Characterization of arbitrary distributions—a new method

For a realistic evaluation of an arbitrary distribution, the fluctuations of the magnitudes as well as its spatial distribution have to be considered. Therefore, a new key figure (CoD—coefficient of distribution) has been found that is able to cover both attributes of the distribution/mixture. First tests with artificial tracer distributions as well as with tracer distributions gained from CFD-calculations show reasonable results. The new key figure provides a realistic evaluation of any arbitrary distribution. The use of this powerful tool can, therefore, improve the possibilities in the design and development phase of products as well as help create more precise definitions for the requirements of the customers.

The mixing of components is one of the oldest processes within mechanical process engineering. Industrial mixing processes are challenging—especially for liquids and, in particular, for liquids with high viscosities. Since more mixing effort is necessary to achieve better homogeneity, the characterization of the state of the mixture is of special interest.

The homogeneity, or the degree of mixing, is commonly evaluated with figures that are based on statistical methods. A well-introduced and commonly accepted value is the CoV, the coefficient of variation, which describes the ratio between standard deviation and expectation.

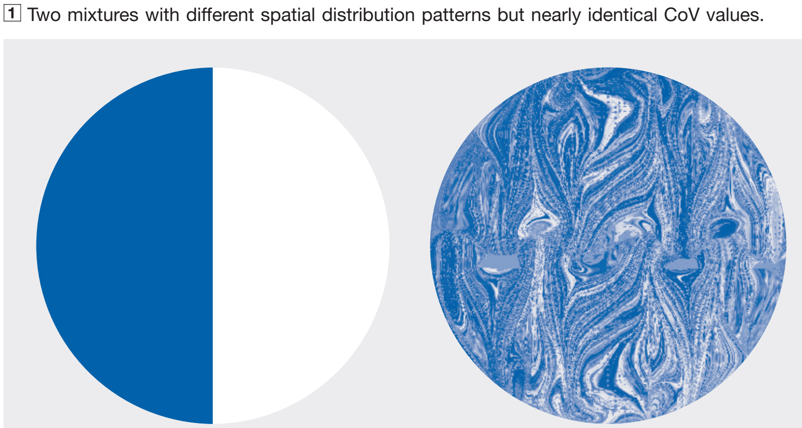
Since the CoV value is an averaged quantity over a region (area or space) and, therefore, not sensitive to spatial differences, a quantification of mixtures only with the CoV can sometimes lead to less expressiveness or to misconstructions. Mixtures that only differ within the spatial distribution of the describing quantities will lead to the same CoV value even though the properties of the mixtures are obviously different 1. In case of, e.g., chemical reactions, the different mixing states can lead to enormous differences in yield and composition.

Two mechanisms of mixing

Two mechanisms are able to increase the quality of the mixing—one is distributive mixing and the other is the diffusive equalization of differences within a concentration field. The latter is a spontaneous, unsolicited process that needs no additional energy to take place.

The result of the diffusive transport can be measured directly via the CoV value. However, as important as diffusive equalization is distributive mixing—the second mechanism for mixing processes. It is a requirement for effective mixing because it enlarges the contact area between higher and lower concentrated regions. Since diffusive transport is proportional to that contact area and to the concentration gradient, an increasing spatial distribution has a direct positive impact on the quality of the mixture and should, therefore, additionally have an impact on the quantity of the mixing quality.

1 Two mixtures with different spatial distribution patterns but nearly identical CoV values.



CoV for the diffusion—ϕ for the distribution

The aim is to have a single method with which to evaluate both mixing mechanisms: diffusive transport and distributive mixing. To incorporate both mechanisms, several artificial tracer distributions have been analyzed. Figure 2 shows nine different mixed situations differing in mixedness and spatial distribution. On the vertical axis, the CoV value decreases, since the state becomes more mixed due to an equalization of the values (simulating a diffusive transport mechanism). In these cases, the spatial distribution remains constant. On the horizontal axis, the CoV value remains constant, but the length scale on which segregation occurs, decreases; therefore, the spatial distribution of the tracer increases in the horizontal direction (simulating distributive mixing processes).

The diffusive equalization can be quantified with the coefficient of variation. Applied to the artificial distributions in figure 2, the mixedness in the first row has a CoV value of 100%, the second row of 60%, and the third of 20%. These values are independent of the spatial distribution.

In this example, the size of the colored squares serves the purpose of characterizing the length scale on which these fluctuations occur. The smaller the individual squares are, the better the distribution is. A good measure of the size of these squares is the length of the contact line between regions of different concentrations. In real cases, this contact line (or contact area) is of special interest as well, since diffusive and dispersive equalization strongly depend on it. The length of contact line is made dimensionless by relating it to a characteristic length scale, e.g., the hydraulic diameter. Applied to the different distributions in figure 2, this dimensionless number ϕ is 2 (=16/8) for the right column, 6 (=48/8) for the middle column, and 14 (=112/8) for the left column. The respective width of each square is 8. These values are independent of the degree of mixing or CoV.

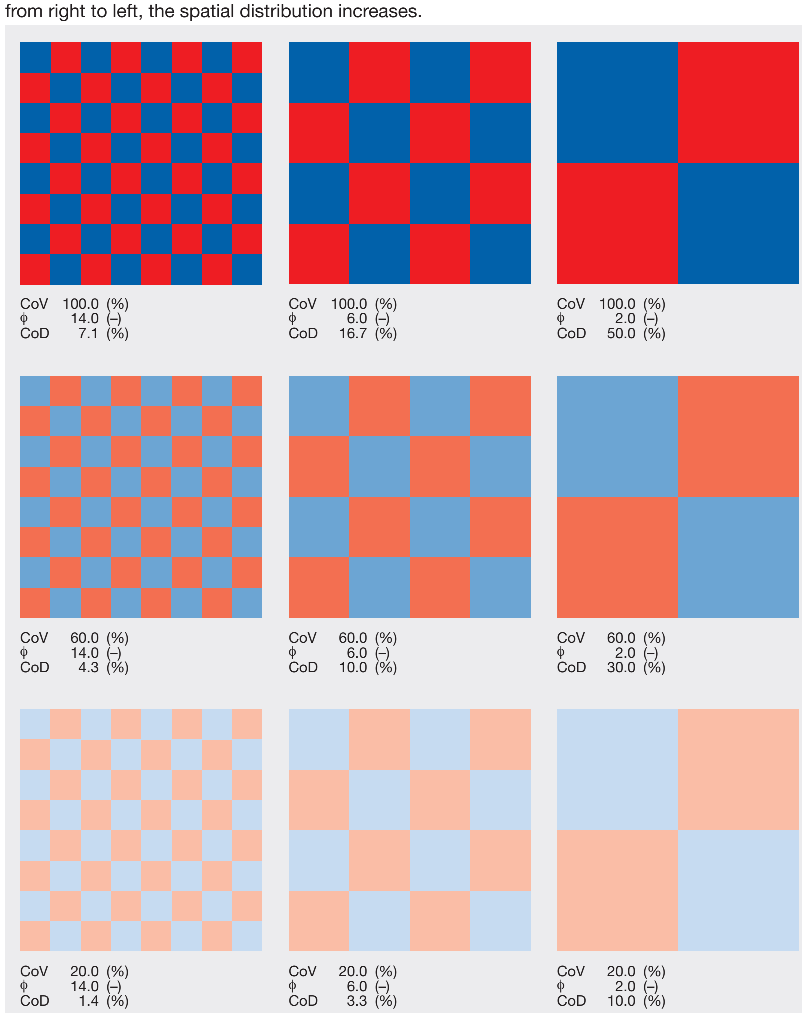
CoD for comparing distributions of different degrees and extents of mixing

Here, two key figures are available to characterize different aspects of a scalar distribution—the commonly used CoV value, used to characterize the magnitude of the fluctuations, and the ϕ value, used to characterize the spatial distribution. The combination of both values leads intuitively to the definition of the coefficient of distribution (CoD)—being the quotient of the CoV and the ϕ value—and allows distributions of different mixing degrees and extents (diagonal directions within figure 2) to be compared. The value of the coefficient of distribution (combining diffusive and distributive mixing effects) in figure 2 ranges from 50% for the worst mixing state down to approx. 1% for the best mixing state (bottom, left).

In contrast to the situation in artificial distributions like this example, in real systems, the contact line is not necessarily easy to determine. Here, measure theory helps. It is known that for a completely segregated system, the integration of the norm of the gradient of a normalized value leads exactly to the length of its contact line (between value 0 and value 1). Applied to real systems, the distributions will be made dimensionless and be scaled by a division by 2 σ. The characteristic length scale is obtained as the ratio of cross section and hydraulic diameter. The fundamental formulas can be seen within figure 3.

A restriction for the calculation of the length of the contact line appears for systems with a massive increasing diffusive equalization. There, the contact line loses its significance, but the values achieved get smaller, so the key value of the CoD is conservative.

2 Sketches of different artificial tracer distributions. From top to bottom, the mixedness increases; from right to left, the spatial distribution increases.



Formula	Scalar quantity	Vectorial quantity
Mean value	$\bar{c} = \frac{1}{n}\sum_i c_i$	$\bar{\vec{u}} = \frac{1}{n}\sum_i \vec{u}_i$
Standard deviation	$\sigma = \sqrt{\frac{1}{\|A\|}\int_A (c-\bar{c})^2 dA}$	$\sigma = \sqrt{\frac{1}{\|A\|}\int_A (\vec{u}-\bar{\vec{u}})^2 dA}$
Coefficient of variation	$CoV = \frac{\sigma}{\bar{c}}$	$CoV = \frac{\sigma}{\|\bar{u}_{FD}\|}$
Norm of the gradient	$\\|\nabla c\\|_2 = \sqrt{\sum_i (\partial_i c)^2}$	$\\|\nabla \vec{u}\\|_2 = \sqrt{\sum_i \sum_j (\partial_i u_j)^2}$
Length scale	$\phi = \frac{\ell}{\ell_{ref}} = \frac{d_h}{A} \frac{\int_A \\|\nabla c\\|_2 dA}{2\sigma}$	$\phi = \frac{\ell}{\ell_{ref}} = \frac{d_h}{A} \frac{\int_A \\|\nabla \vec{u}\\|_2 dA}{2\sigma}$
Coefficient of distribution	$CoD = \frac{CoV}{\phi}$	$CoD = \frac{CoV}{\phi}$

3 Formulas that are necessary in order to calculate the new key value for characterizing a mixture, the coefficient of distribution.

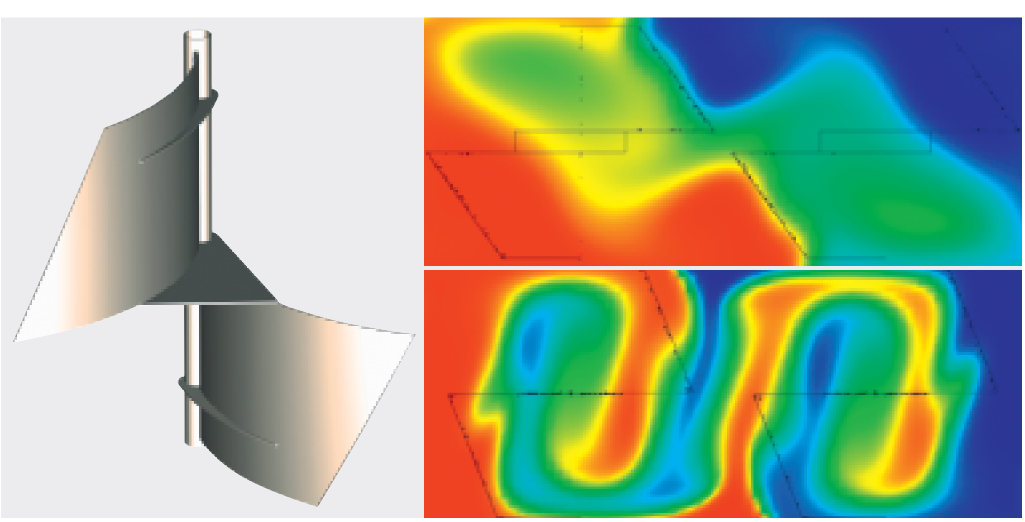
Application to industrial relevant cases

The applicability of the theory developed above can be tested using results gained form CFD calculations. In figure 4, left, tracer distributions gained from mixing processes with alternative ContourMixer™ designs (by Sulzer Chemtech) can be seen. The starting distribution of the tracer was the same in both cases: a totally segregated system with tracer concentration of unity in the left half of the channel and zero in the right half (1 left). 4 (right, top and bottom) shows the distributions on a cross section of the channel at some distance behind the mixing devices. Although the CoV value is nearly identical in both cases (70%), one would intuitively think that the bottom one is better mixed. By incorporating the concept of length of the contact line, one can calculate that the quality of these two distributions differs by a factor of three.

The concept of evaluating the distribution of magnitudes together with the spatial distributions of the quantity of a given distribution is not limited to scalar distributions like concentration or temperature fields, but can also be applied to vectorial distributions like velocity fields.

The new key figure, the coefficient of distribution (CoD) is a powerful tool to be able to give a realistic evaluation of any arbitrary distribution. This advancement opens new possibilities in the design and development phase of products and helps create more precise definitions for the requirements of the customers.

4 Different designs have been tested for the Sulzer Chemtech Contour™ Mixer (left), a static mixer for high turbulent gas flows. For two of the designs, tracer distributions after the mixer are shown (right). In both cases, there was a start configuration of left/red – right/blue.



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