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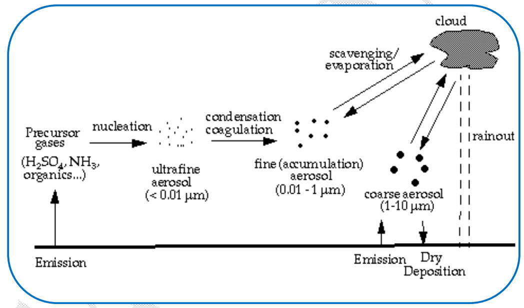
HETROMOLECULAR NUCLEATION OF H_2SO_4 AEROSOLE

Anurag Kumar , Vikas Mishra and Prakash Mishra
D.B.S college ,Kanpur (U.P.)

ABSTRACT :

In the present paper the values of the critical radius (r) and the Gibb's free energy of formation for a critical nucleus (ΔG*)as a function of no. of molecules of H_2SO_4 (n_B)and weight percentage (X) of H_2SO_4 at different temperature for no .of molecules of water (n_A=900) is calculated from the result we concluded that in nucleation process of H_2SO_4 .nH_2O the cluster depends on the relative values of n_A and n_B. The molar volume of solution depends on the vcalue of molar fraction (X)of sulphuric acid. At a given constant value of n_A as weight percent age (X) increases the critical radius (r^*),Gibb's free energy of formation of critical nucleus and the values of n_B will increased.*



KEYWORDS : *Aerosole, Hetromolecular, Embryo.*

INTRODUCTION

With the help of observation done by Friend et .al. [1] it is clear that during the formation of sulphuric acid the trimolecular process is first stage . After this stage reactions takes place. During the varies conversions(which takes place in the lower atmosphere) sulphuric acid plays an important role at the time of gas to particle conversion process. Many workers [2-4] studied effect of presence of H_2So_4 in water vapour .

THEORETICAL CONSIDERATION

In the binary homogeneous nucleation process of $H_2SO_4.nH_2o$ the composition of cluster depends on relative values of n_A and n_B . The molar volume of solution depends on the molar fraction X of sulphuric acid solution.

The formation and growth of special droplets through binary hetromolecular nucleation are controlled by Gibb's free energy change

$$\Delta G(n_i)=n_A(\mu^l{}_A - \mu^g{}_A)+ n_B(\mu^l{}_B - \mu^g{}_B)+4\pi r^2\sigma \quad \text{\_\_\_\_\_\_\_\_\_\_\_\_(1)}$$

Where n_i is the no. of moles of species "I" (A and B), r is the radius of embryo,□□ is the macroscopic surface tension . Subscript A refer's to water and subscript B refer's to solute or acid. Subscript 'I' refer's to liquid phase . Superscript 'g' refer's to gas phase

The weight percentage of acid is

$$X=100\, n_B.M_B /(n_A M_A + n_B M_B) \quad \text{\_\_\_\_\_\_\_\_\_\_\_\_(2)}$$

Where M_A is the molecular weight of H_2O and M_B is the molecular weight of H_2SO_4.

For a given environmental conditions,the critical composition n_A, n_B. the values of r*at the critical point (saddle point) are obtained by the solving the following equations

$(\partial \Delta G/\delta n_A)\ n_B = 0$
And $(\partial \Delta G/\delta n_B)\ n_A = 0$

When saddle point is found from the corresponding values of n_A , n_B the value of r* is

$$r^* = [3(n_A M_A + n_B M_B) / 4\pi \rho N_0]^{1/3}$$

Where N_0 is the Avogadro number.

We observe that as the weight percentage X increase the critical radius is increased and Gibb's free energy formation of critical nucleus increases for a given value of n_A. The calculations are made for H_2SO_4.

For the calculations we have to use relations for Gibb's free energy (**ΔG***), critical radius **(r*) by using the formulas for critical radius**

$$r^* = [3(n_A M_A + n_B M_B) / 4\pi \rho N_0]^{1/3} \quad \_\_\_\_\_\_\_\_\_\_\_\_ (3)$$

and Gibb's free energy

$$\Delta G^* = 4\pi r^* \sigma /3 \quad \_\_\_\_\_\_\_\_\_\_\_\_ (4)$$

RESULT AND DISCUSSION

Using equation 2,3 and 4 , we calculated the values of X, r*and ΔG* at different temperatures and listed in table -1 .

From the result it is concluded that in nucleation process of $H_2SO_4 .nH_2O$ the clusters depends on the relative values of n_A and n_B. The molar volume of solution depends on the value of molar fraction X of sulphuric acid .

At a given constant value of n_A , as the weight percentage X increase the critical radius (r*) , Gibb's free energy of formation of critical nucleus and the value of n_B will increased .

Table-1

S.No.	Temperature (K)	n_B	ρ	X	r*(10^{-8}) A^0	ΔG*(10^{-12}) erg
1.		5	1.0184	3	18.651	10.8062
2.		7	1.0250	4	18.695	10.8573
3.	283	27	1.0947	14	18.971	11.1802
4.		30	1.1020	15	19.035	11.2568
5.		34	1.1168	17	19.071	11.2984
6.		36	1.1243	18	19.085	11.1015
7.		39	1.1318	19	19.148	11.1749
8.	293	44	1.1471	21	19.212	11.2498
9.		52	1.1704	24	19.324	11.3873
10.		55	1.1783	25	19.369	11.4344
11.		58	1.1862	26	19.418	11.2397
12.	303	61	1.1942	27	19.456	11.2838
13.		64	1.2023	28	19.498	11.3325

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Anurag Kumar
D.B.S college , Kanpur (U.P.).