

CONDENSATION OF METALLIC VAPOUR IN FREE TURBULENT JETS

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Abstract—The method of computation of metal vapour condensation admixed to a free heated jet issued into cold stagnant gaseous medium is described. The method is based on numerical integration of a system of differential equations describing the time dependences of concentrations of molecular aggregates and of particles of different sizes together with the equation for the kinetics of turbulent mixing. The free energy of small molecular aggregate formation is expressed in terms of parameters of intermolecular forces. The influence of the Van der Waals forces on the coagulation rate is also accounted for. It is shown that the total particle concentration must be decreasing with time according to the law $t^{-6/5}$. The shape of the asymptotic self-preserving size distribution is determined for the free-molecule coagulation with account for the influence of the Van der Waals interactions. The results of the computation expressed in terms of the specific surface area S of the condensed particles are compared with previously obtained experimental results on condensation of silver vapour. The theory predicts reasonable values of S , but the theoretical dependence of S on the initial vapour concentration has a shape which differs slightly from those observed in experiments. The reasons of the disagreement between the theory and experiment are discussed.

NOMENCLATURE

C_1, C_2 , heat capacities of heated and cold gases;
 c_1 , concentration of singlet molecules;
 c_1^0 , initial concentration of singlets;
 c_1' , concentration of singlets at the beginning of integration step;
 c_g , concentration of clusters of g molecules (g -clusters);
 $c^0(g)$, equilibrium concentration of g -clusters;
 C^* , total particle concentration;
 d , nozzle diameter;
 \bar{g} , mean particle mass;
 h , the Boltzmann constant;
 $K(j, k)$, rate constant for collisions between clusters of j and k molecules, respectively;
 m , mass of vapour molecules;
 M , the factor for the influence of the Van der Waals forces on coagulation;
 M_1, M_2 , molecular weights of heated and cold gases;
 Q_g , partition function of g -cluster;
 R , radial distance from the jet pole;
 S , specific surface of the particle deposit;
 T , absolute temperature;
 t , time;
 u , time-averaged gas velocity;
 V , volume;
 w , ratio of mass fraction of heated and cold gas;
 y_n , concentration of particles of 2^n singlets;
 $\alpha(i, j)$, sticking probability (efficiency) for the collision between i -cluster and j -cluster;
 ${}_2\alpha(i, j)$, sticking probability for binary collision;
 ${}_3\alpha(i, j)$, ratio of the number of efficient three-body collisions to the number of binary collisions;
 η, ψ , the Friedlander functions;

λ , rate constant for the concentration change due to cooling and dilution of the vapour-gas mixture;
 μ_g , chemical potential of g -cluster;
 μ_g^0 , standard chemical potential;
 ρ_0 , cluster density;
 ρ , gas density (R, φ);
 ρ_0 , density of heated gas at the nozzle outlet;
 φ , angle between the direction of R and the nozzle exit plane.

Subscripts

g, i, j, k , the molecule number in clusters;
 n , power of two in the number of molecules in particles having concentration y_n .

PROCESS of condensation of metallic vapour which is contained as admixture to a heated noncondensable gas has some distinct features when compared with condensation of vapour of a volatile liquid. The latter can be described by the classical nucleation theory or by its more recent modifications [1-4]. The large supersaturation ratio, the small size of a critical embryo and the rapid change of temperature during condensation of metallic vapours do not permit usage of the steady-state solutions of the conventional nucleation theory for calculation of condensation. The particle coagulation causes further complication, for it overlaps in time the nucleation process as follows from [5]. Computation of disperse phase formation under such conditions therefore requires a special model that would account for the above mentioned consideration.

In this paper condensation of vapours is considered which are admixed to noncondensable gas in a sufficiently small quantity for its phase transition to

have no effect on the properties of a turbulent flow. The case when the critical embryo contains only several molecules can be treated as a "rapid condensation" [6] and characterized by the Zeldovich nonequilibrium factors close to unity, so that concentrations of critical and pre-critical nuclei are almost equal to the equilibrium ones which correspond to the instantaneous environmental conditions. In this case the nucleation rate can be expressed as the product of the equilibrium concentration of the critical embryos and the frequency of their collisions with the vapour molecules and the collision efficiency (sticking probability) $\alpha(g^*)$:

$$\frac{dc(g^*+1)}{dt} = K(1, g^*)\alpha(g^*)c(1)c^0(g^*) - K(1, g^*+1)\alpha(g^*+1)c(1)c(g) \quad (1)$$

where $c(1)$ is the concentration of singlet molecules. Equilibrium cluster concentration $c^0(g)$ can be found from the condition of equality of the cluster chemical potentials μ_g and also of their equality to the chemical potential of g singlet molecules $g\mu_1$. Since μ_g can be expressed as the sum of a "standard potential" related to a definite concentration $\mu_g^0 = kT \ln Q_g$ and of concentration-dependent term $kT \ln c(g)$ where Q_g is the cluster partition function and c_g^0 may be written as follows:

$$c^0(g) = c_g^0 Q_g Q_1^{-g} \quad (2)$$

Hence the time change of concentrations of the pre-critical and supercritical clusters is described by the following set of the first-order differential equations:

$$c(g) = C^0[T(t), c_1(t)], \quad 1 < g \leq g^* \quad (3)$$

$$\frac{dc(g)}{dt} = 1/2 \sum_{j+k=g} K(j, k)\alpha(j, k)c(j)c(k) - c(g) \sum_{i=1}^{\infty} K(i, g)\alpha(i, g)c(i) - \lambda_g c(g), \quad g > g^* \quad (4)$$

where λ is the rate constant of the concentration change due to cooling and dilution of the vapour-gas mixture. The set of the g values corresponding to the sizes of particles formed during the condensation process is enormously large and the number of equations (3) and (4) should be reduced to a reasonable quantity to make calculations possible. Since the main factor in the process under consideration is known to be coagulation, the number of equations in (3) can be diminished in the way described by Rosinski and Snow [5, 7] and based on substitution of the natural set of g values by the set of natural powers of two: 2^n , $n = 0, 2 \dots$. It can be shown that this procedure implies that all particles with masses from $0.75 \times (2^n + 1)$ to 1.5×2^n singlet molecules are replaced by their mass equivalent of particles with masses of 2^n molecules. Originally [7] this method was applied to the description of completely irreversible condensation, i.e. with each collision even between singlet molecules leading to their combination. In a general case the early stages of molecule agglomeration are reversible and the concentrations of small clusters never exceed the

equilibrium values. Moreover, the sticking probability is not equal to unity in the general case and must depend on the size of colliding particles and on the energy of their relative motion. In such circumstances natural set of g may be preferable for the initial interval of the g axis a set of 2^n values for larger sizes of particles. That is, we write twenty-four equations for the concentration of clusters of 1–24 molecules and eighteen equations for the concentrations of particles containing from $2^{5-2^{23}}$ singlet molecules.

In accordance with the spirit of the Rosinski-Snow approximation we accept that the collisions $g+2^n$ ($g > 0.75 \times 2^n$) lead to formation of particles with 2^{n+1} molecules and the number of these new particles is equal to $(g+2^n)/2^{n+1}$ of the number of such collisions. Furthermore, collisions $g+2^n$ ($g \leq 0.75 \times 2^n$) do not change the size of particles consisting of 2^n molecules but instead increase their number by the factor $(g+2^n)/2^{n+1}$. With these assumptions the terms

$$-c(g) \sum_{n=5}^{23} K(g, n)y_n \quad (5)$$

appear in equations (4) here y_n are the concentrations of particles with masses of 2^n molecules. Simultaneously the superscripts of the summation sign over i in equations (4) must be replaced by 24. For y_n we have a set of differential equations:

$$\begin{aligned} \frac{dy_n}{dt} = & 0.75 K''(n, n-1)y_n y_{n-1} M(n, n-1) \\ & + K''(n-1, n-1)y_{n-1}^2 M(n-1, n-1) \\ & - y_n \sum_{l \geq n-1} K''(n, l)y_l M(n, l) \\ & + y_n \sum_{g \leq (3/8)2^n} (1+g/2^n)K'(n, g)c(g) \\ & + y_n \sum_{g > (3/8)2^n} (g+2^n)/2^{n+1} K'(n, g)c(g) \\ & - \lambda_g c(g). \quad (6) \end{aligned}$$

The factor M accounts for the influence of the Van der Waals forces on the coagulation rate. Let us specify the forms of the functions K , Q , M , α and λ .

The particles whose size is small in comparison with the free path of gas molecules can be treated as molecules of Lorentzian gas [9]. The rate of collisions between such particles is given by expression of the number of collisions between gas molecules:

$$K(i, j) = (i^{1/3} + j^{1/3})^2 [(i+j)/ij]^{1/2} \times (3/\rho)^{2/3} (m/\pi)^{1/6} (kT)^{1/2}$$

where ρ is cluster density and m is mass of molecule. In the cases of $K''(n, g)$ and $K'(n, m)$ the expression in the square brackets must be replaced by $(2^{n/3} + g^{1/3})^2 \times [(2^n + g)/2^n g]^{1/2}$ and $(2^{n/3} + 2^{m/3})^2 [(1 + 2^{n-m})/2^n]^{1/2}$, respectively. A method of calculation of the partition functions Q for clusters consisting of molecules interacting via the Lennard-Jones potential has been proposed by Reed [10]. Application of the Lennard-Jones potential to clusters of metal atoms is a rather

crude approximation but other method for evaluation of Q [11–13] being much more complicated are nevertheless based on a number of dubious assumptions. As will be clear from the present authors' results, though the features of the initial stage of condensation which are affected by Q have but a slight influence on the final result. We use here Reed's method of partition function evaluation for silver clusters. The force constant values are assumed the same as in [5]. It is concluded [8, 14] that the sticking probability $\alpha(i, j)$ for collisions of particles with masses of i and j singlets to decrease quickly when the sum $i + j$ is less than a certain value, perhaps, less than ten. It can be explained by the fact that formation of a dimer from two singlet molecules proceeds only through the three-body collisions with the participation of the carrier-gas molecules as a third body. The probability for two atoms to form a diatomic cluster after a binary collision is only about 10^{-14} even if the activation energy of the recombination process is equal to zero [15]. In view of large excess of neutral gas over the vapour, the three-body reaction can be treated as a pseudo-bimolecular one: the rate of this reaction can be written as ${}_3\alpha(i, j)K(i, j)c(i)c(j)$ where ${}_3\alpha(i, j)$ is equal to the ratio of the number of efficient three-body collisions to the total number of binary collisions. As follows from theoretical and experimental studies of the three-body recombination rate [16], the reaction cross-section differs only but slightly from the cross-section of three-body collisions, so that ${}_3\alpha$ values cannot depend strongly on $i + j$. Sticking probability in binary collisions ${}_2\alpha(i, j)$ increases rapidly with $i + j$ due to growth of probability of the excess kinetic energy of relative motion of clusters to be dissipated on the internal degrees of freedom. The resultant function $\alpha(i, j) = {}_2\alpha(i, j) + {}_3\alpha(i, j)$ must therefore have a large jump at a certain $i + j$ from the value close to ${}_3\alpha(i, j)$ to the microscopic value of the condensation coefficient.

In the present authors' computations use has been made of three different assumptions about the form of $\alpha(i, j)$. In the largest part of calculations we assume $\alpha(i, j)$ to be large enough to provide the equilibrium concentrations of pre-critical clusters. For one set of initial conditions we also used two other assumptions. In the first of them the process was treated as completely irreversible, i.e. (i, j) was always equal to unity and the possibility of evaporation from clusters was neglected. With the other it was assumed that $\alpha(i, j) = 10^{-3}$, $i, j \leq 9$ and $\alpha(i, j) = 1.0$ for $i + j \geq 10$ (a sticking-controlled process). In this case evaporation was also neglected, so that Q were not computed.

As it has been shown [17] the Van der Waals forces could enhance appreciably the coagulation rate of highly disperse aerosols. Earlier [18] collision integral have been computed for the Lorentz particles interacting via the attractive potential described by Hamaker's formula [19] for a wide range of the Hamaker constant. We fitted these data by the approximate relation for M :

$$M(n, n) = 149^{-0.976} + 1 = M(n, n-1) \quad (7)$$

For particles whose mass differs by a factor larger than two:

$$M(n, 1) = M(n, n) - 0.034|n-1|, \quad |n-1| > 1 \quad (8)$$

where n and 1 are the exponents of two in values of the averaged masses of particles.

In this paper we are concerned with the condensation in the free turbulent axisymmetrical jet. The process of turbulent mixing is assumed to be described in terms of Reichardt's theory. First of all we notice that function λ (see equation (4)) is related with the volume of the vapour-gas mixture by

$$\lambda = -d \ln V/dt. \quad (9)$$

Starting from the Reichardt theory we have obtained [5] the expressions for the distributions of time-averaged concentrations and axial components of velocity in the mixing zone of a free jet:

$$\chi = 5.14(\rho_0/\rho)^{1/2}d(R \sin \varphi)^{-1} \exp(-48 \cotan^2 \varphi) \quad (10)$$

$$u = 1.34 u_0 \exp(-41 \cotan^2 \varphi) \quad (11)$$

where $\chi = (w+1)^{-1}$, w is the ratio of mass fractions of hot and cold components of the gas mixture at the point (R, φ) , u is the time-averaged axial component of the velocity, d is the nozzle diameter, u_0 is the initial velocity of the hot gas, R is the distance from the jet pole, φ is the angle between the direction of R and the plane of the nozzle exit, ρ_0 and ρ are the time-averaged densities of mixture in the nozzle exit and at point (R, φ) , respectively. Assuming the time-averaged motion of the fluid particles in the mixing zone to coincide with radial directions we get the equation describing the kinetics of mixing:

$$\frac{dw(\varphi)}{dt} = \frac{dR}{u(R, \varphi) \sin \varphi} = \frac{0.261 \exp(7 \cotan^2 \varphi)}{(w+1)(d/dt)(w \sqrt{[\rho_0/\rho]})}. \quad (12)$$

Averaging over angle φ gives

$$\frac{d\bar{w}}{dt} = \frac{4}{\rho_0 u_0 \pi d^2} \int_0^{\pi/2} 2 \frac{dw}{dt} \pi \rho \chi u R^2 \tan \varphi d\varphi. \quad (13)$$

λ is determined from the equation of state of ideal gas mixture and from the equation of material balance:

$$\lambda = \left[\frac{(w+1)^3}{T_1 + awT_2} \right] \left[\frac{(aT_1 - T_2)w}{(1-aw)} - \frac{M_1/M_2}{1+(M_1/M_2)w} \right] \quad (14)$$

where $a = M_1 C_2 / M_2 C_1$, M_1 and M_2 are the molecular weights of hot and cold gases, C_1 and C_2 are their heat capacities, respectively.

Our method of computation of the condensation process includes the following stepwise procedure. For the moment $t = 0$ at $w = 0$ the equilibrium concentrations of clusters containing up to 6 molecules are determined from the solution of equations (2). Then the size of critical embryo is found as corresponding to the minimum of concentration $c^0(g)$ vs g . The concentrations of precritical and critical clusters as well as of singlet molecules are calculated from equations (2) together with the equation of material balance:

$$\sum_{g=1}^g gc(g)c_1^0 \quad (15)$$

where c_1^0 is the concentration of singlets corresponding to the beginning of step of integration. Then the values of $c(g)$ obtained from (2) and (15) are used in numerical integration of the right-hand sides of equations (3, 4, 6, 7) in a single step. After that all the operations are repeated again and again.

Computations of condensation of silver vapour admixed to a free jet of hot argon which is issued into cold stagnant air were carried out on electronic computer Minsk-32. Initial concentration of silver molecules were 3.16×10^{14} , 10^{15} , 3.16×10^{15} , 10^{16} and 3.16×10^{16} molecules/cm³. Temperatures of hot argon and stagnant air were 1663°K and 297°K, respectively. Nozzle diameter was 0.08 cm, initial jet velocity was 410 ms⁻¹. All the parameters listed are in accordance with the experimental conditions of paper [5]. Integration of the equations (3), (4), (6), (7) was carried out by the Runge-Kutta procedure with periodically increasing step of integration in time interval 0-0.2 s. The term $(d/dw)(\rho_0/\rho)^{1/2}$ in the denominator of equation (14) was neglected. The mixing process was assumed to be described by equation (14) up to $w = 20$ and then mixing was assumed to cease abruptly and condensation continued at the isothermal conditions.

The time dependence of c_1 and of the concentrations of clusters of different sizes for the case $c_1^0 = 3.16 \times 10^{16}$ are shown in Fig. 1. The monomer concentration is exhausted in very early stages of the process and the further evolution of the size distribution proceeds through coagulation. For the whole range of c_1^0 the dimers become the critical embryos before the slightest exhaustion of monomeric vapour. Time dependence of dimensionless particles concentration which is defined as $C^* = (\sum c(g) + \sum y_n)c_1^{0-1}$ is shown in Fig. 2. The mixing being completed, this dependence approaches asymptotically the form $C^* \sim t^{-6/5}$ which has been predicted by Lai *et al.* [20] for free-molecule

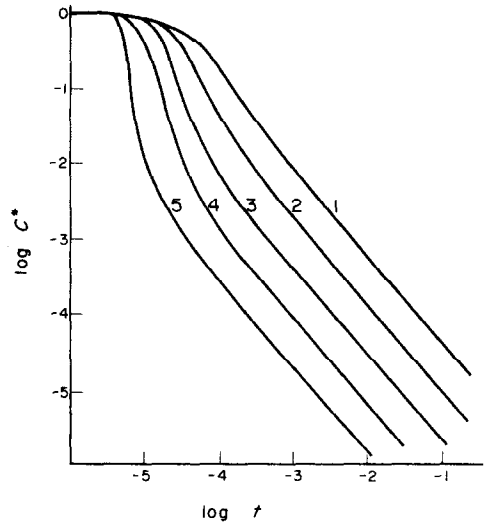


FIG. 2. Time dependence of the total particle concentration. The values of c_1^0 : 1, 3.16×10^{14} ; 2, 10^{15} ; 3, 3.16×10^{15} ; 4, 10^{16} ; 5, 3.16×10^{16} molecules cm⁻³.

coagulation without account for the Van der Waals interactions. Since these forces do not affect homogeneity of the size dependence of coefficients $K(i, j)$, i.e. independent of Van der Waals interactions there exists the relation

$$K(g, g) = g^{1/6}K(1, 1),$$

the appearance of the $t^{-6/5}$ law is not surprising. As far as the $t^{-6/5}$ law is approached, the so-called self-preserving size distribution is established the shape of which in Friedlander's plot [21] $\psi = f(\eta)$ does not depend on time. Here ψ and η are

$$\psi = c_g \sum g c_g / (\sum c_g)^2, \quad \eta = g \sum c_g / \sum g c_g.$$

The shape of our $\psi(\eta)$ distribution which is shown in Fig. 3 differs somewhat from that of Lai [20] due to account made for the Van der Waals forces. The latter accelerate the coagulation of particles with near-equal size in much more pronounced manner than the coagulation of particles which greatly differ in size. Contrary to the results of Lai 29 our size distribution can be fitted with log-normal function only as a crude

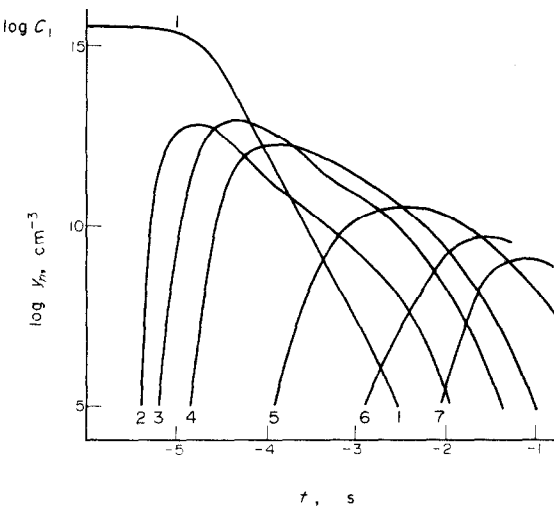


FIG. 1. Time dependence of particle concentrations. The masses of particles in mass of a singlet molecule: 1, 1; 2, 8; 3, 16; 4, 64; 5, 256; 6, 1024; 7, 4096; 8, 8192; 9, 32768; 10, 131068.

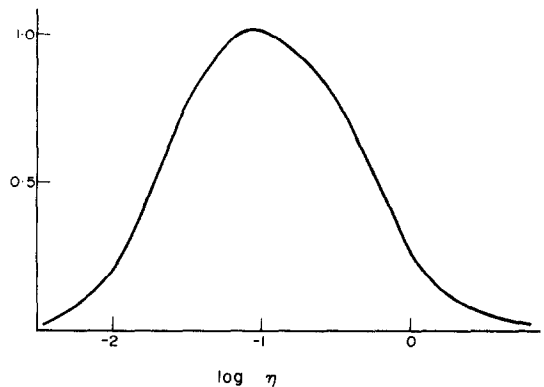


FIG. 3. Self-preserving size distribution.

approximation. In our case with reversible character of early stages of the molecules agglomeration the establishing of the self-preserving distribution takes place at much larger mean particle sizes than in the case of completely irreversible processes. From Fig. 3 it also follows that computations for three different models, namely, instantly equilibrium condensation, completely irreversible condensation and sticking-controllable process, differ from each other only at early stages of the process. Then all the three curves $C^*(t)$ converge in a single dependence $C^* \sim t^{-6/5}$, and the shape of size distributions become identical as well. This fact leads to a very important conclusion concerning the choice of an approach to the computation of condensation. It permits the exact calculation of Q_0 and $\alpha(i, j)$ to be avoided, because the determination of these functions does not affect the final result. The only thing which is required from the theory in this situation is to assess the time-lag between evolution of the real and completely irreversible systems, the latter can be computed readily.

The results of our computation were compared with experimental data on specific surface S of silver powders [5] produced by condensation at the conditions corresponding to those accepted in the calculations. The theoretical predictions for S were made in terms of bulk values for the particle density. The comparison with the experiment is impeded by uncertainty in the choice of lifetime of the system. At the experimental conditions the coagulation was not stopped abruptly but proceeded during the particle deposition in the electrostatic precipitator. The lifetime of the condensing system corresponding to the entrance and to the outlet was about 0.1 and 0.4, respectively. The calculation predicts S values of the same order as those found experimentally but the trend of the $S(c_1^0)$ dependence for theoretical results is somewhat different from that obtained in the experiments. For the fixed lifetime of the condensing system the mean particle size $\bar{g} = 1/C^*$ must be proportional to $c_1^{0/5}$. (The lifetime is assumed to be large in comparison with the time of establishing of the $t^{-6/5}$ law.) Therefore, S must be proportional to $c_1^{0-2/5}$ just like as it was found from the above computation. But the best fit for the experimental results is function $S \sim c_1^{0-1/3}$. This disagreement can be readily ascribed to incomplete coalescence of particles in the coagulation process. When particle collisions lead to the growth of sintered aggregates rather than to formation of larger spheres, S is no more proportional to $g^{-2/3}$ but depends on the particle size in a much more weaker manner. Another complication arises from the uncertainty of the density of a small particle. As follows from numerous calculations, small particles of the condensation origin must have the density value smaller than the bulk value. Recently it has been confirmed for sodium chloride particles [22]. However in spite of these difficulties the method proposed here, as it has been demonstrated, yields quite reasonable results.

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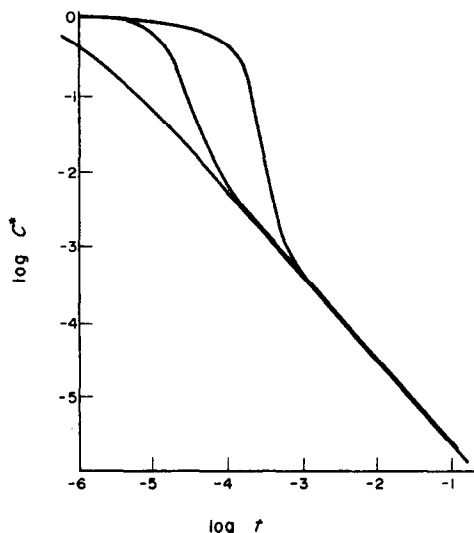


FIG. 4. The results of computation by three different schemes for $c_1^0 = 3.16 \times 10^{15}$ molecules cm^{-3} : 1, completely irreversible process; 2, instantly equilibrium; 3, sticking-controlled condensation.

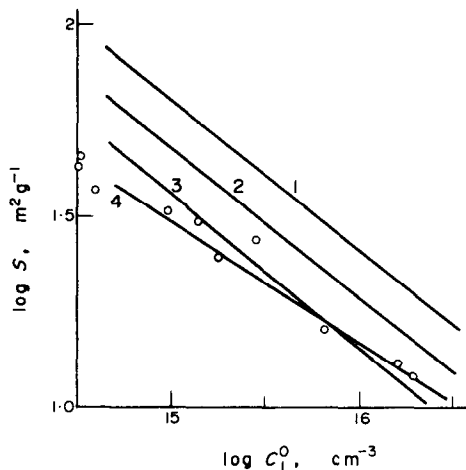


FIG. 5. Theoretical and experimental data on the $S(c_1^0)$ dependence. Theoretical curves $S \sim c_1^{0-2/5}$; lifetime of condensing system: 1, 0.1s; 2, 0.2s; 3, 0.4s; 4, the best fit for experimental data.

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CONDENSATION DE VAPEUR METALLIQUE DANS LES JETS LIBRES TURBULENTS

Résumé—On décrit une méthode de calcul de la condensation d'une vapeur métallique incorporée à un jet libre chaud s'écoulant dans une atmosphère froide immobile. La méthode est basée sur l'intégration numérique d'un système d'équations différentielles qui décrit l'évolution temporelle des concentrations des agrégats moléculaires et des particules de dimensions différentes simultanément avec l'équation cinétique du mélange turbulent. L'énergie libre de formation de petits agrégats moléculaires est exprimée en fonction des paramètres des forces intermoléculaires. On tient également compte de l'influence des forces de Van der Waals sur la vitesse de coagulation. On montre que la concentration totale des particules doit décroître dans le temps suivant une loi en $t^{-6/5}$. La forme de la loi de distribution asymptotique en similitude est déterminée pour la coagulation à molécules libres en tenant compte de l'influence des forces d'interaction de Van der Waals. Les résultats du calcul exprimés en fonction de l'aire S de la surface spécifique des particules condensées sont comparés à des résultats expérimentaux obtenus antérieurement sur la condensation de la vapeur d'argent. La théorie prévoit des valeurs raisonnables de S , mais la courbe théorique de S en fonction de la concentration initiale de vapeur présente une forme qui diffère légèrement de celle observée dans les expériences. Les raisons du désaccord entre théorie et expérience sont discutées.

KONDENSATION VON METALLDÄMPFEN IN TURBULENTEN FREISTRÄHLEN

Zusammenfassung—Es wird eine Methode zur Berechnung der Kondensation von Metaldämpfen beschrieben, die einem erhitzten Freistrahle beigemischt sind, der in ein kaltes, ruhendes, gasförmiges Medium austritt. Die Methode besteht in der numerischen Integration eines Systems von Differentialgleichungen, welche die Zeitabhängigkeit der Konzentrationen von Molekülanhäufungen und von Partikeln unterschiedlicher Größe beschreiben, zusammen mit der Gleichung, welche die Kinetik der turbulenten Mischung beschreibt. Die freie Bildungsenergie kleiner Molekülgruppen wird durch Parameter intermolekularer Kräfte ausgedrückt. Der Einfluß der Van der Waals'schen Kräfte auf die Koagulationsgeschwindigkeit wird ebenfalls berücksichtigt. Es wird gezeigt, daß die Gesamtkonzentration der Partikel mit der Zeit nach dem $t^{-6/5}$ -Gesetz abnehmen muß. Der Verlauf der endgültig stabilen Größenverteilung wird für die Koagulation freier Moleküle unter Berücksichtigung Van der Waals'scher Wechselwirkungskräfte bestimmt. Die Ergebnisse der Rechnung, ausgedrückt als Funktion der spezifischen Oberfläche S der kondensierten Partikel werden mit früher gewonnenen experimentellen Ergebnissen für die Kondensation von Silberdampf verglichen. Die Theorie liefert brauchbare Werte für S , aber die theoretische Abhängigkeit der Größe S von der anfänglichen Dampfkonzentration hat einen Verlauf, der leicht von dem in den Experimenten beobachteten abweicht. Die Gründe für die Widersprüche zwischen Theorie und Experiment werden diskutiert.

КОНДЕНСАЦИЯ ПАРА МЕТАЛЛА ПРИ ОХЛАЖДЕНИИ ЗАТОПЛЕННОЙ СТРУИ

Аннотация — Описан метод расчета конденсации паров металла, содержащихся в виде примеси к свободной струе горячего газа, истекающей в холодную покоящуюся среду. Метод основан на численном интегрировании системы дифференциальных уравнений, описывающих изменение во времени концентраций молекулярных агрегатов и частиц различного размера совместно

с уравнением, описывающим кинетику турбулентного смешения. Свободная энергия образования малых молекулярных агрегатов выражена через параметры потенциала межмолекулярного взаимодействия. Принималось во внимание влияние сил Ван-дер-Вальса на кинетику коагуляции частиц. Показано, что общая концентрация частиц асимптотически приближается к временной зависимости $t^{-6/5}$. Определена форма самосохраняющегося распределения по размерам при свободномолекулярной коагуляции частиц с учетом влияния сил Ван-дер-Вальса. Результаты расчетов представлены в виде значений удельной поверхности конденсированных частиц и сопоставлены с ранее полученными экспериментальными результатами по конденсации паров серебра. Расчет показывает разумные значения удельной поверхности, но форма зависимости удельной поверхности от исходной концентрации пара несколько отличается от найденного экспериментально. Обсуждены причины этого расхождения.