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# CAPTIVE EMULSION POLYMERIZATION

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A final mechanism that was treated was inertial impaction. This was considered, on the basis of experimental data, to be a minor factor in tobacco smoke filtration. It is found to account for less than five percent of observed particle removal efficiencies. Accordingly, the previous and present theory utilized broad approximations to handle this component of the filtration process.

In the present development, the basis established previously has been utilized, with the important modification in the computation of diffusion times and distances. Besides this modification, the previous theory has been extended in two ways. One of these is that the effect of non-cylindrical fibers has been accounted for by computing an "effective" fiber radius. This is necessary for a practical filtration theory since studies of particle deposition on filter fibers, such as those reported last year (7), show that most particles appear to be initially deposited on the extremities of the lobes of actual fibers. This deposition pattern led to an intuitive concept that the "effective" fiber radius for filtration purposes was that of a circle circumscribed about the fiber cross section. This is diagrammatically illustrated in the next figure. The reasoning behind this is essentially that the fiber lobes are the prime collection points for particles and that the valleys represent still air spaces. Particles which happen to be present in these spaces will not be swept along with the moving smoke stream and will eventually be deposited on the fiber. The net effect is that all particles within an area approximately described by a circumscribed circle are very likely subject to capture by the fiber.

To compute such an "effective" fiber radius, two approaches have been taken. The first utilizes experimentally determined filter pressure drop data. This accounts not only for the non-circular perimeter of most fibers, but also includes contributions from fiber touching and coalescence and the non-uniform spatial distribution of fibers which are universally present in practical filters. The computation essentially involves a back-calculation from pressure drop theory (5), combining all effects into an effective fiber radius. Because pressure drop is a commonly used, simple measurement, and because most of the real departures from a model system are effectively treated in this manner, this is the preferred method of computation.

A second method of computing an "effective" fiber radius is to consider individual fiber cross sections as regular geometric shapes. For example, a fiber with a Y cross section can be considered as a composite of a triangle, three rectangles, and three semi-circles, as shown in the next figure. With a fixed geometry such as this, it is possible from surface area or perimeter data and the denier of the fiber to calculate the width and length of the fiber lobes. These dimensions can in turn be used to calculate the radius of the circumscribed circle or "effective" fiber radius.

Possibly the most significant point is that all three methods provide reasonable and fairly close agreement in calculated particle removal efficiencies. For example, a fairly high efficiency 2.4 denier tow has computed particle removal efficiency (PRE) values given in the next figure. Even though the alpha values, which are a volume fraction of the filter occupied by fiber or "effective" fiber differ depending on the method of calculation, there is little real difference between the computed efficiencies. The three methods are a fiber weight, pressure drop, and fiber dimension calculation. This suggests that factors other than fiber dimensions are more important in controlling efficiency, but also indicates that these are reasonable models of the real situation. This indication is considerably fortified by the agreement between the computed efficiencies and the nicotine removal efficiency (NRE) value estimated by regression analysis of experimental data. NRE is thought to be the most readily measureable quantity which approximates a particulate removal efficiency.

The second major extension of previous theory has been the establishment of a function which duplicates a particle size distribution for cigarette smoke. This function was determined by curve fitting with experimental particle size data (8) and the close fit is illustrated in the next figure. The equation describes a Beta function which generally finds use in highly skewed probability distributions. The value of this distribution function is that it allows an integration or summation over all smoke particle sizes, and hence a computation of an overall efficiency. In practice, this distribution is converted to a mass distribution which is multiplied by the particle size dependent single fiber filter efficiency. Integration over the size range of interest, 0.1 to 1.1 microns, yields a weight of filtered smoke. When this is divided by a similarly computed weight of unfiltered smoke, a single fiber efficiency for a smoke with a tobacco smoke range of sizes is obtained. The final step in the process is to suitably sum over all fibers in the smoke stream to obtain an overall particle removal efficiency. This is accomplished by use of the iterative or logarithmic formula described by Fordyce et al (9).

For simplicity, we have omitted the considerable mathematical computations from this presentation. These are included in an appendix which is available to interested parties. A few details are, however, necessary. Because of the complexity of the equations for determining the particle diffusion distance and the "effective" fiber radius from pressure drop theory, it was necessary to utilize numerical approximation techniques. The diffusion and the pressure drop functions were numerically solved using Newton's rule, and the integrations were performed using Simpson's rule. These types of computations are particularly suitable for a computer. Thus the whole calculation of particle removal efficiencies and their comparison with regression data has been incorporated into a program requiring about 45 seconds of computer time for calculation of the efficiency of a given filter.

One of the critical factors in the computation is the determination of the time of travel of a particle around the fiber. This determines the distance that the particle may diffuse because of kinetic bombardment by the surrounding gas molecules. After a number of attempts at an exact solution for this time or equivalently distance, an approximate solution was chosen, mainly because of its simplicity and its analogy with other physical problems. This appears to be a reasonable approach from the agreement between computed and experimental efficiencies.

In both the previous and present developments, the smoke stream is considered as crossing the fiber at right angles to the fiber axis. This intuitively seems correct in regions close to the fiber surface because of the differential drag on the moving stream. Two experimental observations fortify this intuition. One is the finding that filters with fibers purposely oriented perpendicular to the smoke stream do not have improved smoke removal efficiencies over ordinary filters of equivalent pressure drops. A second is illustrated in the next figure. Here a fresh smoke stream was expelled from a jet onto a parallel fiber array oriented at 45° from the jet. As can be seen, the stream coming through the fibers has turned 45° from its initial direction and is consequently perpendicular to the plane of the fiber array.

To further demonstrate the agreement between the theoretically derived particle removal efficiencies and experimentally based efficiencies, the next figure illustrates the correlation for a wide variety of filters. This is a plot of theoretical PRE values as a function of experimental NRE values for filters ranging in pressure drop from 10 to 220 millimeters of water. A wide range of filter weights, circumferences, lengths, fiber deniers and cross sections are represented in the indicated data points. In an overall sense, an excellent agreement between theory and experiment was achieved. The uppermost line represents a 1:1 correlation, while the lower line represents the regression line through the 20 mm filter data. The slope of this line is 1.11 and the intercept is -8.3 PRE units. The departure of the regression line from the 1:1 correlation line is reasonable if a small portion of the nicotine is, as expected, present in the vapor phase and the filter is selective in its removal of nicotine vapor. Lipp (10) has shown that acetate filters are in fact selective for nicotine vapor. From the slope and intercept of the regression line, we compute that 10% of the nicotine is present in the vapor phase, and that a 20 mm filter removes 73% of this vapor. These values are in reasonable agreement with Lipp's findings.

When the filter length is changed, one would expect a shift not only in the particulate efficiency but also in the vapor absorption efficiency. Thus, a departure from the main regression line is expected, with longer filters falling below the line. This is evident in the dashed lines branching off from the main regression line. These represent the effect of changing filter length from 15 to 35 mm for a low, medium, and high dpf tow item, and are in the expected pattern.

The agreement between theory and experiment, and the explainable departures led us to the conclusion that the theory does in fact provide a real particle removal efficiency. If this is the case, then we have a baseline for the estimation of filter selectivity, and a means of separating particulate and vapor filtration processes.

One final point which can be considered is an estimation of the contributions of the three filtration mechanisms to the overall PRE values. This was done by eliminating one or more of the mechanisms from the filtration equation, and the last figure presents the pertinent results. The computed efficiencies for a low and high pressure drop filter are presented, and the figures in brackets represent the expected contribution of each mechanism to the overall efficiency. It is evident that diffusion is the most important filtration mechanism accounting for almost two thirds of the filtration, while direct interception provides most of the rest of the filtration. Impaction is an almost negligible filtration mechanism, contributing only 1 to 1.5% of the calculated efficiency.

In summary, it has been shown that basic filtration mechanisms can be combined in a logical fashion to predict the removal efficiency for particles of practical filters. These calculated efficiencies agree well with observed nicotine removal efficiencies, and the slight deviations are accountable on the basis of a portion of the nicotine being in the vapor phase. Diffusion and direct interception are found to be the most important filtration mechanisms, the former being the primary mechanism.

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REPRESENTATION OF FILTRATION MECHANISMS

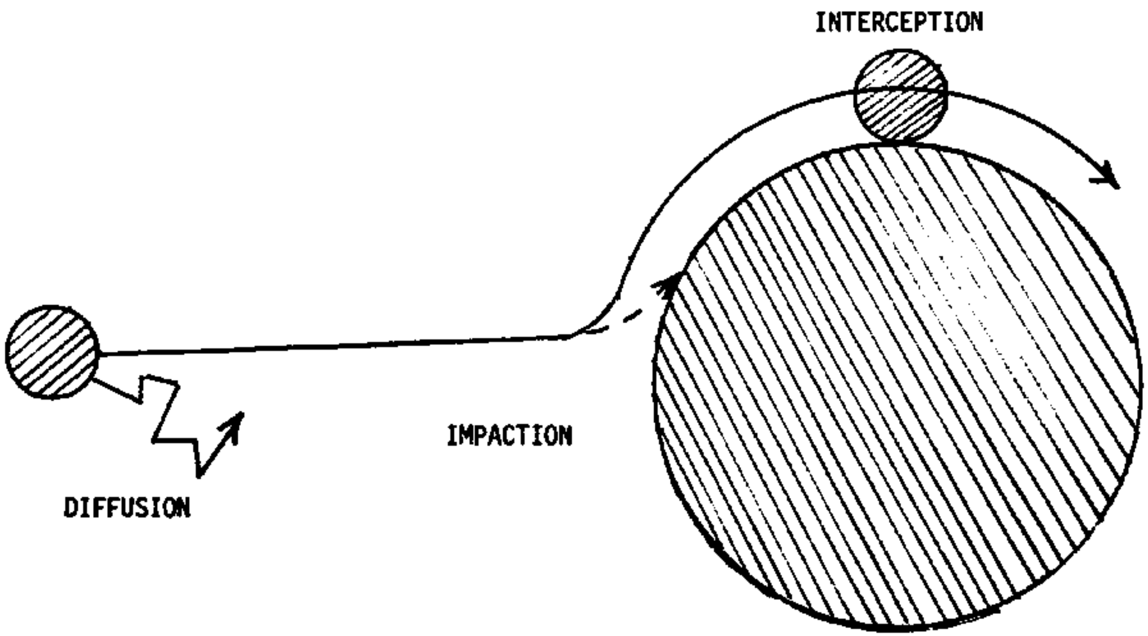



FIGURE 1

FILTER MODEL

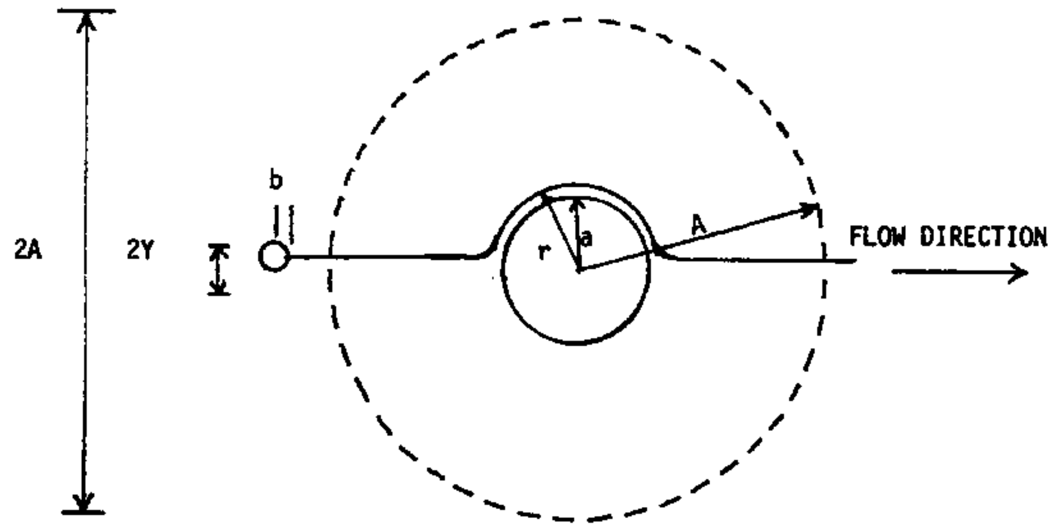



FIGURE 2

r = RADIAL DISTANCE TO A STREAMLINE

2Y = AREA OF A UNIT LENGTH OF FIBER CLEANED OF PARTICLES BY CONTACT WITH THE FIBER

a = RADIUS OF THE FIBER

b = RADIUS OF THE PARTICLE, ADJUSTED FOR DIFFUSIONAL DISPLACEMENT

A = RADIUS OF THE CHANNEL ASSOCIATED WITH EACH FIBER

$e_f = \frac{2y}{2A}$ = THE PARTICULATE REMOVAL EFFICIENCY OF THE FIBER

FIGURE 3

DEFINITION OF "EFFECTIVE"

FIBER RADIUS

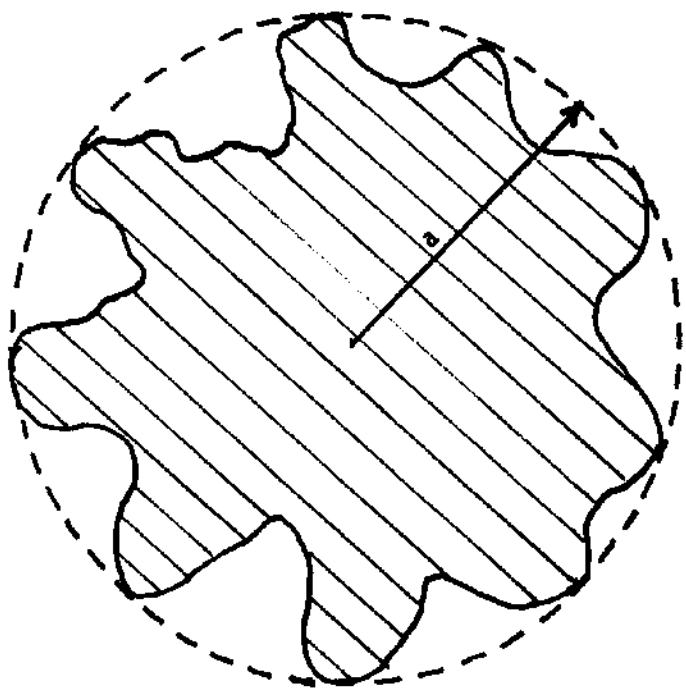


FIGURE 4

GEOMETRIC REPRESENTATION

OF A Y CROSS SECTION FIBER

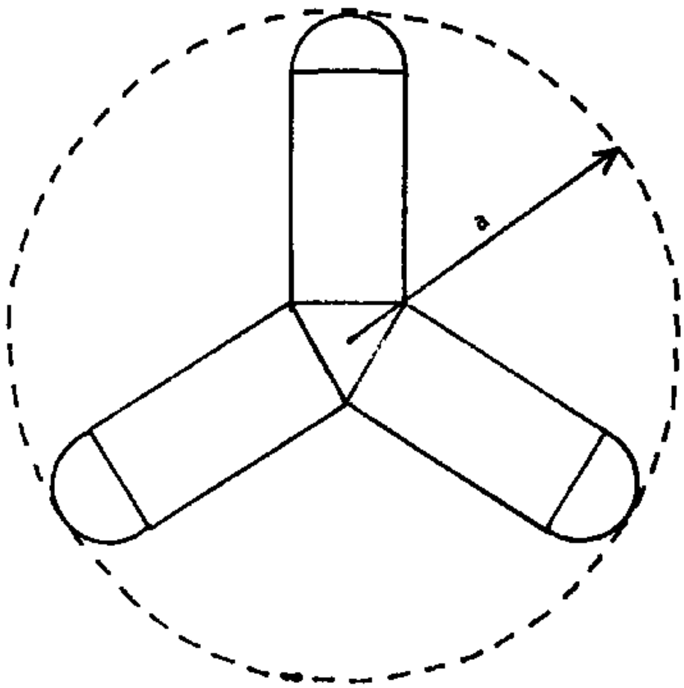


FIGURE 5

PARTICULATE REMOVAL EFFICIENCY CALCULATION

2.4/Y / 46000

| | |
|---|---|
| LENGTH = | 20 MM |
| CIRCUMFERENCE = | 24.8 MM |
| PRESSURE DROP = | 98 MM $H_2O$ |
| F W BASIS, ALPHA = | .1045, PRE = 42.8 PCT |
| P D BASIS, ALPHA = | .1404, PRE = 43.2 PCT |
| F D BASIS, ALPHA = | .1557, PRE = 43.4 PCT |

COMPARATIVE VALUES FROM REGRESSION ANALYSIS OF DATA

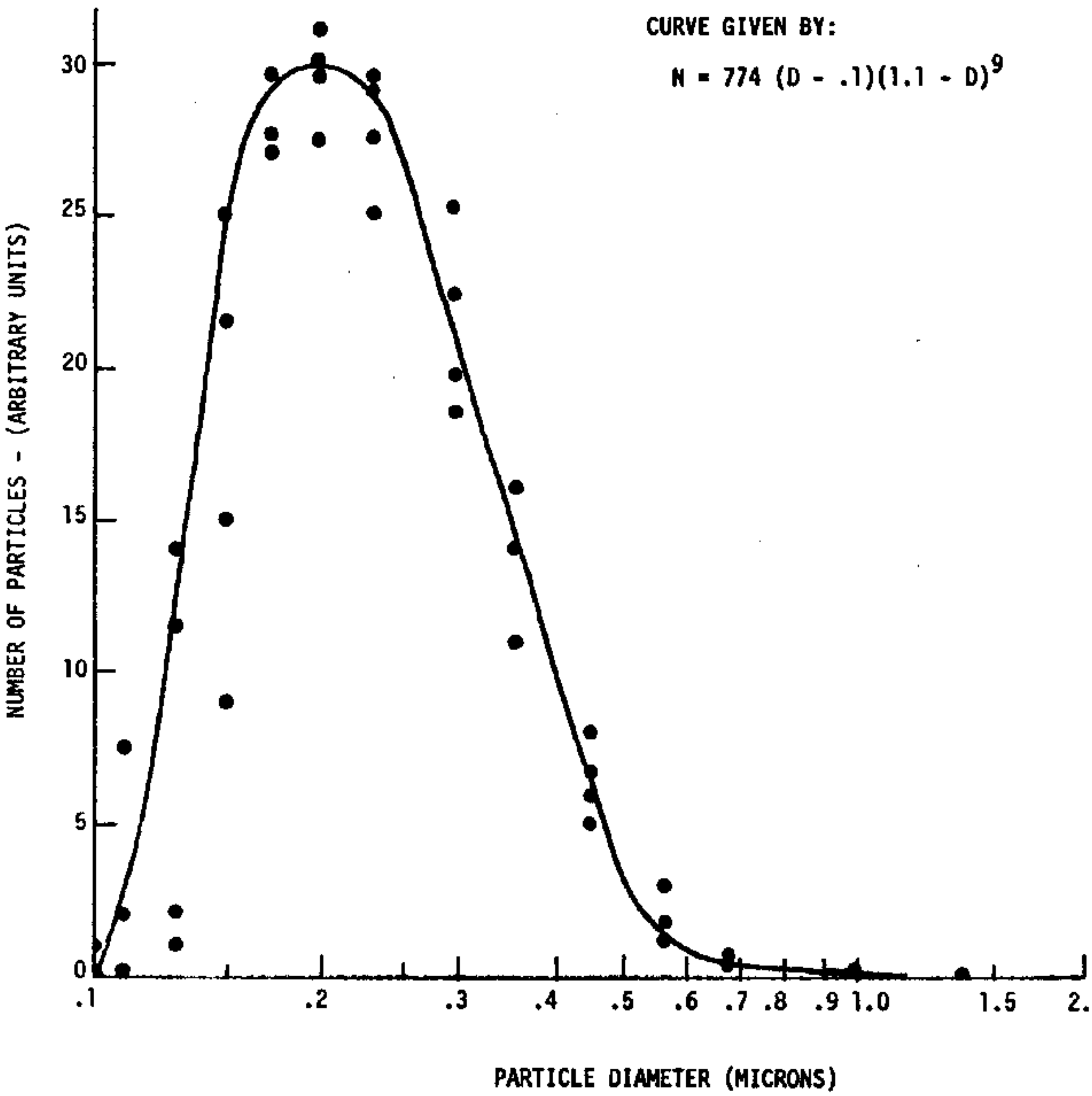
| | |
|---|---|
| SRE = | 56.8 PCT |
| NRE = | 46.0 PCT |
| TRE = | 51.8 PCT |

FIGURE 6

PARTICLE SIZE DISTRIBUTION OF UNFILTERED SMOKE

4th PUFF, 4 RUNS

DATA FROM: KEITH & DERRICK, J. COL. SCI., 15, 340, (1960)



DEFLECTION OF A SMOKE STREAM PASSING THROUGH PARALLEL FIBERS

FIGURE 8

CORRELATION OF COMPUTED PARTICLE
REMOVAL EFFICIENCIES WITH EXPERIMENTAL
NICOTINE REMOVAL EFFICIENCIES

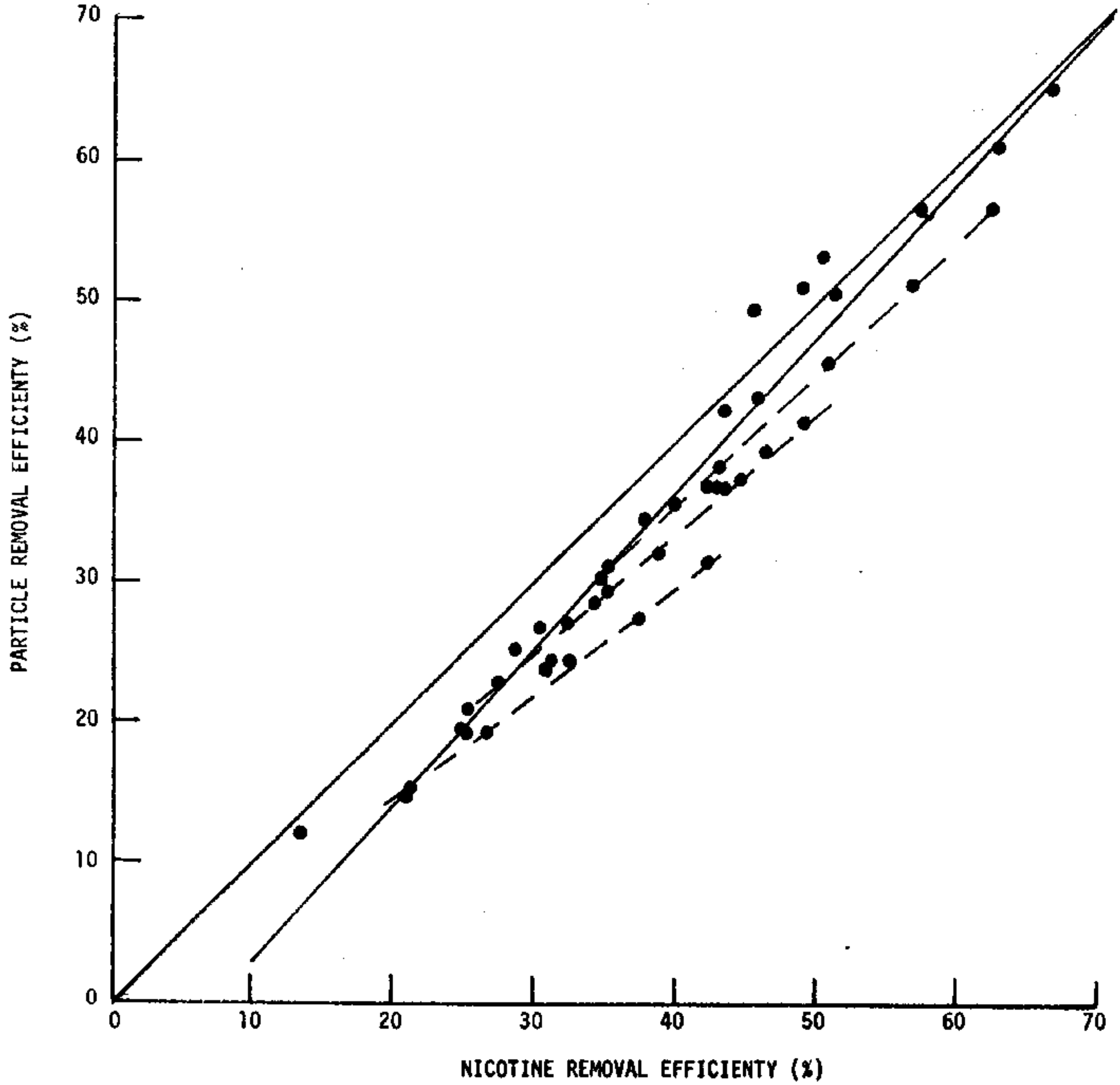


FIGURE 9

CONTRIBUTION OF FILTRATION MECHANISMS TO OVERALL FILTER EFFICIENCY

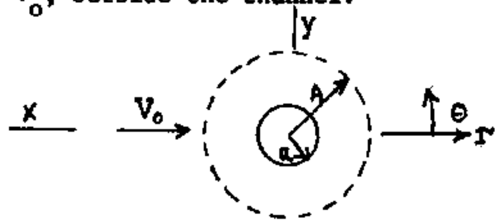
| MECHANISM | LOW P.D. FILTER | | HIGH P.D. FILTER | |
|---|---|---|---|---|
| | COMPUTED EFFICIENCY | CONTRIBUTION | COMPUTED EFFICIENCY | CONTRIBUTION |
| DIRECT INTERCEPTION | 5.9% | (30.3%) | 11.0% | (34.5%) |
| DIFFUSION | 13.3% | (67.5%) | 20.4% | (64%) |
| DIFFUSION + INTERCEPTION | 42.6% | (98.5%) | 24.8% | (98.8%) |
| IMPACTION | - | ( 1.5%) | - | ( 1.2%) |
| ALL MECHANISMS | 43.2% | (100%) | 25.1% | (100%) |

## Appendix

## Derivation of Particle Removal Efficiency Equation

1. Direct Interception

Consider an array of circular fibers of radius, a, surrounded by a flow channel, A, oriented perpendicularly to a fluid stream moving at a steady velocity, $V_o$, outside the channel.




According to Happel (A.I.Ch.E. Journal, 5, 174-177, 1959) the flow is characterized by a stream function, $\Psi$, which is defined by the relationships:

$$V_r = \frac{1}{r}\frac{\partial\Psi}{\partial\theta} \qquad (1)$$

$$V_\theta = -\frac{\partial\Psi}{\partial r} \qquad (2)$$

Where: $\Psi$ = the stream function

$V_r$ = a linear velocity in the radial or r direction

$V_\theta$ = a linear velocity in the angular or θ direction.

The stream function must satisfy the equation:

$$\nabla^4\Psi = 0 \qquad (3)$$

for which a suitable general solution is:

$$\Psi = \sin\theta(Gr^3 + Hr\ln r + Jr + K/r) \qquad (4)$$

or: $$V_r = \frac{1}{r}\frac{\partial\Psi}{\partial\theta} = \cos\theta(Gr^2 + H\ln r + J + K/r^2) \qquad (5)$$

$$V_\theta = -\frac{\partial\Psi}{\partial r} = -\sin\theta(3Gr^2 + H\ln r + H + J - K/r^2) \qquad (6)$$

Where G, H, J, and K are constants to be determined by the boundary conditions:

at $r = a$, $V_r = 0$, $V_\theta = 0$

at $r = A$, $V_r = V_o \cos\theta$, $V_\theta = -V_o \sin\theta$

Where $V_o$ is the average stream flow outside the channel.

Substituting the boundary conditions into (5) and (6) we get:

$$Ga^2 + H\ln a + J + K/a^2 = 0 \quad (7)$$

$$3Ga^2 + H\ln a + H + J - K/a^2 = 0 \quad (8)$$

$$GA^2 + H\ln A + J + K/A^2 = V_o \quad (9)$$

$$3GA^2 + H\ln A + H + J - K/A^2 = V_o \quad (10)$$

Solving simultaneously we find that:

$$G = \frac{V_o}{2\phi} \quad (11)$$

$$H = -\frac{V_o(A^2 + a^2)}{\phi} \quad (12)$$

$$J = \frac{V_o}{2\phi}(A^2 - a^2) + \frac{V_o}{\phi}(A^2 + a^2)\ln a \quad (13)$$

$$K = \frac{-V_o}{2\phi} a^2 A^2 \quad (14)$$

$$\text{Where } \phi = (A^2 - a^2) + (A^2 + a^2)\ln\frac{a}{A} \quad (15)$$

Therefore:

$$\Psi = \frac{V_o \sin\theta}{2\phi}\left\{r^3 - 2(A^2 + a^2)r\ln\frac{r}{a} - \frac{A^2 a^2}{r} + (A^2 - a^2)r\right\} \quad (16)$$

At the outer boundary A,

$$\Psi_A = V_o A\sin\theta = V_o y \quad (17)$$

Where y is a vertical distance.

Near the fiber a particle of radius, b, would touch when $\theta = 90°$ and $r \leq a + b$.

The stream function at this point, F, is:

$$\Psi_f = \frac{V_o}{2\Phi}\left\{(a+b)^3 - 2(A^2+a^2)(a+b)\ln\left(\frac{a+b}{a}\right) - \frac{A^2a^2}{(a+b)} + (A^2-a^2)(a+b)\right\} \quad (18)$$

Letting $R = b/a$ and $\alpha = a^2/A^2$ and substituting in (18) we get:

$$\Psi_F = \frac{V_o a}{2(1-\alpha) + (1+\alpha)\ln\alpha}\left\{\alpha(1+R)^3 - 2(1+\alpha)(1+R)\ln(1+R) - \frac{1}{1+R} + (1-\alpha)(1+R)\right\} \quad (19)$$

Since the particle is much smaller than the fiber, R is much less than unity. Accordingly we can suitably approximate the various functions by series expansions ending in terms containing $R^2$. Using such approximations we get:

$$\Psi_f = V_o a R^2 \cdot \frac{\alpha-1}{(1-\alpha) + \left(\frac{1+\alpha}{2}\right)\ln\alpha} = -\frac{V_o b^2/a}{1+\frac{1}{2}\left(\frac{1+\alpha}{1-\alpha}\right)\ln\alpha} \quad (20)$$

Since the particles follow streamlines, which are defined by a constant value of $\Psi$, we can equate $\Psi_A$ with $\Psi_F$ to obtain the vertical distance, y, which contains particles which will contact the upper half of the fiber during passage around it.

$$y = \frac{-b^2/a}{1+\frac{1}{2}\frac{(1+\alpha)}{(1-\alpha)}\ln\alpha} \quad (21)$$

Since 2y represents a vertical distance from which all particles are removed, and 2A represents the total distance over which the fiber has an effect on the stream, the fractional filtration efficiency resulting from direct interception, $e_f$ is simply 2y/2A. Using (21), we get:

$$e_f = y/A = -\frac{b^2}{aA} \cdot \frac{1}{1+\frac{1}{2}\frac{(1+\alpha)}{(1-\alpha)}\ln\alpha} \quad (22)$$

$$\text{or: } e_f = -\frac{b^2}{a^2}\ \frac{\alpha^{\frac{1}{2}}}{1+\frac{1}{2}\frac{(1+\alpha)}{(1-\alpha)}\ln\alpha} \quad (23)$$

N.B. The minus sign in (23) disappears as $1 + \frac{1}{2}\frac{(1+\alpha)}{(1-\alpha)}\ln\alpha$ is negative. Therefore $e_f$ is positive and less than one for all $\alpha$'s of interest.

2. Diffusion

To include diffusion in the previous expression (22) for interceptional filtration, we need to adjust the particle radius, b, to take account of the distance that the particle diffuses during its passage around a fiber, i.e.

$$b = r_p + r_d \tag{24}$$

Where $r_p$ = the particle radius

$r_d$ = the average diffusional displacement of a particle during its passage around a fiber. From Langmuir (OSRD Report No. 865, 1942), we have an approximate expression for the average displacement of a particle in time, t, this being derived from Einstein's diffusion equation.

$$r_d = \left(\frac{4}{\pi}Dt\right)^{\frac{1}{2}} \quad \text{or} \quad t = \frac{\pi r_d^2}{4D} \tag{25}$$

Where D is the diffusion coefficient for Brownian motion. From Einstein (Ann. Physik, 17, 549 (1905), and 19, 371, (1906)) the diffusion coefficient for a particle is given by:

$$D = \frac{CkT}{6\pi\mu r_p} \tag{26}$$

Where C = Cunningham's correction for slip flow = $1 + 1.25\ \lambda/r_p$ (Pich, J., Aerosol Science, C. N. Davies, ed., Chapt. IX, p. 249, Academic Press, N. Y., 1966).

$\lambda$ = Mean free path of air molecules = $6.5 \times 10^{-6}$ cm.

k = Boltzman's constant = $1.38 \times 10^{-16}$ dyne-cm$^{o}$k

T = Absolute temperature = $300^{o}$k

$\mu$ = Viscosity of air = $1.8 \times 10^{-4}$ dyne-sec/cm$^2$.

To determine $r_d$ in equation 25, it is necessary to determine the time that it takes for a particle to travel in a semi-circle around the fiber. In the region close to the fiber, the velocity of the particle can to a good approximation be considered as $V_\theta$ during this travel around the fiber. As in equation 6

$$V_\theta = r\frac{d\theta}{dt} = -\sin\theta(3Gr^2 + H\ln r + H + J - K/r^2) \tag{27}$$

$$t = \frac{r}{(3Gr^2 + H\ln r + H + J - K/r^2)}\int_0^\pi \frac{d\theta}{\sin\theta} \tag{28}$$

Since the integral goes to infinity at either extreme, the problem cannot be directly or easily solved. An approximation can however be devised from analogy with alternating current electricity. This is to consider the average velocity as being analogous to an RMS current, which is equal to the maximum velocity divided by the square root of two. Thus the sin θ term disappears and

$$t = \frac{2^{\frac{1}{2}} r \cdot \pi}{(3Gr^2 + H\ln r + H + J - K/r^2)} \tag{29}$$

A further refinement to this approximation can be made by considering that the limits of the integration are not 0 and π as given in (28), but are $+\frac{\pi}{2}(\frac{r-a}{r})$ and $\pi - \frac{\pi}{2}(\frac{r-a}{r})$, which is essentially saying that the particle travels around the fiber from a point 1.5 $r_d$ units above the X axis to another point almost 180° away which is also about 1.5 $r_d$ units above the X axis. Using these limits we obtain:

$$t = \frac{2^{\frac{1}{2}} a \cdot \pi}{(3Gr^2 + H\ln r + H + J - K/r^2)} \tag{30}$$

Equating this time with that given in (25), and substituting r-a for $r_d$, we get:

$$(r-a)^2 \cdot (3Gr^2 + H\ln r + H + J - K/r^2) = 4 \cdot 2^{1/2} \cdot a \cdot D \quad (31)$$

Unfortunately an analytic solution of this equation is not feasible, and numerical techniques have to be utilized. Using Newton's rule, a function

$$Z = (r-a)^2 (3Gr^2 + H\ln r + H + J - K/r^2) - 4 \cdot 2^{1/2} \cdot a \cdot D \quad (32)$$

is defined. The derivative of Z with respect to r is:

$$\frac{dZ}{dr} = 2(r-a)(3Gr^2 + H\ln r + H + J - K/r^2) + (r-a)^2(6Gr + H/r + 2K/r^3) \quad (33)$$

Repetitive trials in which new approximations to r are determined by:

$$r_n = r_{n-1} - Z/\frac{dZ}{dr} \quad (34)$$

Where $r_n$ = the nth value of r and $r_{n-1}$ = the previous approximation of r. This gives a value of r to any desired degree of accuracy.

To provide an initial value reasonably close to the final value, an approximation of r was obtained using substitutions of the type used in equations 19 and 20. The appropriate value is given by:

$$r = a + \left\{\frac{D\,\alpha\,\phi}{(\alpha-1)V_o}\right\}^{1/3} \quad (35)$$

This type of numerical solution of (31) is particularly suited for computer techniques, which have been extensively used throughout this development.

From the numerically determined value of r and the fiber radius a we obtain:

$$r_d = r-a \quad \text{or} \quad b = r_p + (r-a) \tag{36}$$

which when substituted in (23) gives the single fiber efficiency for diffusion and interception

$$e_f = -\frac{(r_p + r_d)^2}{a^2} \frac{\alpha^{1/2}}{(1 + \frac{1}{2}\frac{(1+\alpha)}{(1-\alpha)}\ln\alpha)} \tag{37}$$

3. Inertial Impaction:

The equation of motion of a particle of mass, m, moving in a viscous fluid free of external forces is:

$$\frac{d(m\vec{u})}{dt} = -\frac{6\pi\mu r_p}{C}(\vec{u} - \vec{v}) \tag{38}$$

Where m = the mass of the particle = $\frac{4}{3}\pi\rho r_p^3$

- $\rho$ = the density of the particle
- $r_p$ = the radius of the particle
- $\mu$ = viscosity of the fluid
- C = Cunningham correction for slip flow
- $\vec{u}$ = Vector velocity of the particle
- $\vec{v}$ = Vector velocity of the fluid
- t = time.

Rearranging and substituting for the mass of the particle, we get

$$\frac{2C\rho r_p^2}{9\mu}\frac{d\vec{u}}{dt} + \vec{u} = \vec{v} \tag{39}$$

letting $I = \frac{2}{9}\frac{C\rho r_p^2}{\mu}$ and resolving into polar coordinates r and θ we have:

$$I\frac{du_r}{dt} + u_r = v_r \tag{40}$$

and $$I\frac{du_\theta}{dt} + u_\theta = v_\theta \tag{41}$$

Since it can be shown by plotting streamlines that the particles which are collected are those flowing close to the horizontal axis until they are almost at the surface of the fiber, we can ignore the angular velocity components and approximate the inertial contribution with the radial equation of motion.

Since $v_r = \frac{dr}{dt}$ we can eliminate dt from (39), so we get $$\frac{du_r}{dr} + \frac{u_r}{Iv_r} = \frac{1}{I} \tag{42}$$

$$u_r e^{\frac{1}{I}\int\frac{dr}{v_r}} = \frac{1}{I}\int e^{\frac{1}{I}\int\frac{dr}{v_r}}\, dr \tag{43}$$

Since $v_r$ as given in (5) is a complicated function of r and θ, analytical integration of $\frac{dr}{v_r}$ is not possible. A suitable approximation of $v_r$ is:

$$v_r = V_o m(\alpha)(\frac{r}{a} - 1)\cos\theta \qquad (44)$$

This applies in the region where $m(\alpha)(\frac{r}{a} - 1)$ is less than one. When $m(\alpha)(\frac{r}{a} - 1)$ reaches unity, it maintains this value, so that $v_r = V_o \cos\theta$ when r/a is greater than the value which gives $m(\alpha)(\frac{r}{a} - 1) = 1$. This approximation is equivalent to saying that along the x axis $v_r = V_o$ for a distance into the channel about the fiber and then decreases linearly until it reaches zero at the fiber surface. It is found by computer techniques and linear regression that:

$$m(\alpha) = .2214 + 2.011\alpha \qquad (45)$$

and that $(\frac{r}{a})'$, which is the value of r/a at which the function goes to unity, is given by the expression

$$(\frac{r}{a})' = .5733 + .6363/\alpha^{\frac{1}{2}} \qquad (46)$$

Again considering that most of the particles that will be filtered are originally located close to the horizontal axis, we may ignore the angular components of velocity and approximate $v_r$ by the expression:

$$v_r = V_o m(\alpha)(\frac{r}{a} - 1) \qquad (47)$$

This last approximation is not entirely necessary but it does considerably simplify the forthcoming integrations, and the results obtained by using it are found to essentially agree with those obtained using the more rigorous expression. Using (42) in (43), we get

$$e^{\frac{1}{I}\int\frac{dr}{v_r}} = (\frac{r}{a} - 1)^{\frac{a}{IV_o m(\alpha)}} \qquad (48)$$

and $u_r = \frac{a}{I}\left(\frac{1}{\frac{a}{IV_o m(\alpha)} + 1}\right)(\frac{r}{a} - 1) + \text{constant}$ (49)

when $\frac{r}{a} = 1$, $u_r = o$, so that the constant is zero. Rearranging and reintroducing $v_r = V_o m(\alpha)(\frac{r}{a} - 1)$, we get:

$$u_r = \frac{v_r}{1 + \frac{IV_o m(\alpha)}{a}} = \frac{v_r}{1 + I'} \qquad (50)$$

Where $I' = \frac{IV_o m(\alpha)}{a}$, an inertial parameter similar to that described by Chen (Chem. Rev., 55, 595-623, 1955).

Since $u_r = \frac{dx_r}{dt}$ and $v_r = \frac{dr}{dt}$

Where $x_r$ = the position of the particle

$$dx_r = \frac{dr}{1 + I'} \text{ and } x_r = \frac{r}{1 + I'} + \text{const.} \qquad (51)$$

As $r_p$ becomes smaller, I and I' approach zero so that $x_r$ approaches r as would be physically expected. Therefore the constant in (51) must be zero. Now $r - x_r$ is the distance, $s_r$, that the particle moves from inertial forces alone.

$$s_r = r - x_r = r - \frac{r}{1 + I'} = \frac{I'}{1 + I'} r \qquad (52)$$

This distance, $s_r$, is an approximate measure of how far the particle moves across streamlines under the effect of inertia.

Previously we had in (4) and (5) expressions for $\Psi$, the stream function which describes a given streamline, and $v_r$, the radial component of velocity. These were $v_r = F(r) \cos\theta$ and $\Psi = rF(r)\sin\theta$, where:

$$\frac{V_o}{2\phi}\left\{r^2 - 2(A^2 + a^2)\ln\frac{r}{a} - \frac{A^2a^2}{r^2} + (A^2 - a^2)\right\} = F(r)$$

If we describe two streamlines 1 and 2 by means of the stream function $\Psi$,

we have: $\Psi_1 = r_1 F(r_1)\sin\theta$ (53)

and $\Psi_2 = r_2 F(r_2)\sin\theta$ (54)

and in the region of interest close to the x axis, we can say that $r_2 = r_1 + s_r$,

so that $\Psi_2 = (r_1 + s_r) F(r_1 + s_r)\sin\theta$ (55)

Since $s_r \ll r_1$, $F(r_1 + s_r)$ approximately equals $F(r_1)$ and $\Psi_2 = (r_1 + s_r) F(r_1)\sin\theta$ (49)

Since $s_r = \frac{I'}{1 + I'} r_1$, $\Psi_2 = (\frac{I' + 2I'}{1 + I'})r_1F(r_1)\sin\theta = \frac{1 + 2I'}{1 + I'} \Psi_1$ (56)

and since $I' \ll 1$, we can approximate with $\Psi_2 = (1 + I')\Psi_1$ (57)

Now letting $\Psi_2 = \Psi_A$, we obtain from (17) and (20)

$$y = -(1 + I')\cdot\frac{b^2}{a}\cdot\frac{1}{1 + \frac{1}{2}(\frac{1+\alpha}{1-\alpha})\ln\alpha} \qquad (58)$$

and $e_f$, the single fiber efficiency for interception, diffusion, and impaction becomes:

$$e_f = -\frac{(1 + I')\,(r_p + r_d)^2}{A^2 \alpha^{1/2}} \cdot \frac{1}{1 + \frac{1}{2}\left(\frac{1+\alpha}{1-\alpha}\right)\ln\alpha} \qquad (59)$$

Where $I' = \frac{2}{9} \quad \frac{C\rho r_p^{\,2} Q}{\mu a F(1-\alpha)} \quad (.2214 + 4.011\alpha)$

4. Non-Circular Fiber Effects

In the previous derivations, the fibers have been considered as being perfect cylinders arranged in a uniform array throughout the filter. In a cellulose acetate filter this is usually not the case as the fibers have a lobe structure caused by shrinkage of the fiber during evaporation of the polymer solvent. The number of these lobes can either be random as in a regular cross section fiber or can be controlled by the configuration of the spinning jet as in fancy cross section fibers. As was shown by Keith and Mayer ("The Deposition of Particles on Fibrous Filters", paper presented at the 23rd Tobacco Chemists Research Conference, Philadelphia, Pa., October 22-24, 1969), the primary deposition of particles is on the extremities of these lobes. This being the case, the appropriate fiber radius for filtration purposes is that of a circle circumscribed about the fiber cross section.

There are several ways of computing this "effective" fiber radius. The first and simplest is that which has been used in the past, i.e., considering the fiber to be a cylinder. The computation involves dividing the face area of the filter into individual fiber channels and determining the fiber area from $\alpha$, the volume fraction of the filter occupied by fiber. The appropriate equations are:

$$\alpha = \frac{W}{FL\rho} = \frac{a^2}{A^2} \qquad (60)$$

$$a = \left\{\frac{\alpha \cdot F \cdot \delta}{T\pi}\right\}^{\frac{1}{2}} \qquad (61)$$

Where: W = the weight of fiber (gm)

F = the face area of the filter = $\frac{\pi d^2}{4} = \frac{C^2}{4\pi}$ ($cm^2$)

L = the filter length (cm)

$\rho$ = the density of the fiber ($gm/cm^3$)

$\delta$ = the fiber denier per filament (gm/9000 m.)

T = the total denier of the filter (gm/9000 m.)

A second, more realistic computation utilizes the pressure drop of the filter to compute an "effective" fiber radius. This essentially accounts not only for the irregularity of the fiber cross section, but also for the non-uniformity of fiber distribution and fiber touching. Keith, Reynolds, and Dalton ("The Pressure Drop of Cigarette Filters, A Theoretical Development", Paper presented at the 21st Tobacco Chemists Research Conference, Durham, N. C., October 19-20, 1967) presented an equation which closely predicts the pressure drop of conventional cigarette filters.

This was:

$$\Delta p = \frac{K \cdot Q \cdot L}{F \cdot \delta} \cdot \frac{S_x}{bS_o} \cdot \frac{\alpha}{(2\alpha^2-1-\ln\alpha)+(4\alpha-3\alpha^2-2-\ln\alpha)\cos\theta} \qquad (62)$$

Where: $\Delta p$ is the filter pressure drop in mm $H_2O$

$Q$ is the volumetric flow rate in $cm^3/sec$

$S_x$ is the specific surface area of the fiber in $cm^2/gm$

$b$ is an agglomeration factor (unitless)

$S_o$ is the specific surface area of cylindrical fibers of equivalent dpf

$\theta$ is the crimp angle, $\cos\theta = \frac{TL}{9x10^5 W}$

$L$, $F$, $\delta$, $\alpha$, $T$, and $W$ are as indicated previously.

If we incorporate all irregularities in $\alpha$, i.e., adjust the fiber radius to include non-circularity, non-uniformity and fiber touching, the term $S_x/bS_o$ goes to unity. Similarly $\alpha/\delta$ can be replaced by $1/A^2$ with an appropriate change in the constant K. Rearranging to an equation which needs to be solved for $\alpha$, we have:

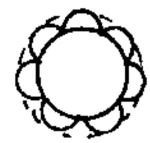
$$(2-3\cos\theta)\alpha^2 - (1+\cos\theta)\ln\alpha + 4\cos\theta\alpha - (1+2\cos\theta + \frac{KQL}{F \cdot A^2 \cdot \Delta p}) = 0 \quad (63)$$

Again, the most convenient solution is provided by Newton's rule, as outlined in equations (32) - (35). The operational function Z is defined as the left hand side of (63), and the initial approximation of $\alpha$ is provided by (60). The final $\alpha$ values are generally .04 to .05 units greater than the initial values. These can be transformed into an "effective" fiber radius by using equation (61).

A second method of computing an "effective" fiber radius is to consider the fibers as regular geometric shapes. A few examples of such regular shapes are given in Table 1. Using surface area (i.e., perimeter) and dpf data

Table 1

Regular Shape Approximations of Fiber Cross Sections

| Nominal Fiber Cross Section | Approximation | |
|---|---|---|
| Regular | Central circle with n semi-circular lobes |  |
| Y | Equilateral triangle, 3 rectangles, and 3 semi-circles |  |
| I | Rectangle and 4 semi-circles |  |
| X | Square, 4 rectangles, and 4 semi-circles |  |

allows a computation of the radius, a, of the circle circumscribed about the shape approximation. An example for a Y cross section fiber will suffice to demonstrate this type of computation.

$$\frac{S_x \cdot \delta}{9 \times 10^5} = \text{Perimeter} = 6\ell + \frac{3}{2}\pi m$$

Where $\ell$ = the length of the rectangle

$m$ = the width of the rectangle

$$\frac{\delta}{9 \times 10^5 \rho} = \text{Fiber Area} = 3\ell m + \frac{3}{8}\pi m^2 + .433m^2 \qquad (65)$$

Solving the simultaneous equations (64) and (65) provides values of $\ell$ and m. The "effective" fiber radius a is then the radius of the circle circumscribed about the regular geometric shape and is given by:

$$a = .289\ m + \ell + \frac{m}{2} \qquad (66)$$

These values of a can be combined with the known channel radii to compute effective $\alpha$ values.

Utilization of these "effective" fiber radii and $\alpha$ values in (59) provides a single fiber filtration efficiency for non-circular fibers.

5. Particle Size Distribution

Since the single fiber filtration efficiency computed in (59) is dependent on particle radius, it is necessary to approximate the particle size distribution of smoke to properly weight the filtration of different sizes. From Keith and Derrick's data (J. Colloid Sci., 15, 340-356, 1960) a close approximation to the measured size distribution of unfiltered tobacco smoke is given by a highly skewed Beta distribution between particle diameters of .1 and 1.1 microns. The appropriate function is

$$\text{No. of particles} = \text{Const.} \cdot (r_p - .05) \cdot (.55 - r_p)^9 \qquad (67)$$

This function goes to zero at diameters of .1 and 1.1 microns and is peaked at a diameter of .2 micron. Since filtration is a mass removal process, it is necessary to convert this number distribution to a mass distribution by multiplication by $r_p^3$.

$$\text{Mass of particles} = \text{Const.} \cdot (r_p - .05) \cdot (.55 - r_p)^9 \cdot r_p^3 \qquad (68)$$

6. Integration

Since filtration efficiency is defined as the ratio of the weight of smoke removed by a filter to the weight presented to the filter, the single fiber efficiency would be obtained by the equation

$$e_f = \frac{\int_{.05}^{.55} (r_p-.05)(.55-r_p)^9 \cdot r_p^3 \cdot \frac{(1+I')(r_p+r_d)^2}{A^2 \cdot \alpha^{\frac{1}{2}}} \cdot \frac{1}{1+\frac{1}{2}\frac{(1+\alpha)}{(1-\alpha)}\ln\alpha} \cdot dr_p}{\int_{.05}^{.55} (r_p-.05)(.55-r_p)^9 \, r_p^3 \, dr_p} \qquad (69)$$

Although it is technically possible to analytically integrate this if an appropriate function describing $r_d$ in terms of $r_p$ is empirically determined, the considerable number of terms (66) involved makes it easier to use approximate numerical integration techniques. A Simpson's Rule integration computer program (CAC program SMPSNX***) was adapted for this purpose. This uses 64 intervals and provides an integrand accurate to within $\pm$.04%. It should be noted that the quality of this integration is important as the result will be multiplied many fold to obtain the final filtration efficiency.

7. Calculation of Overall Efficiency

Since the fibers are reasonably randomly oriented throughout a real filter, the chance of encountering another fiber is equivalent in all directions, so that the fiber-to-fiber spacing should be 2A in the longitudinal as well as transverse directions. Since the smoke stream crosses individual fibers at a 90° angle, the path of the stream should follow a zig-zag pattern in going through the filter. The length of the path is thus $L/\cos\theta$, and $L/2A\cos\theta$ fibers should be encountered during the passage of the stream through the filter, each having an efficiency $e_f$.

As indicated by Fordyce et al (Tob. Sci., 5, 70-75 (1961), each fiber does not remove a constant fraction of the total stream, but increasing the number of fibers or length of the filter causes a logarithmic increase in filtration. This can be demonstrated by conducting a stepwise filtration computation. The first fiber in the filter removes a fraction $e_f$ of the influent smoke, so that the fraction passing this fiber is $1-e_f$. The second fiber removed $e_f(1-e_f)$ of the original stream, so that the fraction passing is $1-e_f - e_f(1-e_f)$ or $(1-e_f)^2$ of the original quantity. Similarly the third fiber removes $e_f(1-e_f)^2$ and allows $(1-e_f)^2 - e_f(1-e_f)^2$ or $(1-e_f)^3$ to pass. Continuing this to the last or $L/2A^{th}$ fiber gives an effluent fraction which is $(1-e_f)^{L/2A\cos\theta}$. If E is the overall efficiency of the filter, the effluent fraction is also equal to 1-E, so that $1-E = (1-e_f)^{L/2A\cos\theta}$. (70)

Converting this to a logarithmic form gives an equation similar to that advanced by Fordyce et al.

$$\ln(1-E) = \frac{L}{2A\cos\theta}\ln(1-e_f) \qquad (71)$$

or: $E = 100 \cdot \left\{1-e^{L\cdot\ln(1-e_f)/2A\cos\theta}\right\}$

A final minor correction to the particle removal efficiency should be made, this involving the small (3%) amount of smoke left in the filter at the end of the puff. This residual smoke settles out on the filter surface during the interval between puffs. Letting $V_f$ = the volume of the filter, and for a 35 ml puff, we have:

$$E_{corr.} = \left\{ \frac{E}{100} \cdot (1 - V_f/35) + V_f/35 \right\} \cdot 100 \qquad (72)$$

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