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Mathematical Modeling and Human Nutrition

Jean Mayer's article "Toward a national nutrition policy" (*1*) is an impressive report on the recent history and accomplishments of social contributions to the improvement of nutritional health in this country. Mayer is right in pointing out the causal relations between *improper diet* and malnourishment, and he is also right in listing the potentialities of institutional feeding programs, food labeling, education, and research as possible means of achieving improvement on a national scale. However, he is not specific as to how these factors can significantly affect the following of "proper diets" and thus eliminate the causes of malnutrition.

Most nutritionists seem to share the mistaken assumption that the knowledge of the nutrient composition of foods and the recommended dietary allowances is somehow sufficient to plan a diet, when in fact this information contains only part of the coefficients of the system of mathematical equations that must be solved to determine nonnegative quantities of food. Contrary to popular belief, the problem of diet *planning* is not a nutritional, but a mathematical one (*2*). Moreover, the term "proper diet" defies definition, both conceptually and operationally, unless the problem is cast into some mathematical model built upon the concepts of constrained optimization techniques. The scientific methodology to plan diets which are "proper" in the sense of satisfying consumers while meeting nutritional and budgetary allowances is already well developed (*3, 4*). Years of research and repeated comparisons in many institutions (*4, 5*) have consistently shown that diets planned with mathematical techniques on computers will cost less (by 10 to 30 percent), be preferred, and be better balanced nutritionally than diets planned by conventional means. It is laudable that increased federal funding is now available to extend participation in the school lunch and other volume feeding programs. But by changing from the conventional to the mathematical (computerized) method of diet planning, these programs could be extended to about 20 percent more people without extra funds.

Other disturbing signs point to the existing shortcomings in diet planning methods. One is the proposed rule of the Food and Drug Administration for nutrition labeling (*6*). Nutritionists without mathematical models have limited use for precise nutrient composition data; more data means only that more information will have to be ignored. The proposed labeling formally advocates shortcuts in determining the precision of nutrient values that do not benefit the consumer, yet place unnecessary constraints on the food packagers. In this process, the issue of the consumer's right to know and the method of using the information are confused.

It is consistent with this picture that the majority of the population is ignorant or indifferent about proper diets. Of the millions who "eat out," no one can purchase a balanced meal. A fixed combination of menu items that explicitly guarantees some specified fraction of recommended daily allowances (*7*) is yet to be included in the menus of our food service industry.

A move toward mathematical methods for meal planning will require an interdisciplinary approach, with the participation of fields not traditionally linked to that of human nutrition. Only with the aid of mathematics, mathematical statistics, psychometrics, operations research, and computer science can the vast amount of information generated by nutrition science be fully utilized in medical or economic decisions. Mathematical modeling is the key to the perspective Mayer envisions when he calls for the cooperation of the scientific community in reexamining "our policies and habits concerning food." Within this broad framework, however, three specific issues emerge that must have top priority in our national nutrition policy. These are the problems of data, education, and research.

Nutrition science is a quantitative field, routinely producing and using a large amount of tabulated data. It should be a fundamental part of our national nutrition policy to see that a reliable source of food nutrient composition data is available and easily accessible to the public through a central computerized data bank.

To help nutritionists begin to conceive diet problems in mathematical terms, a complete overhaul of the curriculum in dietary education is necessary. The recent report of a study commission on dietetics (*8*) omits any reference to this need. The recognition of the role and value of scientific methods in diet planning is the responsibility of the leading educators and researchers in nutrition science. Until this responsibility is met, cooperation between experts and other scientists who are now often considered "outsiders" will be hindered.

The art of mathematical modeling in the field of human nutrition is still in a developmental stage. With more and better data and with improved interdisciplinary cooperation, research teams could develop more sophisticated and acceptable models of diet planning that could be applied in hospitals, supermarkets, restaurants, and even to the cost-of-living index (*9*). Research in these areas demands both talent and funds, but the return in benefits to the public far outweighs the investment. The extension of funding for diet planning research should be an integral part of any program or policy which is aimed at the revitalization of nutrition science and the increase of its potential contributions to our life.

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2 January 1973

Precipitation of Phosphates in a Primeval Sea

Handschuh and Orgel (*1*) have reported experiments in which struvite ($MgNH_4PO_4 \cdot 6H_2O$) was produced by the addition of ammonia to simulated (artificial) modern seawater. On this basis they surmise "that struvite may have precipitated from evaporating seawater on the primitive earth, and may have been important for prebiotic phosphorylation."

Although their speculation is interesting, it contains several unmentioned assumptions that do not seem to have attracted their attention. What precipitates from modern seawater, presumably under biochemical influences (*2*), is not hydroxyapatite but a carbonate apatite (*2, 3*). Under these circumstances it becomes difficult to understand why "Carbon dioxide was excluded from the system by means of a tube containing granules of BaO." Both present-day seawater and the phosphatic solid which forms in contact with it contain CO_2, and one wonders why Handschuh and Orgel should assume that primeval seawater did not.

The chemistry of seawater appears to be extremely complex, and the francolite (carbonate fluorapatite) which usually forms—in addition to carbonate minerals and others—cannot be predicted from a simple knowledge of the ionic activities. This is true because the types and extents of complexing are not known but probably are related to organic components of seawater that behave as positive or negative catalysts (*2*).

Although the concentration of Cl^- in seawater exceeds that of F^- by a factor of more than 10,000, it has been estimated that F^- is being removed from seawater about a hundred times faster than Cl^-, principally as phosphates and carbonates of calcium (*4*), and, while phosphorites may contain a few percent fluorine, their chlorine contents usually are almost negligible (*5*). Although it has been estimated that the concentration of F^- in vitro would have to be 100 to 1000 times greater in order for the precipitation of fluorapatite to occur (*6*), the marine brachiopod genus *Lingula* apparently does not know this and forms its shell of francolite (the fluorine content of the ash is 2.44 percent) (*7*).

Shifting consideration from seawater to physiological solutions of vertebrates can lead to some interesting analogies; with the exception of their fluorine contents, these solutions have several similarities. Whereas Handschuh and Orgel (*1*) were concerned with the greater insolubility of apatite and felt compelled to consider struvite as an alternative, there appears to be no problem connected with the resorption of deciduous teeth among mammals, and this raises a question of the extremely complex organic-inorganic relationships.

Finally, even the most ancient phosphatic sediments (phosphorites) generally contain less than 1 percent MgO, so speculations concerning relict struvite receive no support from this direction. Indeed, as Handschuh and Orgel (*1*) admit in the last sentence of their report, struvite is uncommon even as a biomineral (*8*), and it is difficult to believe that primeval seawater would behave in any such manner as their in vitro experiment implies even after the exclusion of CO_2, which was found by McConnell *et al.* (*9*) to be one of the most important factors in the precipitation of dahllite (carbonate hydroxyapatite).

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5 February 1973

In our report we suggested that struvite would have precipitated during the evaporation of tide pools if ammonia was present in seawater at a concentration in excess of $10^{-2}M$. We did not question that apatite would also have been present in the oceans, but, since Mg^{2+} inhibits the direct precipitation of apatite, we believed that prebiotic apatites would have formed by *slow* replacement, for example, from calcium carbonate (*1*). Since the direct formation of apatites nowadays is believed to be a biological process, this process throws no light on the dynamics of prebiotic phosphate precipitation.

We did not consider the possibility that, in the presence of carbonate, carbonate apatite would precipitate in place of struvite. We took it for granted that, during evaporation, calcium carbonate would have deposited first. In view of the acknowledged complexity of such systems, we believe that it is now up to McConnell to show by experiment that this reasonable assumption (*2*) was incorrect.

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2. The same assumption seems to have been implicit in earlier studies. See, for example, (*1*), in which Mg^{2+} was shown to inhibit the precipitation of apatite, apparently in the presence of CO_2.

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