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Graphical Presentation of Results from Scientific Computer Models

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With the advent of high-speed digital computers, scientific model computations expanded from short systems of equations capable of being solved by hand to much larger systems requiring machine solution. Systems of 30 or 40 partial differential equations requiring simultaneous solution are now common; systems of several hundred equations are capable of being treated with modern computational equipment.

Summary. The graphical presentation of the results of complex computer model calculations is frequently as important as the computation, since it is generally through such presentations that the modeler and the modeler's audience derive the maximum amount of information. In this article graphical techniques for presenting multidimensional model results are reviewed and examples are given of the most useful forms of presentation. Color graphics is used increasingly for the presentation of model results, and three types of color displays are discussed here: the chromatic plot, the binary chromatic plot, and the ternary chromatic plot. Their use is illustrated with examples from computer modeling of air quality in the urban atmosphere.

The amount of information contained in the results of a large model computation is very great. A dual challenge thus faces the modelers: how to present the results to themselves so that the maximum amount of information can be perceived, and how to present the results to others so that the maximum amount of information can be transmitted. The solutions to this challenge have been diverse, but are nearly always graphical. Tables have proved not nearly as useful to the modeler in perceiving qualitative results; their function is to present detailed quantitative results, the information transferred by means of graphical displays being semiquantitative in nature.

The degree of sophistication needed in the presentation of results is a strong function of the dimensionality involved. With the exception of equilibrium calculations, most models include time as an independent, continuous variable. The spatial detail of models depends on their application; efforts have ranged from no spatial dimensions (one homogeneous volume) to three spatial dimensions. The spatial dimensions may be discretized into convenient volumes, but are often thought of and presented as continuous variables. Often a computation is performed several times, each computation differing by the value of a parameter such as one of the initial conditions. This adds one more dimension in a discrete variable. The dimensionality thus may range from zero to five or more—a wide range indeed in a world of two-dimensional paper and projection screens.

Our purpose in this article is to survey the graphical techniques that have been used for the presentation of scientific computer model results, to present new techniques we have developed, and to examine the merits of the various approaches. New techniques involving chromatic presentations of data are described. Because of our interest and experience, the examples that we present are drawn from chemical kinetics, one of the fields that has experienced rapid growth in model complexity and sophistication. A similar situation occurs, however, in solid-state physics, meteorology, and many other fields. A single set of data is used in this article for many of the presentations so that the relative merits of the presentations can be evaluated by the reader.

Dependent Variables in Chemical Kinetic Computations

The central variable whose values must always be presented in some fashion is the species concentration. The concentration is often plotted as a function of one or more independent variables such as time or space. A number of other dependent variables related to concentration are also commonly used, such as change in concentration (*1*), ratio of two concentrations (*2*), length of a growing polymer chain (*3*), nucleation rate (*4*), opacity (*5*), length of a radical reaction chain (*6*), or temperature (in calculations where temperature is a dependent variable) (*7*).

Once the concentrations of the important species and their variation with space and time variables are known, it is generally desirable to study why the concentrations behave as they do. Two subdivisions are common. The first is the presentation of the principal rates (time derivatives of a concentration as a result of a specific reaction). The rates are usually plotted as a function of time, but can also be plotted as a function of a space variable (*8*). Unlike concentrations, the absolute values of rates are generally of less interest than their ratios, for the latter show which reactions or processes control the concentration results. Although chemical reaction rates or physical source or sink processes or their ratios are the computational varia-

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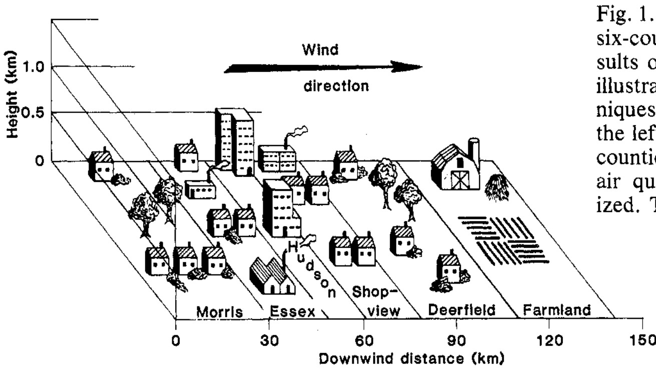

Fig. 1. Schematic diagram of the six-county air quality model, results of which are used here to illustrate graphical display techniques. The three counties to the left are existing New Jersey counties whose emissions and air quality are well characterized. The three to the right are fictitious and are used to study air quality downwind of an urban area while avoiding the complexities of the actual meteorology in the area.

bles most commonly displayed, a number of alternatives have been used: energy release rate (*9*), residence time (*10*), surface loss (*11*), and conversion rate (*12*). A second behavioral subdivision is the concentration dependence on parameters, such as initial conditions or reactant injection rates (*13*). Although modern mathematical techniques show promise of deriving such dependence from a single calculation (*14*), results of this type have traditionally required a series of independent calculations for different choices of the parameter of interest. As mentioned above, this approach adds a dimension to the calculation, the dimension being discrete rather than continuous.

A final but crucial requirement is the comparison of results with data in order to assess the degree to which the model reproduces observable characteristics. These comparisons are almost always made with the concentration results rather than the rates or processes that produce those results, since the latter are generally not observable. Comparisons of model results with data are often made by superimposing the data on one of the calculated concentration plots. Among the variations on this procedure are displays of some form of the residuals between model and data, such as the ratios of calculated and observed concentrations as a function of one of the independent parameters of the model (*15*), or the logarithmic ratios in the approach of Olson and Gardiner (*16*).

Graphical Displays of Concentration

To demonstrate alternative graphical displays of concentration, we use results from a three-dimensional (two spatial, one temporal) model of air quality in the urbanized northern New Jersey region. The model, pictured schematically in Fig. 1, has a grid of six geographic areas (the horizontal variable) with three altitude ranges (the height variable; 1.5 kilometers is the altitude to which the atmospheric boundary layer is well mixed). The chemical reactions involving the interactions among atmospheric trace species are computed within each volume at each time step, interactions among volumes being produced by advective and diffusive air motions. The calculations are performed for the entire day from midnight to midnight. Further details of the model and some of its results have been presented (*17*).

The simplest concentration display one can make from the computation described above is to choose a single volume (or several volumes) and plot the variation in the concentration of a chosen species (or several species) with time. As an illustration of interest in atmospheric chemistry, we examine the computed concentrations of ozone at ground level in several geographic areas (Fig. 2). The ozone concentration is seen to increase rapidly in midmorning, reaching a maximum value in midafternoon. The ozone in Morris County, upwind from the urban area, is similar in pattern and slightly higher in concentration than that in Hudson County. In Farmland County, downwind from the urban area, the concentration is substantially higher and the pattern is distinctly different (for reasons that will become apparent). Comparison displays such as this can be of great value, but distinctions can be difficult to see if the results in adjacent volumes are very similar. If they show the concentrations of several species, the results for only one geographic area can be shown in such a graph.

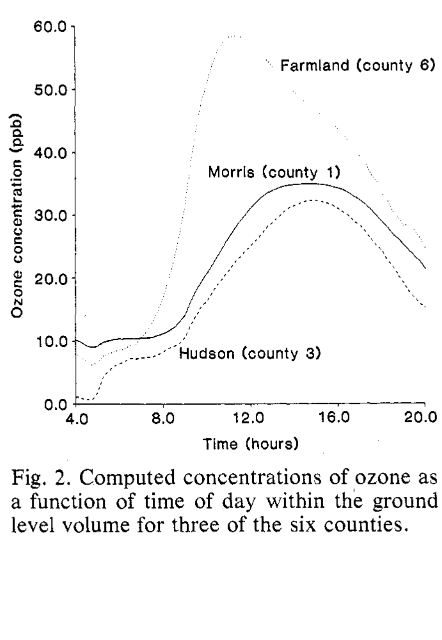

Fig. 2. Computed concentrations of ozone as a function of time of day within the ground level volume for three of the six counties.

The results from two-dimensional calculations (or those of higher dimensionality expressed in two dimensions) are conveniently displayed by using the two independent variables as x and y axes and indicating the concentrations of a dependent variable of choice at each point x_i, y_j. The dependent variable values are most often presented by contour plots, as shown in Fig. 3a. Here we see that ozone concentrations in Hudson County are lower near the ground and that the diurnal pattern has two maxima at the higher altitudes. The lower concentrations near the ground result from the emission of NO from ground-based sources. The two maxima at high altitudes result from the scavenging of ozone by NO from rush-hour traffic; the NO is brought to these altitudes in late morning by atmospheric motions. Although these plots are useful (*17, 18*), they have the disadvantage that attention is drawn not to the concentration values themselves but to their derivatives; that is, one's eye is caught by the bunching of the contour lines rather than by their numerical values. The use of shading (through black to gray and white) or cross-hatching is an aid to the viewer, but the limited number of tones is restrictive and perceptually difficult. An alternative presentation is the projection of a surface in two dimensions, shown in Fig. 3b. This display enhances extreme values in the results (*19*) and is particularly good for the detection of trends (note the concentration increase as a function of height in the early morning hours and the interplay of height and time at the peak concentrations), but the required masking of some regions causes details in the "valleys" of the surface to be hidden behind the "mountains"; a second difficulty is that it is hard to compare two such plots made for different species or different independent variables.

A presentation that avoids the difficulties of both of the types of displays discussed above is the chromatic contour plot, on which the concentration value z_{ij} at each point x_i, y_j is indicated by color. As with traditional contour plots, the z_{ij} are discretized within a series of ranges, each of which in this case is assigned a color. The choice of

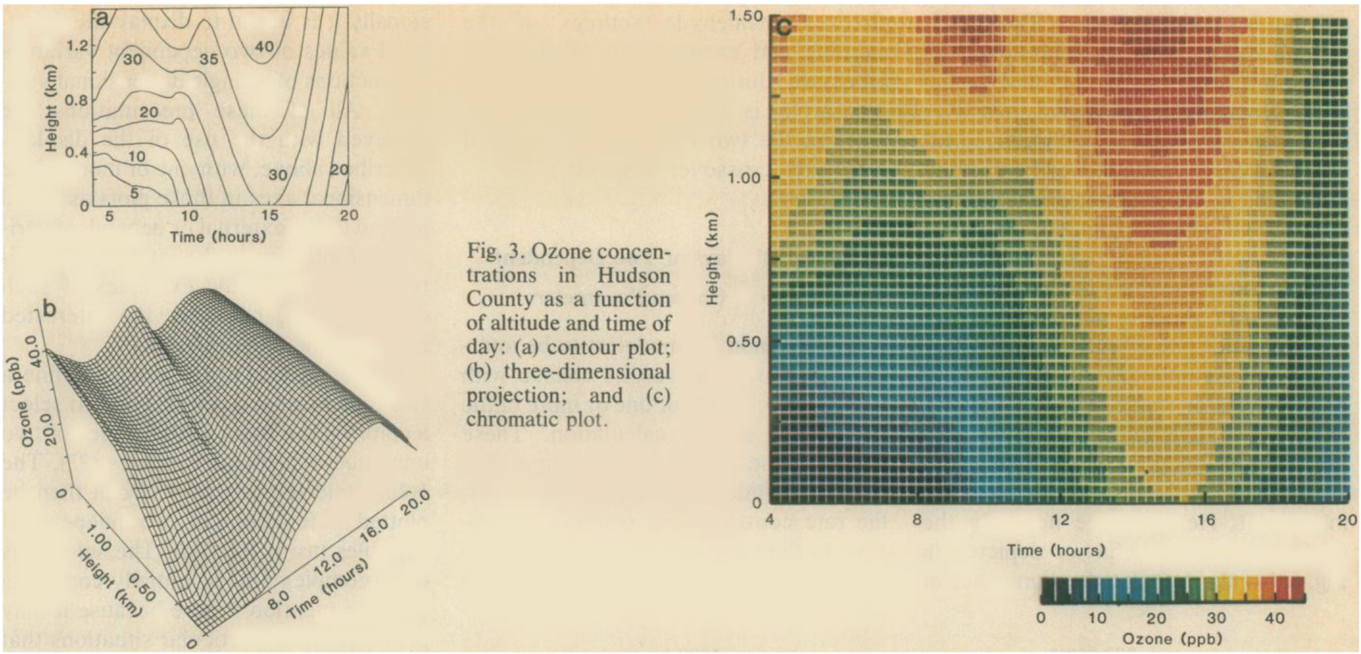

Fig. 3. Ozone concentrations in Hudson County as a function of altitude and time of day: (a) contour plot; (b) three-dimensional projection; and (c) chromatic plot.

colors is not straightforward and is discussed below; here we will simply note our choice of red for high values of z_{ij} and blue for low values. Chromatic contour plots are commonly seen on topographic maps and NASA has utilized them for data collected by satellites, but they have heretofore seen relatively little use in scientific model applications. They have many advantages. As seen in Fig. 3c, they permit a wide range of concentration values to be instantly comprehended and permit the results for any x_i, y_j point of interest to be readily perceived. Plots for different species or different dimensions can be compared more easily and accurately than either contour plots or three-dimensional projections, provided there is consistency of scale and color association across plots.

No existing graphical method appears capable of presenting on a single plot the concentration for a calculation of dimensionality higher than two. The presentation of a sequence of plots, however, can permit concentrations for a three-dimensional computation to be shown. In general, such presentations have two spatial dimensions as the independent variables on each plot, with time as the sequence variable. A restricted form of such a presentation is shown in Fig. 4, where time "snapshots" of interest to the analyst have been selected. A much better approach is to put together a large sequence of such frames into a motion picture, where frame-to-frame changes can easily be detected.

Several features of the computational results are readily conveyed by Fig. 4. Perhaps the most striking is the occurrence of the highest concentration downwind of the urban area (see Fig. 1) and at the highest altitudes within the mixed boundary layer. The lowest concentrations occur in the morning near the ground, where ozone is lost by reaction with NO from rush-hour traffic.

Another approach to the high-dimensionality problem is to plot binary information in three dimensions. Such displays are commonly used to plot the positions in space of atoms (*20*), molecules (*21, 22*), or polymer chains (*23*) or to plot the direction of time in coordinates representing three dependent variables (*24*). The binary nature of this display (that is, is there something at position x_i, y_j, z_k or isn't there?) limits its applicability. It can be applied to continuous variables, however, by plotting excursions above a selected cutoff value. Such a plot is shown in Fig. 5 for ozone values above 50 parts per billion in the six-county calculation. The tendency for high ozone values to occur downwind at altitudes above ground level at midday is clearly shown in a single display.

Graphical Displays of Principal Rates

It is often advantageous as part of a model presentation to include schematic diagrams of the processes involved. The rates of these processes (or, in a calculation without time dependence, their equilibrium values) are the factors that determine the concentration results. A dual purpose can thus be served by adding rate information to a schematic process diagram, either numerically or by a device such as width of arrows (*25*). Such a diagram provides insight into both the processes and their relative importance. A limitation of the display is its restriction to a single spatial and temporal point. Edelson and Chambers (*26*) surmounted this difficulty for a one-dimensional calculation with a motion picture presentation of a flow diagram. For calculations of greater dimensionality, however, other techniques must be employed. The most common is to plot one or more rates as functions of time or space, as was done for concentration in Fig. 2. This presentation, which expresses dependence on only a single independent variable, allows several rates to be directly compared and numerical values to be derived.

The magnitude of a reaction rate can also be shown as a function of two dimensional variables. To illustrate such a plot, we use the rates of generation of formaldehyde in the six-county calculation. As shown in Fig. 6a, there is a chemical reaction chain that begins with hydrocarbons (RCH_3) and ends with formaldehyde (HCHO, the species produced when R = H). A key reaction is the photolysis of ozone to yield HO· radicals, a process possible only during the daytime. Aldehydes are also directly emitted from a number of sources, including motor vehicles. We thus anticipate peak direct aldehyde emission during the rush-hour traffic periods. These effects are shown by the contour plots in Fig. 6, b and c. That of Fig. 6b demonstrates that the formaldehyde emission rate is a maximum at 7 to 9 a.m. and 3 to 6 p.m. and that its spatial intensity follows the industrial and population patterns indicated in Fig. 1. The chemical production of formaldehyde, on the other hand, is a midday process. The chemical rate is thus at its maximum over the period 10 a.m. to 2 p.m. and has a broader maximum downwind than over the urban area. Just as with concentration data, these features may be usefully presented in three-dimensional projections or chromatic plots, as described above.

Rather than the rates themselves, it is often rate or process ratios that are of interest, since one often wishes to know which rate dominates at a particular point in time or space. Figure 6d shows how the relative contributions of two processes as functions of two dimensional variables can be displayed on a chromatic plot. Here we see not only the qualitative source behavior depicted in Fig. 6, b and c, but also the dominance of direct formaldehyde sources in the morning and evening and of chemical processes during midday. (Note that such a plot is useful only if the magnitudes of the two rates being compared show such crossover behavior.)

Graphical Displays of Two Dependent Variables or of Chosen Parameters

It is common for modelers to be interested in how their results change with the values selected for one or more of the parameters in the calculation. These might be the initial concentration of a reactant, a ratio of initial concentrations, the rate constant of a reaction or process, or the value of a physical condition such as pressure or temperature. Occasionally it is useful to display the calculated values of two dependent variables as functions of a single dimensional variable. All of these presentations are achieved with the use of the displays described above, with one or more of the dimensional axes in those plots assigned instead to the external or dependent variables of interest. In the interest of brevity, we do not show examples of such displays here, but refer the interested reader to the cited references.

In principle, it is possible to define a two-dimensional color grid and to select a color on the basis of the values of two unrelated dependent variables (*27*). The colors selected in this way can then be plotted as functions of two independent variables (as in Fig. 6d). The scheme is quite complex and potentially confusing (*28*); we mention it here because it may prove useful in particular situations that arise.

In examining the dependence of results on the values of selectable parameters, practical considerations of time and computer capacity generally limit the range of values that can be considered. The values are often used to predict results as though the variable had been treated as continuous, a process that involves interpolation before presentation. Such an approach is generally satisfactory, but users must be alert to its possible failure when results are not linearly dependent on the parametric value. In such cases, regions of rapid change may have to be investigated in more detail than regions where the results are changing slowly.

Graphical Displays of Three Related Variables

In certain applications it is useful to display the mutual relationship of three variables as a function of several space and time dimensions. For this purpose we have devised the ternary chromatic plot, illustrated in Fig. 7. In this display the color square plotted at each point is selected by computing the relative proportions of the three variables and using these values to define a position within the ternary color key. The color selections should be made in accordance with psychological color perception theory (*29*). In the example shown here, we illustrate the relative concentrations of NO, NO_2, and HNO_3 (the "odd nitrogen" species) in the six-county region. These relative concentrations are directly related to the chemical state of the atmosphere, since NO is directly emitted from sources, NO_2 represents a chemi-

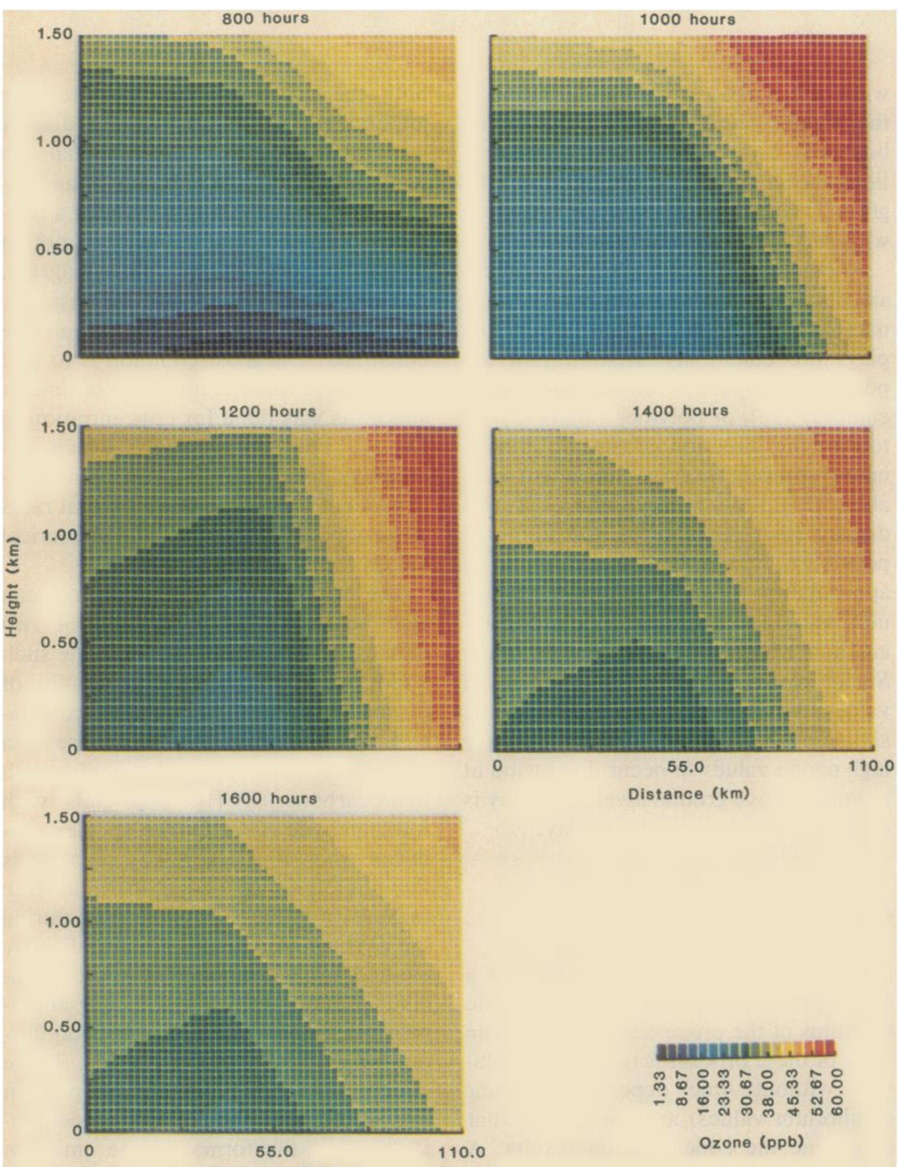

Fig. 4. Ozone concentrations within the six-county region as a function of position along the west-to-east airflow trajectory and of altitude. When a sequence of these chromatic plots is presented in motion picture form, the concentration variations in three independent dimensions are displayed.

cally intermediate state of oxidation, and HNO_3 is the terminal oxidation phase of atmospheric nitrogen, a phase reached only during the photochemically active periods when HO· is produced. In Fig. 7 the relative proportions of the three nitrogen-containing species are color-coded as functions of downwind distance and altitude: a point at which the odd nitrogen is primarily NO is coded magenta (lower left corner of the triangle), a point dominated by NO_2 is coded cyan (lower right corner), and a point dominated by HNO_3 is coded yellow. The intermediate points are coded as combinations of the subtractive primary colors. The display in Fig. 7 reflects the dependence of the odd nitrogen species both on direct sources and on chemical reactions, NO being the dominant species in urban areas during rush-hour traffic periods, NO_2 becoming dominant as the NO is oxidized during transport downwind, and HNO_3 becoming more abundant away from the ground and far downwind of the urban center during the daytime. In that location the photochemical source of the HNO_3 is optimized, while the deposition to the ground is not a factor. The interplay of the nitrogen chemistry with that of ozone can be studied in more detail by comparing Fig. 7 with Fig. 4.

Ternary chromatic plots can be tremendously effective in communicating information, but their applicability is quite restricted. They are suitable if three variables (species, rates, and so on) are each of concern, if each becomes or may become dominant at some time or location of interest, and if they have a close conceptual relationship. Our experience suggests that the latter requirement is the most crucial; its neglect produces a display with more diverse information than can readily be assimilated and promotes confusion rather than communication.

Comparison of Results with Data

The true test of a model is the degree to which it reproduces observational data. This agreement can be expressed numerically as the value of a selected correlation function or graphically as a function of a dimensional variable. The latter is perhaps more common and is generally restricted to comparisons of concentration values. (Although in principle there is no reason why comparisons could not be made between observed and calculated rates, rates are seldom observed.) More sensitive graphical procedures involve plotting the ratio of observed and computed values as a function of a dimensional variable, or constructing a scatterplot of observed and computed values. As models of increased dimensionality are used, comparison with observations becomes more complex. Frequently (as with the air quality examples used here), insufficient data are available to permit detailed comparison. If detailed observations have been made, recourse to some of the graphical methods shown above are likely to be useful. A particularly promising display is the chromatic rate plot of Fig. 6d, with the chromatic scale keyed to the ratios of observed and calculated values.

Use of Color Graphics

The recent increase of interest in the use of color graphics for scientific purposes has been largely motivated by two factors—the increasing ease of obtaining filled color areas (as opposed to colored lines), and the greatly reduced cost of producing and reproducing hard-copy color output. The former are currently provided most efficiently by color cathode-ray tube terminals, the latter by color copiers operating under computer control.

The increasing availability of a color graphics capability (*30*) is no guarantee of its optimum use, since the appropriate use of color is highly complex and few scientists have experience in this field. This is particularly true in the areas of psychological color perception and esthetics, both important in the successful use of color in graphical displays. The complexity results from the three-dimensional nature of color space, one dimension being darkness (black to white), the second individual color (or hue), and the third chroma (or intensity of the hue). Recognition of this nature suggests cer-

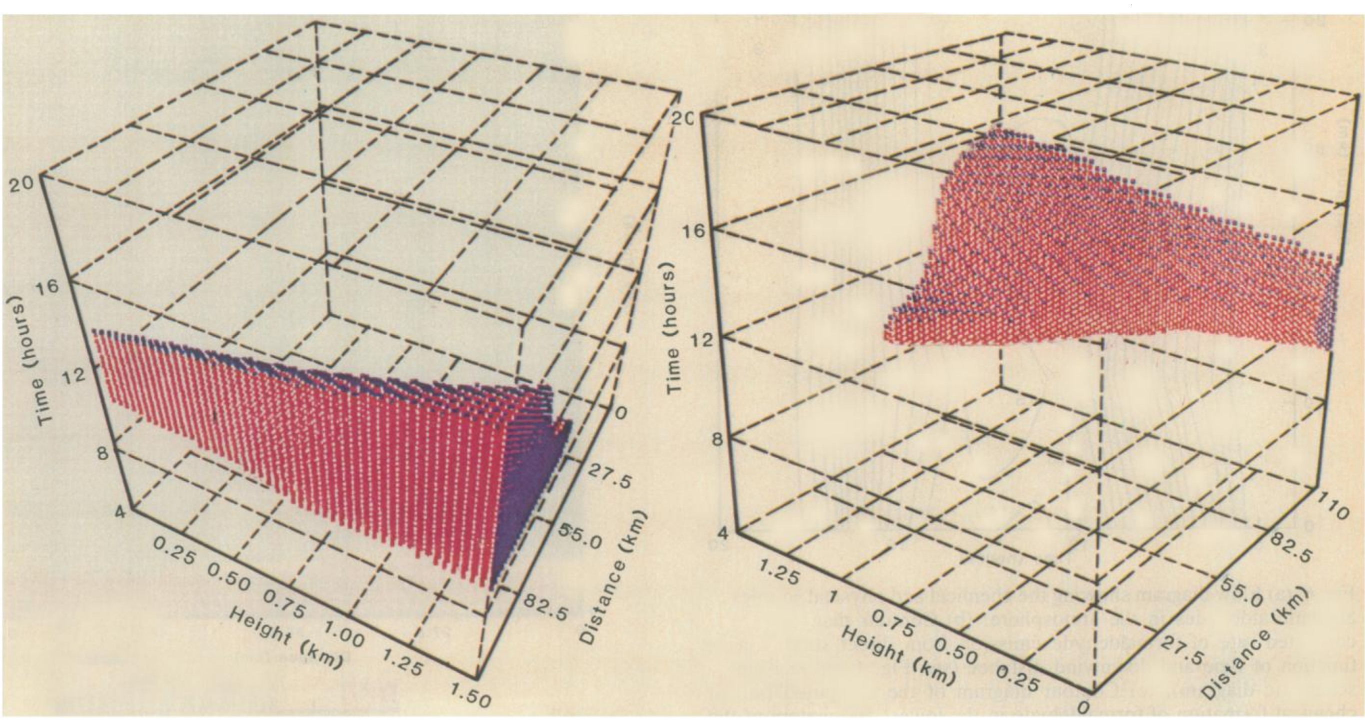

Fig. 5. Three-dimensional "binary" diagrams of ozone concentrations throughout the day for the six-county calculation, as viewed from two different perspectives. A small rectangle is plotted at the x_i, y_j, z_k points for which the ozone concentration is greater than 50 parts per billion. The two colors indicate the "top" and "sides" of the solid and are not related to concentration.

tain guidelines in the selection of color scales. In a typical application, a color scale encodes values from low to high. Experience shows that the data are better conveyed if a chromatically sequential scale is employed. Thus the sequence blue, green, yellow, red (which follows the natural ordering of color space) is preferable to yellow, blue, green, red (which does not). Further, care must be taken that the scale selected is not chromatically circular, an error that frequently arises when all available hues are used. Consider the scale green, cyan, blue, magenta, red, yellow as an encoding of low to high values. Yellow, which encodes the highest value, is chromatically (and perceptually to many)

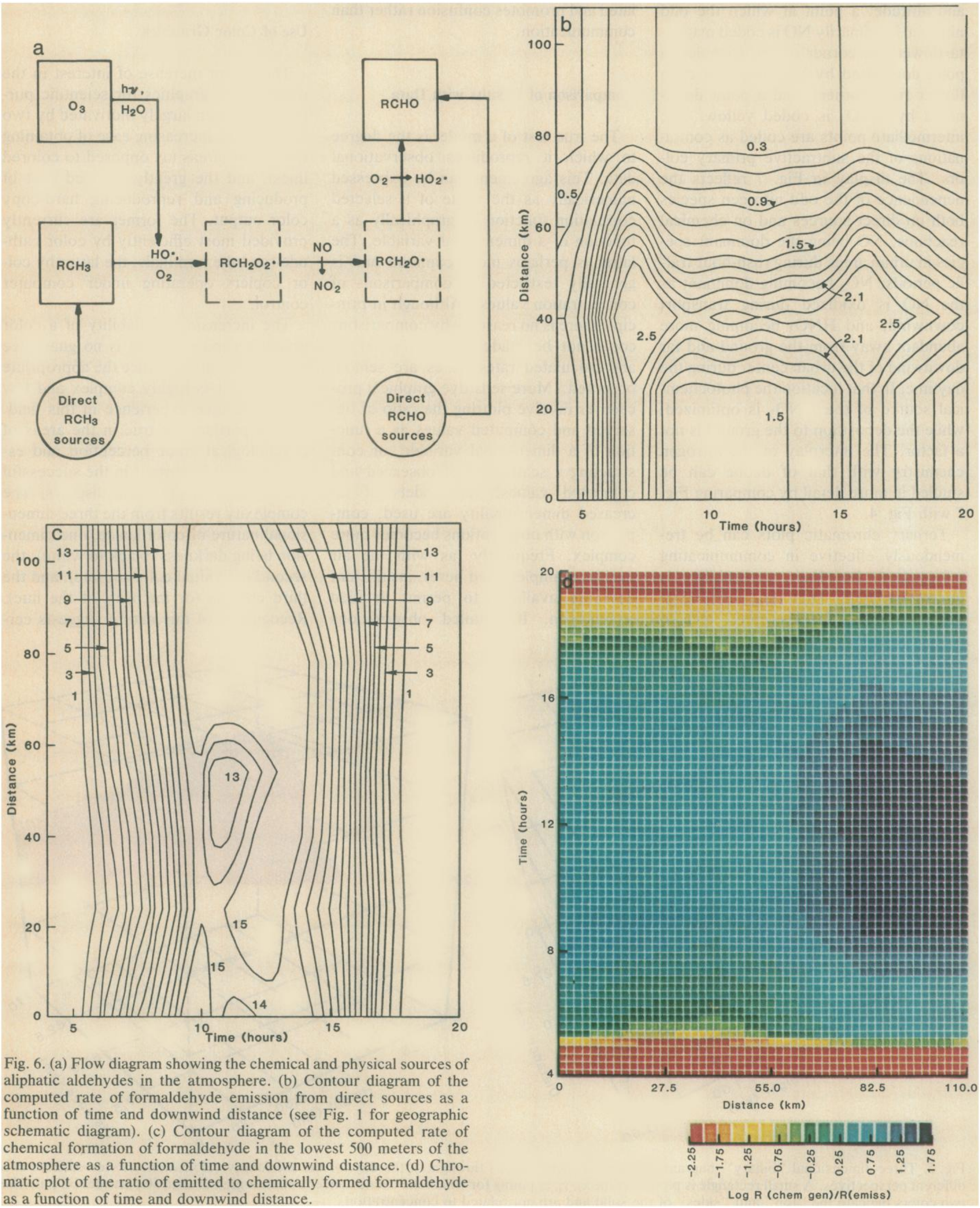

Fig. 6. (a) Flow diagram showing the chemical and physical sources of aliphatic aldehydes in the atmosphere. (b) Contour diagram of the computed rate of formaldehyde emission from direct sources as a function of time and downwind distance (see Fig. 1 for geographic schematic diagram). (c) Contour diagram of the computed rate of chemical formation of formaldehyde in the lowest 500 meters of the atmosphere as a function of time and downwind distance. (d) Chromatic plot of the ratio of emitted to chemically formed formaldehyde as a function of time and downwind distance.

closer to green, the lowest, than to magenta. The solution is to omit part of the spectrum, perhaps yellow in this example. Similarly, in Figs. 3c, 4, and 6d we have omitted magenta. In contrast, we use all the primary hues in Fig. 7, since the continuous chromatic scale complements the information to be conveyed.

Another common problem in color graphics is the garishness of the displays, which results in part from the limitation of many color devices to six or eight hues of very high saturation. We have found two techniques useful in minimizing this problem. The first is to use a form of halftone in which an area is filled with alternate pixels of two colors. A mixture of red and yellow, for example, produces a visual impression of orange, a color of lower chroma. A second technique is to superimpose a white grid over the display. In addition to serving as a positional reference, the grid produces a more pleasing display because hues do not directly abut one another.

The limitation of many color devices to a half-dozen or so hues may not be very serious in practice; Bertin (*31*) suggests that no more than six colors can be used successfully on any one display. Their choice may control the viewers' perceptions, however. Red is a particularly important color, since studies show that it is perceived out of proportion to its surface area (*32*). Regardless of the current availability of colors and the appropriateness of those available, one can expect a wider range to be common in the near future. Chromatic plot development should thus anticipate future extension to this richer palette.

Discussion

In this article we have illustrated and discussed a number of techniques for presenting results from scientific computer models. Here we discuss the results with emphasis on the dimensionality involved in the calculation.

One-dimensional models. The independent variable in these models may be either space or time. Results are appropriately presented as shown in Fig. 2, with the independent variable as the abscissa and one or more dependent variables on the ordinate scale or scales. This is the only display in which more than one unrelated dependent variable can be usefully shown, but only if they have a common vertical scale. Such plots may be useful for calculations with higher dimensionality; the cost is sacrifice of some dimensional information.

Two-dimensional models. One spatial and one temporal independent variable are generally used in these models, but equilibrium calculations with two spatial variables are also common. Results containing the full dimensionality of the calculation may be presented in any of the forms shown in Figs. 3, a to c, 6d, and 7. The dependent variable may be a concentration value or a rate, the ratio of two such values (if related to each other in a readily understood way), or the relative proportions of three closely related variables.

Three-dimensional models. These calculations generally comprise two or three spatial dimensions and one or no time dimension. The full dimensionality can be retained on a single display only if the dependent variable is binary in nature (see Fig. 5). In the more usual case, a series of plots of the type shown in Figs. 3, a to c, and 6d are presented in sequence, as in Fig. 4.

Models of dimensionality ≥ four. No graphical displays can be constructed for these models without loss of information. A possibility offering perhaps the smallest loss for four-dimensional models is a sequence of binary displays (a combination of Figs. 4 and 5), which retains the dimensionality while reducing a semiquantitative dependent variable result to a binary result. Another option, which is particularly good if one of the dimensions is an external parameter rather than a spatial or temporal vari-

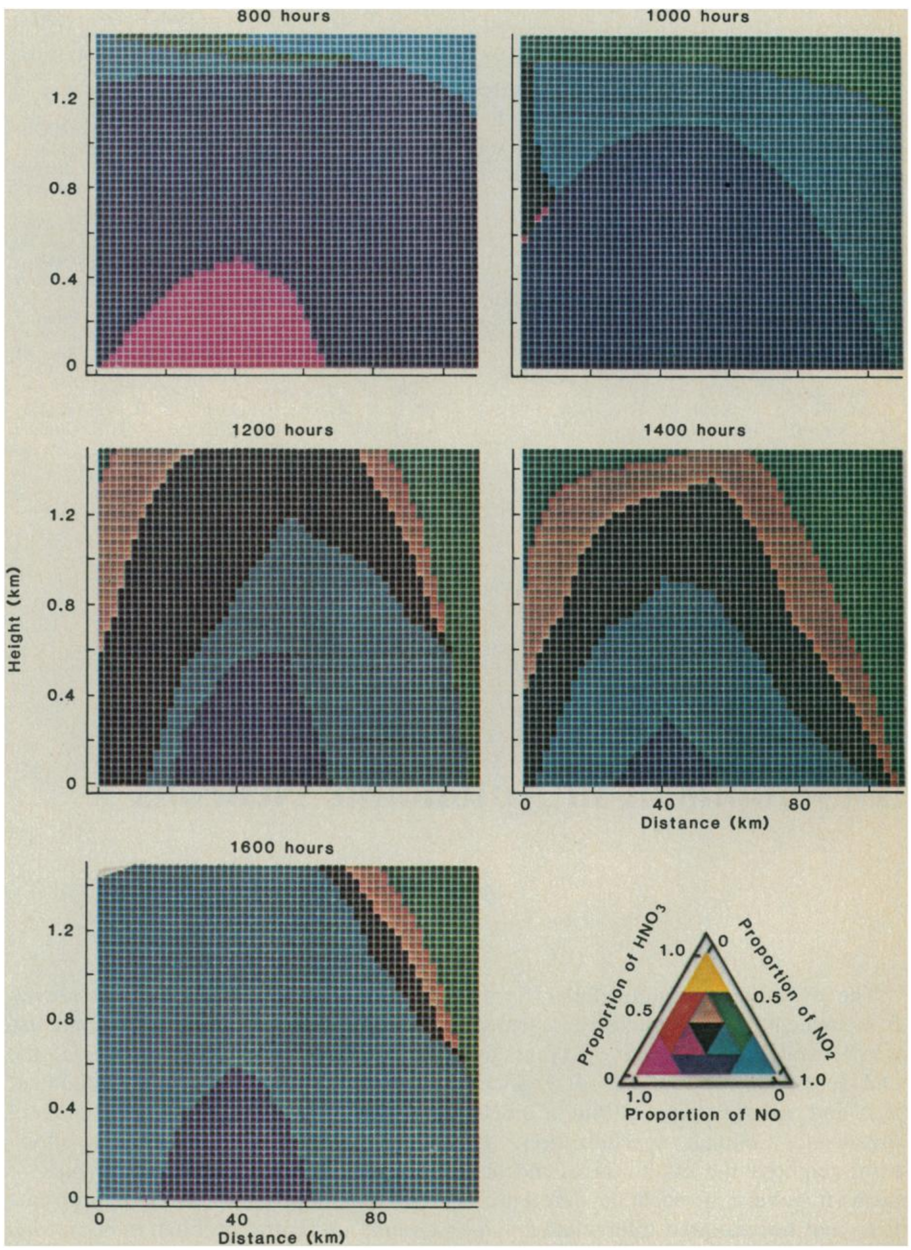

Fig. 7. Relative concentrations of NO, NO_2, and HNO_3 within the six-county region as functions of height and downwind distance. When a sequence of these plots is presented in motion picture form, the relative process strengths in three independent dimensions are displayed.

able, is to use several sequence plots as in Fig. 4, each for a selected discrete value of that parameter. The results of models with high dimensionality are inherently difficult to display by any technique, however, and careful thought and innovation are crucial to success.

General conclusions. It seems possible to draw several general conclusions from this work. First, scientific computer models often benefit from utilizing displays of results that present the full dimensionality or the maximum presentable dimensionality of the calculation. Second, routine plotting of results should be made as automatic as possible. If these two principles are followed, the analyst will often discover features of the results that would otherwise have gone unnoticed. Finally, color is very effective as a medium of information transfer and should be used freely in the displays, provided it is used with sufficient discretion that the viewer is not overloaded with information. Color graphics for the display of scientific model results, it would seem, has come of age.

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Stages of Neurotransmitter Development in Autonomic Neurons

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The evolution of multicellular forms from unicellular progenitors represented a new strategy for selective advantage, and foreshadowed cellular diversification and specialization within a single organism. Cellular specialization, in turn, required the evolution of mechanisms to govern intracellular differentiation, and necessitated intercellular synchronization during development and maturity. The processes of differentiation and cellular synchronization reach a remarkable level of complexity in the nervous system: different neurons develop the capacity to synthesize and use different specific chemical signals, the neurotransmitters. Moreover, billions of individual neurons form thousands of highly specific interconnections, allowing the different transmitter signals to function in physiologically appropriate circuits. A central problem in neurobiology concerns the mechanisms generating such specificity.

One approach to this problem has involved study of the relatively simple, peripheral autonomic nervous system. Autonomic neurons use a number of well-characterized transmitters, including norepinephrine and acetylcholine. The availability of sensitive techniques to measure noradrenergic and cholinergic gene products, such as their biosynthetic enzymes, has allowed examination of individual transmitter phenotypic characters. Analysis of individual phenotypic characters is critical for elucidation of mechanisms governing transmitter ontogeny, since expression of any given transmitter depends on development of multiple individual characters (such as the foregoing enzymes).

Emerging evidence suggests that autonomic neurons pass through a sequence of distinct stages during neurotransmitter differentiation. The stages may be distinguished by the specific transmitter gene products expressed, and by the mechanisms influencing phenotypic expression of these transmitter charac-

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