23   CCCCC WFCN=STABILITY CALCULATED BY SUBROUTINE WVFCN
  24   CCCCC VFCN=POTENTIAL CALCULATED BY SUBROUTINE WVFCN
  25   CCCCC FA=FUNCTION VALUE AT A
  26   CCCCC FB=FUNCTION VALUE AT B
  27   CCCCC DX=WIDTH OF SECTIONS
  28   CCCCC ODDS=SUM OF FUCTION VALUES AT ODD SECTIONS
  29   CCCCC EVENS=SUM OF FUCTION VALUES AT EVEN SECTIONS
  30   CCCCC AREAO=AREA CALCULATED IN PREVIOUS ITERATION
  31   CCCCC AREAN=AREA CALCULATED IN PRESENT ITERATION
  32   CCCCC DIFFN=DIFFERENCE BETWEEN PRESENT AND PREVIOUS
       CCCCC       ITERATION
  33   CCCCC CONTMX=MAXIMUM CONTRIBUTION TO TOTAL AREA
  34   CCCCC        BEFORE A MATH OVERFLOW ERROR CAUSES
       CCCCC        PROGRAM TERMINATION
  35   CCCCC SUMMAX=MAXIMUM POSITVE VALUE FOR A REAL
  36   CCCCC        VARIABLE BEFORE A MATH OVERFLOW ERROR
       CCCCC        OCCURS AND CAUSES PROGRAM TERMINATION
  37   CCCCC SUMMARG=ARGUMENT USED TO CALCULATE SUMMAX
  38   CCCCC SUMMIN=MINIMUM POSITVE VALUE FOR A REAL
  39   CCCCC        VARIABLE BEFORE A MATH OVERFLOW ERROR
       CCCCC        OCCURS AND CAUSES PROGRAM TERMINATION
  40   CCCCC V=INTERPARTICLE POTENTIAL AT A COORESPONDING
```

Line# Source Line

```
CCCCC   DISTANCE XV(ARRAY)
CCCCC XV=INTERPARTICLE SEPARATION DISTANCE (ARRAY)
CCCCC VN=COUNTER FOR TRACKING POSITION IN V AND XV
CCCCC    ARRAYS
CCCCC XN=COUNTER FOR SAVING V AND XV IN VOO,VOT,VTT
CCCCC    AND X ARRAYS


CC----------------------INTIALIZE AREAO TO ZERO----
05    AREAO=0.0

CC----------------------SET DIFF,NSECTS,& NMAX
C-------------------------VALUES--------------------
10    DIFFT = 0.0001
15    NSECTS=64
20    NMAX=2.0E+6
25    SUMARG=663.0
30    SUMMAX=EXP(SUMARG)
35    SUMMAX=SUMMAX*1.0E+20

CC----------------------EVALUATE FUNCTION AT UPPER &
C-------------------------LOWER BOUND---------------
40    CALL WVFCN(WFCN, VFCN, A, APR, TAH, PSI, I, J,
     &           CONCL, HOA, TEMPK)
45    FA=WFCN
50    XV(1)=A
55    V(1)=VFCN
60    CALL WVFCN(WFCN, VFCN, B, APR, TAH, PSI, I, J,
     &           CONCL, HOA, TEMPK)
65    FB=WFCN
70    XV(130)=B
75    V(130)=VFCN

CC----------------------BEGIN ITERATION LOOP--------
80    IF (NSECTS .LE. NMAX) THEN

CC----------------------CALCULATE WIDTH OF SECTIONS-
85       DX = (B-A)/REAL(NSECTS)

CC----------------------RE-INITIALIZE ODDS & EVENS
C-------------------------TO ZERO-------------------
90       ODDS = 0.0
95       EVENS = 0.0
100      VN=1

CC----------------------CALCULATING SUM OF ALL ODD
C-------------------------FUNCTION VALUES-----------
105      DO 170 L=1,NSECTS-1,2
110       SEP = A+(L*DX)
115       CALL WVFCN(WFCN, VFCN, SEP, APR, TAH, PSI,
```

Source Line

```
      &               I, J, CONCL, HOA, TEMPK)
 120       CONTMX=SUMMAX-ODDS
 125       IF (WFCN.GE.CONTMX)THEN
 130         ODDS=SUMMAX
 135       ELSE
 140        ODDS=ODDS + WFCN
 145       END IF
 150       IF(NSECTS.EQ.128)THEN
 155         XV(VN+L)=SEP
 160         V(VN+L)=VFCN
 165       END IF
 170      CONTINUE

 CC----------------------CALCULATING SUM OF ALL EVEN
 C-------------------------FUNCTION VALUES-----------
 175      DO 240 L=2,NSECTS-2,2
 180       SEP = A+(L*DX)
 185       CALL WVFCN(WFCN, VFCN, SEP, APR, TAH, PSI,
      &               I, J, CONCL, HOA, TEMPK)
 190       CONTMX=SUMMAX-EVENS
 195       IF(WFCN.GE.CONTMX)THEN
 200         EVENS=SUMMAX
 205       ELSE
 210         EVENS=EVENS + WFCN
 215       END IF
 220       IF(NSECTS.EQ.128)THEN
 225         XV(VN+L)=SEP
 230         V(VN+L)=VFCN
 235       END IF
 240      CONTINUE

 CC----------------------SAVING V DATA FOR WRITING TO
C-------------------------FILE----------------------
 245      IF (NSECTS.EQ.128 .AND. B.LT.300.0E-9)THEN
 C-----------------------FOR INTERACTION OF PARTICLE
 C-------------------------ONE WITH ONE--------------
 250        IF (I+J.EQ.2)THEN
 255          VOO(XN)=V(1)
 260          X(XN)=XV(1)
 265          XN=XN+1
 270          DO 290 L=20,100,20
 275            VOO(XN)=V(L)
 280            X(XN)=XV(L)
 285            XN=XN+1
 290          CONTINUE
 295          VOO(XN)=V(130)
 300          X(XN)=XV(130)
 305          XN=XN+1
 C-----------------------FOR INTERACTION OF PARTICLE
 C-------------------------ONE WITH TWO--------------
```

Line# Source Line

```
310        ELSE IF (I+J.EQ.3)THEN
315          VOT(XN)=V(1)
320          XN=XN+1
325          DO 340 L=20,100,20
330            VOT(XN)=V(L)
335            XN=XN+1
340          CONTINUE
345          VOT(XN)=V(130)
350          XN=XN+1
C----------------------FOR INTERACTION OF PARTICLE
C------------------------TWO WITH TWO-------------
355        ELSE IF (I+J.EQ.4)THEN
360          VTT(XN)=V(1)
365          XN=XN+1
370          DO 385 L=20,100,20
375            VTT(XN)=V(L)
380            XN=XN+1
385          CONTINUE
390          VTT(XN)=V(130)
395          XN=XN+1
400        END IF
405      END IF

CC----------------------ADDING ALL FUNCTION VALUES
C------------------------THIS TO FIND AREA OF
C------------------------ITERATION----------------
410      IF (ODDS.GE.SUMMAX .OR.
     &                         EVENS.GE.SUMMAX)THEN
415        AREAN=SUMMAX
420      ELSE
425        AREAN = (DX/3.0)*
     &                    (FA+FB+4.0*ODDS+2.0*EVENS)
430      END IF

CC----------------------RETURNING AREA VALUE IF
C------------------------DIFFERANCE BETWEEN
C------------------------SUCCESSIVE ITERATIONS IS
C------------------------TOLERABLE----------------
435      IF (AREAN.EQ.0.0)THEN
440        DIFFN=0.0
445      ELSE
450        DIFFN = ABS( (AREAN-AREAO) / AREAN)
455      END IF
460      IF (DIFFN.LT.DIFFT)THEN
465        SIMP = AREAN
470        RETURN

CC----------------------SINCE DIFFERENCE IS NOT
C------------------------WITHIN TOLERANCE THEN
C------------------------PREPARE FOR ANOTHER
```

```
Line#  Source Line

       C--------------------------ITERATION-----------------
   169 475      ELSE
   170 480        AREAO = AREAN
   171 485        NSECTS = NSECTS*2
   172 490      ENDIF
   173 495      GOTO 80
   174
   175 CC----------------------RETURNING AREA VALUE SINCE
       C--------------------------NSECTS TOO LARGE----------
   176 500   ELSE
   177 505      SIMP=AREAN
   178 510      WRITE(*,*)'NSECTS TOO LARGE IN SIMPSONS',
            &             'INTEGRATION,'
   179 515      WRITE(*,*)'RETURNING AREA(LOW,HIGH) FOR',
            &            'PH:'
   180 520      WRITE(*,*)'(',A,',',B,')','FOR:',CPH
   181 525      PAUSE
   182 530   ENDIF
   183
   184 CCC---------------------RETURNING TO WCALC
       C--------------------------SUBPROGRAM----------------
   185 998   RETURN
   186 999   END
```

```
SI  Local Symbols

Name                      Class   Type        Size   Offset

TEMPK . . . . . . . . . . param                       0006
XN. . . . . . . . . . . . param                       000a
X . . . . . . . . . . . . param                       000e
VTT . . . . . . . . . . . param                       0012
VOT . . . . . . . . . . . param                       0016
VOO . . . . . . . . . . . param                       001a
CPH . . . . . . . . . . . param                       001e
HOA . . . . . . . . . . . param                       0022
CONCL . . . . . . . . . . param                       0026
J . . . . . . . . . . . . param                       002a
I . . . . . . . . . . . . param                       002e
PSI . . . . . . . . . . . param                       0032
TAH . . . . . . . . . . . param                       0036
APR . . . . . . . . . . . param                       003a
B . . . . . . . . . . . . param                       003e
A . . . . . . . . . . . . param                       0042
SIMP. . . . . . . . . . . param                       0046
V . . . . . . . . . . . . local   REAL*8      1120    0000
EVENS . . . . . . . . . . local   REAL*8         8    0002
FA. . . . . . . . . . . . local   REAL*8         8    000a
FB. . . . . . . . . . . . local   REAL*8         8    0012
```

```
SI  Local Symbols

Name                          Class   Type        Size   Offset

L . . . . . . . . . . . . . . local   INTEGER*4     4     001a
SUMARG. . . . . . . . . . . . local   REAL*8        8     001e
NSECTS. . . . . . . . . . . . local   INTEGER*4     4     0026
CONTMX. . . . . . . . . . . . local   REAL*8        8     002a
SUMMAX. . . . . . . . . . . . local   REAL*8        8     0032
DX. . . . . . . . . . . . . . local   REAL*4        4     003a
VN. . . . . . . . . . . . . . local   INTEGER*4     4     003e
DIFFN . . . . . . . . . . . . local   REAL*8        8     0042
AREAN . . . . . . . . . . . . local   REAL*8        8     004a
AREAO . . . . . . . . . . . . local   REAL*8        8     0052
SEP . . . . . . . . . . . . . local   REAL*4        4     005a
ODDS. . . . . . . . . . . . . local   REAL*8        8     005e
VFCN. . . . . . . . . . . . . local   REAL*8        8     0066
DIFFT . . . . . . . . . . . . local   REAL*8        8     006e
WFCN. . . . . . . . . . . . . local   REAL*8        8     0076
NMAX. . . . . . . . . . . . . local   INTEGER*4     4     007e
XV. . . . . . . . . . . . . . local   REAL*4      560     0460


Global Symbols

Name                          Class   Type        Size   Offset


SI. . . . . . . . . . . . . . FSUBRT  ***          ***    0000
WVFCN . . . . . . . . . . . . extern  ***          ***     ***

Code size = 0a5e (2654)
Data size = 00a7 (167)
Bss size  = 0082 (130)

No errors detected
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```
      Microsoft FORTRAN Optimizing Compiler Version 5.00.03

Line#  Source Line

     1        SUBROUTINE WVFCN(WFCN, VFCN, SSEP, APR, TAH,
     2       & PSI, I, J, CONCL, HOA, TEMPK)
     3
     4  CCCCC REV. 05-04-92
     5
     6  CCC---------------------EVALUATING THE FCN.S W AND V
         CC-----------------------AT GIVEN SEPERATIONS------
     7        IMPLICIT NONE
     8        INTEGER I,J
     9        REAL EC, BOC, SSEP, PIE, CONCL, CONCM, NA
              REAL APRM, DIEL, PSEP
    10        REAL APR,TAH,PSI,HOA,RSEP,RSEPSD,TEMPK
    11        REAL*8 EARGMX,EARGMN,EXARG,EXAMAX,X,Y
    12        REAL*8 TTWKT,TTH,FR,FV,KAP
              REAL*8 DIELM,DIELV,EXW,WFCN,VFCN
    13        REAL*8 TTWN,TTWNKT,TTWD,SI,SE,VRKT,FRE,FVNE
    14        REAL*8 TTHN,TTHD,FRN,FRD,FVN,VTKT
              REAL*8 VAKT,VANKT,VAD,KAPN,KAPD,KAPS
    15        DIMENSION APR(2),PSI(2),APRM(2),TAH(2:4)
    16
    17  CCCCC EC=ELECTRON CHARGE (COUL)
    18  CCCCC PIE=NUMERIC VALUE OF PIE (UNITLESS)
    19  CCCCC DIELM=RELATIVE DIELECTRIC CONSTANT OF MEDIUM
    20  CCCCC       (@25 C)(DIMENSIONLESS)
    21  CCCCC DIELV=DIELECTRIC CONSTANT OF VACUUM (C^2/JM)
    22  CCCCC DIEL=DIELECTRIC CONSTANT OF MEDIUM (C^2/JM)
    23  CCCCC BOC=BOLTZMAN CONSTANT (J/ATOM K)
    24  CCCCC NA=AVAGADRO'S CONSTANT (ATOMS/MOLE)
    25  CCCCC CONCL=CONCENTRATION OF ELECTROLYTE (MOLE/L)
    26  CCCCC CONCM=CONCENTRATION OF ELECTROLYTE (MOLE/M^3)
    27  CCCCC APR=ATOMIC PARTICLE RADIUS (NM)
    28  CCCCC APRM=ATOMIC PARTICLE RADIUS (M)
    29  CCCCC SSEP=SEPERATION DISTANCE [BETWEEN STERN
        CCCCC                                 SURFACES] (M)
    30  CCCCC PSEP=SEPERATION DISTANCE [BETWEEN PARTICLE
        CCCCC                                 SURFACES] (M)
    31  CCCCC RSEP=SEPERATION DISTANCE [BETWEEN CENTERS] (M)
    32  CCCCC RSEPSD=RSEP SQUARED (M^2)
    33  CCCCC TAH=TOTAL HAMAKER CONSTANT (J)
    34  CCCCC HOA=MINIMUM SURFACE SEPERATION FOR VAN DER
    35  CCCC      WAALS ATTRACTION (M)
    36  CCCCC HOR=MINIMUM SURFACE SEPERATION FOR REPULSION
        CCCCC     (M)
    37  CCCCC VTKT=TOTAL INTERACTION POTENTIAL IN UNITS
                   OF KT
    38  CCCCC VAKT=ATTRACTION INTERACTION POTENTIAL IN UNITS
                   OF KT
    39  CCCCC VRKT=REPULSION INTERACTION POTENTIAL IN UNITS
```

```
Line#  Source Line

                OF KT
       CCCCC KAP=KAPPA THE DEBYE-HUCKEL PARAMETER (1/M)
       CCCCC X,Y,VAN,VAD=VARIABLES USED TO BREAK DOWN
       CCCC                EQUATION FOR THE ATTRACTION
       CCCC                INTERACTION POTENTIAL SO IT MAY BE
       CCCC                SOLVED IN FORTRAN CODE WITH
       CCCC                LIMITED LINE LENGTH
       CCCCC TTWKT,TTWNKT,TTWN,TTWD,TTH,TTHN,TTHD,FR,FRN
       CCCC & FRD,FRE,FV,FVN, SI,SE,KAP,KAPN,KAPD,KAPS
       CCC   = VARIABLES USED TO BREAK DOWN
       CCC     LARGE EQUATION FOR THE REPULSION
       CCC     INTERACTION POTENTIAL SO IT MAY
       CCC     BE SOLVED IN FORTRAN CODE WITH
       CCC     LIMITED LINE LENGTH


       CC----------------------INITIALIZING THE CONSTANTS-
       10     CONCM = CONCL*1.0E+3
       20     EC = 1.602E-19
       30     NA = 6.02E+23
       40     PIE = 3.1416
       50     DIELM = 78.54
       60     DIELV = 8.8542E-12
       70     DIEL = DIELM*DIELV
       80     BOC = 1.381E-23
       90     APRM(I) = APR(I)/1.0E+9
       100    APRM(J) = APR(J)/1.0E+9
       110    PSEP=SSEP+HOA
       120    EARGMX=709.0
       130    EARGMN=-745.0

       CC----------------------EVALUATING FCN. BY BREAKING
       C------------------------INTO SMALLER TERMS &
       C------------------------RECOMBING THEM------------

       CC----------------------CALCULATING VA--------------
       140    X=PSEP/(APRM(I)+APRM(J))
       150    Y=APRM(I)/APRM(J)
       160    VANKT=0.0-(TAH(I+J)/(12.0*BOC*TEMPK))
       170    VAD=(Y/(X**2+(X*Y)+X))+(Y/(X**2+(X*Y)+X+Y))
       180    VAD=VAD+(2.0*LOG(X**2+(X*Y)+X) /
             &                             (X**2+(X*Y)+X+Y))
       190    VAKT=VANKT*VAD

       CC----------------------CALCULATING VR TERMS--------
       200    TTWN=PIE*DIEL*APRM(I)*APRM(J) *
             &                       (PSI(I)**2+PSI(J)**2)
       210    TTWNKT=TTWN/(BOC*TEMPK)
       220    TTWD=(APRM(I)+APRM(J))
       230    TTWKT=TTWNKT/TTWD
```

```
Line#  Source Line

240   IF (PSI(1).EQ.0.0 .OR. PSI(2).EQ.0.0)THEN
250      TTH = 0.0
260   ELSE
270      TTHN = 2*PSI(I)*PSI(J)
280      TTHD = PSI(I)**2+PSI(J)**2
290      TTH = TTHN/TTHD
300   END IF

310   KAPN = 2.0*CONCM*EC**2*NA
320   KAPD = DIEL*BOC*TEMPK
330   KAPS = KAPN/KAPD
340   KAP = SQRT(KAPS)

350   FRE = 0.0 -(KAP*SSEP)
360   IF (FRE.LT.EARGMN) THEN
370      FRE=EARGMN
C-----------------------PREVENTING MATH OVERFLOW
C-------------------------ERROR---------------------
380   ELSE IF (FRE.LT.1.0E-4 .AND.
     &                        FRE.GT.-1.0E-4)THEN
390      IF (FRE.GE.0.0)THEN
400        FRE=1.0E-4
410      ELSE
420        FRE=-1.0E-4
430      END IF
440   END IF
450   FRN = 1.0 + EXP(FRE)
460   FRD = 1.0 - EXP(FRE)
470   FR = LOG(FRN/FRD)

480   FVNE =(0.0-(2.0*KAP*SSEP))
490   IF (FVNE.LT.EARGMN)THEN
500      FVNE=EARGMN
C-----------------------PREVENTING MATH OVERFLOW
C-------------------------ERROR---------------------
510   ELSE IF (FVNE.GT.-1.0E-16)THEN
520      FVNE=-1.0E-16
530    END IF
540   FVN = 1.0 - EXP(FVNE)
550   FV = LOG(FVN)

560   SI=TTH*FR

570   SE=SI+FV

CC----------------------RECOMBINING TERMS TO
C------------------------------ CALCULATE VR--------
580   VRKT=TTWKT*SE

```

```
 Line#  Source Line

   129  CC----------------------CALCULATING VT FROM VA & VR-
   130  590   VTKT = VAKT+VRKT
   131  600   VFCN=VTKT
   132
   133
   134  CC----------------------CALCULATING VT OVER KT AND
   135  C---------------------------PREVENTING MATH OVERFLOW
        C---------------------------ERRORS------------------
   136  610   IF (VTKT.GT.EARGMX)THEN
   137  620      EXW=EARGMX
   138  630   ELSE IF (VTKT.LT.EARGMN)THEN
   139  640      EXW=EARGMN
   140  650   ELSE
   141  660      EXW=VTKT
   142  670   END IF
   143  680   EXARG=EXP(EXW)
   144
   145  CC----------------------CALCULATING WFCN------------
   146  690   RSEP = PSEP+APRM(I)+APRM(J)
   147  700   RSEPSD=RSEP**2
   148  710   EXAMAX=EXP(EARGMX)*RSEPSD
   149  720   IF (EXARG.GT.EXAMAX)THEN
   150  730      WFCN=EXP(EARGMX)
   151  740   ELSE
   152  750      WFCN=EXP(EXW)/RSEPSD
   153  760   END IF
   154
   155  CC----------------------RETURNING FUNCTION TO
        C-------------------------SUBPROGRAM----------------
   156  998   RETURN
   157  999   END
```

```
WVFCN  Local Symbols

Name                         Class   Type        Size   Offset

TEMPK . . . . . . . . . . . . param                      0006
HOA . . . . . . . . . . . . . param                      000a
CONCL . . . . . . . . . . . . param                      000e
J . . . . . . . . . . . . . . param                      0012
I . . . . . . . . . . . . . . param                      0016
PSI . . . . . . . . . . . . . param                      001a
TAH . . . . . . . . . . . . . param                      001e
APR . . . . . . . . . . . . . param                      0022
SSEP. . . . . . . . . . . . . param                      0026
VFCN. . . . . . . . . . . . . param                      002a
WFCN. . . . . . . . . . . . . param                      002e
```

```
WFCN

Name

TWD.
TANKT
DIRMA
DARGM
TRET.
IC. .
TCKT.
TOWN.
SA. .
ESEPS
ICC .
SE. .
FR. .
I . .
I . .
TAD .
FRD .
SL. .
KAP .
FN. .
FRE .
TWKT
DIEL.
PIE .
FAPD.
FRN .
FAPN.
FWN .
DIELM
TWNKT
FAPS.
FNE.
TH .
APPM.
CONCM
TTHD.
IW .
DIELV
TAKT.
EARG
PSEP.
EARGM
PSEP.
TGN.
```

```
WVFCN  Local Symbols

Name                      Class   Type          Size   Offset

TTWD. . . . . . . . . . . local   REAL*8        8    0000
VANKT . . . . . . . . . . local   REAL*8        8    0008
EXAMAX. . . . . . . . . . local   REAL*8        8    0010
EARGMX. . . . . . . . . . local   REAL*8        8    0018
VRKT. . . . . . . . . . . local   REAL*8        8    0020
EC. . . . . . . . . . . . local   REAL*4        4    0028
VTKT. . . . . . . . . . . local   REAL*8        8    002c
TTWN. . . . . . . . . . . local   REAL*8        8    0034
NA. . . . . . . . . . . . local   REAL*4        4    003c
RSEPSD. . . . . . . . . . local   REAL*4        4    0040
BOC . . . . . . . . . . . local   REAL*4        4    0044
SE. . . . . . . . . . . . local   REAL*8        8    0048
FR. . . . . . . . . . . . local   REAL*8        8    0050
X . . . . . . . . . . . . local   REAL*8        8    0058
Y . . . . . . . . . . . . local   REAL*8        8    0060
VAD . . . . . . . . . . . local   REAL*8        8    0068
FRD . . . . . . . . . . . local   REAL*8        8    0070
SI. . . . . . . . . . . . local   REAL*8        8    0078
KAP . . . . . . . . . . . local   REAL*8        8    0080
FV. . . . . . . . . . . . local   REAL*8        8    0088
FRE . . . . . . . . . . . local   REAL*8        8    0090
TTWKT . . . . . . . . . . local   REAL*8        8    0098
DIEL. . . . . . . . . . . local   REAL*4        4    00a0
PIE . . . . . . . . . . . local   REAL*4        4    00a4
KAPD. . . . . . . . . . . local   REAL*8        8    00a8
FRN . . . . . . . . . . . local   REAL*8        8    00b0
KAPN. . . . . . . . . . . local   REAL*8        8    00b8
FVN . . . . . . . . . . . local   REAL*8        8    00c0
DIELM . . . . . . . . . . local   REAL*8        8    00c8
TTWNKT. . . . . . . . . . local   REAL*8        8    00d0
KAPS. . . . . . . . . . . local   REAL*8        8    00d8
FVNE. . . . . . . . . . . local   REAL*8        8    00e0
TTH . . . . . . . . . . . local   REAL*8        8    00e8
APRM. . . . . . . . . . . local   REAL*4        8    00f0
CONCM . . . . . . . . . . local   REAL*4        4    00f8
TTHD. . . . . . . . . . . local   REAL*8        8    00fc
EXW . . . . . . . . . . . local   REAL*8        8    0104
DIELV . . . . . . . . . . local   REAL*8        8    010c
VAKT. . . . . . . . . . . local   REAL*8        8    0114
EXARG . . . . . . . . . . local   REAL*8        8    011c
PSEP. . . . . . . . . . . local   REAL*4        4    0124
EARGMN. . . . . . . . . . local   REAL*8        8    0128
RSEP. . . . . . . . . . . local   REAL*4        4    0130
TTHN. . . . . . . . . . . local   REAL*8        8    0134
```

```
Global Symbols

Name                          Class    Type        Size   Offset

WVFCN . . . . . . . . . . . . FSUBRT   ***          ***    0000

Code size = 086e (2158)
Data size = 0074 (116)
Bss size  = 013c (316)

No errors detected
```

```
       Microsoft FORTRAN Optimizing Compiler Version 5.00.03

Line#  Source Line

     1        SUBROUTINE WVFCN(WFCN, VFCN, SSEP, APR, TAH,
             & PSI, I, J, CONCL, HOA, TEMPK)
     2
     3  CCCCC---------CONSTANT CHARGE CALCULATIONS----------

     4  CCCCC REV. 05-04-92
     5
     6  CCC---------------------EVALUATING THE FCN.S W AND V
         CC-----------------------AT GIVEN SEPERATIONS------
     7        IMPLICIT NONE
     8        INTEGER I,J
     9        REAL EC, BOC, SSEP, PIE, CONCL, CONCM, NA
              REAL APRM, DIEL, PSEP
    10        REAL APR,TAH,PSI,HOA,RSEP,RSEPSD,TEMPK
    11        REAL*8 EARGMX,EARGMN,EXARG,EXAMAX,X,Y
    12        REAL*8 TTWKT,TTH,FR,FV,KAP
              REAL*8 DIELM,DIELV,EXW,WFCN,VFCN
    13        REAL*8 TTWN,TTWNKT,TTWD,SI,SE,VRKT,FRE,FVNE
    14        REAL*8 TTHN,TTHD,FRN,FRD,FVN,VTKT
              REAL*8 VAKT,VANKT,VAD,KAPN,KAPD,KAPS
    15        DIMENSION APR(2),PSI(2),APRM(2),TAH(2:4)
    16
    17  CCCCC EC=ELECTRON CHARGE (COUL)
    18  CCCCC PIE=NUMERIC VALUE OF PIE (UNITLESS)
    19  CCCCC DIELM=RELATIVE DIELECTRIC CONSTANT OF MEDIUM
    20  CCCCC       (@25 C)(DIMENSIONLESS)
    21  CCCCC DIELV=DIELECTRIC CONSTANT OF VACUUM (C^2/JM)
    22  CCCCC DIEL=DIELECTRIC CONSTANT OF MEDIUM (C^2/JM)
    23  CCCCC BOC=BOLTZMAN CONSTANT (J/ATOM K)
    24  CCCCC NA=AVAGADRO'S CONSTANT (ATOMS/MOLE)
    25  CCCCC CONCL=CONCENTRATION OF ELECTROLYTE (MOLE/L)
    26  CCCCC CONCM=CONCENTRATION OF ELECTROLYTE (MOLE/M^3)
    27  CCCCC APR=ATOMIC PARTICLE RADIUS (NM)
    28  CCCCC APRM=ATOMIC PARTICLE RADIUS (M)
    29  CCCCC SSEP=SEPERATION DISTANCE [BETWEEN STERN
        CCCCC                                  SURFACES] (M)
    30  CCCCC PSEP=SEPERATION DISTANCE [BETWEEN PARTICLE
        CCCCC                                  SURFACES] (M)
    31  CCCCC RSEP=SEPERATION DISTANCE [BETWEEN CENTERS] (M)
    32  CCCCC RSEPSD=RSEP SQUARED (M^2)
    33  CCCCC TAH=TOTAL HAMAKER CONSTANT (J)
    34  CCCCC HOA=MINIMUM SURFACE SEPERATION FOR VAN DER
    35  CCCC      WAALS ATTRACTION (M)
    36  CCCCC HOR=MINIMUM SURFACE SEPERATION FOR REPULSION
        CCCCC     (M)
    37  CCCCC VTKT=TOTAL INTERACTION POTENTIAL IN UNITS
                   OF KT
    38  CCCCC VAKT=ATTRACTION INTERACTION POTENTIAL IN UNITS
```

Line# Source Line

```
           OF KT
CCCCC VRKT=REPULSION INTERACTION POTENTIAL IN UNITS
           OF KT
CCCCC KAP=KAPPA THE DEBYE-HUCKEL PARAMETER (1/M)
CCCCC X,Y,VAN,VAD=VARIABLES USED TO BREAK DOWN
CCCC              EQUATION FOR THE ATTRACTION
CCCC              INTERACTION POTENTIAL SO IT MAY BE
CCCC              SOLVED IN FORTRAN CODE WITH
CCCC              LIMITED LINE LENGTH
CCCCC TTWKT,TTWNKT,TTWN,TTWD,TTH,TTHN,TTHD,FR,FRN
CCCC & FRD,FRE,FV,FVN, SI,SE,KAP,KAPN,KAPD,KAPS
CCC   = VARIABLES USED TO BREAK DOWN
CCC     LARGE EQUATION FOR THE REPULSION
CCC     INTERACTION POTENTIAL SO IT MAY
CCC     BE SOLVED IN FORTRAN CODE WITH
CCC     LIMITED LINE LENGTH


CC----------------------INITIALIZING THE CONSTANTS-
10    CONCM = CONCL*1.0E+3
20    EC = 1.602E-19
30    NA = 6.02E+23
40    PIE = 3.1416
50    DIELM = 78.54
60    DIELV = 8.8542E-12
70    DIEL = DIELM*DIELV
80    BOC = 1.381E-23
90    APRM(I) = APR(I)/1.0E+9
100   APRM(J) = APR(J)/1.0E+9
110   PSEP=SSEP+HOA
120   EARGMX=709.0
130   EARGMN=-745.0

CC----------------------EVALUATING FCN. BY BREAKING
C-------------------------INTO SMALLER TERMS &
C-------------------------RECOMBING THEM------------

CC----------------------CALCULATING VA--------------
140   X=PSEP/(APRM(I)+APRM(J))
150   Y=APRM(I)/APRM(J)
160   VANKT=0.0-(TAH(I+J)/(12.0*BOC*TEMPK))
170   VAD=(Y/(X**2+(X*Y)+X))+(Y/(X**2+(X*Y)+X+Y))
180   VAD=VAD+(2.0*LOG(X**2+(X*Y)+X) /
     &                             (X**2+(X*Y)+X+Y))
190   VAKT=VANKT*VAD

CC----------------------CALCULATING VR TERMS--------
200   TTWN=PIE*DIEL*APRM(I)*APRM(J) *
     &                       (PSI(I)**2+PSI(J)**2)
210   TTWNKT=TTWN/(BOC*TEMPK)
```

```
Line#  Source Line

220   TTWD=(APRM(I)+APRM(J))
230   TTWKT=TTWNKT/TTWD

240   IF (PSI(1).EQ.0.0 .OR. PSI(2).EQ.0.0)THEN
250      TTH = 0.0
260   ELSE
270      TTHN = 2*PSI(I)*PSI(J)
280      TTHD = PSI(I)**2+PSI(J)**2
290      TTH = TTHN/TTHD
300   END IF

310   KAPN = 2.0*CONCM*EC**2*NA
320   KAPD = DIEL*BOC*TEMPK
330   KAPS = KAPN/KAPD
340   KAP = SQRT(KAPS)

350   FRE = 0.0 -(KAP*SSEP)
360   IF (FRE.LT.EARGMN) THEN
370      FRE=EARGMN
C-----------------------PREVENTING MATH OVERFLOW
C-------------------------ERROR---------------------
380   ELSE IF (FRE.LT.1.0E-4 .AND.
     &                         FRE.GT.-1.0E-4)THEN
390      IF (FRE.GE.0.0)THEN
400        FRE=1.0E-4
410      ELSE
420        FRE=-1.0E-4
430      END IF
440   END IF
450   FRN = 1.0 + EXP(FRE)
460   FRD = 1.0 - EXP(FRE)
470   FR = LOG(FRN/FRD)

480   FVNE =(0.0-(2.0*KAP*SSEP))
490   IF (FVNE.LT.EARGMN)THEN
500      FVNE=EARGMN
C-----------------------PREVENTING MATH OVERFLOW
C-------------------------ERROR---------------------
510   ELSE IF (FVNE.GT.-1.0E-16)THEN
520      FVNE=-1.0E-16
530    END IF
540   FVN = 1.0 - EXP(FVNE)
550   FV = LOG(FVN)

560   SI=TTH*FR

570   SE=SI-FV

CC----------------------RECOMBINING TERMS TO
C------------------------------ CALCULATE VR--------
```

```
Line#  Source Line

       580   VRKT=TTWKT*SE

       CC---------------------CALCULATING VT FROM VA & VR-
       590   VTKT = VAKT+VRKT
       600   VFCN=VTKT


       CC---------------------CALCULATING VT OVER KT AND
       C------------------------PREVENTING MATH OVERFLOW
       C------------------------ERRORS------------------
       610   IF (VTKT.GT.EARGMX)THEN
       620      EXW=EARGMX
       630   ELSE IF (VTKT.LT.EARGMN)THEN
       640      EXW=EARGMN
       650   ELSE
       660      EXW=VTKT
       670   END IF
       680   EXARG=EXP(EXW)

       CC---------------------CALCULATING WFCN-----------
       690   RSEP = PSEP+APRM(I)+APRM(J)
       700   RSEPSD=RSEP**2
       710   EXAMAX=EXP(EARGMX)*RSEPSD
       720   IF (EXARG.GT.EXAMAX)THEN
       730      WFCN=EXP(EARGMX)
       740   ELSE
       750      WFCN=EXP(EXW)/RSEPSD
       760   END IF

       CC---------------------RETURNING FUNCTION TO
       C-----------------------SUBPROGRAM---------------
       998   RETURN
       999   END
```

```
WVFCN  Local Symbols

Name                          Class   Type       Size   Offset

TEMPK . . . . . . . . . . . . param                      0006
HOA . . . . . . . . . . . . . param                      000a
CONCL . . . . . . . . . . . . param                      000e
J . . . . . . . . . . . . . . param                      0012
I . . . . . . . . . . . . . . param                      0016
PSI . . . . . . . . . . . . . param                      001a
TAH . . . . . . . . . . . . . param                      001e
APR . . . . . . . . . . . . . param                      0022
SSEP. . . . . . . . . . . . . param                      0026
VFCN. . . . . . . . . . . . . param                      002a
WFCN. . . . . . . . . . . . . param                      002e
```

```
WVFCN  Local Symbols

Name                      Class   Type          Size   Offset

TTWD. . . . . . . . . . . local   REAL*8        8    0000
VANKT . . . . . . . . . . local   REAL*8        8    0008
EXAMAX. . . . . . . . . . local   REAL*8        8    0010
EARGMX. . . . . . . . . . local   REAL*8        8    0018
VRKT. . . . . . . . . . . local   REAL*8        8    0020
EC. . . . . . . . . . . . local   REAL*4        4    0028
VTKT. . . . . . . . . . . local   REAL*8        8    002c
TTWN. . . . . . . . . . . local   REAL*8        8    0034
NA. . . . . . . . . . . . local   REAL*4        4    003c
RSEPSD. . . . . . . . . . local   REAL*4        4    0040
BOC . . . . . . . . . . . local   REAL*4        4    0044
SE. . . . . . . . . . . . local   REAL*8        8    0048
FR. . . . . . . . . . . . local   REAL*8        8    0050
X . . . . . . . . . . . . local   REAL*8        8    0058
Y . . . . . . . . . . . . local   REAL*8        8    0060
VAD . . . . . . . . . . . local   REAL*8        8    0068
FRD . . . . . . . . . . . local   REAL*8        8    0070
SI. . . . . . . . . . . . local   REAL*8        8    0078
KAP . . . . . . . . . . . local   REAL*8        8    0080
FV. . . . . . . . . . . . local   REAL*8        8    0088
FRE . . . . . . . . . . . local   REAL*8        8    0090
TTWKT . . . . . . . . . . local   REAL*8        8    0098
DIEL. . . . . . . . . . . local   REAL*4        4    00a0
PIE . . . . . . . . . . . local   REAL*4        4    00a4
KAPD. . . . . . . . . . . local   REAL*8        8    00a8
FRN . . . . . . . . . . . local   REAL*8        8    00b0
KAPN. . . . . . . . . . . local   REAL*8        8    00b8
FVN . . . . . . . . . . . local   REAL*8        8    00c0
DIELM . . . . . . . . . . local   REAL*8        8    00c8
TTWNKT. . . . . . . . . . local   REAL*8        8    00d0
KAPS. . . . . . . . . . . local   REAL*8        8    00d8
FVNE. . . . . . . . . . . local   REAL*8        8    00e0
TTH . . . . . . . . . . . local   REAL*8        8    00e8
APRM. . . . . . . . . . . local   REAL*4        8    00f0
CONCM . . . . . . . . . . local   REAL*4        4    00f8
TTHD. . . . . . . . . . . local   REAL*8        8    00fc
EXW . . . . . . . . . . . local   REAL*8        8    0104
DIELV . . . . . . . . . . local   REAL*8        8    010c
VAKT. . . . . . . . . . . local   REAL*8        8    0114
EXARG . . . . . . . . . . local   REAL*8        8    011c
PSEP. . . . . . . . . . . local   REAL*4        4    0124
EARGMN. . . . . . . . . . local   REAL*8        8    0128
RSEP. . . . . . . . . . . local   REAL*4        4    0130
TTHN. . . . . . . . . . . local   REAL*8        8    0134
```

```
Global Symbols

Name                         Class   Type       Size   Offset

WVFCN . . . . . . . . . . .  FSUBRT  ***         ***    0000

Code size = 086e (2158)
Data size = 0074 (116)
Bss size  = 013c (316)

No errors detected
```

```
      Microsoft FORTRAN Optimizing Compiler Version 5.00.03

Line#  Source Line

    1         SUBROUTINE DATA STORAGE(V, APR, ZPQ, AHM, AHP,
    2        & PHCZI, NZP1, NZP2, ZPPH1, ZPDP1, ZPPH2,
    3        & ZPDP2, WT, PH, CONCL, WOO, WOT, WTT,CDATE,
             & STIME, FTIME, TEMP)
    4
    5  CCCCC REV. 06-22-92
    6
    7  CCC----------------------SUBPROGRAM TO STORE INPUT &
     CC-----------------------CALCULATED DATA------------
    8
    9         IMPLICIT NONE
   10         CHARACTER IFLNM*17,FLDSC*100,ZPQ*1,FLNME*20
              CHARACTER FLXT*4,TEMPC*34,AHMC*33,CONCC*42
   11         CHARACTER APRC*35,PHCZIC*28,RICS*16,AHPC*33
   12         CHARACTER TFLNME*34
   13         INTEGER K,L,NZP1,NZP2
   14         INTEGER*2 CDATE,STIME,FTIME
   15         DIMENSION CDATE(3),STIME(4),FTIME(4)
   16         REAL PH,APR,PHCZI,AHP,AHM,ZPPH1,ZPDP1,CONCL
   17         REAL ZPPH2,ZPDP2,TEMP,V
   18         REAL*8 WT,WOO,WOT,WTT,WMAX
   19         DIMENSION WT(200),PH(200),APR(2),AHP(2),
              DIMENSION PHCZI(2), ZPPH1(200),ZPDP1(200)
   20         DIMENSION ZPPH2(200), ZPDP2(200)
   21         DIMENSION WOO(200),WOT(200),WTT(200)
   22
   23  CCCCC IFLNM=INPUT FILE NAME FOR DATA STORAGE
   24  CCCCC FLXT=FILE EXTENSION FOR DATA STORAGE FILE
   25  CCCCC FLNME=COMPLETE FILE NAME (I.E. FILE NAME &
       CCCCC       EXTENSION)
   26  CCCCC TFLNME=TOTAL FILE NAME FOR DATA STORAGE
       CCCCC        (INCLUDES DIRECTORY)
   27  CCCCC FLDSC=DESCRIPTION OF FILE
   28  CCCCC WMAX=MAXIMUM W VALUE ALLOWABLE FOR PLOTTING
       CCCCC      PROGRAMS
   29
   30  CCC----------------------ASSIGNING CHARACTER
       CC-----------------------VARIABLES-----------------
   31  05     APRC = 'ATOMIC PARTICLE RADIUS OF COMPONENT'
   32  10     PHCZIC = 'POINT-OF-ZERO-CHARGE OF COMPONENT'
   33  15     RICS = 'VALUE(S) INPUT :'
   34  20     AHPC = 'HAMAKER CONSTANT OF COMPONENT'
   35  25     AHMC = 'HAMAKER CONSTANT OF MEDIUM ='
   36  30     CONCC = 'CONCENTRATION OF 1-1 ELECTROLYTE IN'
             &        'SYSTEM'
   37  35     TEMPC = 'TEMPERATURE OF SYSTEM (IN DEG. C.)'
   38
   39  CCC----------------------COLLECTING A FILE NAME AND
```

Line# Source Line

```
C-------------------------SYSTEM DESCRIPTION FOR THE
C-------------------------DATA FILE TO STORE
C-------------------------INFORMATION IN------------
40    READ(14,800)FLDSC
45    READ(14,810)IFLNM
50    TFLNME(1:14)='C:\JK\LL\DATA\'

CCC---------------------WRITING DATA TO A PRINTABLE
CC------------------------DATA FILE-----------------
55    FLXT = '.PDF'
60    FLNME(1:16)=IFLNM(2:17)
65    FLNME(17:20)=FLXT(1:4)
70    TFLNME(15:34)=FLNME(1:20)
75    OPEN(4,FILE=TFLNME,STATUS='UNKNOWN')
80      WRITE(4,875)
85      WRITE(4,880)
90      WRITE(4,885)
95      WRITE(4,890)FLNME,FLDSC
100     WRITE(4,895)CDATE(2),CDATE(3),CDATE(1)
105     WRITE(4,900)STIME(1),STIME(2),STIME(3),
     &              STIME(4)
110     WRITE(4,905)FTIME(1),FTIME(2),FTIME(3),
     &              FTIME(4)
115     WRITE(4,910)V,CONCC,CONCL,APRC,APR(1),
     &              APRC,APR(2)
120     WRITE(4,915)TEMPC,TEMP
125     WRITE(4,930)AHMC,AHM,AHPC,AHP(1),AHPC,AHP(2)
130    IF (ZPQ.EQ.'P')THEN
135       WRITE(4,920)
140       WRITE(4,925)PHCZIC,PHCZI(1),PHCZIC,
     &                PHCZI(2)
145     ELSE
150         WRITE(4,935)
155         WRITE(4,940)1
160        DO 170 K=1,NZP1,1
165           WRITE(4,945)ZPDP1(K),ZPPH1(K)
170         CONTINUE
175         WRITE(4,940)2
180         DO 190 K=1,NZP2,1
185           WRITE(4,945)ZPDP2(K),ZPPH2(K)
190         CONTINUE
195     END IF
200     WRITE(4,955)
205     DO 225 K=1,200,1
210       IF (PH(K).NE.0.0) THEN
215         WRITE(4,960)WOO(K),WOT(K),
     &                  WTT(K),WT(K),PH(K)
220       END IF
225     CONTINUE
230   CLOSE(4)
```

Source Line

```
CCC---------------------WRITING DATA TO DATA FILE
CC------------------------FOR PLOTTING--------------

CC----------------------WRITING DATA FILE WITH ALL W
C-------------------------VALUES--------------------
235   FLXT = '.DAT'
240   TFLNME(31:34)=FLXT
245   OPEN(3,FILE=TFLNME,STATUS='UNKNOWN')
250     WRITE(3,850)FLNME,FLDSC
255     DO 275 L=1,200,1
260       IF (PH(L).NE.0.0)THEN
265         WRITE(3,860)PH(L),WOO(L),WOT(L),WTT(L),
     &                  WT(L)
270       END IF
275     CONTINUE
280   CLOSE(3)

CC----------------------WRITING DATA TO FILE WITH
C----------------------------ALL W VALUES WITH A
C----------------------------MAXIMUM OF WMAX--------
285   FLXT='.DAM'
290   TFLNME(31:34)=FLXT
295   OPEN(3,FILE=TFLNME,STATUS='UNKNOWN')
300     WRITE(3,850)FLNME,FLDSC
305     WMAX=9.9999E+30
310     DO 350 L=1,200,1
315       IF (PH(L).NE.0.0)THEN
320         IF(WOO(L).GT.WMAX)WOO(L)=WMAX
325         IF(WOT(L).GT.WMAX)WOT(L)=WMAX
330         IF(WTT(L).GT.WMAX)WTT(L)=WMAX
335         IF(WT(L).GT.WMAX)WT(L)=WMAX
340         WRITE(3,860)PH(L),WOO(L),WOT(L),WTT(L),
     &                  WT(L)
345       END IF
350     CONTINUE
355   CLOSE(3)


CC----------------------WRITING DATA FILE WITH ONLY
C-------------------------WT VALUES-----------------
360   FLXT='.DWT'
365   TFLNME(31:34)=FLXT
370   OPEN(3,FILE=TFLNME,STATUS='UNKNOWN')
375     WRITE(3,850)FLNME,FLDSC
380     DO 400 L=1,200,1
385        IF (PH(L).NE.0.0)THEN
390          WRITE(3,860)PH(L),WT(L)
395        END IF
400     CONTINUE
```

Source Line

```
405   CLOSE(3)

CC----------------------WRITING DATA FILE WITH ONLY
C---------------------------WT VALUESWITH A MAXIMUM
C---------------------------OF WMAX---------------
410   FLXT = '.DWM'
415   TFLNME(31:34)=FLXT
420   OPEN(3,FILE=TFLNME,STATUS='UNKNOWN')
        WRITE(3,850)FLNME,FLDSC
        DO 455 L=1,200,1
           IF (PH(L).NE.0.0)THEN
             IF(WT(L).GT.WMAX)WT(L)=WMAX
             WRITE(3,860)PH(L),WT(L)
           END IF
        CONTINUE
460   CLOSE(3)

CCC---------------------FORMATTING READ STATEMENTS--
800   FORMAT(A70)
810   FORMAT(A17)

CCC---------------------FORMATTING WRITE STATEMENTS-
850   FORMAT(1X,A70)
855   FORMAT(1X,24(/),
     & 1X,'TYPE IN A NAME FOR A FILE TO STORE DATA',
     & 'IN.'/,
     & 1X,'(MUST BE 8 CHARACTERS IN LENGTH WITH NO',
     & 'SPACES.)',15(/))
860   FORMAT(1X,F5.2,1X,',',1X,E12.4,1X,',',1X,
     & E12.4,1X,',',1X,
     & E12.4, 1X,',',1X,E12.4)
865   FORMAT(1X,24(/),
     & 1X,'DO YOU WANT A PRINTED COPY OF DATA?(Y',
     & 'or N)',15(/))
870   FORMAT(1X,24(/),
     & 1X,'READY PRINTER FOR PRINTING.'/,
     & 1X,'WHEN PRINTER IS READY FOR PRINTING',
     & 'TYPE: "Y"'/,
     & 1X,'IF PRINTER IS IN-OPERABLE TYPE:',
     & '"N"',13(/))
C----------------------FORMATTING TITLE BLOCK------
875   FORMAT(/,/,/,/,/,/,/,/,11X, 58('C')/,
     & 11X,'C',40X,'Rev. 06-22-92',3X,'C'/,
     & 11X,'C',4X,'MASTERS THESIS RESEARCH',
     & 29X,'C'/,
     & 11X,'C',4X,'BRETT A. WILSON',37X,'C'/,
     & 11X,'C',4X,'MICHIGAN STATE UNIVERSITY',
     & 27X,'C'/,
     & 11X,'C',4X,'COLLEGE OF ENGINEERING',30X,'C'/,
     & 11X,'C',4X,'DEPARTMENT OF METALLURGY,',
```

```
Line#  Source Line

            & 'MECHANICS, ',16X,'C'/,
            & 11X,'C',4X,5X,'AND MATERIAL SCIENCE',
            & 27X,'C'/,
            & 11X,'C',56X,'C'/,
            & 11X,58('C'),/,/,/,/,/,/,/)
       C-----------------------FORMATTING PROGRAM
       C-----------------------DESCRIPTION----------------
       880   FORMAT(/,/,11X,58('C')/,
            & 11X,'C',56X,'C'/,
            & 11X,'C',4X,'THIS PROGRAM USES MEASURABLE',
            & 'MATERIAL DATA TO',
            & 7X,'C'/,
            & 11X,'C',4X,'CREATE INFORMATION WHICH SHOULD',
           & 'PREDICT THE',9X,'C'/
            & 11X,'C',4X,'FLOCCULATION STATE OF TWO',
            & 'COMPONENT COLLOIDAL',
            & 7X,'C'/,
            & 11X,'C',4X,'SUSPENSIONS.',40X,'C'/,
            & 11X,'C',56X,'C'/,
            & 11X,'C',4X,'THE PROGRAM RELIES ON A METHOD',
            & 'WHICH IS A MOD-',
            & 6X,'C'/,
            & 11X,'C',4X,'IFICATION OF THE H.H.F. METHOD,',
           & 'WHICH IS BASED ON',
            & 3X,'C'/,
            & 11X,'C',4X,'THE DEBYE-HUCKEL APPROXIMATION',
          & 'FOR THE REPULSION',
            & 4X,'C'/,
            & 11X,'C',4X,'BETWEEN TWO PLATES OF CONSTANT',
          & 'POTENTIAL.',11X,'C'/,
            & 11X,'C',56X,'C')
       885   FORMAT(11X,'C',4X,'MODIFICATIONS INCLUDE:',
            & 30X,'C'/,
#           & 11X,'C',5X,'-USING AN EFFECTIVE HAMAKER',
            & 'CONSTANT FOR TWO',7X,'C'
            & 11X,'C',6X,'PARTICLES IN A DISPERSING',
            & 'MEDIUM.',18X,'C'/,
            & 11X,'C',5X,'-USING ZETA POTENTIAL DATA',
            & 'INSTEAD OF CALCULAT-',
            & 4X,'C'/,
#           & 11X,'C',6X,'ING THE SURFACE POTNTIAL FROM',
            & 'POINT-OF-ZERO-',6X,'C'
            & 11X,'C',6X,'CHARGE DATA.',38X,'C'/,
            & 11X,'C',56X,'C'/,
            & 11X,58('C'),/)
       890   FORMAT(1X,'FILE NAME:',A12/,
            & 1X,'FILE DESCRIPTION:'/,
            & 1X,A70)
       895   FORMAT(1X,'THIS DATA WAS AQUIRED ON:',
            & 1X,I2.2,'/',I2.2,'/',I4.4)
```

```
Line#  Source Line

       900    FORMAT(1x,'AQUISITION BY THE PROGRAM STARTED',
             & 'AT...',
             & 1X,I2.2,':',I2.2,':',I2.2,':',I2.2)
       905    FORMAT(1X,21X,'AND FINISHED AT...',
             & 1X,I2.2,':',I2.2,':',I2.2,':',I2.2)
       910    FORMAT(1X,'OVERALL PROPORTION OF COMPONENT 1',
             & 'IN SYSTEM =',
             & F4.3/,
             & 1X,A42,1X,'=',1X,F7.5/,
             & 1X,A35,1X,'1',1X,'=',1X,F7.1/,
             & 1X,A35,1X,'2',1X,'=',1X,F7.1)
       915    FORMAT(1X,A34,1X,'=',1X,F4.1)
       920    FORMAT(1X,'ZERO-POINT-OF-CHARGE DATA WAS',
             & 'USED',
             & ' FOR CALCULATIONS.')
       925    FORMAT(1X,A33,1X,'1',1X,'=',1X,F5.2/,
             & 1X,A33,1X,'2',1X,'=',1X,F5.2)
       930    FORMAT(1X,A28,1X,E10.2/,
             & 1X,A29,1X,'1 =',1X,E10.2/,
             & 1X,A29,1X,'2 =',1X,E10.2)
       935    FORMAT(1X,'ZETA POTENTIAL DATA WAS USED FOR',
             & ' CALCULATIONS.')
       940    FORMAT(1X,'ZETA POTENTIAL DATA FOR PARTICLE',
             & 1X,I1,':'/,
             & 1X,'ZETA POTENTIAL VALUES:',10X,
             & 'CORESPONDING PH VALUES:')
       945    FORMAT(23X,F5.1,29X,F5.1)
       950    FORMAT(1X,'CALCULATED OVERALL STABILITY',
             & 'RATIO DATA:'/,
             & 1X,'OVERALL STABILITY RATIO:',28X,
             & 'CORESPONDING PH',/,
             & 1X'(W11,W12,W22,WT)',44X,'VALUES:')
       955    FORMAT(1X,/,/,/,/,/,/,/,'CALCULATED OVERALL',
             & 'STABILITY RATIO',
             & 1X,'DATA:'/,
             & 1X,'OVERALL STABILITY RATIO:',28X,
             & 'CORESPONDING PH',/,
             & 1X'(W11,W12,W22,WT)',44X,'VALUES:')
       960    FORMAT(1X,E12.4,', ',E12.4,', ',E12.4,', ',
             & E12.4,8X,F5.2)

       CCC---------------------RETURNING TO MAIN PROGRAM---
      998    RETURN
       999    END
```

```
DATASTORAGE  Local Symbols

Name                          Class   Type          Size   Offset

TEMP. . . . . . . . . . . . . param                        0006
FTIME . . . . . . . . . . . . param                        000a
STIME . . . . . . . . . . . . param                        000e
CDATE . . . . . . . . . . . . param                        0012
WTT . . . . . . . . . . . . . param                        0016
WOT . . . . . . . . . . . . . param                        001a
WOO . . . . . . . . . . . . . param                        001e
CONCL . . . . . . . . . . . . param                        0022
PH. . . . . . . . . . . . . . param                        0026
WT. . . . . . . . . . . . . . param                        002a
ZPDP2 . . . . . . . . . . . . param                        002e
ZPPH2 . . . . . . . . . . . . param                        0032
ZPDP1 . . . . . . . . . . . . param                        0036
ZPPH1 . . . . . . . . . . . . param                        003a
NZP2. . . . . . . . . . . . . param                        003e
NZP1. . . . . . . . . . . . . param                        0042
PHCZI . . . . . . . . . . . . param                        0046
AHP . . . . . . . . . . . . . param                        004a
AHM . . . . . . . . . . . . . param                        004e
ZPQ . . . . . . . . . . . . . param                        0052
APR . . . . . . . . . . . . . param                        0056
V   . . . . . . . . . . . . . param                        005a
PHCZIC. . . . . . . . . . . . local   CHAR*28         28   0002
TFLNME. . . . . . . . . . . . local   CHAR*34         34   001e
K   . . . . . . . . . . . . . local   INTEGER*4        4   0040
L   . . . . . . . . . . . . . local   INTEGER*4        4   0044
AHMC. . . . . . . . . . . . . local   CHAR*33         33   0048
AHPC. . . . . . . . . . . . . local   CHAR*33         33   006a
CONCC . . . . . . . . . . . . local   CHAR*42         42   008c
APRC. . . . . . . . . . . . . local   CHAR*35         35   00b6
FLDSC . . . . . . . . . . . . local   CHAR*100       100   00da
RICS. . . . . . . . . . . . . local   CHAR*16         16   013e
FLNME . . . . . . . . . . . . local   CHAR*20         20   014e
IFLNM . . . . . . . . . . . . local   CHAR*17         17   0162
TEMPC . . . . . . . . . . . . local   CHAR*34         34   0174
WMAX. . . . . . . . . . . . . local   REAL*8           8   0196
FLXT. . . . . . . . . . . . . local   CHAR*4           4   019e

Global Symbols

Name                          Class   Type          Size   Offset

DATASTORAGE . . . . . . . . . FSUBRT  ***            ***   0000

Code size = 0c65 (3173)
Data size = 0311 (785)
Bss  size  = 01a2 (418)
No   errors detected
```

Microsoft FORTRAN Optimizing Compiler Version 5.00.03

Line# Source Line

```
      PROGRAM VARYN

CCCCC REV. 07-07-92

CCC----------PROGRAM TO CALCULATE OVERALL STABILITY
C--------------RATIO FOR VARYING VALUES OF V USING
C--------------DATA FROM PROGRAM RUNS WITH V=0.5----

      IMPLICIT NONE
      CHARACTER NDIRNAME*7,NWFLNAME*34,TNFLNAME*34
      CHARACTER A*70,B*70,PSC*1
      INTEGER L,K,NFLS,I,J
      REAL*8 WT,WOO,WOT,WTT,OOWT,WTN,AZP,AZN,AZ,WMAX

      REAL N,PH,V,PR,OON,PRC
      DIMENSION PH(200),WT(200),WTN(5),V(5)
      DIMENSION N(5),PR(2),PRC(2)
      DIMENSION WOO(200),WOT(200),WTT(200)

CCCCC N=OVERALL PROPORTION OF PARTICLES OF COMPONENT
CCCCC   ONE IN SYSTEM
CCCCC V=VOLUME PERCENT OF COMPONENT ONE IN SYSTEM
CCCCC WT=OVERALL STABILTY RATIO
CCCCC OOWT=ONE OVER WT
CCCCC WOO,WOT,WTT=INVERSE OF THE PROBABILITY THAT A
CCCCC                  GIVEN PARTICLE COLLISION LEADS TO
CCCCC                  ADHESION
CCCCC NFLS=NUMBER OF FILES TO RUN PROGRAM ON
CCCCC NDIRNAME=NEW DIRECTORY NAME WHERE WILL FIND
CCCCC          DATA FILE
CCCCC NWFLNAME=NEW FILE NAME
CCCCC TNFLNAME=TOTAL NEW FILE NAME INCLUDING DRIVE
CCCCC          AND PATH
CCCCC K=INTEGER VARIABLE USED AS A COUNTER FOR DO
CCCCC   LOOP WHICH CALCULATES OVERALL STABILITY AT
CCCCC   EACH SPECIFIED PH
CCCCC L,I,J=INTEGERS USED AS COUNTER FOR VARIOUS DO
CCCCC       LOOPS
CCCCC AZ=VARIABLE REPRESENTING ALMOST ZERO
CCCCC   =(1.0E-309)
CCCCC AZP=POSITIVE VALUE OF AZ USED TO PREVENT AN
CCCCC     INVERSE FROM GOING TO INFINITY WHICH
CCCCC     CAUSES A MATH OVERFLOW ERROR RESULTING IN
CCCCC     PROGRAM TERMINATION
CCCCC AZN=NEGATIVE VALUE OF AZ USED AS AZP IS
CCCCC PR=PARTICLE RADIUS
CCCCC PRC=PARTICLE RADIUS CUBED
CCCCC OON=ONE OVER N
```

Line# Source Line

```
  CCCCC PSC=PARTICLE SIZE CHARACTER WHICH INDICATES
  CCCCC     PARTICLE SIZE
  CCCCC WTN=NEW WT VALUES CALCULATED FOR DIFFERENT
  CCCCC     VALUES OF N (OR V)
  CCCCC WMAX=MAXIMUM W VALUE ALLOWED BY PLOTTING
  CCCCC      PROGRAM


  CC----------------------CALCULATING VALUES FOR
  C-------------------------AZP,AZN-------------------
  10    AZ = 1.0E-25
  20    DO 40 K=1,11,1
  30       AZ = AZ/1.0E+25
  40    CONTINUE
  50    AZP = AZ/1.E9
  60    AZN = -1.0*AZP
  70    WMAX=9.9999E+30

  CC----------------------INITIALIZING DRIVE AND PATH
C-------------------------FOR TNFLNAME--------------
  80    TNFLNAME(1:14) = 'C:\JK\LL\DATA\'
  90    TNFLNAME(22:23) = '\B'
  100   TNFLNAME(31:34) = '.DAT'

  CC----------------------INITIALIZING VALUES OF V FOR
  C-------------------------CALCULATIONS--------------
  110   V(1) = 0.001
  120   V(2) = 0.25
  130   V(3) = 0.5
  140   V(4) = 0.75
  150   V(5) = 0.999

  CC----------------------READING DATA FILE WITH LIST
C-------------------------OF FILES------------------
  160   OPEN(14,FILE='C:\JK\LL\DATA\FILELST',
       &                                  STATUS='OLD')
  170   READ(14,800)NFLS


  CC----------------------RUNNING CALCULATIONS FOR
  C-------------------------EACH FILE-----------------
  180   DO 670 I=1,NFLS,1

  C-----------------------READING NEW DIRECTORY NAME--
  190      READ(14,810)NDIRNAME
  200      TNFLNAME(15:21) = NDIRNAME
  210      TNFLNAME(24:30) = NDIRNAME
  220      NWFLNAME = TNFLNAME
  230      NWFLNAME(20:21)='VN'
  235      NWFLNAME(29:30)='VN'
```

Line# Source Line

```

C-----------------------DETERMINING PARTICLE SIZE
C------------------------FROM DIRECTORY NAME--------
240      PSC = NDIRNAME(4:4)
250      PR(2) = 250
260      IF(PSC.EQ.'1')PR(1)=2750
270      IF(PSC.EQ.'2')PR(1)=900
280      IF(PSC.EQ.'3')PR(1)=400
290      PRC(1) = PR(1)**3
300      PRC(2) = PR(2)**3

C-----------------------READING DATA FROM N=0.5 DATA
310      OPEN(15,FILE=TNFLNAME,STATUS='OLD')
320      READ(15,820)A
330      READ(15,820)B
340      OPEN(16,FILE=NWFLNAME,STATUS='NEW')
350      NWFLNAME(31:34)='.DAM'
360      OPEN(17,FILE=NWFLNAME,STATUS='NEW')
370      WRITE(16,900)A,B
380      DO 630 K=1,15,1
390        READ(15,830)PH(K),WOO(K),WOT(K),WTT(K)

C-----------------------CALCULATING N VALUES FROM V
C-------------------------VALUES--------------------
400        DO 570 L=1,5,1
410          OON = ((PRC(1))-(V(L)*PRC(1))) /
    &                                (V(L)*PRC(2))
420          OON = OON + 1.00
430          N(L) = 1.00/(OON)

CC----------------------FINDING THE OVERALL
C-------------------------STABILITY RATIO AT CURRENT
C--------------------------PH-----------------------
C------------------------PREVENTING MATH OVERFLOW
C---------------------------ERRORS AND PROGRAM
C---------------------------TERMINATION-------------
440          IF(WOO(K).LE.AZP .AND.
    &                            WOO(K).GE.AZN)THEN
450            WT(K)=WOO(K)
460          ELSE IF(WOT(K).LE.AZP .AND.
    &                            WOT(K).GE.AZN)THEN
470            WT(K)=WOT(K)
480          ELSE IF(WTT(K).LE.AZP .AND.
    &                            WTT(K).GE.AZN)THEN
490            WT(K)=WTT(K)
500          ELSE
510            OOWT = (N(L)*N(L)/WOO(K))
520            OOWT=OOWT+
    &                  ((1.0-N(L))*(1.0-N(L))/WTT(K))
530            OOWT=OOWT+
```

```
 Line#  Source Line

             &                   (2.0*N(L)*(1.0-N(L))/WOT(K))
   121  540               WT(K)=1.0/OOWT
   122  550             END IF
   123  560             WTN(L) = WT(K)
   124  570           CONTINUE
   125
   126  CCC---------------------WRITING NEW DATA TO A
        CC-------------------------STORAGE FILE--------------
   127  580           WRITE(16,910)PH(K),WTN(1),WTN(2),WTN(3),
             &                                     WTN(4),WTN(5)
   128  590           DO 610 J=1,5,1
   129  600             IF(WTN(J).GT.WMAX)WTN(J)=WMAX
   130  610           CONTINUE
   131  620           WRITE(17,910)PH(K),WTN(1),WTN(2),WTN(3),
              &                                    WTN(4),WTN(5)
   132  630         CONTINUE
   133  640         CLOSE(17)
   134  650         CLOSE(16)
   135  660         CLOSE(15)
   136  670      CONTINUE
   137  680      CLOSE(14)
   138
   139  800      FORMAT(I2)
   140  810      FORMAT(A7)
   141  820      FORMAT(A70)
   142  830      FORMAT(1X,F5.2,3X,E12.4,3X,E12.4,3X,E12.4)
   143
   144  900      FORMAT(1X,A70,/,1X,A70)
   145  910      FORMAT(1X,F5.2,',',E12.4,',',E12.4,',',
   146          & E12.4,',',E12.4,',',E12.4)
   147
   148  999      END


main  Local Symbols

Name                          Class    Type        Size    Offset

PH. . . . . . . . . . . . . . local    REAL*4       800     0000
A . . . . . . . . . . . . . . local    CHAR*70       70     0002
B . . . . . . . . . . . . . . local    CHAR*70       70     0048
OOWT. . . . . . . . . . . . . local    REAL*8         8     008e
I . . . . . . . . . . . . . . local    INTEGER*4      4     0096
J . . . . . . . . . . . . . . local    INTEGER*4      4     009a
K . . . . . . . . . . . . . . local    INTEGER*4      4     009e
L . . . . . . . . . . . . . . local    INTEGER*4      4     00a2
N . . . . . . . . . . . . . . local    REAL*4        20     00a6
NDIRNAME. . . . . . . . . . . local    CHAR*7         7     00ba
TNFLNAME. . . . . . . . . . . local    CHAR*34       34     00c2
V . . . . . . . . . . . . . . local    REAL*4        20     00e4
```

```
main  Local Symbols

Name                          Class   Type        Size   Offset

NWFLNAME. . . . . . . . . . . local   CHAR*34       34     00f8
AZ. . . . . . . . . . . . . . local   REAL*8         8     011a
PR. . . . . . . . . . . . . . local   REAL*4         8     0122
PRC . . . . . . . . . . . . . local   REAL*4         8     012a
PSC . . . . . . . . . . . . . local   CHAR*1         1     0132
AZN . . . . . . . . . . . . . local   REAL*8         8     0134
AZP . . . . . . . . . . . . . local   REAL*8         8     013c
OON . . . . . . . . . . . . . local   REAL*4         4     0144
NFLS. . . . . . . . . . . . . local   INTEGER*4      4     0148
WTN . . . . . . . . . . . . . local   REAL*8        40     014c
WMAX. . . . . . . . . . . . . local   REAL*8         8     0174
WT. . . . . . . . . . . . . . local   REAL*8      1600     0320
WOO . . . . . . . . . . . . . local   REAL*8      1600     0960
WOT . . . . . . . . . . . . . local   REAL*8      1600     0fa0
WTT . . . . . . . . . . . . . local   REAL*8      1600     15e0


Global Symbols

Name                          Class   Type        Size   Offset

main. . . . . . . . . . . . . FSUBRT  ***          ***    0000

Code size = 06ef (1775)
Data size = 016d (365)
Bss size  = 017c (380)

No errors detected
```

```
FILE NAME:SS213SD\BSS213SD
FILE DESCRIPTION: RUN USING BMTHFWVB.EXE.
     THIS DATA WAS AQUIRED ON: 07/08/1992
AQUISITION BY THE PROGRAM STARTED AT... 00:21:33:16
                     AND FINISHED AT... 01:17:26:97
VOLUME FRACTION OF COMPONENT 1 IN SYSTEM =.500
CONCENTRATION OF 1-1 ELECTROLYTE IN SYSTEM =  .00100
ATOMIC PARTICLE RADIUS OF COMPONENT 1 =  2750.0
ATOMIC PARTICLE RADIUS OF COMPONENT 2 =   250.0
TEMPERATURE OF SYSTEM (IN DEG. C.) = 25.0
HAMAKER CONSTANT OF MEDIUM =    .45E-19
HAMAKER CONSTANT OF COMPONENT 1 =    .30E-18
HAMAKER CONSTANT OF COMPONENT 2 =    .16E-18
ZETA POTENTIAL DATA WAS USED FOR CALCULATIONS.
ZETA POTENTIAL DATA FOR PARTICLE 1:
ZETA POTENTIAL VALUES:         CORESPONDING PH VALUES:
                        5.8                           2.0
                       -2.2                           2.5
                      -15.0                           3.0
                      -26.0                           3.5
                      -34.0                           4.0
                      -40.0                           4.5
                      -44.0                           5.0
                      -48.0                           5.5
                      -51.0                           6.0
                      -53.0                           6.5
                      -54.0                           7.0
                      -56.0                           7.5
                      -57.0                           8.0
                      -58.0                           8.5
                      -59.0                           9.0
                      -60.0                           9.5
                      -60.0                           10.0
                      -61.0                           10.5
                      -61.0                           11.0
ZETA POTENTIAL DATA FOR PARTICLE 2:
ZETA POTENTIAL VALUES:         CORESPONDING PH VALUES:
                       44.0                            2.9
                       38.9                            4.0
                       29.4                            5.0
                        9.1                            6.1
                      -24.0                            7.1
                      -33.0                            8.0
                      -43.0                            9.0
                      -43.0                            10.0
                      -45.0                            11.0
```

```
CALCULATED OVERALL STABILITY RATIO DATA:
 OVERALL STABILITY RATIO:
CORESPONDING PH (W11,W12,W22,WT)
              VALUES:
.1819+248,    .2738E+00,    .1105E+77,    .1825E+03    4.00
.4761+303,    .2738E+00,    .1257E+55,    .1825E+03    4.50
.4761+303,    .2738E+00,    .4842E+36,    .1825E+03    5.00
.4761+303,    .2738E+00,    .9557E+09,    .1825E+03    5.50
.4761+303,    .2738E+00,    .5053E+00,    .5047E+00    6.00
.4761+303,    .2738E+00,    .4998E+00,    .4992E+00    6.50
.4761+303,    .2738E+00,    .4468E+13,    .1825E+03    7.00
.4761+303,    .2738E+00,    .4563E+31,    .1825E+03    7.50
.4761+303,    .2738E+00,    .7460E+49,    .1825E+03    8.00
.4761+303,    .3677E-04,    .6029E+72,    .2451E-01    8.50
.4761+303,    .8836E+18,    .6955E+99,    .5889E+21    9.00
.4761+303,    .8792E+22,    .3959+101,    .5860E+25    9.50
.4761+303,    .8792E+22,    .3959+101,    .5860E+25    10.00
.4761+303,    .2195E+30,    .4755+107,    .1463E+33    10.50
.4761+303,    .1257E+35,    .8488+113,    .8378E+37    11.00
```

```
FILE NAME:SS213ES\BSS213ES
FILE DESCRIPTION: RUN USING BMTHFWVB.EXE.
THIS DATA WAS AQUIRED ON: 07/08/1992
AQUISITION BY THE PROGRAM STARTED AT... 14:43:32:87
                     AND FINISHED AT... 16:38:15:92
VOLUME FRACTION OF COMPONENT 1 IN SYSTEM =.500
CONCENTRATION OF 1-1 ELECTROLYTE IN SYSTEM =  .00100
ATOMIC PARTICLE RADIUS OF COMPONENT 1 =  2750.0
ATOMIC PARTICLE RADIUS OF COMPONENT 2 =   250.0
TEMPERATURE OF SYSTEM (IN DEG. C.) = 25.0
HAMAKER CONSTANT OF MEDIUM =    .45E-19
HAMAKER CONSTANT OF COMPONENT 1 =    .30E-18
HAMAKER CONSTANT OF COMPONENT 2 =    .16E-18
ZETA POTENTIAL DATA WAS USED FOR CALCULATIONS.
ZETA POTENTIAL DATA FOR PARTICLE 1:
ZETA POTENTIAL VALUES:       CORESPONDING PH VALUES:
                      -13.0                           3.9
                      -14.0                           4.0
                      -15.0                           4.1
                      -16.0                           4.2
                      -18.0                           4.3
                      -19.0                           4.4
                      -20.0                           4.5
                      -21.0                           4.6
                      -23.0                           4.7
                      -23.0                           4.8
                      -23.0                           4.8
                      -25.0                           4.9
                      -26.0                           5.0
                      -27.0                           5.1
                      -28.0                           5.2
                      -28.0                           5.3
                      -30.0                           5.4
                      -31.0                           5.6
                      -32.0                           5.7
                      -33.0                           5.9
                      -34.0                           6.1
                      -35.0                           6.2
                      -35.0                           6.4
                      -36.0                           6.6
                      -37.0                           6.7
                      -38.0                           6.9
                      -38.0                           7.0
                      -39.0                           7.2
                      -40.0                           7.3
                      -40.0                           7.4
                      -41.0                           7.6
                      -41.0                           7.7
                      -42.0                           7.8
                      -42.0                           7.9
                      -44.0                           8.1
                      -45.0                           8.3
```

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                      -47.0                           8.4
                      -48.0                           8.6
                      -48.0                           8.6
                      -48.0                           8.8
                      -49.0                           8.9
                      -49.0                           9.0
                      -49.0                           9.1
                      -50.0                           9.2
                      -50.0                           9.3
                      -50.0                           9.4
                      -50.0                           9.5
                      -51.0                           9.6
                      -51.0                           9.7
                      -51.0                           9.8
                      -52.0                           9.9
                      -52.0                          10.0
                      -52.0                          10.2
                      -53.0                          10.3
                      -53.0                          10.4
                      -54.0                          10.5
                      -55.0                          10.7
                      -56.0                          10.8
                      -57.0                          10.9
                      -59.0                          11.1
                      -61.0                          11.2
ZETA POTENTIAL DATA FOR PARTICLE 2:
ZETA POTENTIAL VALUES:      CORESPONDING PH VALUES:
                        8.0                           3.9
                        8.0                           4.0
                        7.8                           4.1
                        7.5                           4.2
                        7.4                           4.3
                        7.0                           4.4
                        6.8                           4.6
                        6.6                           4.7
                        6.4                           4.8
                        6.1                           4.9
                        5.7                           5.0
                        5.5                           5.1
                        5.4                           5.1
                        5.2                           5.2
                        4.8                           5.3
                        4.4                           5.4
                        4.1                           5.5
                        3.8                           5.7
                        3.3                           5.8
                        2.7                           5.9
                        2.1                           6.1
                        1.5                           6.2
                         .8                           6.3
                         .2                           6.4
                        -.7                           6.6
```

-1.5	6.7
-2.3	6.8
-2.9	6.9
-3.5	7.0
-4.0	7.2
-4.4	7.3
-4.8	7.5
-5.2	7.8
-5.3	8.0
-5.5	8.2
-5.7	8.4
-5.9	8.6
-6.0	8.7
-6.2	8.8
-6.2	8.9
-6.5	8.9
-6.5	9.0
-6.7	9.1
-6.9	9.2
-7.0	9.3
-7.1	9.4
-7.1	9.5
-7.3	9.6
-7.5	9.7
-7.5	9.8
-7.7	9.9
-7.7	9.9
-8.0	10.1
-8.0	10.2
-8.1	10.3
-8.5	10.4
-8.6	10.5
-8.9	10.6
-8.9	10.7
-9.4	10.8
-9.6	10.9
-9.7	11.0
-10.0	11.1

```
CALCULATED OVERALL STABILITY RATIO DATA:
 OVERALL STABILITY RATIO:                          CORESPONDING PH
 (W11,W12,W22,WT)                                      VALUES:
.2269E+00,     .2738E+00,     .5009E+00,     .5003E+00       4.00
.2269E+00,     .2738E+00,     .5004E+00,     .4998E+00       4.50
.5914E+21,     .2738E+00,     .5000E+00,     .4994E+00       5.00
.7792+134,     .2738E+00,     .4997E+00,     .4991E+00       5.50
.1725+236,     .2738E+00,     .4994E+00,     .4988E+00       6.00
.4761+303,     .2738E+00,     .4993E+00,     .4987E+00       6.50
.4761+303,     .2738E+00,     .4996E+00,     .4989E+00       7.00
.4761+303,     .2738E+00,     .4998E+00,     .4992E+00       7.50
.4761+303,     .2738E+00,     .4999E+00,     .4993E+00       8.00
.4761+303,     .2738E+00,     .5000E+00,     .4994E+00       8.50
.4761+303,     .2738E+00,     .5003E+00,     .4996E+00       9.00
.4761+303,     .2738E+00,     .5005E+00,     .4999E+00       9.50
.4761+303,     .2738E+00,     .5009E+00,     .5002E+00      10.00
.4761+303,     .2738E+00,     .5014E+00,     .5008E+00      10.50
.4761+303,     .2738E+00,     .5027E+00,     .5020E+00      11.00
```

```
FILE NAME:SS213CC\BSS213CC
FILE DESCRIPTION: RUN USING BMTHFWVB.EXE.
THIS DATA WAS AQUIRED ON: 07/08/1992
AQUISITION BY THE PROGRAM STARTED AT... 11:04:37:77
                      AND FINISHED AT... 11:51:44:57
VOLUME FRACTION OF COMPONENT 1 IN SYSTEM =.500
CONCENTRATION OF 1-1 ELECTROLYTE IN SYSTEM =  .00100
ATOMIC PARTICLE RADIUS OF COMPONENT 1 =  2750.0
ATOMIC PARTICLE RADIUS OF COMPONENT 2 =   250.0
TEMPERATURE OF SYSTEM (IN DEG. C.) = 25.0
HAMAKER CONSTANT OF MEDIUM =    .45E-19
HAMAKER CONSTANT OF COMPONENT 1 =    .30E-18
HAMAKER CONSTANT OF COMPONENT 2 =    .16E-18
ZETA POTENTIAL DATA WAS USED FOR CALCULATIONS.
ZETA POTENTIAL DATA FOR PARTICLE 1:
ZETA POTENTIAL VALUES:        CORESPONDING PH VALUES:
                        5.8                           2.0
                       -2.2                           2.5
                      -15.0                           3.0
                      -26.0                           3.5
                      -34.0                           4.0
                      -40.0                           4.5
                      -44.0                           5.0
                      -48.0                           5.5
                      -51.0                           6.0
                      -53.0                           6.5
                      -54.0                           7.0
                      -56.0                           7.5
                      -57.0                           8.0
                      -58.0                           8.5
                      -59.0                           9.0
                      -60.0                           9.5
                      -60.0                          10.0
                      -61.0                          10.5
                      -61.0                          11.0
ZETA POTENTIAL DATA FOR PARTICLE 2:
ZETA POTENTIAL VALUES:        CORESPONDING PH VALUES:
                       44.0                           2.9
                       38.9                           4.0
                       29.4                           5.0
                        9.1                           6.1
                      -24.0                           7.1
                      -33.0                           8.0
                      -43.0                           9.0
                      -43.0                          10.0
                      -45.0                          11.0
```

```
CALCULATED OVERALL STABILITY RATIO DATA:
 OVERALL STABILITY RATIO:                          CORESPONDING PH
 (W11,W12,W22,WT)                                        VALUES:
.4761+303,    .2738E+00,    .4336+302,    .1825E+03      4.00
.4761+303,    .2738E+00,    .4336+302,    .1825E+03      4.50
.4761+303,    .2738E+00,    .4336+302,    .1825E+03      5.00
.4761+303,    .2738E+00,    .7502+144,    .1825E+03      5.50
.4761+303,    .2738E+00,    .6674E+00,    .6660E+00      6.00
.4761+303,    .2738E+00,    .4998E+00,    .4992E+00      6.50
.4761+303,    .9751E-07,    .5189+181,    .6499E-04      7.00
.4761+303,    .2597+303,    .4336+302,    .4341+302      7.50
.4761+303,    .2597+303,    .4336+302,    .4341+302      8.00
.4761+303,    .2597+303,    .4336+302,    .4341+302      8.50
.4761+303,    .2597+303,    .4336+302,    .4341+302      9.00
.4761+303,    .2597+303,    .4336+302,    .4341+302      9.50
.4761+303,    .2597+303,    .4336+302,    .4341+302     10.00
.4761+303,    .2597+303,    .4336+302,    .4341+302     10.50
.4761+303,    .2597+303,    .4336+302,    .4341+302     11.00
```

```
FILE NAME:SS223SD\BSS223SD
FILE DESCRIPTION: RUN USING BNHTFWVB.EXE.
THIS DATA WAS AQUIRED ON: 07/08/1992
AQUISITION BY THE PROGRAM STARTED AT... 01:17:28:56
                     AND FINISHED AT... 01:48:04:33
VOLUME FRACTION OF COMPONENT 1 IN SYSTEM =.500
CONCENTRATION OF 1-1 ELECTROLYTE IN SYSTEM =  .00100
ATOMIC PARTICLE RADIUS OF COMPONENT 1 =   900.0
ATOMIC PARTICLE RADIUS OF COMPONENT 2 =   250.0
TEMPERATURE OF SYSTEM (IN DEG. C.) = 25.0
HAMAKER CONSTANT OF MEDIUM =    .45E-19
HAMAKER CONSTANT OF COMPONENT 1 =    .30E-18
HAMAKER CONSTANT OF COMPONENT 2 =    .16E-18
ZETA POTENTIAL DATA WAS USED FOR CALCULATIONS.
ZETA POTENTIAL DATA FOR PARTICLE 1:
ZETA POTENTIAL VALUES:        CORESPONDING PH VALUES:
                        5.8                           2.0
                       -2.2                           2.5
                      -15.0                           3.0
                      -26.0                           3.5
                      -34.0                           4.0
                      -40.0                           4.5
                      -44.0                           5.0
                      -48.0                           5.5
                      -51.0                           6.0
                      -53.0                           6.5
                      -54.0                           7.0
                      -56.0                           7.5
                      -57.0                           8.0
                      -58.0                           8.5
                      -59.0                           9.0
                      -60.0                           9.5
                      -60.0                          10.0
                      -61.0                          10.5
                      -61.0                          11.0
ZETA POTENTIAL DATA FOR PARTICLE 2:
ZETA POTENTIAL VALUES:        CORESPONDING PH VALUES:
                       44.0                           2.9
                       38.9                           4.0
                       29.4                           5.0
                        9.1                           6.1
                      -24.0                           7.1
                      -33.0                           8.0
                      -43.0                           9.0
                      -43.0                          10.0
                      -45.0                          11.0
```

```
CALCULATED OVERALL STABILITY RATIO DATA:
 OVERALL STABILITY RATIO:                            CORESPONDING PH
 (W11,W12,W22,WT)                                         VALUES:
.1185E+85,     .2926E+00,     .1105E+77,     .7121E+01       4.00
.1126+168,     .2926E+00,     .1257E+55,     .7121E+01       4.50
.7627+235,     .2926E+00,     .4842E+36,     .7121E+01       5.00
.1559+303,     .2926E+00,     .9557E+09,     .7121E+01       5.50
.1559+303,     .2926E+00,     .5053E+00,     .4909E+00       6.00
.1559+303,     .2926E+00,     .4998E+00,     .4859E+00       6.50
.1559+303,     .1057E+12,     .4468E+13,     .1658E+13       7.00
.1559+303,     .1524E+39,     .4563E+31,     .4760E+31       7.50
.1559+303,     .4540E+63,     .7460E+49,     .7783E+49       8.00
.1559+303,     .9818E+91,     .6029E+72,     .6290E+72       8.50
.1559+303,     .7745+122,     .6955E+99,     .7257E+99       9.00
.1559+303,     .4593+127,     .3959+101,     .4131+101       9.50
.1559+303,     .4593+127,     .3959+101,     .4131+101      10.00
.1559+303,     .7530+136,     .4755+107,     .4961+107      10.50
.1559+303,     .1342+143,     .8488+113,     .8855+113      11.00
```

```
FILE NAME:SS223ES\BSS223es
FILE DESCRIPTION: RUN USING BNHTFWVB.EXE.
THIS DATA WAS AQUIRED ON: 07/08/1992
AQUISITION BY THE PROGRAM STARTED AT... 16:38:17:89
                     AND FINISHED AT... 18:02:57:18
OVERALL PROPORTION OF COMPONENT 1 IN SYSTEM =.500
CONCENTRATION OF 1-1 ELECTROLYTE IN SYSTEM =  .00100
ATOMIC PARTICLE RADIUS OF COMPONENT 1 =   900.0
ATOMIC PARTICLE RADIUS OF COMPONENT 2 =   250.0
TEMPERATURE OF SYSTEM (IN DEG. C.) = 25.0
HAMAKER CONSTANT OF MEDIUM =    .45E-19
HAMAKER CONSTANT OF COMPONENT 1 =    .30E-18
HAMAKER CONSTANT OF COMPONENT 2 =    .16E-18
ZETA POTENTIAL DATA WAS USED FOR CALCULATIONS.
ZETA POTENTIAL DATA FOR PARTICLE 1:
ZETA POTENTIAL VALUES:        CORESPONDING PH VALUES:
                      -10.0                         4.0
                      -11.0                         4.1
                      -12.0                         4.2
                      -13.0                         4.3
                      -14.0                         4.4
                      -15.0                         4.5
                      -16.0                         4.6
                      -17.0                         4.7
                      -18.0                         4.8
                      -19.0                         4.8
                      -20.0                         5.0
                      -21.0                         5.0
                      -22.0                         5.1
                      -22.0                         5.3
                      -23.0                         5.3
                      -24.0                         5.4
                      -25.0                         5.5
                      -25.0                         5.6
                      -27.0                         5.7
                      -29.0                         5.8
                      -30.0                         6.0
                      -31.0                         6.1
                      -32.0                         6.2
                      -33.0                         6.3
                      -35.0                         6.4
                      -36.0                         6.5
                      -36.0                         6.6
                      -37.0                         6.7
                      -38.0                         6.9
                      -39.0                         7.0
                      -39.0                         7.1
                      -40.0                         7.2
                      -41.0                         7.3
                      -42.0                         7.4
                      -43.0                         7.5
                      -43.0                         7.6
```

```
                -44.0                            7.7
                -45.0                            7.8
                -47.0                            7.9
                -48.0                            8.0
                -49.0                            8.1
                -49.0                            8.2
                -51.0                            8.3
                -50.0                            8.4
                -51.0                            8.4
                -52.0                            8.5
                -53.0                            8.6
                -53.0                            8.7
                -55.0                            8.8
                -54.0                            8.8
                -55.0                            8.9
                -55.0                            8.9
                -55.0                            9.1
                -56.0                            9.1
                -57.0                            9.3
                -57.0                            9.3
                -57.0                            9.5
                -59.0                            9.6
                -59.0                            9.6
                -59.0                            9.8
                -61.0                           10.0
                -61.0                           10.1
                -62.0                           10.2
                -63.0                           10.3
                -63.0                           10.4
                -64.0                           10.6
                -65.0                           10.7
                -68.0                           10.8
                -70.0                           11.1
                -70.0                           11.1
ZETA POTENTIAL DATA FOR PARTICLE 2:
ZETA POTENTIAL VALUES:       CORESPONDING PH VALUES:
                  8.0                            3.9
                  8.0                            4.0
                  7.8                            4.1
                  7.5                            4.2
                  7.4                            4.3
                  7.0                            4.4
                  6.8                            4.6
                  6.6                            4.7
                  6.4                            4.8
                  6.1                            4.9
                  5.7                            5.0
                  5.5                            5.1
                  5.4                            5.1
                  5.2                            5.2
                  4.8                            5.3
                  4.4                            5.4
```

4.1	5.5
3.8	5.7
3.3	5.8
2.7	5.9
2.1	6.1
1.5	6.2
.8	6.3
.2	6.4
-.7	6.6
-1.5	6.7
-2.3	6.8
-2.9	6.9
-3.5	7.0
-4.0	7.2
-4.4	7.3
-4.8	7.5
-5.2	7.8
-5.3	8.0
-5.5	8.2
-5.7	8.4
-5.9	8.6
-6.0	8.7
-6.2	8.8
-6.2	8.9
-6.5	8.9
-6.5	9.0
-6.7	9.1
-6.9	9.2
-7.0	9.3
-7.1	9.4
-7.1	9.5
-7.3	9.6
-7.5	9.7
-7.5	9.8
-7.7	9.9
-7.7	9.9
-8.0	10.1
-8.0	10.2
-8.1	10.3
-8.5	10.4
-8.6	10.5
-8.9	10.6
-8.9	10.7
-9.4	10.8
-9.6	10.9
-9.7	11.0
-10.0	11.1

```
CALCULATED OVERALL STABILITY RATIO DATA:
 OVERALL STABILITY RATIO:                       CORESPONDING PH
(W11,W12,W22,WT)                                         VALUES:
.2285E+00,     .2926E+00,     .5009E+00,     .4865E+00    4.00
.2285E+00,     .2926E+00,     .5004E+00,     .4860E+00    4.50
.2285E+00,     .2926E+00,     .5000E+00,     .4856E+00    5.00
.1357E+02,     .2926E+00,     .4997E+00,     .4858E+00    5.50
.1510E+46,     .2926E+00,     .4994E+00,     .4856E+00    6.00
.8030+108,     .2926E+00,     .4993E+00,     .4855E+00    6.50
.4518+152,     .2926E+00,     .4996E+00,     .4857E+00    7.00
.3056+214,     .2926E+00,     .4998E+00,     .4859E+00    7.50
.1559+303,     .2926E+00,     .4999E+00,     .4860E+00    8.00
.1559+303,     .2926E+00,     .5000E+00,     .4861E+00    8.50
.1559+303,     .2926E+00,     .5003E+00,     .4863E+00    9.00
.1559+303,     .2926E+00,     .5005E+00,     .4865E+00    9.50
.1559+303,     .2926E+00,     .5009E+00,     .4868E+00   10.00
.1559+303,     .2926E+00,     .5014E+00,     .4873E+00   10.50
.1559+303,     .2926E+00,     .5027E+00,     .4885E+00   11.00
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FILE NAME:SS223CC\BSS2223CC
FILE DESCRIPTION: RUN USING BNHTFWVB.EXE.
THIS DATA WAS AQUIRED ON: 07/08/1992
AQUISITION BY THE PROGRAM STARTED AT... 11:51:46:16
                     AND FINISHED AT... 12:22:28:47
VOLUME FRACTION OF COMPONENT 1 IN SYSTEM =.500
CONCENTRATION OF 1-1 ELECTROLYTE IN SYSTEM =   .00100
ATOMIC PARTICLE RADIUS OF COMPONENT 1 =    900.0
ATOMIC PARTICLE RADIUS OF COMPONENT 2 =    250.0
TEMPERATURE OF SYSTEM (IN DEG. C.) = 25.0
HAMAKER CONSTANT OF MEDIUM =     .45E-19
HAMAKER CONSTANT OF COMPONENT 1 =    .30E-18
HAMAKER CONSTANT OF COMPONENT 2 =    .16E-18
ZETA POTENTIAL DATA WAS USED FOR CALCULATIONS.
ZETA POTENTIAL DATA FOR PARTICLE 1:
ZETA POTENTIAL VALUES:        CORESPONDING PH VALUES:
                        5.8                             2.0
                       -2.2                             2.5
                      -15.0                             3.0
                      -26.0                             3.5
                      -34.0                             4.0
                      -40.0                             4.5
                      -44.0                             5.0
                      -48.0                             5.5
                      -51.0                             6.0
                      -53.0                             6.5
                      -54.0                             7.0
                      -56.0                             7.5
                      -57.0                             8.0
                      -58.0                             8.5
                      -59.0                             9.0
                      -60.0                             9.5
                      -60.0                            10.0
                      -61.0                            10.5
                      -61.0                            11.0
ZETA POTENTIAL DATA FOR PARTICLE 2:
ZETA POTENTIAL VALUES:        CORESPONDING PH VALUES:
                       44.0                             2.9
                       38.9                             4.0
                       29.4                             5.0
                        9.1                             6.1
                      -24.0                             7.1
                      -33.0                             8.0
                      -43.0                             9.0
                      -43.0                            10.0
                      -45.0                            11.0
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CALCULATED OVERALL STABILITY RATIO DATA:
 OVERALL STABILITY RATIO:                              CORESPONDING PH
 (W11,W12,W22,WT)                                             VALUES:
.1559+303,     .2926E+00,     .4336+302,     .7121E+01       4.00
.1559+303,     .2926E+00,     .4336+302,     .7121E+01       4.50
.1559+303,     .2926E+00,     .4336+302,     .7121E+01       5.00
.1559+303,     .2926E+00,     .7502+144,     .7121E+01       5.50
.1559+303,     .2926E+00,     .6674E+00,     .6343E+00       6.00
.1559+303,     .2450+161,     .4998E+00,     .5215E+00       6.50
.1559+303,     .9961+302,     .5189+181,     .5414+181       7.00
.1559+303,     .9961+302,     .4336+302,     .4440+302       7.50
.1559+303,     .9961+302,     .4336+302,     .4440+302       8.00
.1559+303,     .9961+302,     .4336+302,     .4440+302       8.50
.1559+303,     .9961+302,     .4336+302,     .4440+302       9.00
.1559+303,     .9961+302,     .4336+302,     .4440+302       9.50
.1559+303,     .9961+302,     .4336+302,     .4440+302      10.00
.1559+303,     .9961+302,     .4336+302,     .4440+302      10.50
.1559+303,     .9961+302,     .4336+302,     .4440+302      11.00
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FILE NAME:SS233SD\BSS233SD
FILE DESCRIPTION: RUN USING BMTHFWVB.EXE.
     THIS DATA WAS AQUIRED ON: 07/08/1992
AQUISITION BY THE PROGRAM STARTED AT... 01:48:06:04
                     AND FINISHED AT... 02:12:19:64
VOLUME FRACTION OF COMPONENT 1 IN SYSTEM =.500
CONCENTRATION OF 1-1 ELECTROLYTE IN SYSTEM =  .00100
ATOMIC PARTICLE RADIUS OF COMPONENT 1 =   400.0
ATOMIC PARTICLE RADIUS OF COMPONENT 2 =   250.0
TEMPERATURE OF SYSTEM (IN DEG. C.) = 25.0
HAMAKER CONSTANT OF MEDIUM =    .45E-19
HAMAKER CONSTANT OF COMPONENT 1 =    .30E-18
HAMAKER CONSTANT OF COMPONENT 2 =    .16E-18
ZETA POTENTIAL DATA WAS USED FOR CALCULATIONS.
ZETA POTENTIAL DATA FOR PARTICLE 1:
ZETA POTENTIAL VALUES:        CORESPONDING PH VALUES:
                        5.8                            2.0
                       -2.2                            2.5
                      -15.0                            3.0
                      -26.0                            3.5
                      -34.0                            4.0
                      -40.0                            4.5
                      -44.0                            5.0
                      -48.0                            5.5
                      -51.0                            6.0
                      -53.0                            6.5
                      -54.0                            7.0
                      -56.0                            7.5
                      -57.0                            8.0
                      -58.0                            8.5
                      -59.0                            9.0
                      -60.0                            9.5
                      -60.0                           10.0
                      -61.0                           10.5
                      -61.0                           11.0
ZETA POTENTIAL DATA FOR PARTICLE 2:
ZETA POTENTIAL VALUES:        CORESPONDING PH VALUES:
                       44.0                            2.9
                       38.9                            4.0
                       29.4                            5.0
                        9.1                            6.1
                      -24.0                            7.1
                      -33.0                            8.0
                      -43.0                            9.0
                      -43.0                           10.0
                      -45.0                           11.0
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CALCULATED OVERALL STABILITY RATIO DATA:
 OVERALL STABILITY RATIO:                          CORESPONDING PH
 (W11,W12,W22,WT)                                         VALUES:
.1765E+40,     .3193E+00,     .1105E+77,     .1012E+01       4.00
.1920E+77,     .3193E+00,     .1257E+55,     .1012E+01       4.50
.3301+107,     .3193E+00,     .4842E+36,     .1012E+01       5.00
.1497+142,     .3193E+00,     .9557E+09,     .1012E+01       5.50
.1161+171,     .3193E+00,     .5053E+00,     .4412E+00       6.00
.5052+191,     .3194E+00,     .4998E+00,     .4385E+00       6.50
.2729+202,     .1514E+29,     .4468E+13,     .6917E+13       7.00
.5347+224,     .7590E+55,     .4563E+31,     .7062E+31       7.50
.1938+236,     .1654E+79,     .7460E+49,     .1155E+50       8.00
.1324+248,     .4834+105,     .6029E+72,     .9332E+72       8.50
.1707+260,     .1116+134,     .6955E+99,     .1077+100       9.00
.4147+272,     .1254+138,     .3959+101,     .6128+101       9.50
.4147+272,     .1254+138,     .3959+101,     .6128+101      10.00
.1900+285,     .1611+146,     .4755+107,     .7360+107      10.50
.1900+285,     .8486+151,     .8488+113,     .1314+114      11.00
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FILE NAME:SS233ES\BSS233ES
FILE DESCRIPTION: RUN USING BMTHFWVB.EXE.
THIS DATA WAS AQUIRED ON: 07/08/1992
AQUISITION BY THE PROGRAM STARTED AT... 09:27:50:39
                     AND FINISHED AT... 11:04:35:90
VOLUME FRACTION OF COMPONENT 1 IN SYSTEM =.500
CONCENTRATION OF 1-1 ELECTROLYTE IN SYSTEM =  .00100
ATOMIC PARTICLE RADIUS OF COMPONENT 1 =   400.0
ATOMIC PARTICLE RADIUS OF COMPONENT 2 =   250.0
TEMPERATURE OF SYSTEM (IN DEG. C.) = 25.0
HAMAKER CONSTANT OF MEDIUM =    .45E-19
HAMAKER CONSTANT OF COMPONENT 1 =    .30E-18
HAMAKER CONSTANT OF COMPONENT 2 =    .16E-18
ZETA POTENTIAL DATA WAS USED FOR CALCULATIONS.
ZETA POTENTIAL DATA FOR PARTICLE 1:
ZETA POTENTIAL VALUES:        CORESPONDING PH VALUES:
                       -2.2                           4.0
                       -2.6                           4.1
                       -2.9                           4.2
                       -3.2                           4.3
                       -3.6                           4.4
                       -3.9                           4.5
                       -4.5                           4.6
                       -4.7                           4.7
                       -5.0                           4.8
                       -5.3                           4.9
                       -5.5                           5.0
                       -6.0                           5.1
                       -6.3                           5.2
                       -6.4                           5.2
                       -6.6                           5.3
                       -6.9                           5.4
                       -7.2                           5.5
                       -7.3                           5.6
                       -7.4                           5.6
                       -7.7                           5.7
                       -8.0                           5.8
                       -8.1                           5.8
                       -8.2                           5.9
                       -8.6                           6.0
                       -8.8                           6.1
                       -8.9                           6.1
                       -9.1                           6.2
                       -9.3                           6.3
                       -9.5                           6.3
                       -9.8                           6.4
                      -10.0                           6.5
                      -10.0                           6.6
                      -10.0                           6.7
                      -11.0                           6.8
                      -11.0                           6.8
                      -11.0                           6.9
```

-11.0	7.0
-12.0	7.1
-12.0	7.2
-12.0	7.2
-12.0	7.3
-13.0	7.4
-13.0	7.4
-13.0	7.5
-13.0	7.6
-14.0	7.6
-14.0	7.7
-14.0	7.8
-14.0	7.8
-15.0	7.9
-15.0	8.0
-15.0	8.0
-15.0	8.1
-15.0	8.1
-15.0	8.2
-15.0	8.3
-16.0	8.3
-16.0	8.4
-16.0	8.5
-16.0	8.6
-16.0	8.7
-17.0	8.8
-17.0	8.9
-17.0	9.0
-17.0	9.1
-17.0	9.2
-17.0	8.3
-17.0	9.4
-18.0	9.5
-18.0	9.6
-18.0	9.7
-18.0	9.9
-18.0	9.9
-19.0	10.0
-19.0	10.1
-19.0	10.2
-19.0	10.4
-20.0	10.5
-20.0	10.6
-21.0	10.7
-21.0	10.9
-21.0	11.0
-21.0	11.1

ZETA POTENTIAL DATA FOR PARTICLE 2:

ZETA POTENTIAL VALUES:	CORESPONDING PH VALUES:
8.0	3.9
8.0	4.0
7.8	4.1
7.5	4.2
7.4	4.3
7.0	4.4
6.8	4.6
6.6	4.7
6.4	4.8
6.1	4.9
5.7	5.0
5.5	5.1
5.4	5.1
5.2	5.2
4.8	5.3
4.4	5.4
4.1	5.5
3.8	5.7
3.3	5.8
2.7	5.9
2.1	6.1
1.5	6.2
.8	6.3
.2	6.4
-.7	6.6
-1.5	6.7
-2.3	6.8
-2.9	6.9
-3.5	7.0
-4.0	7.2
-4.4	7.3
-4.8	7.5
-5.2	7.8
-5.3	8.0
-5.5	8.2
-5.7	8.4
-5.9	8.6
-6.0	8.7
-6.2	8.8
-6.2	8.9
-6.5	8.9
-6.5	9.0
-6.7	9.1
-6.9	9.2
-7.0	9.3
-7.1	9.4
-7.1	9.5
-7.3	9.6
-7.5	9.7
-7.5	9.8

-7.7	9.9
-7.7	9.9
-8.0	10.1
-8.0	10.2
-8.1	10.3
-8.5	10.4
-8.6	10.5
-8.9	10.6
-8.9	10.7
-9.4	10.8
-9.6	10.9
-9.7	11.0
-10.0	11.1

```
CALCULATED OVERALL STABILITY RATIO DATA:
 OVERALL STABILITY RATIO:                          CORESPONDING PH
 (W11,W12,W22,WT)                                        VALUES:
.2293E+00,     .3193E+00,     .5009E+00,     .4089E+00     4.00
.2293E+00,     .3193E+00,     .5004E+00,     .4087E+00     4.50
.2293E+00,     .3193E+00,     .5000E+00,     .4085E+00     5.00
.2293E+00,     .3193E+00,     .4997E+00,     .4084E+00     5.50
.2293E+00,     .3193E+00,     .4994E+00,     .4083E+00     6.00
.2293E+00,     .3193E+00,     .4993E+00,     .4082E+00     6.50
.2293E+00,     .3193E+00,     .4996E+00,     .4083E+00     7.00
.2293E+00,     .3193E+00,     .4998E+00,     .4084E+00     7.50
.2293E+00,     .3193E+00,     .4999E+00,     .4085E+00     8.00
.2293E+00,     .3193E+00,     .5000E+00,     .4085E+00     8.50
.2293E+00,     .3193E+00,     .5003E+00,     .4086E+00     9.00
.2293E+00,     .3193E+00,     .5005E+00,     .4088E+00     9.50
.2293E+00,     .3193E+00,     .5009E+00,     .4089E+00    10.00
.2293E+00,     .3193E+00,     .5014E+00,     .4091E+00    10.50
.2293E+00,     .3193E+00,     .5027E+00,     .4097E+00    11.00
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FILE NAME:SS233CC\BSS233CC
FILE DESCRIPTION: RUN USING BMTHFWVB.EXE.
THIS DATA WAS AQUIRED ON: 07/08/1992
AQUISITION BY THE PROGRAM STARTED AT... 12:22:30:01
                     AND FINISHED AT... 12:49:50:91
VOLUME FRACTION OF COMPONENT 1 IN SYSTEM =.500
CONCENTRATION OF 1-1 ELECTROLYTE IN SYSTEM =  .00100
ATOMIC PARTICLE RADIUS OF COMPONENT 1 =   400.0
ATOMIC PARTICLE RADIUS OF COMPONENT 2 =   250.0
TEMPERATURE OF SYSTEM (IN DEG. C.) = 25.0
HAMAKER CONSTANT OF MEDIUM =    .45E-19
HAMAKER CONSTANT OF COMPONENT 1 =    .30E-18
HAMAKER CONSTANT OF COMPONENT 2 =    .16E-18
ZETA POTENTIAL DATA WAS USED FOR CALCULATIONS.
ZETA POTENTIAL DATA FOR PARTICLE 1:
ZETA POTENTIAL VALUES:        CORESPONDING PH VALUES:
                        5.8                           2.0
                       -2.2                           2.5
                      -15.0                           3.0
                      -26.0                           3.5
                      -34.0                           4.0
                      -40.0                           4.5
                      -44.0                           5.0
                      -48.0                           5.5
                      -51.0                           6.0
                      -53.0                           6.5
                      -54.0                           7.0
                      -56.0                           7.5
                      -57.0                           8.0
                      -58.0                           8.5
                      -59.0                           9.0
                      -60.0                           9.5
                      -60.0                          10.0
                      -61.0                          10.5
                      -61.0                          11.0
ZETA POTENTIAL DATA FOR PARTICLE 2:
ZETA POTENTIAL VALUES:        CORESPONDING PH VALUES:
                       44.0                           2.9
                       38.9                           4.0
                       29.4                           5.0
                        9.1                           6.1
                      -24.0                           7.1
                      -33.0                           8.0
                      -43.0                           9.0
                      -43.0                          10.0
                      -45.0                          11.0
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CALCULATED OVERALL STABILITY RATIO DATA:
 OVERALL STABILITY RATIO:                          CORESPONDING PH
 (W11,W12,W22,WT)                                         VALUES:
.6932+302,    .3193E+00,    .4336+302,    .1012E+01      4.00
.6932+302,    .3193E+00,    .4336+302,    .1012E+01      4.50
.6932+302,    .3193E+00,    .4336+302,    .1012E+01      5.00
.6932+302,    .3193E+00,    .7502+144,    .1012E+01      5.50
.6932+302,    .3193E+00,    .6674E+00,    .5113E+00      6.00
.6932+302,    .2417+283,    .4998E+00,    .7737E+00      6.50
.6932+302,    .5634+302,    .5189+181,    .8032+181      7.00
.6932+302,    .5634+302,    .4336+302,    .4750+302      7.50
.6932+302,    .5634+302,    .4336+302,    .4750+302      8.00
.6932+302,    .5634+302,    .4336+302,    .4750+302      8.50
.6932+302,    .5634+302,    .4336+302,    .4750+302      9.00
.6932+302,    .5634+302,    .4336+302,    .4750+302      9.50
.6932+302,    .5634+302,    .4336+302,    .4750+302     10.00
.6932+302,    .5634+302,    .4336+302,    .4750+302     10.50
.6932+302,    .5634+302,    .4336+302,    .4750+302     11.00
```

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