On the Optimal Utilization of Experimental Data

Frediano V. Bracco*
Guggenheim Laboratories, Princeton University, Princeton, N.J.

Theme

An analysis and generalization of the so called "inverse method is undertaken. The inverse method consists of determining some variables experimentally and in using them in equations to compute other variables. When generalized, this method becomes a procedure to obtain maximum information out of a set of experimental data. It can even be considered a method of investigating physical problems which combines the advantages, and limits the disadvantages of solely experimental or theoretical approaches. The logic of the method is outlined and its properties are listed. An introductory example is given while complete and incomplete examples can be found in the backup paper.

Contents

This synoptic, and its backup paper, do not deal with a specific research problem but rather with the question of how to get the most out of experiment and theory. Advantages are shown to derive from coupling them closely in the explained manner. It consists of initially avoiding the use of the more uncertain assumptions and equations in the formulation of theoretical models by replacing them with experimental data.

The concept of measuring some variables and using them in equations to determine other variables is not a new one. It is often called the "inverse approach." However, in all the applications of which this author is aware, the full advantages of this approach were never exploited; they were *ad hoc*, incomplete applications. This is because the method itself was never formalized, i.e., a logic for its application was never outlined, and its properties were never identified and listed. It is the purpose of the paper to make a first step toward such a formalization. This method is here called the Experimental Data Optimal Utilization Method, or briefly, the EDOU method since this name best represents what is perhaps the most outstanding of its many properties.

In this synoptic, the EDOU method is defined and its properties are listed in summary forms. Also given is an introductory, schematic application. A complete, practical application is summarized in the backup paper (with details given in Ref. 1) where other examples of similar uses of experimental data, mostly by other authors, and from the field of reactive fluid dynamics, are also briefly reviewed to point out the generality and usefulness of the EDOU method. These examples include applications to steady spray combustion,[2,3] unsteady combustion of solid propellants,[4] detonation of solid explosives,[5] chemical kinetics,[6] internal combustion engines,[7] and flame structure studies.[8] The EDOU method and its properties.

Given a physical problem, the Experimental Data Optimal Utilization Method to study it consists of: 1) a study of the equations to indentify the weakest assumptions, the measurable variables, and the possibility of splitting the system of equations into subsystems; 2) the collection of experimental data to determine some of the variables; 3) the solution of subsystems of equations with the direct use of the experimentally determined variables; and 4) the reconstruction of the complete solution.

This method is particularly useful when some of the controlling processes of a complex problem are either unknown or subject to inaccurate representation. Then it allows one to approach the complete solution by successive steps. At each step, maximum information is extracted from the experimental data and the accuracy of the assumptions and of the experimental data themselves is checked. More specifically, the properties of this method are: 1) Experimental Data Information Optimization: The direct substitution of some experimentally determined variable in the equations often allows one to evaluate other unknowns readily, thus extracing maximum information from the experimental data; 2) Experimental Data Check: When the experimentally determined variables are used in the general equations and the equations are solved, the newly determined variables often take on unrealistic values if the data used are in error. Researchers using the conventional theoretical approach often do not closely evaluate the accuracy of the experimental data. On the other hand, experimentalists do not always select the most informative parameters to be measured or may be unaware of their experimental errors. Practice has shown that in using the EDOU method, seemingly consistent data were actually found to be in error, and, subsequently, the source of error was identified; 3) Set Splitting: An important property of the EDOU method is its splitting of the equations into uncoupled groups. The unknowns are also split into groups and some of them are completely determined, while others remain bound by functional relationships; 4) Mathematical Simplification: Both the conventional approach and the EDOU approach require the same amount of experimental data and the solution of the same equations but for different unknowns. Actually, in the EDOU method, one often has to solve fewer equations than in the conventional one. This is so for two reasons. First, one or more of the unknowns is determined via measurements and, therefore, one or more of the equations can be dropped (except for being used later to check the accuracy of the experimental data and of the assumptions). Second, the equations are split into subgroups which are solved in series. The solution of each subsystem is generally easier than the solution of the complete sytem. Furthermore it is not always necessary to solve all the subgroups. Finally, in the conventional approach, a primary source of error may be hidden in the mathematical approximations which are often made to obtain the more difficult solution of the complete set of equations; 5) Assumption Splitting: Associated with the property of splitting the equations into uncoupled groups, is the property of splitting the assumptions into groups as well. This property is important and, therefore, is given separate heading. The EDOU method leads to the solution of subsets of equations which incorporate only subsets of assumptions. The validity of the smaller number of assumptions involved in each subset of equations can be evaluated independently. This is much easier than having to evaluate the validity of all assumptions appearing in all of the equations simultaneously; 6) Parameterization: It may occur that it is not possible or practical to measure enough of the variables and that only an underspecified subset of equations can be isolated, i.e., the subset contains more unknowns than equations. In this case, it is often possible and advantageous to solve the underspecified subset for specific values of some of the nonmeasured unknowns. A parametric set of restricted solutions is thus obtained. It is found that the study of these parametric solutions is very useful in helping one to determine the physical and mathematical properties of the problem. In particular, the family of solutions could be sufficiently narrow so as to be used as a unique solution. Obviously, the existence of useful parametric solutions is related to the physical nature of the

Received January 29, 1975; synoptic received July 28, 1975. Full paper available from National Technical Information Service, Spring field, Va., 22151 as N75-28955 at the standard price (available upon request).

Index categories: Reactive Flows; Combustion in Heterogeneous Media; Thermochemistry and Chemical Kinetics.

*Assistant Professor. Member AIAA.

problem. However, the existence of such solutions is more likely to unfold during the application of the EDOU method because it is based on the search for restricted solutions from its inception; 7) Maximum Information: This last property is possibly the most important yet the most difficult to define specifically, Having a complex problem, there is always some variable which can be readily measured (like pressure in many fluid dynamics problems). The basic equations can then be studied using directly the measured variable. In so doing, a wealth of information about the *nature* of the problem, the *properties* of its solution, the *ordering* of the terms in the various equations, and the *mathematical techniques* to be used in the study of the complete set of equations becomes available; so does experience show.

An Introductory Example: Consider a one-dimensional, steady flow in a duct of slowly varying cross-sectional area. Assume that both the termal and the caloric equations of state of the fluid are unknown. Assume also that thermal energy is added to the flow by some process of unknown nature or rate. The following conservation equations can then be written between any two sections of the duct

$$\rho_1 u_1 A_1 = \rho_2 u_2 A_2 \tag{1}$$

$$\rho_1 u_1^2 A_1 + p_1 A_1 + \int_{A_1}^{A_2} p dA = \rho_2 u_2^2 A_2 + p_2 A_2 \tag{2}$$

$$e_1 + p_1/\rho_1 + u_1^2/2 + \xi = e_2 + p_2/\rho_2 + u_2^2/2 \tag{3}$$

$$p = p(\rho, T) \tag{4}$$

$$e = e(\rho, T) \tag{5}$$

$$\xi = \xi(?) \tag{6}$$

where the first three equations represent the conservation of mass, momentum and energy (with the unknown energy source, ξ), and the next two represent the missing thermal and caloric equations of state (ρ = density; u = velocity; A = cross-sectional area; p = pressure; e = internal energy; T = temperature).

The conventional theoretical way of attacking the problem would be to postulate controlling physical processes and to write down expressions for the energy source and for the equations of state (and may require the introduction of additional equations as for the conservation of chemical species, for example). The resulting equations would then be solved. Finally, a quantity would be measured, say, the pressure along the duct and compared with the predicted one. The model would then be modified until theoretical and experimental results match. Notice the following: 1) The experimental data were used to check the theoretical results and not directly in the process of formulating the model; 2) There is no way of knowing how accurate the experimental data are. The experimental data could be in error and the model might be adjusted to predict the wrong data; 3) In the theoretical study, a system of at least six coupled equations must be solved. To reach the solution certain mathematical approximations might be necessary; 4) In the formulation of the model, many assumptions may have to be made. If the model yields results not quite in agreement with the experimental ones, some difficulty may arise in deciding which of the assumptions should be modified.

In the EDOU method, the formulation of a complete model is temporarily postponed and the equations are studied to see if quantities could be measured which would allow one to solve some of the equations for some of the unknowns without having to use the most uncertain of the assumptions. It is then noticed that the first two equations contain only three unknowns. Thus, if one of the unknowns is measured, the other two can be determined without any assumption about the energy source and the equations of state. Accordingly, if p is measured along the duct, ρ and u can then be computed provided initial values are known. Setting $\rho = \rho_2/\rho_1$, $u = u_2/u_1$, $p = p_2/p_1$, $A = A_2/A_1$ one finds

$$u = 1 - (pA - 1 - \int_1^A p dA)\, p_1/\rho_1 u_1^2 \tag{7}$$

$$\rho = (uA)^{-1} \tag{8}$$

Now one knows not only p, but also ρ and u, and more information is available on which to base further exploration. Notice the following: 1) Experimental data are needed sooner or later in both approaches. In the EDOU approach one obtains more information out of the experimental data since the knowledge of p led to the knowledge of ρ and u without any more assumptions than were already imbedded in the equations (Experimental Data Information Optimization); 2) After having determined ρ and u, one can make a few measurements of u and see if it agrees with that calculated by the first two equations. If it does, the first two equations are correct and pressure measurements are reliable. If it does not, either there is an error in the measurements or more terms must be added in the first two equations (for example, viscosity effects should not have been neglected). (Experimental Data Check); 3) The system of six equations has been split into two subsystems. A subsystem of two equations (already solves) and a subsystem containing the remaining equations still to be solved. The mathematics is then simpler. (Set Splitting and Mathematical Simplification); 4) When the equations were split so were the assumptions. The assumptions going into the first two equations can be checked independently of the asumptions going into the remaining four equations (Assumption Splitting).

The previous, schematic example is an incomplete application of the EDOU method because it does not exemplify two important properties of the method, parameterization and maximum information, and because it leaves out the fourth, conclusive, step of the method, i.e., the reconstruction of the complete solution. As previously stated, a complete, practical application is summarized in the backup paper and the details are given in Ref. 1.

In conclusion, the EDOU method, particualrly when applied to complex physical problems (involving differential and partial differential equations), offers several advantages with respect to the solely theoretical and experimental approaches. They stem from the fact that one can solve for some of the unknowns even if he does not know many aspects of his problem. Then the unknown aspects can be investigated more easily, since more information is available and some features or properties of the problem have already been determined.

References

[1]Bracco, F. V., "The Direct Method as Applied to the Liquid Rocket Engine Combustion and Explosion Problems," Ph. D. thesis, Rept. AMS 902T, 1970; Princeton University, Princeton, N. J. Available as Rept. 71-14359 at the University Microfilms, Xerox Comp., 300 N. Zeeb Rd., Ann Arbor, Mich., 48106

[2]Bracco, F. V., "An Experimental-Analytical Method to Study Steady Spray Combustion," *Journal of Spacecraft and Rockets*, Vol. 10, June 1973, pp. 353-354.

[3]Bracco, F. V., "Applications of Steady-State Spray Equations to Combustion Modeling," *AIAA Journal*, Vol. 12, Nov. 1974, pp. 1534-1540.

[4]Zel'dovich, Ya. B., "Theory of Burning of Powders and Explosives," *Zhurnal Eksperimental' Noi i Tekhnicheskoi Fiziki* (Russian Journal of Experimental and Theoretical Physics), Vol. 12, 1942, pp. 498-524.

[5]Bracco, F. V., "Comments on the Equation of State of the Products of High Density Explosives," *Combustion and Flame*, Vol. 22, Feb. 1974, pp. 9-11.

[6]Ball, W. E. and Groenweghe, L. C. D., "Determination of Best-Fit Rate Constants in Chemical Kinetics," *Industrial and Engineering Chemistry Fundamentals*, Vol. 5, May 1966, pp. 181-184.

[7]Lavoie, G. A., Heywood, J. B., and Keck, J. C., "Experimental and Theoretical Study of Nitric Oxide Formation in Internal Combustion Engines," *Combustion Science and Technology*, Vol. 1, Feb. 1970, pp. 313-326.

[8]Lovatchev, L. A., Basevich, W. Y., Kogan, A. M., and Posvyanskii, S. V., *Transactions of the Acadamie of Sciences of U. S. S. R.*, Chem. Series #6, 1970.