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NASA TECH BRIEF

Computer Program Calculates and Plots Surface Area and Pore Size Distribution Data

A computer program has been developed for the calculation of surface area and pore size distribution of powders, metals, ceramics, catalysts, and other substances. The program performs all calculations, then prints and plots the desired data directly. The directions for using the program, including the format of the experimental data that must be supplied with the program deck, are also described.

The calculations of surface area are based on the gas adsorption technique of Brunauer, Emmett, and Teller (BET). The calculations of pore size distribution are based on the gas adsorption technique of Pierce. Both techniques are adequately described and the field of particle measurement is demonstrated.

The BET multilayer theory results in an equation which can be used to establish the point at which monomolecular coverage occurs and to determine the volume of gas adsorbed in reaching this point. The resultant volume is related to the surface area of the material under investigation. The BET expression is $V = VaCp/((Ps-P2)[1 + (C-1)P/Ps])$ where V is the volume of gas adsorbed at equilibrium pressure P2, Va is the volume of gas adsorbed when the entire surface is covered with a monomolecular layer, Ps is saturation pressure of the gas, C is a constant related to the energy of adsorption of the first layer and to liquifaction of the absorbing gas.

The surface area Sw can be calculated from $Sw = (Va\ \sigma N)/M$ where σ is the area of an adsorbed molecule, N is Avogadro's number, and M is the molar volume.

The pore volume and pore size distribution can also be calculated using the gas adsorption technique. This is done by first increasing the adsorbing gas pressure to the saturation point, then desorbing in increments. As the saturation pressure of the gas is reached, pores up to a certain size are filled by capillary condensation, taking into consideration multilayer adsorption on the pore surface. Through use of the Kelvin equation the size of pores having different radii can be calculated by knowing the relative pressure and the volume desorbed incrementally. The thickness of the adsorbed layers at various relative pressures can be theoretically estimated. The pore size distribution can be determined by graphic or numerical integration of the Wheeler equation

$$Vp - Va = \int_{Rc}^{\infty} \pi(rw-t)^2 L\, drw,$$

using the desorption data where Vp is the total pore volume, Va the volume adsorbed, Rc the critical radius, t the film thickness, and L is the total length of all pores of radius rw per unit weight of adsorbent.

Notes:

1. This program is written in Fortran H for use on the IBM 360 computer.
2. Inquiries concerning this program may be made to:
   COSMIC
   Computer Center
   University of Georgia
   Athens, Georgia 30601
   Reference: B68-10009

Patent status:

No patent action is contemplated by NASA.

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