

Sales and technical service personnel are briefed on how the IBM machine will serve the fertilizer field

## Formulation by Electronic Computer

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**A rapid, systematic appraisal of the numerous variables involved in formulating a granular fertilizer can be made by electronic computer**

**T**HE HIGHLY COMPLEX and highly competitive fertilizer business of today has come a long way from the simple blending of dry raw materials which was the common practice not many years ago. Lengthening lists of raw materials and product varieties, coupled with changes in production techniques, have made necessary scores of management decisions where previously no alternatives existed. With the strong trend toward the manufacture of granular fertilizers, other complexities are being added. It is time that some modern tools be

used to simplify rather than further complicate this business.

Among the many problems facing the fertilizer manufacturer are:

- Selection of the best raw materials
- Improvement of plant operation and control
- Lowering of costs
- Revision of formulations to keep up with changing raw material prices
- Continual demand for new and generally higher analysis grades

These problems are interrelated; their

answers are interdependent. A change in any one of them may require a new attack on any or all of the others. The frequency with which formulation changes are made in modern fertilizer plants and the complexity of the calculations involved point directly to the need for a method of calculating formulations not only accurately but quickly.

As a supplier of phosphorus and nitrogen raw materials for fertilizer manufacture, Monsanto Chemical Co. has become increasingly concerned over this need, and has sought some

way to simplify and speed up the work of calculating formulations while preserving—and preferably improving—the usefulness of the answers obtained. A firm grasp of the intricacies of successful formulation is essential if the basic supplier is to produce the raw materials best suited to the advancing technology of fertilizer manufacture.

### A Progress Report

Although the program is not completed, Monsanto has made considerable progress in adapting the IBM 702 electronic computer to the task of formulating granular fertilizers. A second step—formulation of nongranular fertilizers by a similar method—is being developed. Success in the first step will not necessarily be the solution to all granular fertilizer problems, but it should prove a useful contribution to the industry.

The objective is to be able to calculate formulations with a variety of different raw materials, for any given plant operating under specified conditions. Each formulation must meet all of the requirements for good granulation. To achieve this objective requires all the technical information available, as well as some educated guesses which have been partially confirmed by plant tests. The method of calculation must be rapid because a wide range of conditions and materials must be considered; with such a method, a systematic appraisal of the numerous variables can be made in order to minimize cost and improve plant operation.

In order to change formulation from an art to a science, it is necessary to use mathematics, the basic tool of science, rather than trial and intuition,

the basic tools of art. Only after defining the requirements of a formulation in terms of mathematical equations can high speed electronic computers be used to solve the mathematical relationships.

Before any attempt at calculation can be made, the general features of the granulation plant must be known, such as whether a batch or continuous ammoniation system is used. It is necessary to know the range of recycle normally handled in the plant in pounds of recycle to pounds of finished product. It is assumed that the temperature of the recycled material will be 120° to 130° F. Deviations from this range should be noted. Moisture content of the finished product should be specified, as well as moisture content of the recycled material if the two differ significantly.

Raw materials analyses should be specified as accurately as possible. Specifications should be included for all materials presently used, and those which may be considered for future use. Finally, an intelligent study of the formulation problem will require a knowledge of the costs of raw materials, including both purchased goods and those produced, such as normal superphosphate. With such information, it should be possible to formulate various grades mathematically to determine the best operating conditions and lowest raw materials costs.

There are seven requirements for a good granulation formula if one considers only how well the formulation will behave in a plant: material balance, nitrogen balance, phosphate balance, potash balance, ammoniation balance, water balance, and heat balance.

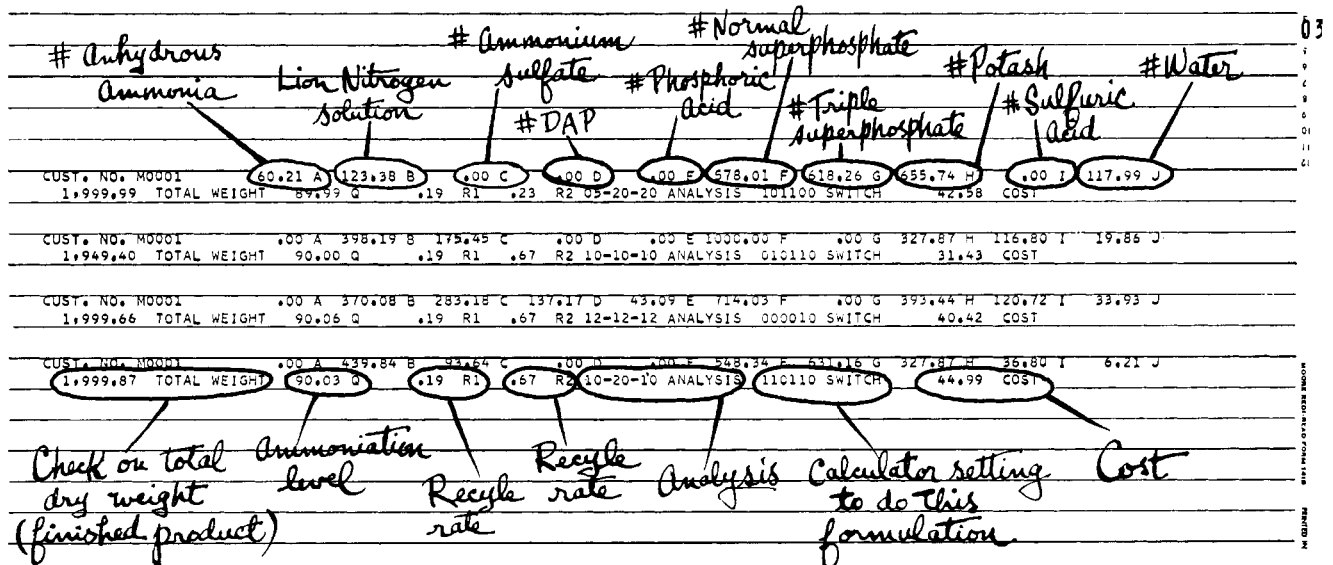
The first four are easily defined mathematically. The material balance must be such that one ton of product from the specified raw materials, after drying to the desired moisture level, contains the desired nitrogen, available phosphate, and potash content to meet the requirements of the grade.

Degree of ammoniation has been extensively studied for superphosphates. Although there is not complete agreement, the amount of uncertainty is small in comparison with other variables. For purposes of electronic computation, it becomes necessary to extend this theory of ammoniation in order to predict the results which will be achieved when phosphoric acid or diammonium phosphate is used as a raw material.

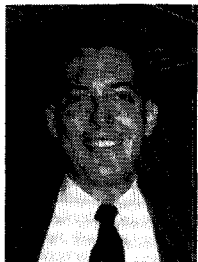
By working backward from the figures used in plant practice for the ammoniation of normal and triple superphosphate, the chemical reactions which previous investigators have proposed were studied. It was found possible to assign equilibrium constants for the reactions taking place in such a manner that ammoniation practice on normal and triple superphosphates could be explained. It seems logical to assume that various combinations of normal and triple superphosphates and diammonium phosphate and phosphoric acid will behave in a similar manner. That is, while the relative importance of the various reactions taking place will differ with the phosphate sources being used, the basic chemistry of the reactions as defined by the equilibrium constants will stay unchanged.

This approach seems reasonable since the constituents of the final mixture do not know from which raw materials they initially came. How-

Some typical granular fertilizer formulations as they come out of the IBM 702; handwriting shows how figures are read



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ever, since the theory was used only as a guide to practice, it was necessary to confirm the theory by running tests in widely different types of plants. These tests confirmed that theory and actual practice were in fairly good agreement. Further experimental studies under more carefully controlled conditions in a laboratory or pilot plant will be required in order to obtain more detailed information, but the present theory is believed adequate to permit formulation with these raw materials.

Moisture content for granulation is an extremely critical factor, because there is only a narrow margin between a too-dry consistency in which large amounts of fines are formed, and a too-muddy consistency in which plant difficulties and large amounts of oversize result. Moisture requirements for granulation depend primarily on the amounts of soluble salts present to dissolve and form the liquid phase, and secondarily upon the temperature at which granulation occurs.

The solubility of ammonium nitrate (or urea) is much greater than the solubility of the other salts. As a first approximation, it may be assumed that the moisture content required will be dependent upon the amount of ammonium nitrate (or urea) added to the formulation, usually in the form

of a nitrogen solution. Other soluble salts, particularly the ammonium phosphates produced, for example, from diammonium phosphate or ammoniation of phosphoric acid, also have an effect on the amount of water required for granulation. These differences become most pronounced in low nitrogen grades where their effect is not obscured by the effects of ammonium nitrate. However, in these low nitrogen grades, the water balance is generally not an important cost factor since additional water is usually required to achieve granulation. Thus, for practical purposes, it has been possible to define mathematically in terms of ammonium nitrate concentration the moisture content required for granulation.

The heat required to produce granulation is somewhat less critical than the moisture, since satisfactory granulation can take place over a range of temperatures. The temperature limitations are somewhat dependent upon the type of equipment being employed. In general, at temperatures below about 160° F., granulation becomes progressively more difficult to control. The amount of oversize produced increases significantly at low temperatures, and there is greater tendency for caking to occur in the dryer because the particles then become more fluid as their temperature increases. On the other hand, at high temperatures (about 220° F.) problems are encountered with the decomposition of ammonium nitrate and urea. There is also increasing danger of flash fires when ammonium nitrate is present. If only ammoniacal nitrogen is being used, somewhat higher temperatures may be employed, but eventually the evaporation of water becomes so rapid there is not time to achieve granulation before the product becomes too dry.

The heat of ammoniation of normal and triple superphosphates has been carefully studied. Furthermore, heats of formation of monoammonium and diammonium phosphates and of ammonium sulfate are known. Consequently, it is possible to write a satisfactory mathematical relationship between the chemical heat produced from the components of the formulation and the temperature rise experienced in plant practice in the mixing and granulating operations.

### Recycle Requirements

The requirements for granulation apply not to the raw materials alone but rather to the combination of raw materials and recycle being granulated together. Recycle is used for reworking the granules of undesired particle size, for drying and cooling

the mixture so that greater quantities of liquid raw materials (generally cheaper) can be used, and in some plants for controlling granulation.

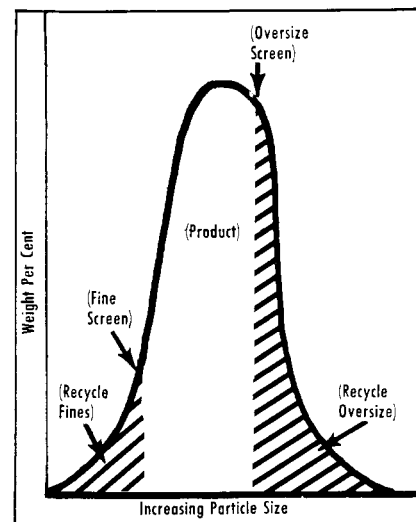
Amount of recycle, the product particle size requirements of the manufacturer, and formulation are closely related factors. A distribution of particle size is characteristic of granulation, even though the shape of the distribution curve (Figure 1) will vary with the equipment and formulation used. The amount of fines and oversize removed will depend upon the mesh size of the screens selected. Consequently, a closely screened product and high recycle must go together. If a closely sized product is required, proper formulation can improve, but not drastically change, the amount of recycle. On the other hand, if close screening is used only as a means of producing recycle for wet formulations, then the production rate can be increased markedly by screening between wider limits and formulating for lower recycle.

### Raw Materials

Eleven different raw materials may be used in the proposed method of formulation: anhydrous ammonia, triple superphosphate, phosphoric acid, diammonium phosphate (DAP), nitrogen solution, ammonium sulfate, normal superphosphate, potash, sulfuric acid, water, and filler. The last seven of these are assumed to be available in all plants.

Since it is possible to combine 11 raw materials in 2047 different ways, considerable selection must be made with respect to the different raw material combinations which can be con-

Figure 1. Distribution of particle size is characteristic of granulation, but shape of the curve will vary with equipment and formulation used



sidered for formulation. It has been assumed, therefore, that all plants will have the seven more common raw materials available, and that the various selections will be made by adding one or more of the remaining four raw materials. All possible cases for these four added raw materials (i.e., anhydrous ammonia, phosphoric acid, DAP, and triple superphosphate) would give a total of 15 different combinations. Present work is concentrated on seven of these 15 possible combinations.

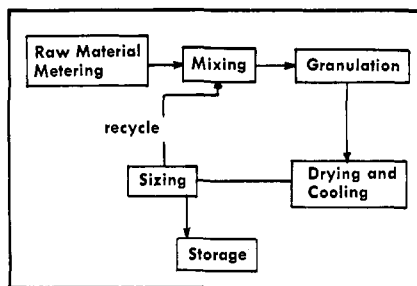
Because a given material is "available" for formulation does not necessarily mean the formulation will call for its use. For example, filler is never used in combination with the three more concentrated forms of phosphate. Water is often not needed. Also, combinations of anhydrous ammonia and sulfuric acid are less likely to be found. Thus, a given raw material is used only if needed for the formulation.

### Why a Computer is Employed

With the problem defined in mathematical terms, it is then necessary to find its solution. In this problem, the raw materials are the unknowns, and the seven requirements for formulation give seven equations which must be solved simultaneously. The raw material specifications and the various operational parameters are the physical constants which must fit into these equations.

The solution of seven simultaneous equations for seven unknowns is impractical with a slide rule or desk calculator because of the time required. On the other hand, a high speed computer—such as the IBM 702—can quickly solve problems that require many man-hours of "hand" calculations. Often, there is more than one solution to a problem since, with eight or more unknowns, there can be an infinite number of solutions. As a result, it is possible to obtain more than one formulation for a given grade from the same group of raw materials.

Monsanto's IBM 702 is called "the brain" by many who have watched it perform, but more often "the idiot" by those who work with it. Actually, both are right. It is a "brain" on speed and accuracy, but an "idiot" on the extent of detailed instructions it requires and on its lack of discretion in performing ridiculously if instructed to do so. The machine requires about 2500 separate instructions to learn how to formulate fertilizers. If a single instruction is written incorrectly, almost any kind of answer may result. However, since not every instruction is used for every formulation, it is possible to have some correct results and some that are completely in error.



There are still some incorrect instructions to be tracked down in Monsanto's granular formulation program.

The IBM 702 is used for several types of calculation at Monsanto, and must be retaught to formulate each time it is changed from some other job back to the job of formulation. This lesson takes about one minute if the instruction is conducted from punched cards, or about 1/100 of a second if the instructions are given from magnetic tape. Alterations are now being made to increase the memory of the machine from 10,000 to 20,000 spaces for yes-or-no type answers. The memory can be extended to a much larger extent by using magnetic tape, although in this case magnetic tape is slower in response.

The problem of formulating granular fertilizers presently requires about 12,000 memory spaces. Each formulation to be calculated requires the insertion of two standard punch cards for machine instructions. Most of the raw material specifications will remain the same for a given formulator as different grades are set up with different raw materials and plant operating conditions. Therefore, most of the punches will remain the same from card to card. The punches which remain the same can be automatically duplicated; the variable punches are put in by hand. The time required for punching a pair of formulation cards is less than one minute.

After automatically feeding in a pair of problem cards, approximately 10 to 30 seconds of computation is required before the completed formulation is printed out. The expanded memory capacity will greatly shorten this time. The results are printed in two lines, a complete line being printed at a time. The first line contains the pounds of raw materials to be used. The second line back-calculates the total weight of product (after drying to the desired moisture content), the estimated recycle rate to be used, the per cent of the maximum theoretical ammoniation which has been utilized, and the grade and calculator settings used to select raw materials. The machine calculates the total cost of the formulation

by multiplying the price of each raw material by the pounds used, and summing up the total. If given an impossible problem to formulate, the machine will keep trying indefinitely until instructed to stop.

A good comparison of the costs of using different raw materials and different nitrogen solutions can be made by formulating so that the operational values will remain constant. In other words, the attempt is made to compare formulations which will operate at essentially the same recycle rate. Having selected the best raw materials, one then determines the best combination of production rate and raw materials cost by comparing the same raw materials formulated to give different recycle rates.

It frequently may be desirable to use different formulations for off-season production from those used during peak-production periods. For example, raw materials cost would be the predominating factor during off-season production, whereas during the peak of the season maximum production rate would be the primary consideration. Furthermore, it often will be desirable to have a series of closely related formulations so that seasonal variations in temperature and humidity as well as variations in raw materials, such as the moisture content of normal superphosphate, can be taken into account. Also, special formulations may be developed for starting up a plant with no recycle available, or for consuming any existing recycle supply at the end of a run.

Monsanto hopes to be able to use studies of this type to determine which nitrogen solutions and other raw materials should be produced in order better to meet the needs of the granular fertilizer industry.

### Present Status

Formulations for some grades and raw material combinations are now being correctly formulated by the IBM 702. Other formulations are still giving trouble. The problem of finding errors in calculator instructions is a slow, painful process and will require additional time before all errors are completely eliminated. The resulting formulations must be thoroughly evaluated, and their limitations carefully defined. It is anticipated that some further modifications and changes in the methods of calculation will be required to improve the results obtained. This approach to the problem, however, promises to be at least a step in the right direction, and efforts are being made to make an electronic formulation service available at the earliest possible date.