LETTERS TO THE EDITOR

To the Editor:

Hartounian et al. December 1993, p. 1976, in their article titled "Effect of Temperature on the Phase Equilibrium of Aqueous Two-Phase Polymer Systems," characterize the polydispersity of polymers with the log-normal distribution of molar masses (the so-called Lansing-Kraemer function, Lansing and Kraemer, 1935):

$$F = \frac{1}{\beta\sqrt{\pi}} \exp\left(-\frac{1}{\beta^2} \ln^2 \frac{M}{M_0} \right) \qquad (1)$$

From this function, the number average molar mass of the polymer is determined to be

$$M_n = \int_{M=0}^{M=\infty} MF d\ln M = M_o e^{\beta^2/4} \qquad (2)$$

the mass-average molar mass is

$$M_w = (1/M_n) \int_{M=0}^{M=\infty} M^2 F d\ln M = M_o e^{3\beta^2/4} \qquad (3)$$

and, therefore, the "polydispersity" is:

$$b \equiv M_w / M_n = e^{\beta^2/2} \qquad (4)$$

Hartounian et al. present an incorrect expression for the polydispersity index. Incorrect versions for all three above expressions appear in earlier related articles of Sandler and his coworkers (such as Kang and Sandler, 1988).

In Hartounian et al. (1993) (and in the earlier articles), the parameters in the log-normal distribution, M_o and β, are recovered from reported values of the polydispersity index and the mass-average molar mass of dextran polymers. These values are used to construct a discrete analog of the polydisperse polymer through Hermitian quadrature.

Hermitian quadrature permits approximation of certain integrals through function evaluations at a few points. The quadrature formula is

$$M = \int_{-\infty}^{\infty} \exp(-x^2) G(x) dx \cong \sum_{k=1}^{n} (W_k/\sqrt{\pi}) G(x_k) \sqrt{\pi} \qquad (5)$$

Values of W_k and x_k for various numbers of quadrature points, n, are commonly available in mathematical tables. We have included $\sqrt{\pi}$ in this expression as a normalizing factor, since $\Sigma_k W_k = \sqrt{\pi}$ for all n. Apparently, Hartounian et al. interpret $G(x_k)\sqrt{\pi}$ as the molar mass of a discrete polymer component present at fraction $W_k/\sqrt{\pi}$.

If M in Eq. 5 is taken to be the number-average molar mass, M_n, then on manipulation of Eq. 2, the molar mass of the kth discrete component would be

$$M_k = M_o \exp(\beta x_k) \qquad (6)$$

and $W_k/\sqrt{\pi}$ should be interpreted as the *mole* fraction. It is also possible to rearrange Eq. 3 for the mass-average molar mass into the form of Eq. 5, in which case the molar mass of the kth discrete component would be

$$M_k = M_o b \exp(\beta x_k) \qquad (7)$$

and $W_k/\sqrt{\pi}$ should be interpreted as the *mass* fraction.

Hartounian et al. use Eq. 6 for the molar masses of the pseudo-components but report interpreting the fractions $W_k/\sqrt{\pi}$ as *mass* fractions. This process is apparently not self-consistent.

Consider the Dextran 500,000 (M_w = 500,000) with polydispersity index b = 2.75 (corresponding to $M_n = 181{,}818$) that is described by Hartounian et al. If three discrete pseudo-components are determined from the mass-average molar mass, their *mass* fractions are 1/6, 2/3 and 1/6 with molar masses of 52,812 301,511 and 1,721,371. This mixture of pseudo-components has M_w = 496,705 and $M_n = 183{,}024$, values that are close to, but that do not match exactly, the original quantities.

If the same dextran is divided into pseudo-components using Hermitian quadrature for the number-average molar mass, the components have *mole* fractions of 1/6, 2/3 and 1/6 with molar masses of 19,204, 109,640 and 625,953. This discrete mixture has M_w = 406,260 and $M_n = 180{,}619$.

The molar masses of the pseudo-components used by Hartounian et al. are 2.06×10^5, 8.40×10^5, and 2.08×10^6. Taking the *mass* fractions as 1/6, 2/3, and 1/6, we calculate M_w = 941,000 and M_n = 594,233 for this mixture, values quite different from the original polymer information. We are not sure how Hartounian et al. arrived at the molar masses used in their article but there may be other considerations than the error noted in their equation for the polydispersity index or the noted internal inconsistencies of their method.

In any case, the rather extreme differences between the two characterizations we obtained (one based on the number-average molar mass and other on the mass-average molar mass), in our view, expose a certain underlying arbitrariness and ambiguity in the use of quadrature as a procedure for setting up discrete analogs of a few components to represent a disperse polymer.

Literature cited

Kang, C. H., and S. I. Sandler, "Effects of Polydispersivity on the Phase Behaviour of Aqueous Two-Phase Polymer Systems," *Macromol.*, **21**, 3088 (1988).

Lansing, W. D., and E. O. Kraemer, "Molecular Weight Analysis of Mixtures by Sedimentation Equilibrium in the Svedberg Ultracentrifuge," *J. Am. Chem. Soc.*, **57**, 1369 (1935).

Robert A. Heidemann
Naveen Koak
Chemical and Petroleum Engineering
University of Calgary
Calgary, Alberta T2N 1N4, Canada

Reply:

Heidemann and Koak raise two questions in their letter. The first relates to whether the equations we use for the mass- and number-average molecular weights are correct, and the second with an interpretation of mass and mole fractions. The proper expression for the log normal or Lansing and Kraemer (1935) distribution is

$$f = \frac{1}{\beta\sqrt{\pi}} \frac{1}{M} \exp\left(- \frac{1}{\beta^2} \ln^2 \frac{M}{M_0} \right) \quad (1)$$

Kang and Sandler (1988), in a typographical error, omitted the factor of $(1/M)$ *in the pre-exponential term.* However, the distribution above was used for all our calculations. Further, as shown by Tung (1967) and others, the expressions we used for the mass- and number-average molecular weights and for the polydispersivity index of the Lansing-Kraemer distribution are correct. The same typographical error in Eq. 1 was repeated in the subsequent article by Hartounian et al. (1993), though again all other equations and our calculations are correct.

The Lansing-Kraemer distribution was originally written and used in terms of the molecular weight of each incremental range of mass fraction, as we have done. To do otherwise from analytical data is very difficult. For consistency the weight factors when using the quadrature method should then be interpreted as mass fractions, which is what we have done.

Literature cited

Tung, L. H., *Polymer Fractionation*, M. J. R. Cantow, ed., Academic Press, New York, p. 385 (1977).

Stanley I. Sandler
Dept. of Chemical Engineering
University of Delaware
Newark, DE 19716

To the Editor:

In the article titled "Direct Simulation of Turbulent Particle Transport in Electrostatic Precipitators" (November 1993, p. 1910), Soldati et al. mention our work. Therefore, I would like to make some comments or ask questions. (My coauthor Prof. Löffler died unexpectedly in January 1994.)

1. In the case of electrostatic precipitation particle separation occurs in an electrofluid (sometimes called electrohydrodynamical flowfield). The fluid phase consists of two subfluids: gas ions and neutral gas molecules. The dynamics of the former is described by Maxwell Equations, and the behavior of the latter is described by Navier-Stokes-Equations. As the authors say, the coupling between both is decisive but unfortunately not (yet) considered. The fundamental and excellent works on this topic had been published by *Shaugnessy and coworkers (1985, 1986),* but were not included in the reference of Soldati et al. Shaugnessy et al., in coupling the equation sets mentioned above, found that dedimensionalization leads to two dimensionless numbers: the Reynolds number and (what they call) the electrical Froude number. In my opinion, the square of that number (Eq. 1) represents energies brought into the precipitator by the neutral fluid (ρv^2) and by the electrical field ($j2s/b \sim QU$). Therefore, the definition of the electrical Froude number (Eq. 9) by Soldati et al. could be confusing (in Mechanical Process Engineering a particle Froude number sometimes is used in analogy to the classical Froude number which characterizes a pressure ratio in fluids).

$$Fr_{el}^2 = \frac{b \cdot \rho_F \cdot v_0^2}{j_{NE} \cdot 2s} \quad (1)$$

2. The "electrical Froude number" and the particle relaxation time as introduced by Soldati et al. look slightly different as usual (Friedlander, 1977). This is presumably caused by dedimensionalizing the equation of particle motion with the shear velocity and the kinematic viscosity. Otherwise, one would get (Riehle, 1992):

$$m_p \frac{d\vec{w}}{dt} = 3\pi\eta d_p(\vec{v} - \vec{w})\left(\cdot \frac{1}{Cu} \right) + Q_p^\infty \vec{E} \quad (2a)$$

$$\frac{d\vec{w}'}{dt'} = \xi(\vec{v}' - \vec{w}') + \zeta \vec{E}' \quad (2b)$$

with

$$\xi = \frac{18\eta}{\rho_p d_p^2} \cdot \frac{s}{v_0}\left(\cdot \frac{1}{Cu} \right) = \frac{s}{\tau_p \cdot v_0} = \frac{1}{\Psi} \quad (3)$$

$$\zeta = \frac{Q_p^\infty E_{ps}}{\rho_p \frac{\pi}{6} d_p^3} \cdot \frac{s}{v_0^2} \quad (4)$$

$$\vec{w}' = \vec{w}/v_0, \quad \vec{v}' = \vec{v}/v_0,$$

$$\vec{E}' = \vec{E}/E_{ps}, \quad t' = t/(s/v_0)$$

where τ_p is relaxation parameter and Ψ the Stokes parameter, respectively, both well known in characterizing particle behavior (Friedlander, 1977; Löffler and Raasch, 1992). τ_p results when solving the equation of motion for fluid velocity zero (and without gravity) and it is the constant in the exponential function describing the time behavior of a particle (Eq. 5).

$$w(t) = w_{th}\left[1 - \exp\left(-\frac{t}{\tau_p} \right) \right] \quad (5)$$

Furthermore, it is difficult to understand Eq. 8 of Soldati's article which shows the dependence of the relaxation time on the Reynolds number, rather I can see its dependence on the Cunningham correction (function of particle diameter to mean free path of gas molecules), as shown in our Eq. 3.

3. Soldati et al. call the migration velocity w_e (Eq. 10) a reference velocity which may lead the reader to the assumption that this is equivalent to the so-called effective migration velocity. In this context, the authors refer to Riehle and Löffler's article (1992), from which they have not drawn the correct conclusions. Actually Eq. 10 represents a particle velocity called theoretical migration velocity which emerges as steady-state value w_{th} (our Eq. 5) when solving our Eq. 2 with gas velocity zero. It should be clarified (Riehle and Löffler, 1992) that while the theoretical migration velocity can really describe the local movement of a particle for certain circumstances, the effective migration is *not* capable to do so.

I felt that Soldati et al. are confused about both things because they said: "the actual migration velocity decreases as particle collection proceeds" and "the actual migration velocity gives a measure of the mass transfer." The actual particle migration velocity has to decrease when moving downstream because the particles are increasingly closer to the walls, that is, they see a correspondingly decreasing electrical field (Riehle, 1992; Miller et al., 1993). The decrease in the electrical field is especially strong when calculating pure electrostatically, neglecting space charge (Miller et al., 1993). In industrial electrical precipitators, effective migration velocities (sectionalized) decrease with the precipitator length; however, it should be noted that this is a completely different issue since w_{eff} does *not* characterize particle transport in the fluid phase. It characterizes the mass flux toward the collecting plates (Riehle and Löffler, 1992; Riehle, 1994).

4. Finally, Soldati et al. refer to the Deutsch equation and the excellent work done by Self and coworkers. In this context, it is worth noting that the difference between the two extreme cases, Deutsch model and laminar model (covered by convective diffusion models with eddy diffusivities from infinity to zero), is surprisingly low in fractional efficiencies (Riehle and Löffler, 1991). We measured fractional efficiencies higher than the predictions of the Deutsch model too, in the fine particle even higher than the predictions of the laminar model (Riehle and Löffler, 1991, 1993). This trend can be verified by simulation of efficiencies by calculating particle trajectories (Riehle, 1992) similar to work presented here.

Self et al. proposed to term the exponent in the Deutsch model "Deutsch number" (Eq. 12), but I think it is not correct to say that the "Deutsch number represents a dimensionless length" for several reasons. For example, the ratio x/d already is a dimensionless length. And one dimensionless number can be multiplied by another arbitrary one. Obviously the product remains dimensionless, but its meaning will not remain that of a length in general. The second ratio in Eq. 12 is formed by two velocities: the theoretical migration velocity (characterizing the local particle transport toward the collecting plates) and the mean gas velocity (usually identical with the particle velocity in main gas flow direction). Therefore, this ratio of velocities can be interpreted as a ratio characterizing the particle transport conditions perpendicular to each other (cross flow to main flow). In analogy to the Stokes parameter in inertial separators we termed this ratio electrical drift parameter (Riehle, 1992; Riehle and Löffler, 1993). Combining both ratios as it happens in the Deutsch exponent therefore has to be interpreted as a ratio of times. We called it dimensionless residence time of a particle (w_{th} is a function of particle size) because x/v_0 is the time a particle (or a fluid element) needs to pass the precipitation zone and s/w_{th} is the critical time for a particle of size d_p if it is to be deposited at the collecting plates. [This simple idea implies straight particle trajectories as happening in laminar flows; therefore, it does not match reality, but it helps its interpretation (Riehle and Löffler, 1993).]

5. Soldati et al. do not mention the equation with which the particle charge was calculated. We use the well-known Cochet equation and calculated for the values in Table 1 (assuming an electrical permittivity of $\epsilon_r = 10$) a theoretical migration velocity w_{th} (4μm, 2.4 kV/cm) = 9.8 cm/s which is 94% more than 5.05 cm/s. What's the reason for that?

Literature cited

Friedlander, S. K., *Smoke, Dust and Haze*, Wiley, New York (1977).

Löffler, F., and J. Raasch, *Grundlagen der Mechanischen Verfahrenstechnik*, Vieweg (1992).

Miller, J., C. Riehle, A. J. Schwab, and F. Löffler, "Numerical Field Calculations in Electrostatic Precipitators with Respect to Electrically Similar Operating Conditions," *J. of Electrostatics*, **33**, 213 (1994).

Riehle, C., "Bewegung und Abscheidung von Partikeln im Elektrofilter," Diss. Universität Karlsruhe (1992).

Riehle, C., "Mass Flux and Effective Migration Velocity in Electrical Precipitators," *Powder Technol.*, submitted (1993).

Riehle, C., and F. Löffler, "The Effective Migration Rate in Electrostatic Precipitators," *Aerosol. Sci. & Technol.*, **16**, 1 (1992).

Riehle, C., and F. Löffler, "Grade Efficiency and Eddy Diffusivity Models," *Proc. of Symp. on Transfer and Utilization of Particulate Control Technology*, Williamsburg, VA (1991).

Riehle, C., and F. Löffler, "Grade Efficiency in Electrical Precipitators of Different Size," *Proc. Symp. on Particulate Control Technology and Int. Conf. Electr. Precipitation*, Washington, DC (Apr., 1993).

Riehle, C., and F. Löffler, "Reflections on Similarity Laws Concerning Particle Transport in Electrical Precipitators," *Powder Technol.*, **77**, 201 (1993).

Self, S. A., M. Mitchner, K. D. Khim, D. H. Choi, and R. Leach, "Effect of Turbulence on Precipitator Performance," *Proc. Int. Conf. Electr. Precip.*, Kyoto, Japan, p. 249 (1984).

Shaughnessy, E. J., J. H. Davidson, and J. C. Hay, "The Fluid Mechanics of Electrostatic Precipitators," *Aerosol Sci. & Technol.*, **4**, 471 (1985).

Shaughnessy, E. J., and J. H. Davidson, "Turbulence Generation by Electrical Body Forces," *Exp. in Fluids*, **4**, 17 (1986).

Claus Riehle
Bayer AG, ZF-TVG3/E41
Partikel-u., Stroemungstechnik
D-51368, Leverkusen, Germany

Reply:

In his analysis of our article titled "Direct Simulation of Turbulent Particle Transport in Electrostatic Precipitators" (December 1993, p. 1910), Dr. Riehle raises a number of points that, in his opinion, need to be clarified. Many of the comments are, however, matter of nomenclature and semantics. We will try to answer all the questions and to clarify the doubts about the consistency of the definitions we adopt. We will respond to Dr. Riehle's remarks in the numerical order he listed.

1. In our article, the transport of aerosol particles was computed in the numerically simulated turbulent flow field under the action of different electrostatic fields. The electrostatic body force was acting only on particles and did not modify the flow field. Consequently, no electrohydrodynamic effect was considered. Therefore, it does not seem appropriate to cite the work done by Shaughnessy et al. (1985) and Davidson and Shaughnessy (1986) to argue about our definition of the particle electrostatic Froude number, Fr_p (where p stands for particle). As a matter of fact, there cannot be any confusion since the contexts are different. We use Fr_p in the particle dynamics equation to quantify the effect of the electrical force compared to the inertial one. Shaughnessy et al. (1985) define F as a measure of the square root of the ratio of the inertial force to the electric body force *acting on the fluid parcel*. The same dimensionless quantity was found also in previous works (Leonard et al., 1983) from a proper nondimensionalization of the momentum balance equations for the fluid considering the electrostatic body force term. In any case, when we define the particle electrical Froude number and it is clearly stated in the Notation section that it represents the square root of the ratio of the inertial force to the electrostatic force *acting on the aerosol particle*.

2. The particle relaxation time, defined elsewhere as the particle time constant or the particle characteristic time, gives a measure of the time necessary to a particle to adapt itself to a modification of the surrounding flow field. This time characterizes particle inertia compared to the fluid drag. In the Stokes regime [$Re_p = (|\vec{u} - \vec{v}|d_p)/\nu_f < 1$] with only viscous and inertial forces acting, the particle relaxation time has the form

$$\tau_p = \frac{d_p^2 \rho_p}{18 \mu_f}. \tag{1}$$

However, for larger particle Reynolds number out of the Stokes regime, the operative definition of τ_p changes and its value can be estimated from the measured particle drag (Rogers and Eaton, 1991). Since we used the relation proposed by Rowe and Henwood (1961) to evaluate the fluid dynamic drag, we defined the particle time constant as:

$$\tau_p = \frac{d_p^2 \rho_p}{18\mu_f} \frac{1}{1.+0.15Re_p^{.697}}. \qquad (2)$$

The dependence on the particle Reynolds number has to be introduced to account for the modification of the drag force since the particle is not in the Stokes regime. Similar definitions can be found in other works (Rogers and Eaton, 1991; Elgobashi and Truesdell, 1993).

About the Cunningham factor, it gives account of the particle/air slip modification due to the particle diameter and the air molecule's mean free path becoming of comparable magnitude. Usually, the Cunningham factor is employed for particles of size smaller than 1 μm in air. Dr. Riehle would like to see the Cunningham factor included in the drag coefficient, but our particles are a bit too large to be affected by such phenomenon. In our analysis, the particle diameter is about two orders of magnitude larger than the air molecules mean free path, giving a negligible correction to the drag force.

3. We cannot possibly have misled the reader in the use of the term migration velocity that is defined without any ambiguity in the article. We used the migration velocity as a reference velocity obtained balancing at steady state, the Stokes drag and the Coulomb force. The term migration velocity does not belong to the jargon of electrostatic precipitation, but it is commonly used in the field of particle dispersion to characterize phenomena like gravity settling or velocity profile effects (Cherukat and McLaughlin, 1990). Riehle and Löffler (1992) used the term *effective migration velocity* (which we did not use) to define the average velocity that particles would have *if* the collection process followed a Deutsch-type equation. This effective migration velocity is indeed determined *a posteriori*, once the collection efficiency is known (experimentally). This is why the effective migration velocity characterizes the mass flux toward the collecting electrodes.

We referred to the work by Riehle and Löffler (1992) to identify an approach completely different from ours. What we call *actual migration velocity* is the particle velocity toward the plate-electrodes as measured from the direct simulation results. The actual migration velocity quantifies the local movement of the particles in the flow field *and* the specific mass flux toward the collecting electrodes.

4. Unfortunately, we do not know of the papers cited by Dr. Riehle (not available in the archival literature). However, at low Deutsch number (*De*) we calculated efficiencies higher than the Deutsch line and extremely close to the limit of the laminar model.

Regarding the definition of *De*, we would like Dr. Riehle to observe that his very same arguments about our interpretation of *De* hold for the one he proposes. We prefer to attribute to *De* the meaning of the nondimensional distance covered by particles in the flow direction. This interpretation appears also in the work by Self et al. (1987) and Kihm et al. (1987), which Dr. Riehle apparently knows.

5. The last equation seems out of context. It is clearly said that in our simulation we neglect all phenomena connected with the ionic discharge and that particles enter the duct precharged. Since we execute a simulation, the charge on each particle is freely assignable (like, for example, with a precharger) with the only constraint being to obtain a reasonable migration velocity, that is, comparable with the one used in the experiments to be simulated. As a reference, we decided to assign the particle charge as if it derived from a field-charging mechanism. To determine the charge on each particle we used the following field charging equation:

$$q_p = 3\pi \frac{\epsilon}{\epsilon + 2} \epsilon_0 |\vec{E}| d_p^2. \qquad (3)$$

In this equation, ϵ_0 is the permittivity of vacuum, $\vec{E}$ is the electrostatic field vector, and ϵ is the dielectric constant of the particle. We simulated a dispersion of an aerosol of oleic acid for which ϵ is about 2. This gives the basis for the numbers we used.

We hope that all the questions posed by Dr. Riehle are answered and thank him for giving us the opportunity to discuss these issues.

Literature cited

Cherukat, P., and J. B. McLaughlin, "Wall-Induced Lift on a Sphere," *Int. J. Multiphase Flow*, **16**, 899 (1990).

Davidson, J. H., and E. J. Shaughnessy, "Turbulence Generation by Electric Body Forces," *Exp. Fluids*, **4**, 17 (1986).

Elgobashi, S., and G. C. Truesdell, "On the Two-Way Interaction between Homogeneous Turbulence and Dispersed Solid Particles," *Phys. Fluids*, **A5**, 1790 (1993).

Kihm, K. D., M. Mitchner, and S. A. Self, "Comparison of Wire-Plate and Plate-Plate Electrostatic Precipitators in Turbulent Flow," *J. of Electrostatics*, **19**, 21 (1987).

Leonard, G. L., M. Mitchner, and S. A. Self, "An Experimental Study of the Electrohydrodynamic Flow in Electrostatic Precipitators," *J. Fluid Mech.*, **127**, 123 (1983).

Riehle, C., and F. Löffler, "The Effective Migration Rate in Electrostatic Precipitators," *Aerosol. Sci. Technol.*, **16**, 1 (1992).

Rogers, C. B., and J. K. Eaton, "The Effect of Small Particles on Fluid Turbulence in a Flat-plate, Turbulent Boundary Layer in Air," *Phys. Fluids*, **A3**, 928 (1991).

Rowe, P. N., and G. A. Henwood, "Drag Forces in Hydraulic Model of a Fluidised Bed: I," *Trans. Instn. Chem. Engrs.*, **39**, 43 (1961).

Self, S. A., K. D. Kihm, and M. Mitchner, "Precipitator Performance Improvement Through Turbulence Control," *Int. Conf. Electrostatic Precipitators*, Avano/Venice, Italy (1987).

Shaughnessy, E. J., J. H. Davidson, and J. C. Hay, "The Fluid Mechanics of Electrostatic Precipitators," *Aerosol Sci. Technol.*, **4**, 471 (1985).

Alfredo Soldati
Paolo Andreussi
Dip. di Scienze e Tecnologie Chimiche
Università di Udine
33100 Udine, Italy
Sanjoy Banerjee
Dept. of Chemical and Nuclear Engineering,
University of California,
Santa Barbara, CA 93106