

# On the potential utility of $2 \times 2$ contingency tables in electrochemical engineering

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**Abstract**  $2 \times 2$  contingency tables are widely used in the statistical analysis of categorical data grouped according to certain (mutually exclusive) attributes, characters or quality. The paper describes three specific applications to electrochemical engineering, employing (i) Fisher's exact test for electrolyzer selection; (ii) the McNemar test to determine improvement in current efficiency, and (iii) the Mantel–Haenszel test to evaluate electrolyzer performance. The subject matter represents a cross-fertilization of two disciplines to facilitate statistically backed design decisions and performance analysis.

**Keywords** Electrolyzers · Electrocatalysts · Contingency tables · Statistical decision

## Nomenclature

$a, b, c, d$	Cell elements of a $2 \times 2$ contingency table
$A, B$	Event categories
$c_1, c_2$	Column sums of the cell elements
$CE$	Current efficiency
$C[m;n]$	Binomial coefficient (also known as combination) defined as $m!/[n!(m-n)!]$
EE	Electrochemical engineering
ERE	Electrochemical reaction engineering
$E[X]$	Expectation of (random) variable $X$
$F_N(z)$	Cumulative distribution function of the standardized normal variate $z$
$k$	Stratum index
$MH$	Mantel–Haenszel statistic
$m, n$	Sample or observation size

$n_{AA}; n_{BB}$	Diagonal elements of a contingency table for paired data dichotomous response test
$n_{AB}; n_{BA}$	Off-diagonal elements of a contingency table for paired data dichotomous response test
$N_k$	Observation total in the $k$ -th stratum
$P[X]$	Probability of occurrence of (random) variable or event $X$
$r_1; r_2$	Row sums of the cell elements
$s$	The number of strata
TAFE	Tank flow electrolyzer
TUFE	Tubular flow electrolyzer
$T_i$	Parameters of the McNemar test, $i = 1, \dots, 4$
$V[X]$	Variance of (random) variable $X$
$X$	Random variable; $x$ its numerical value
$Z$	Standardized normal variate; $z$ its numerical value
$\alpha$	Level of significance; size of the Type I error
$\nu$	Degree of freedom
$\chi^2$	Chi square variate; $\chi^2_\alpha$ its critical value at $\alpha$ and $\nu$

## 1 Introduction

Electrochemical engineering (EE) does not possess a uniform definition, but various experts in the field agree on its fundamental features. Coeuret and Storck [1] state that in EE, all phenomena occurring simultaneously in an electrochemical reactor have to be accorded an overall consideration. Hine [2] affirms that EE is the bridge connecting science and practice in the field of electrochemistry, and that it concerns "... practical subjects related either directly or indirectly to industrial processes..."; EE, therefore, uses principles of electrochemistry and chemical engineering.

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Roušar et al. [3] indicate that EE “... deals with the analysis of complex situations...” implying that transport phenomena and charge transfer have equal importance. According to Pletcher and Walsh [4], “... the design, characterization, and operation of electrolytic devices and processes...” are “... in the province of EE...”, hence fundamental electrochemistry, industrial-scale electrochemistry, “... and the essential link between them...”, electrochemical technology are of utmost importance to the electrochemical engineer. Scott [5] distinguishes electrochemical reaction engineering (ERE) in the sense of a parallel drawn between the ERE to EE relationship and the catalytic reaction engineering to chemical engineering relationship.

Within this framework, a further horizon to EE is opened directly from its design and optimization aspects, by the inclusion of applied probability theory and statistics. Through their various branches they account for our imperfect understanding of the physical world, as well as the inherent randomness of many natural phenomena. The realm of applied electrochemistry and EE has been slow in widely adopting probabilistic approaches with respect to other disciplines (e.g. industrial engineering, biology, and management sciences). On the positive side, an early recognition of the role of queuing theory [6] was followed by an exploration of decision theory in electrochemical process design and performance analysis [7, 8]. A recent overview [9] demonstrates the utility of likelihood functions, confidence intervals of regression model parameters, various Bayesian concepts, conjugate probability distributions and fractiles in EE. The potential of the log-normal [10] and Poisson log-normal distribution [11] portrays the promise of advanced probabilistic techniques for the electrochemical field.

The purpose of this paper is to explore the potential of an additional area: the treatment of categorical data grouped with respect to certain character, attribute, or quality arising in EE practice. In particular, data grouping due to two (mutually exclusive) categories is considered, whose general scheme is depicted by the so-called  $2 \times 2$  contingency table (shown in Table 1). The first illustration deals with the case of fixed marginal totals using Fisher’s Exact Test for choosing a tank-flow or a tubular-flow electrolyzer. In the second illustration, McNemar’s test [13] for paired-comparison analyses of dichotomous responses is employed to evaluate improvement in current efficiency due to the replacement of an electrocatalyst. The third and final illustration shows a performance analysis of electrolyzer operation using stratified contingency tables.

Because of its exploratory nature, and the current paucity of statistically analyzable observations in pertinent literature, data are hypothetical, albeit based on realistic assumptions arising from “core” information provided by experimenters. Such data, if provided in future experimental investigations, will solidify the position of the subject matter in EE.

A fundamental quantity in probability-based tests is the error committed by rejecting the null hypothesis concerning a population parameter. In conventional (“classical”) statistics, this so-called Type I error,  $\alpha$ , is either significant ( $\alpha = 0.05$ , or 5%), or highly significant ( $\alpha = 0.01$ , or 1%); there are no other rejection levels of importance. The modern view holds that the analyst assigns the level of importance to  $\alpha$  found in a test. If the test statistic itself is taken to be critical, then this  $\alpha$  is also the Type I error.

Let, for instance, the chi square statistic be found to have the value of 2.72 in one of the tests described in the

**Table 1** A general  $2 \times 2$  contingency table

	A	not A	Row total
(a) Chi-square test for category independence, including Yates’ continuity correction factor of 1/2 [12] for categories A and B with small numbers			
B	a	b	$r_1$
not B	c	d	$r_2$
Column total	$c_1$	$c_2$	$n = c_1 + c_2 = r_1 + r_2$
(b) Selected critical chi-square values			
$\alpha$	$\chi^2_{\alpha}(1)$	$\alpha$	$\chi^2_{\alpha}(1)$
0.95	0.00393	0.10	2.706
0.90	0.0158	0.05*	3.841
0.80	0.0642	0.025	5.024
0.60	0.275	0.01**	6.635
0.50	0.455	0.005	7.879
0.20	1.642	0.001	10.83

\*Significant level, \*\*highly significant level; Adapted from D. V. Lindley and W. F. Scott, New Cambridge Statistical Tables, Cambridge Univ. Press (1984), Table 8, pp. 40–41

sequel (with degree of freedom  $\nu = 1$ ). Table 1 shows that it is essentially the critical  $\chi^2_\alpha(1)$  value for  $\alpha = 0.1$ , and in classical statistics the related null hypothesis would not be rejected. The chi-square test [14]

$$\chi^2 = \frac{n(|ad - bc| - 0.5n)^2}{r_1 r_2 c_1 c_2} \tag{1}$$

not recommended for cell entries less than five, indicates independence of categories if  $\chi^2 < \chi^2_\alpha(1)$  at an  $\alpha$ -level of significance. In the modern view,  $\chi^2 = 2.72$  might be claimed critical by an analyst willing “to live” with a 10% Type I error, given the particular physical circumstances. Conversely, a test value of  $\chi^2 = 7.9$  would indicate to the conventional analyst that the null hypothesis can be rejected at a highly significant level, whereas a modern analyst might judge even  $\alpha \approx 0.005$  (or 0.5%) not to be a sufficiently small Type I error for rejecting the null hypothesis, for certain reasons.

**2 Illustration 1: current efficiency (CE) of an electrode reaction in tank flow (TAFE) and tubular flow (TUFE) electrolyzers**

Table 2 presents three  $2 \times 2$  contingency tables with numerically different fixed marginal totals and total observation numbers. To ascertain which reactor type would perform better in terms of CE, Fisher’s Exact Test [15–18] is employed by first defining random variable  $X$  as the number of tank flow reactors with substandard (i.e. unacceptable) CE observations. The modified hypergeometric distribution:

$$P[X] = \frac{C[c_1; x]C[c_2; (r_1 - x)]}{C[n; r_1]} \tag{2}$$

yields the probability of occurrence of 0,1,2,...,x number of such reactors, and the cumulative form

$$P[X \leq x_1] = \sum_{x=0}^{x_1} P[X] = \sum_{x=0}^{x_1} \frac{C[c_1; x]C[c_2; (r_1 - x)]}{C[n; r_1]} \tag{3}$$

provides a means of determining whether the TAFE or the TUFE would be a better choice. Evidently, if  $x_1 = 0$ , the TAFE is strongly favoured in all three cases. If  $x_1 = 1$ , the TAFE is a good choice, although in Case (a) only at a significant, but not at a highly significant level. If  $x_1 = 2$ , only Case (c) would warrant the TAFE as a good choice for this process.

**3 Illustration 2: analysis of improvement in current efficiency upon the replacement of an electrocatalyst**

Motivation for this analysis, involving  $2 \times 2$  tables with paired data, originates from the study by Kawaguchi et al. [19] of the electro-oxidation of methanol, where Rh-free PtRu/C catalysts would appear to be better performers than PtRuRh/C catalysts. Table 3 illustrates the results of the McNemar test [20] with hypothetical observation frequencies in 15 independently operating electrolyzers (known also as ‘focus groups’). The premise of the approach is that improvement upon replacement of an *individual* electrocatalyst is essentially a probabilistic (random) entity, although *on an average* such improvement may be evident by inspection. The task here is to ascertain to what

**Table 2** Hypothetical observations of current efficiency in TAFE and TUFE with fixed column and row totals, and analysis via Fisher’s Exact Test

	Substandard CE	Acceptable CE	Row total
(a) $2 \times 2$ contingency table			
TAFE	$x$	$(r_1 - x)$	$r_1$
TUFE	$(c_1 - x)$	$(r_2 - c_1 + x)^a$	$r_2$
Column total	$c_1$	$c_2$	$N = r_1 + r_2 = c_1 + c_2$
(b) Probability $P[X \leq x_1]$ of substandard CE in $x_1$ or less number of TAFE’s			
$x$	Case (a)	Case (b)	Case (c)
0	0.00155	0.000357	0.000141
1	0.02632	0.01025	0.00464
2	0.1563	0.0952	0.0480

<sup>a</sup> or, equivalently,  $(c_2 - r_1 + x)$

Case (a):  $r_1 = 10; r_2 = 12; c_1 = 8; c_2 = 14; n = 22$

Case (b):  $r_1 = 10; r_2 = 10; c_1 = 8; c_2 = 12; n = 20$

Case (c):  $r_1 = 12; r_2 = 10; c_1 = 8; c_2 = 14; n = 22$

**Table 3** McNemar's test of improvement in performance upon an assumed replacement of a PtRuRh/C electrocatalyst by a PtRu/C electrocatalyst in a focus group of fifteen electrolyzers

	Poor CE after replacement	Good CE after replacement
(a) $2 \times 2$ contingency table		
Poor CE before replacement	$n_{AA} = 3$	$n_{AB} = 7$
Good CE before replacement	$n_{BA} = 2$	$n_{BB} = 3$
(b) McNemar's test		
$T_4 = T_3^2 = \{(n_{AB} - n_{BA})^2 / (n_{AB} + n_{BA})\} = 2.778$		

From Table 1,  $\chi_{0.10}^2(1) = 2.706$  and  $\chi_{0.05}^2(1) = 3.841$ , yielding an approximate  $p$ -value =  $0.05 + [(0.10 - 0.05)/(2.706 - 3.841)](2.778 - 3.841) = 0.0968$

extent the observations in Table 3 would justify the conclusion of proven improvement. The  $2 \times 2$  table elements are the number of electrolyzers exhibiting  $n_{AA}$ : poor performance regardless of replacement,  $n_{AB}$ : improved performance upon replacement,  $n_{BA}$ : worse performance upon replacement, and  $n_{BB}$ : good performance regardless of replacement. The McNemar statistic

$$T_4 = T_3^2 = \frac{(n_{AB} - n_{BA})^2}{(n_{AB} + n_{BA})} \quad (4)$$

has an approximately chi-square distribution with one degree of freedom (the nomenclature stemming from pertinent theory defines the  $T$ -parameters as  $T_1 = n_{AB}$ ;  $T_2 = n_{AB} - n_{BA}$ ;  $T_3 = (n_{AB} - n_{BA}) / (n_{AB} + n_{BA})^{1/2}$ ;  $T_4 = T_3^2$ ). Since the  $p$ -value of the test is nearly 0.1, it follows that the assertion of improved CE upon electrocatalyst replacement carries a 10% Type I error with it. In traditional hypothesis-testing improvement would be judged not significant, and a cautious engineering decision would be either to search for a better set of electrocatalysts, or to

carry out repeated replacement tests, hoping that additional samples would indicate otherwise.

#### 4 Illustration 3: analysis of ECO-cell performance via stratified contingency tables

Table 4 contains a number of ECO-cells [21] operating independently under respective conditions, assumed to have been found in a hypothetical study conducted at a specific time at four different locations, called strata. If  $X_k$  is defined as the random number of observations in row 1 and column 1 of the  $k$ -th stratum, the Mantel–Haenszel statistic [22–24] may be written as

$$MH = \frac{\sum_{k=1}^s [X_k - E(X_k)]^2}{\sum_{k=1}^s V(X_k)} \quad (5)$$

in terms of the mean  $E(X_k) = r_{1k}c_{1k}/N_k$  and the variance  $V(X_k) = (r_{1k}c_{1k})(r_{2k}c_{2k})/[N_k^2(N_k - 1)]$  of the permutation distribution of  $X_k$ . The numerator of Eq. 5 is a measure of

**Table 4** The number of ECO-cells operating under hypothesized conditions in four different countries (strata)

	STR-1		STR-2		STR-3		STR-4	
	DC	UC	DC	UC	DC	UC	DC	UC
CO	3	14	2	13	5	10	4	8
IO	7	10	7	15	8	8	6	7
Stratum no. $i$	STR-1		STR-2		STR-3		STR-4	
$N_i$	34		37		31		25	
$r_{1i}$	17		15		15		12	
$r_{2i}$	17		22		16		13	
$c_{1i}$	10		9		13		10	
$c_{2i}$	24		28		18		15	
$E(x_i)$	5		3.6486		6.2903		4.8000	
$V(x_i)$	1.8182		1.6873		1.9480		1.5600	

Legend: DC divided cell; UC undivided cell; CO continuous operation (via automatic stripping and fluidization of metal powder); IO intermittent operation; STR stratum

$$MH = \{[(3 - 5) + (2 - 3.6486) + (5 - 6.2903) + (4 - 4.8000)]^2\} / \{1.8182 + 1.6873 + 1.9489 + 1.5600\} = 4.695$$

Type I error committed by rejecting the null hypothesis of independence:  $0.025 + ((0.05 - 0.025)/(3.84 - 5.02))(4.70 - 5.02) = 0.032(3.2\%)$

how much  $X_k$ ,  $k = 1, \dots, s$  deviate from the values one could expect from the assumption of independence between cell type and mode of operation. Hence, the larger is *MH*, the smaller is the error in rejecting the null-hypothesis of independence. In the case of a large number of observations, the *MH*-distribution is approximately chi square with one degree of freedom. Since  $\chi_{0.05}^2(1) = 3.84$  and  $\chi_{0.025}^2 = 5.02$  (Table 1), linear interpolation yields a Type I error of 3.2%. The conclusion to draw from the *MH*-test is that there is a significant, but not a highly significant association between mode of operation and the utilization of divided cells. In fact, a smaller proportion of divided cells operated continuously at the locations considered in the study, at a specific time.

## 5 Discussion

### 5.1 Illustration No. 1

When the cell entries are larger than five (per cell), the conventional test of independence may be applied as an alternative, inasmuch as the basic tenet of the chi-square distribution, that it is the distribution of the sum of the squares of  $v$  independent standard normal variates, is at least approximately obeyed. Eq. 1 follows from the mathematical statement of this tenet, readily available in the textbook literature. If, for instance, the  $2 \times 2$  contingency table entries were  $a = 7$ ;  $b = 16$ ;  $c = 8$ ;  $d = 9$ , Eq. 1, the chi-square variate:

$$\chi^2 = \frac{(40|63 - 128| - 20)^2}{(23)(17)(15)(25)} = 0.552 \tag{6}$$

would indicate an about 48% error in rejecting the hypothesis of no significant difference between tank-flow and tubular-flow behaviour, Fisher’s Exact Test yields a qualitatively identical result with  $P[X_1 \leq 7] = 0.2284$ , computed via Eq. 3. Fisher’s test does not require that the observations come from a normal distribution, being a distribution-free (i.e. non-parametric) method—this is a distinct advantage for the evaluation of small-size samples.

### 5.2 Illustration No. 2

The McNemar test is one of three variations of the same theme that can be applied to this category of problems. Recognizing that  $n = (n_{AB} + n_{BA})$  is the number of behaviour switches upon replacement, and that if  $n$  is fixed and the *AB* and *BA* probabilities are equal, it follows that the  $A \rightarrow B$  and  $B \rightarrow A$  switches have an equal chance.

Thus, the conditional distribution of  $n_{AB}$  is binomial with mean  $n/2$  and variance  $n/4$  under the null hypothesis of equal switching probability 1/2, and

$$P[n_{AB} \geq k] = 0.5 \sum_{j=k}^n C[n; j] \tag{7}$$

where  $k$  is an arbitrarily (but judiciously) chosen integer. In the third variation, the normal distribution is invoked by approximating with standard variate

$$z = \frac{n_{AB} - 0.5n}{\sqrt{0.25n}} \tag{8}$$

if  $n$  is sufficiently large. If  $n$  is small, the usual continuity correction has to be applied. Here,  $n = 7 + 2 = 9$  (Table 3), and the probability of 8.98% via Eq. 7 is very close to the McNemar probability of 9.69% indicated in Table 3. Thirdly, since  $z = 1.33$ , and  $F_N(1.33) = 0.9082$  (Appendix A), the normal approximation via Eq. 8 yields a 9.18% probability. Discrepancy between the three variations is negligible.

Assuming the hypothetical set  $n_{AB} = 1$ ;  $n_{AB} = 9$ ;  $n_{BA} = 1$ ;  $n_{BB} = 4$ , a stronger replacement effect within the same framework of 15 electrolyzers is obvious. In fact, the results of the McNemar test (1.09%), Eq. 7 (1.10%) and Eq. 8 (1.32%) unanimously indicate, for all practical purposes, a highly significant improvement in current efficiency. As shown in Table 5, the  $n_{AB}/n_{AA}$  ratio is an important factor in determining the beneficial effect of replacing the original electrocatalyst: the higher the ratio, the smaller the Type I error committed in rejecting the null hypothesis of no change in performance.

### 5.3 Illustration No. 3

An important caveat in applying Eq. 5 is its inappropriateness when in some strata the  $X_k$  values tend to be larger than their mean  $E(X_k)$ , while in other strata the opposite is true:  $X_k < E(X_k)$ .

The second comment concerns sample size. If it is small, the permutation distribution of the  $2 \times 2$  contingency table elements is needed, and the  $p$ -value of the independence test is provided by the fraction of the number of permutations whose *MH*-statistic is at least as large as the *MH* pertaining to the experimental permutation, with respect to the total number of permutations. For the entries in Table 4, the size of  $C[34;17]C[37;15]C[31;15]C[25;12] \approx 5.1 \times 10^{30}$  demonstrates the numerical encumbrance characteristic of permutation-based tests [25], whose principle is, however, illustrated in Appendix B for the sake of completeness.

**Table 5** The effect of the  $n_{AA}$  and  $n_{AB}$  elements on performance decision in Illustration 2 when 20 electrolyzers operate independently, with fixed values  $n_{BA} = 2$  and  $n_{BB} = 3$

$n_{AA}$	$n_{AB}$	McNemar's test $p$ -value (%), via	Eq. 7	Eq. 8
1	14	0.28	0.30	0.21
2	13	0.46	0.49	0.37
3	12	0.69	0.80	0.65
4	11	1.3	1.3	1.1
5	10	2.4	2.2	1.9
6	9	3.7	3.5	3.3
7	8	6.1	5.7	5.5
8	7	9.7	9.2	9.0

#### 5.4 Further observations

$2 \times 2$  contingency tables are an important subset of more general  $R \times C$  tables where  $R$  and  $C$  are the row- and column dimension, respectively. The chi-square statistic, although widely used in the analysis of such tables, may not be the preferred tool if e.g. there is an ordering among factor categories. The discussion of singly (i.e. one factor)-ordered, and doubly (i.e. both factors)-ordered tables calls on principles of advanced nonparametric statistics, and is well beyond the scope of this article.

In dealing with stratified contingency tables, the concept of the *odds ratio* yields an alternative means of testing independence. For a particular  $k$ th stratum, the “odds” that an observation from the first row falls in the first column, divided by the “odds” that an observation from the second row falls in the first column, is an odds ratio  $\theta(k)$ . If  $\theta(1) = \theta(2) = \dots = \theta(k) = 1$ , independence is inferred, via an appropriate test of this null hypothesis. Confidence intervals for  $\theta$  at specified significance levels  $\alpha$  can be obtained by the exponentiation of the confidence interval established for  $\ln(\theta)$ , whose variance [26] determines the width of the confidence interval when the sample estimate  $\theta_s$  is known. Large samples require statistical (e.g. StatX-act) computer software.

#### 6 Final remarks

Although by no means exhaustive, the preceding material demonstrates the potential of  $2 \times 2$  contingency tables for specific purposes of analysis in electrochemical engineering. As in all applications of probability theory and statistical methods, the larger is the body of observations, the more reliable are the inferences drawn from tests of hypotheses. In this respect, the study of electrochemical systems still has a long way to go in order to take full advantage of available methods of analysis.

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#### Appendix A

Notes on the cumulative distribution functions  $F_N(z)$  and  $F_N(\chi^2)$

Tabulations of the cumulative distribution function  $F_N(z)$  of the standardized normal variate  $Z$  are readily available in most texts and handbooks on probability theory and statistics. The formula, based on a simple relationship between  $F_N(z)$  and the error function  $\text{erf}(z/\sqrt{2})$ , and a close approximation of the latter by a third-order polynomial [27]:

$$F_N(z) \cong 1 - \frac{1}{2}f(y) \exp\left(-\frac{z^2}{2}\right) \quad (\text{A.1})$$

is at least four-decimal accurate, with

$$y = \frac{\sqrt{2}}{\sqrt{2} + 0.47047z} \quad (\text{A.2})$$

and

$$f(y) = 0.348026y - 0.095878y^2 + 0.74785y^3 \quad (\text{A.3})$$

When  $v$  is large, the cumulative chi square distribution function  $F_v(\chi^2)$ , also widely tabulated, can be approximated [28] as

$$\chi_v^2(\alpha) \cong \sqrt{2v}z_\alpha + v \quad (\text{A.4})$$

or alternatively, with better accuracy [29] as

$$\chi_v^2(\alpha) \cong \frac{1}{2}(z_\alpha + \sqrt{2v-1})^2 \quad (\text{A.5})$$

**Table A.1** Comparison of tabulated and approximate values of the chi square distribution at the significant and the highly significant level

N	$\alpha = 0.05 (z_{0.05} = 1.6449)$			$\alpha = 0.01 (z_{0.01} = 2.3263)$		
	Tables	Eq. A.2	Eq. A.3	Tables	Eq. A.2	Eq. A.3
1	3.84	3.33	3.50	6.63	4.29	5.54
2	5.99	5.29	5.70	9.21	6.65	8.25
3	7.81	7.03	7.53	11.34	8.70	10.41
5	11.07	10.20	10.79	15.09	12.36	14.20
10	18.30	17.36	18.02	23.21	20.40	22.37
15	25.00	24.01	24.71	30.58	27.74	29.76
20	31.41	30.40	31.13	37.57	34.71	36.77
30	43.77	42.74	43.49	50.89	48.02	50.11

where  $z_\alpha$  is the standard normal variate corresponding to significance level  $\alpha$ , and  $\chi^2_\nu(\alpha)$  is the critical chi-square variate with  $\nu$  degrees of freedom at the same  $\alpha$ . At small values of  $\nu$  the approximations are poor, especially at low values of  $\alpha$ . Table A.1 portrays the gradual improvement at increasing values of the degree of freedom, when  $\alpha = 0.05$  and  $\alpha = 0.01$ .

### Appendix B

Illustration of the permutation-distribution approach to chi square based analysis

An experimentally observed cell is assumed to contain elements  $a = 2; b = 1; c = 0; d = 2$ . The  $(a, b)$  set represents a “new” electrolyzer or a “new” technique, while the  $(c, d)$  set represents the “old” counterparts. Written otherwise, the elements are expressed by scores of 1 as  $a_1, a_2, b_3, d_4, d_5$ . If there is no difference between the “new” and the “old”, then all configurations created by a random assignment of three of the scores to the “new” and two of the scores to “old”, have an equal chance of being observed. There are, therefore,  $C[(3 + 2);3] = 10$  such data sets, summarized below.

Permutation	A	b	c	d	Frequency	$\chi^2$ (Eq. 1)
1	0	3	2	0	1	1.701
2	1	2	1	1	6	0.313
3	2	1	0	2	3	0.035

The reasoning is as follows. The experimental observation pattern, rewritten as  $a_1 = 1; a_2 = 1; b_3 = 1; d_4 = 1; d_5 = 1$ , yields the first line/second line structures  $b_3d_4d_5/a_1a_2; a_2d_4d_5/a_1b_3; a_2b_3d_5/a_1d_4; a_2b_3d_4/a_1d_5; a_1d_4d_5/a_2b_3; a_1b_3d_5/a_2d_4; a_1a_2d_5/b_3d_4; a_1a_2d_4/b_3d_5; a_1a_2b_3/d_4d_5; a_1b_3d_4/a_2d_5$ . Consider the first structure, where there is no  $a$

element at the (1,1) position, and there are three elements, namely  $b_3 = 1, d_4 = 1$  and  $d_5 = 1$ , yielding the entry 3 at the (1,2) position. In the second line,  $a_1 = 1$  and  $a_2 = 1$  yield the entry 2 at the (2,1) position, and the entry 0 at the (2,2) position. This is Permutation 1. Similar reasoning leads to the six identical structures of Permutation 2, and the three identical structures of Permutation 3 structures, shown above.

The experimental pattern is one of the three (Permutation 3) obtained upon coalescence. Since all chi-square values equal or higher than 0.035 for Permutation 3, it follows that the  $p$ -value is  $(3 + 6 + 1)/10 = 1$ , indicating independence (i.e. the null-hypothesis of independence can be rejected only at a 100% Type I error). If the cell entries came from a normal population,  $\chi^2 = 0.035$  would imply a  $p$ -value (via Table 1) between 0.90 and 0.95 (i.e. a minimum 90% Type I error), and the test would very strongly indicate independence, similarly to the permutation approach. If the experimental observations fell into the first or second permutation category, the null-hypothesis of independence would still be maintained, but at a lower Type I error (10% and 70%, respectively, via the permutation approach; about 19.5% and 58%, respectively, by the classical chi-square approach).

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