values of \((f_k, k)\) and \((1 - m)\) are never positive so that the second moment divided at \(2\pi^2\) equals
\[
\sum_{k_1} \sum_{k_2} x^{(k_1 - k_2)} = 3 + x. \tag{11}
\]

**NUMERIC MULTIPLICATION**

For the same example

<table>
<thead>
<tr>
<th>Matrix</th>
<th>1</th>
<th>0</th>
</tr>
</thead>
<tbody>
<tr>
<td>(A^{-1})</td>
<td>1</td>
<td>(A^{-1} \delta_{i,k}) vector</td>
</tr>
<tr>
<td>(A^{-1})</td>
<td>1</td>
<td>(1 + x )</td>
</tr>
<tr>
<td>(A^{-1})</td>
<td>1</td>
<td>(3 + x )</td>
</tr>
<tr>
<td>(\delta_{m,k})</td>
<td>0</td>
<td>3 + x</td>
</tr>
</tbody>
</table>

**REFERENCES**


**Solution of population balance equations**

(First received 13 October 1970; accepted 26 October 1970)

The general population balance equation for a particulate system in which the individual particle property is a vector \(X = (X_1, X_2, \ldots, X_n)\) with some range \(V\) in the \(n\)-dimensional property space is given by [1].

\[
\frac{\partial W_X}{\partial t} + \nabla \cdot [\mathbf{X} W_X] = h(W_X, t). \tag{1}
\]

In Eq. (1) \(W_X(x, t)\) is the density of the distribution of particles in \(V\) and \(t\); \(\mathbf{X}\) is the rate of change of property \(X\); the operator on the left hand side of Eq. (1) is a "continuity operator" and the nonzero right hand side reflects the possibility of "spontaneous creation and destruction" of particles in this space. The functional \(h(W_X, t)\) represents the net rate of appearance of new particles with property \(x\). Equation (1) written for the particulate phase may be coupled with another for the continuous phase, when interactions exist between the two phases.

The form of the functional \(h(W_X, t)\) depends on the specific processes by which particles appear and disappear from the system. Generally \(h\) is an integral expression involving \(W_X\) linearly as for fission processes[1, 2] or nonlinearly as for agglomeration processes[1, 3–5].

The solution of Eq. (1) for the general situation, in which particle property is a vector, is a difficult mathematical problem, especially when the equation is integro-differential in nature[2]. We shall restrict our discussion to scalar versions of Eq. (1).

A popular approach to the solution of PBE (for the scalar case) has been via the generation of moment equations directly.
from the PBE[1, 3, 6, 7]. Hulburt and Katz[1] have suggested an estimation of the unknown distribution from a few of its leading integral moments by a "suitably truncated" expansion of the distribution in terms of Laguerre functions. The coefficients of the Laguerre function expansion are related to the integral moments of the distribution in a simple manner. When the moment equations generated contain only integral moments and are also "closed" the solution of moment equations would then yield exact values of as many leading integral of interest. However, evaluation of the leading moments may not be possible when:

(i) The moment equations contain integral moments and are not "closed" (i.e. each moment equation contains higher moments which creates more unknowns than equations; e.g. See [8]).

(ii) The moment equations contain fractional moments[7].

(iii) No moment equations are obtainable directly from the PBE as, for example, in particle fission processes where asymmetric breakage is considered[9,10].

In all of the above situations the Laguerre function expansion suggested by Hulburt and Katz may, at least in principle, permit an approximate evaluation of the leading moments. Hulburt and Akiyama[7] provide a demonstration of this method for the coagulation of aerosols.

The method of moment equations together with a Laguerre function expansion of the distribution is actually a special case of a more general approach to the solution of PBE. This general approach is essentially the method of weighted residuals (MWR). An excellent review of MWR has been given by Finlayson and Scriven[11]. Consider the solution of a scalar version of Eq. (1):

\[ \frac{\partial W}{\partial t} + \frac{\partial}{\partial x}[\hat{W}] = h(W, t) \quad 0 < x < \infty \quad t > 0 \]  
\[ W(x, 0) = g(x). \]  

In MWR the unknown distribution \( W(x, t) \) is expanded in terms of a finite number of trial functions \( \{\varphi_n(x)\} \).

\[ W(x, t) = \sum_{n=1}^{N} C_n(t)\varphi_n(x) \]  
\[ W(x, 0) = \sum_{n=1}^{N} C_n(0)\varphi_n(x) = g(x). \]  

The \( \{\varphi_n(x)\} \) may preferably come from a complete set in an appropriate space to which \( W(x, t) \) belongs (say \( L_2[0, \infty) \) in this case). The trial functions have also been assumed to be time-independent although a more general formulation may eliminate this stipulation.

The trial solution (4) is then substituted into Eq. (2) to obtain a residual function \( R(x, t) \).

\[ R(x, t) = L\left( \sum_{n=1}^{N} C_n(t)\varphi_n(x) \right) - h\left( \sum_{n=1}^{N} C_n(t)\varphi_n(x), (t) \right) \]  

where \( I \) represents the continuity operator in the left hand side of Eq. (2). Also

\[ R(x, 0) = \sum_{n=1}^{N} C_n(0)\varphi_n(x) = g(x). \]  

The functions \( \{C_n(t)\} \) together with their initial values \( \{C_n(0)\} \) must be determined such that the residuals (5) and (6) are as close to zero as possible over the entire semi-infinite interval. The essence of MWR is to accomplish this by orthogonalizing the residuals with a set of functions \( \{\psi_n(x)\} \) also preferably from a complete set in \( L_2[0, \infty) \). Thus

\[ \int_{0}^{\infty} R(x, t)\psi_n(x) \, dx = 0 \quad n = 1, 2, \ldots, N \]  
\[ \int_{0}^{\infty} R(x, 0)\psi_n(x) \, dx = 0. \]  

Equations (7) will lead to a set of \( N \) ordinary differential equations in \( \{C_n(t)\} \) where initial conditions can be obtained from (8). The success of the method hinges on appropriate selection of the trial functions \( \{\varphi_n\} \) and the weighting functions \( \{\psi_n\} \). The number of weighting functions may sometimes be less than \( N \) by incorporation of any additional information available on the solution. Thus the vanishing of \( W(x, t) \) at \( x = 0 \) may yield an algebraic equation in \( \{C_n(t)\} \) requiring only \( (N - 1) \) differential equations and hence \( (N - 1) \) weighting functions.

It is easy to show that when the trial functions \( \{\varphi_n\} \) are taken equal to the Laguerre functions and the weighting functions \( \{\psi_n\} \) are given by

\[ \psi_n(x) = x^n \]  

Eqs. (7) reduce to the moment equations while Eqs. (8) provide the initial moments. Thus the method of moment equations along with a Laguerre function expansion for the distribution due to Hulburt and coworkers[1,7] is indeed a special case of MWR expressed by condition (9).

For the trial solution to satisfy Eq. (2) over the entire semi-infinite interval a proper combination of trial and weighting functions must be found. Thus when Laguerre functions are used as trial functions the choice of weighting functions according to (9) may not be appropriate for all situations. Other weighting functions could and should be tried.

Subramanian[9,10] has used MWR to solve PBE that arise in the description of a microbial population distributed according to their mass and which multiplies by binary fission. Asymmetric division was allowed so that the PBE was an integropartial differential equation involving a breakage kernel. Further, individual cell growth was assumed to depend on the concentration of a nutrient substance in the environment. Thus the PBE was also coupled with an equation for the continuous phase. Subramanian assumed that the trial functions were Laguerre functions and the weighting functions of the form

\[ \psi_n(x) = e^{-\lambda x} x^{n-1} \quad \lambda > 0. \]  

The solutions obtained with the above weighting functions were found to be sufficiently accurate by successive approximation using the generated solution as the initial approximation. Randolph[6] discusses problems in crystallization studies which are closely analogous to microbial systems; the method of moment equations however permitted solutions only under assumptions much more restrictive than those made by
Subramanian[9, 10]. Hulbert and Akiyama observe that the solutions to PBE which arise in the description of Brownian coagulation could be solved by the method of moment equations introducing a Laguerre function expansion for the fractional moments, except when the initial distribution was broadly disperse[7]. This shows that the weighting functions (9) do not provide for an adequate weighting operation for the entire semi-infinite interval and alternative choices must be considered.

Very recently, Bramlette and Mallette have used MWR techniques for the solution of the Boltzmann equation for the linearized Couette flow problem[12].

The solution of PBE must clearly be viewed in the more general light of MWR of which the method of moment equations with a Laguerre function expansion of the distribution represents a special case. Thus the problem of obtaining solutions to PBE could be subjected to the many diverse ramifications of the method of weighted residuals[11]. It may also be worthwhile to investigate the convergence of MWR methods to the exact solutions of population balance equations.

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REFERENCES


Consistency conditions in the extended principle of corresponding states

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The principle of corresponding states, long used by engineers for the prediction of thermodynamic properties of fluids and fluid mixtures, has been extended by numerous investigators by including a third parameter in addition to the critical temperature and pressure (or volume). Although different third parameters are used, most extensions follow the general scheme of Pitzer[1] where a correction term proportional to the acentric factor, \( \omega \), is added to the thermodynamic property in question. This class of extension generally uses one thermodynamic property at a time in their derivation and involve no consistency conditions. However, their application to mixtures is not straightforward because the third parameter is defined only for pure components. Thus, an introduction of an empirical recipe to determine third parameters for mixtures becomes necessary. To overcome this shortcoming, Leland and his colleagues[2] introduced an extended principle of corresponding states based on shape factors which does not require the estimation of third parameters for mixtures. However, since simultaneous use of two the thermodynamic properties is used to determine two shape factors, \( \phi \) and \( \theta \), the dependence of \( \phi \) and \( \theta \) on volume and temperature, as pointed out by Rowlinson and Watson[3], is not arbitrary. This paper is devoted to the derivation of an explicit expression required thermodynamically for consistency between \( \phi \) and \( \theta \) and to a test for consistency for equation for \( \phi \) and \( \theta \) presented previously by Leland and his colleagues.

Leland and coworkers calculate shape factors by requiring that for two substances, 0 and 1,

\[
(t/P)_1 = (t/P)_0 \quad \text{and} \quad Z_1 = Z_0
\]

(1)

when

\[
T_1/\theta_{1.0} T_1^c = T_0/\theta_0^c \quad \text{and} \quad V_1/\phi_{1.0} V_1^c = V_0/V_0^c
\]

(2)

where the subscript, 0, refers to a reference substance and 1 refers to any other substance. Such an approach will yield