Design of Papers for Error Minimization*

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Stimulated by the evidence presented at the recent Symposium on Errors in the Chemical Literature, specific suggestions are made to reduce the number of errors creeping into the chemical literature: 1. Establishment of a mechanized screening system for the determination of errors in molecular structures and stoichiometry and in internal and external consistency of a reported physical property to serve for pre-examination of papers before examination by editors and reviewers. Modes of experimental and final implementation of the proposed scheme are also presented. 2. Establishment of standard formats for technical, especially experimental, papers.

PURPOSE AND SCOPE

The purpose of the present proposal is to design a publication method to reduce the probability of publishing unnecessary errors in the chemical literature, to reduce the volume of printed words accompanying the data to the minimum required for effective communication, and yet to provide for easy access to all of the (experimental) data. The requirement of "complete information" cannot be relaxed because our civilization rests on the premise the the results reported by a scientist or engineer are a legitimate component of knowledge only if they can be duplicated anywhere at any time.

The scope of the present work is set by the self-imposed constraint that its results can be implemented with currently available technology. Moreover, the means required for editorial control are limited to those requiring a minimum of technical judgment—namely, those which can be completely mechanized. Organizational aspects of the implementation of the proposed scheme will also be discussed.

GENERAL PRINCIPLES

Empirical studies of the use of technical literature[1-7] and of its transmission and use[8] have shown that accessibility, ease of use, and perception of its reliability determine the choice of information sources. Only two of these basic "qualities," ease of use and easily perceptible reliability, are subject to editorial control and therefore proper subjects for the present discussion.

The present scheme proposes not only such a paper format to be followed in the presentation of experimental data and their correlation, but also a concurrent limitation on the length of published papers. One consequence of this enforced brevity is the need for periodic review of the resulting information fragments. Such a review of a given area of research may be commissioned by such organizations as the editorial board of *Accounts of Chemical Research* and *Chemical Reviews* upon advice by computer count provided by Chemical Abstract Service whenever, say, more than 50 papers have been published in that area over a three-year (or otherwise fixed) period.

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RAISING THE RELIABILITY LEVEL

The recent symposium on "Errors in the Chemical Literature"[9] brought to light the extent as well as the nature of the most serious errors entering our literature at present. The present work deals primarily with means to reduce this error flux. A major source of error flow past reviewers and editors is obscure presentation or even absence of relevant information. This situation can be remedied by insisting on a format which makes data quality, relevant results, and internal consistency visible on first glance: (The ACS "Handbook for Authors," page 24, makes many of the same points, but in permissive rather than mandatory mode. Hence, few papers in ACS journals meet the recommended standards.)

1. In the case of experimental papers the following information must be presented in mandatory form at the beginning of the paper's section marked Experimental:

a) **Description of Materials Used:** Name, origin, purity analysis (including analytical method employed). The common availability of chromatographic and other convenient methods makes the absence of impurity data wholly inexcusable.

b) **Description of Experimental Equipment:** Only differences from equipment described in the previous literature must be described. Total descriptions should be tolerated only in exceptional cases.

c) **Description of Procedure:** Only differences from published procedures must be described. Total description should be tolerated only when clarity demands it. The method errors must be clearly displayed.

d) **Description of Results:** In an orderly tabulation, including error range, of the data. Display of the error range of the experimental data, including the extent of replication, should be mandatory.

e) **Generalization of Results:** By theory or empirical correlation, should show only the arithmetic, the error range of the coefficients, and a graphical display of the relation between experimental data and calculation.

2. In the case of theoretical papers, the body of the paper must contain the following information in a mandatory format:

a) Short description of the phenomenon giving rise to the need for a new theoretical treatment.

b) Precise statement of the assumptions made in the mathematical formulation of the theory, including the boundary conditions set.

c) Mathematical formulation of the theory, where applicable.

d) Comparison of theoretical calculation with experimental data.

DIRECT ERROR PREVENTION

Chemical Names, Structures, and Stoichiometry. The most frequent source of errors in chemical literature appears to be the incorrect statement of the name of chemical substances used, of their molecular structure, or of the empirical formula, or of all three. Any inconsistency among these three items is easily discovered by machine encodement, using such systems as the Wiswesser Code, the Shell Chemical-Typewriter, etc., and a computer program that converts these into the empirical formula. The correctness of stoichiometry in chemical reaction equations can be checked mechanically by means of simple material balance programs. Computational checks on the correct interpretation of spectroscopic information, especially molecular vibrations and NMR data, should be carried out by means of comparatively simple logic assemblies. In case more than one structure is compatible with the observed spectra, chemical or other physical evidence will generally fix the structure definitively.

Physical Properties. Nearly all physical properties can now be checked for external consistency[11]—i.e., for consistency with accumulated information in the form of physical property correlations of varying degree of reliability by means of existing or easily supplemented computer programs.[11] The majority of equilibrium properties, especially the thermodynamic properties (other than the melting point), must be subjected to well-established yet frequently violated rigorous internal consistency tests. These likewise are or can readily be made available as computer programs.[11]

This error-prevention routine should be executed by the originator of the data. A nationally accessible service bureau should be encouraged to install the described "error filter" routine for nationwide access, particularly for authors whose organizations do not own (large enough) computers for such work. Evidence for an executed data check, manual or mechanical, should be mandatory for the acceptance of any experimental paper. Should the editor or the reviewer be unsatisfied by the data quality and/or the evidence presented, they should ask the author to (report the) check or allow them to apply the mechanical check, at the author's expense.

Publication worthiness requires novelty as well as reliability. In principle the reviewer is chosen on the basis of his expertise in the field of the proposed paper. Hence, he should be able to discern novelty or its absence. In case of disagreement between author and reviewer on this point, the author could ask for a mechanized *CA* search at his expense covering at least the most recent five years, and which could possibly be carried out by CAS.

A summary of the proposed "Error Filter" is shown as Figure 1. The "Final Review" step, whether carried out by author or reviewer, has been inserted to emphasize that the final judgment of the quality of the work must rest with humans and not with computers, since deviations from external consistency may constitute a new discovery.

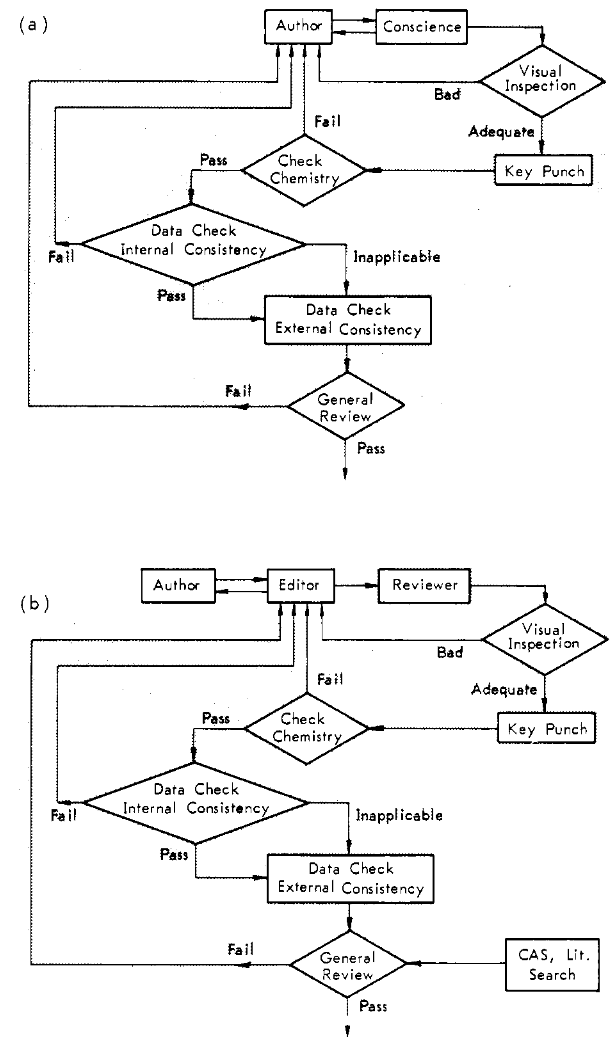

Figure 1. Paper review for errors, (a) operated by the author, (b) operated by the journal editor

GENERAL FORMAT OF TECHNICAL PAPERS

Let's abandon the pretense that technical papers are a contribution to English literature. Management of the physical bulk of publication calls for drastic measures. In that spirit the following suggestions are offered to govern the size of technical papers:

a) Precede the paper with an abstract of less than 200 words.

b) Call the introductory paragraph "Purpose and Scope;" prohibit the term "Introduction" and limit its length to less than 300 words. This should eliminate the ritual of the rambling historical introductions. The absence of this historical introduction can be compensated for by adopting the bibliography style of the engineering journals, namely, to state the title of the reference between the referenced author(s)'s name and the journal reference.

c) The format of the body of the paper as described earlier.
d) Discussion, if any, should be held to less than 500 words.
e) Comparison with previous work should be held to less than 250 words.
f) Suggestions for future work should likewise be held to less than 250 words.

This could add up to a maximum of 1500 words of "frame" plus an unspecified length for the descriptive part or body of the paper. "Comparisons with earlier work" are generally implied in "Purpose and Scope" and in the "Discussion." Few authors nowadays discuss "Future Work." Hence, a more common length limit for the frame will be 1000 words. A concise description of the results or derivation of theory need not exceed 500 words of text plus tables of supporting data and graphs, giving an average maximum length of 1500 words plus tables and graphs.

The proposed restriction of the size of the published paper to barebone essentials, nearly a long abstract, may deprive the editors and the scientific community of access to the raw data and to essential details which the author may not have recognized as essential. Hence, all of the basic data and the conventional length report must be submitted to the editor together with the Standard Format Paper which the author abstracted therefrom. These basic data and the conventional length report are to be deposited (as microfilm) with the American Society for Information Science or similar repository for retrieval when needed. Adoption of the same procedure for "Communications" or "Notes" would improve the level of editorial control over these short contributions to the literature substantially and raise their utility and prestige correspondingly.

The Standard Format plan is offered to help the problem of error accumulation and that of almost unmanageable bulk volume growth of the chemical literature. The many man-hours wasted through the use of incorrect data and the bulging shelves in chemists' offices and homes should argue forcefully in favor of a scheme such as the one presented here. The cooperation of the chemical world should therefore be forthcoming, especially if the editors of the ACS journals provide the required imaginative leadership.

Implementation must, of course, proceed in stages and might consist of the following parallel steps:

a) Publish the proposed Standard Format in the "Instructions for Authors" section of all ACS-owned journals as purely suggestive for voluntary adherence.
b) Contract with a suitable research institute to run through two to four recent years of the *Journal of Physical Chemistry* or of the *Journal of the American Chemical Society* and test the chemistry (structure and stoichiometry) and the physical property data of all appropriate experimental papers for internal and external consistency, etc. Many of the required computer programs are already in being, and the remaining ones are comparatively easy to produce. Thus the extent of the problem will be established experimentally as well as the most expeditious ways to handle it.

Both (a) and (b) should be carried out for a year, and monitored by a committee representing the editors of ACS journals as well as of Chemical Abstract Service. The next stage should be decided upon at the end of that year, and may well involve the taking on of the error control function for one or two journals either by the previously mentioned contractor or by the computer section of Chemical Abstract Service.

Since most authors are also reader-users of the literature, they may come to appreciate the improved utility of papers prepared in the proposed Standard Format by a few enterprising volunteers. Their voluntary or encouraged participation in a general change-over may thus meet decreasing resistance over a period of a few years. Imposition of length restrictions will come probably quite soon anyway simply because there will be no money for indefinite expansion of the chemical literature.

COMPARISON WITH EARLIER WORK

Reduction of the length of papers to "Précis" or Long Abstract form, similar to that prevalent in the French *Comptes Rendus* was proposed in the course of the British Royal Society inquiry into the redesign of the scientific literature.[12] Since the paper shortage, which largely motivated that proposal, has abated, its implementation has not been attempted so far. The need to adapt the mode of information presentation to computer control had not arisen before now. Hence, no precedent was looked for.

APPENDIX I

Survey of "Experimental" Sections of Chemistry Papers

A random sampling of various recent issues of *J. Am. Chem. Soc.* brought to light that in the majority of papers current practices of compound purity characterization show little advance over those of 1867. Typical of 90% of the papers is the satisfaction with recrystallization of the sample *x* times and correspondence of its melting point with that given elsewhere, or "the sample was slowly distilled and the middle 30% retained" without description of the distillation column, if any, and conditions employed, or "the boiling point at 1 mm. is within a few degrees of literature reference" without recognizing that this pressure is hardly a very reproducible condition because of the difficulty of accurate reading of the commonly used manometers and the frequently incorrect attachment of these devices to the distillation train. Chromatography or mass spectroscopy need never have been invented for these authors.

More remarkable is the author who, obviously—and rightfully—concerned about the purity of his samples, zone refines many times, yet does not take the trouble to determine the impurity concentration in his samples (before or) after this laborious procedure.

A large fraction of novel compounds reported is characterized by elemental analysis. Seemingly small deviations in these analyses can have large effects on the postulated compound's stoichiometry. Neither the resulting uncertainty in chemical composition nor the uncertainty due to method error are mentioned by most authors. Once the gross consistency of the elemental composition data with proposed structure has been ascertained within the method and replication error bounds, these data could serve as a rough guide to sample purity. Modern analytical techniques are often adequate for such purity estimation, but their use for this purpose is so rare as to be virtually nonexistent.

The absence of method error and of replication error statements from many experimental investigations makes the reported data virtually useless for testing the validity of the author's own or someone else's mathematical model of the studied process or property. It should be noted in this context that the thought expended on the nature and consequences of error magnitude for testing the proposed interpretation of the data should also lead to better planning of the experiment as a whole, including the proper spacing of points in variable space. Far more than an editor's pedantry is obviously involved here.

Qualitative analysis is equally bedevilled by inadequate characterization of method uncertainty. Typical examples are optical spectroscopy data without measure of resolution, or even of slit width used. Subsequent investigators may then be unable to tell whether their compound truly differs from that reported by an author who gave only a portion of the spectrum without error bounds.

The enumerated examples for mounting numbers of inaccuracies in the reported chemical literature perhaps do not retard the development of chemistry very much because the leading chemists' unmatched intuitive judgment guides the phalanx of their followers nearly unharmed through a morass of inadequate data. However, the lack of emphasis on experimental rigor and thoroughness leaves many of today's graduate students unprepared to deal with the extreme sensitivity of product quality, reaction yield, and selectivity to reactant purity in most modern industrially important chemical processes. This alone seems to me to be sufficient reason for unbending editorial insistence on the indicated criteria of publication-worthiness.

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Experiments with Programmed Learning as a New Literary Form*

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The artful use of computer aids can help us create a wealth of new forms for representing, transmitting, storing, transforming, and displaying knowledge. One such form is a programmed text. A novel kind of programmed text, used as an experimental instrument in behavioral engineering, is described. Its aim is to overcome blocks against mathematics on the part of people who are allergic to the manipulation of abstract symbols, or who are rusty in mathematics, or who have never been exposed to the excitement of mathematical thinking. Experimental findings resulting from its use in class are presented and used to evaluate and improve the instrument in a systematic way.

Some of the more recent new methods of teaching that have been developed or proposed are called programmed learning. There are now almost 300 computer-aided instruction programs in operation and many more book-form programmed texts. In 1961, there were 82, and in 1962, 86 published programmed texts on mathematics alone.[29] By then, over 100 companies were selling programs. Harcourt, Brace, and World alone commissioned the writing of 50 programmed texts, and Encyclopaedia Britannica Films has planned an entire high school curriculum in the newer form. Eight semesters of mathematics materials have been tested on over 1000 students in 1965–67. As early as 1960, Grolier, Inc., added a machine

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Editor's note: Other papers from this symposium were published in the November 1968 issue.