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Computer Modeling in Energy and the Environment

Computer modeling has played a significant role in the evaluation of possible sources of energy as well as the consequences of the use of energy on the environment. In this paper the contributions of IBM scientists to improve models in the fields of air pollution, solar energy, plasma physics, coal gasification, and energy conservation are summarized. These contributions include not only better numerical and programming techniques but improved mathematical models based upon advances in understanding of the physical processes involved.

Introduction

Issues surrounding the utilization and availability of energy resources have been among the principal social issues of the last twenty-five years. As one example, early in this period, the pollution of the atmosphere caused by the use of coal in power plants was reduced by the conversion of many of these plants to the use of the cheap oil and natural gas then available. In this way, it was possible to continue the growth of the use of electrical power deemed necessary to maintain or increase the living standards desired by many. Events of the last decade have made it all too clear that the availability of such energy resources cannot continue to be taken for granted. Increased concern about energy conservation has become evident, while the search for alternative energy sources has been pressed. As we now consider in the United States the conversion of power plants from the use of oil back to coal, debates have continued about the environmental consequences of the use of any of these energy sources, consequences which range far beyond mere air pollution.

Significant studies have been undertaken in the search for a balanced approach to the problem of the meeting of energy requirements while minimizing the environmental consequences of the use of energy. Considerations of cost, safety, and the time scale of the physical phenomena involved have in many cases ruled out purely experimental methods for these studies. Computer models have therefore been used over the past three decades to increase our understanding of the opportunities and problems posed by attempts to meet these human needs. Advances in our knowledge of the physical and engineering processes involved, in the numerical and programming methods used in modeling, and in computer technology itself have permitted the use of the computer as a "laboratory" for the conduct of experiments. This use has in turn contributed to an increased understanding of the underlying principles.

Research workers around the world have contributed to these advances not only through the development of computer technology but also through the development of computer models useful for the above studies. In this paper, we attempt to summarize the contributions of IBM scientists to this effort. We begin with a description of air quality models developed for environmental studies. The second part of the paper describes various studies in the environment and solar energy which are unified by the use of increasingly sophisticated methods which were developed for the solution of the radiative transfer equation. The final part of the paper discusses modeling studies for some alternative energy sources as well as for energy conservation.

The above outline makes clear the unfortunate necessity to omit a number of IBM studies which have been carried out both in the energy and in the environmental area. Notable among these studies have been those in surface and sub-surface hydrology [1–24]. This extensive

work, while not consistent with the limited purpose of this paper, could as well be used to illustrate the contributions that computer modeling has made to the solution of problems of social importance.

Air quality modeling

Heavy fuels with a high sulphur content have been utilized around the world to provide energy for the production of electricity and heat for homes, offices, and factories. The burning of these fuels produces sulphur dioxide, a gaseous compound which, in sufficiently high concentrations, poses health hazards for people exposed to it over a period of time and has also caused serious damage to buildings and monuments of great historical or artistic importance. Sulphur dioxide is just one of many solid, liquid, and gaseous pollutants which contaminate the atmosphere in a modern urban area, but is a good indicator of the level of pollution in an urban environment. Also, for the time scales of importance in urban air pollution models, it may be considered chemically nonreactive. For this reason, the development of mathematical models describing the diffusion of sulphur dioxide has been simpler than for other types of pollutants.

These "air pollution" models not only require an understanding of the dominant physical processes in the atmosphere, that of the random movements of air masses (eddy diffusion) and of the transport of pollutants by the prevailing wind field, but also require knowledge of the ground features of the area ("surface roughness"). Further, the location, height, and time-dependent strength of the emitters of sulphur dioxide must be known or estimated ("source emission inventory"). While other approaches could be used, practical considerations have in general dictated as the basis for the models the use of a partial differential equation frequently called the advection-diffusion equation [25].

IBM scientists, among others, have developed urban pollution models, which may be used both as an aid in determining optimum control strategies for limiting the use of major emitting sulphur dioxide sources during high air pollution potential periods. These models are also useful for planning purposes in connection with land use management and urban development. The IBM models were developed over a period of time in a number of locations and reflect not only the advancement of understanding of the problems involved, but also special geographic and data problems.

- *New York City*

Initial work by IBM researchers on the use of computers in air pollution was done in a study of the New York City area. The first model for that city depended upon the use of an approximation of the solution of the diffusion equation [26] in which it is assumed that the mean concentration in the cross-wind direction for a pollutant emitted from a fixed point source has a Gaussian distribution. The down-wind transport of the pollutant from that source dominates the dilution of the pollutants in that direction. The models derived based on these assumptions are known as Gaussian plume models and contain several parameters which must be evaluated from experimental observation. Since it would not be practical in an urban area to consider all sources as point sources, the concept of an area source and effective height was utilized successfully in studies of an air pollution episode which occurred in New York City on January 11, 1971. This episode was caused by a warm front which became stationary over that area. Initial results were reported in [26], and more extensive results for the period January 10–12, 1971, were reported in [27]. In general, computations based upon the model were in good agreement with actual observations.

- *St. Louis*

A different approach to obtaining an approximation to the solution of the diffusion equation was used for a model for the city of St. Louis [25, 28]. Here, based on earlier work of Shir [29–31], a numerical integration scheme was used to compute concentration distributions in time and three space dimensions. This more detailed treatment was justified by the availability of data from a number of meteorological and sulphur dioxide stations in the area, as well as a source emission inventory. A new method was developed to estimate the turbulent diffusivity and atmospheric stability.

While a number of shortcomings were noted in the model, the flexibility of the model in treating the wide variety of variables (emission rates, eddy diffusion coefficients, mixing heights, etc.) involved was quite important in handling the conditions occurring during a twenty-five day test period. The model performed consistently well during this entire period, and the correlation of the measured and computed values for both two- and twenty-four-hour periods was significantly higher than for a Gaussian plume model (0.899 and 0.873, respectively, *versus* 0.675 for the latter model).

- *Mexico City*

Because of the lack of sufficient data in Mexico City in 1973, a less sophisticated model than that used in New York City was employed in an initial study [32]. An extension to the earlier work of Gifford and Hanna [33] was made in order to account for the fact that the wind is calm in Mexico City about 60% of the time. The results of the calculations were in general agreement with observed

results. However, these results did emphasize the importance of obtaining data from more meteorological stations in order to better account for the spatial dependence of the prevailing wind field caused by the particular topographic features of Mexico City.

Another approach to overcoming the difficulties caused by the lack of data for Mexico City and the frequency of calm winds was taken by Lamb [34]. Lamb developed formulae for the long term mean concentration of linearly reactive air pollutants by subdividing the averaging period into three disjoint domains designated as the plume period, the stagnation period, and the transition period. Events in each domain were modeled separately and superimposed to obtain the final estimate of the mean concentration. Results of computations [35] using the model showed a high correlation between the predicted and measured annual mean sulphur dioxide concentrations in Mexico City. Although it was believed that errors in the input data contributed significantly to the magnitude of the error in the predicted concentrations, it was believed that the model could be used as it then existed for emission control strategy studies.

• *Bilbao*

Bilbao, a highly industrialized city in northern Spain, was the site of another intensive air pollution modeling study [36–42]. Tabular-probabilistic models were used with the ultimate objective of the evaluation of alternative policies for the reduction of emissions on the basis of defined criteria and of prior estimation of the probability distribution of the concentration of pollutants.

There were several components of the model: a factorial analysis model for estimating the meteorological factors contributing to the pollutant concentration; a number of submodels based on multiple linear regression which, by limiting the range of the factors so as to define a particular meteorological situation, avoid the nonlinearity of the meteorological effect on the pollution; a model to estimate which sources in a given situation affect the concentration in a given area; a stochastic regression model to estimate the probability distribution of the pollutant concentration; and a decision model based on mixed integer programming techniques for estimating the reduction of the emission of atmospheric pollutants.

Subsequently, Mantero [43] utilized a Gaussian plume model in order to assist in the design of an air quality monitoring network for the Bilbao area.

• *Venice*

Under certain meteorological conditions which arise notably in winter, the production of sulphur dioxide from industrial plants located on the mainland near the islands on which the city of Venice is situated leads to very high concentrations of that pollutant in Venice itself. This pollution has been of concern, not only because of the associated health problems, but because of the contribution of the sulphur dioxide to the deterioration of the buildings and monuments of Venice.

In 1973, scientists at the IBM Scientific Center in Venice began modeling studies using available data [44]. Methods for building a source emission inventory were developed based on optically readable forms [45] and an extensive study of the meteorological conditions was carried out [46]. A Gaussian plume model was developed [47] in which the normal use of stability classes was modified so as to better take into account the effects of surface nonuniformity and heat islands on the atmospheric turbulence state. This modification allowed a significantly higher correlation of both three-month and annual concentration averages predicted by the model with actual measurements. Similar models were also used in subsequent work [48, 49] which were used to determine values for physical parameters of the systems under consideration.

Consideration was also given to problems of real-time forecasting of air pollution episodes [50]. Here, only the most sophisticated deterministic models of the type considered by Shir and Shieh [29] have had sufficient accuracy to be of value for the short-term predictions required. However, such models have the disadvantages of requiring large amounts of computer time as well as good meteorological and emission data, which were not always available. Very importantly, from their very nature, these models could not handle the unknown variations in emission which do occur. On the other hand, purely stochastic models which would predict future concentrations on the basis of previous pollution levels were unsatisfactory for forecasting pollution episodes. Building upon earlier work of Bankoff and Hanzevack [51], which combined both deterministic models based on numerical integration of the advection-diffusion equation using a method of fractional time steps [52] and statistical methods based on a Kalman filtering method [53, 54], a new model was developed in conjunction with the Politecnico di Milano [55, 56]. Comparisons of the predictions generated from this model with observed values from an episode of August 2, 1973, showed a clear improvement over methods based solely on a purely deterministic or a stochastic model.

• *Himeji City*

Himeji City in Japan is in the center of a large industrial area developed along the coastal region of the Seto Inland

Sea. The availability of meteorological data and emission data from each factory (notably iron and steel plants, electric power plants, and oil refineries) made possible the development of a Gaussian plume model [57], which utilized the concept of two atmospheric stability categorizations for high and low stacks, instead of the single stability class normally used. Predicted results compared favorably with observed concentrations.

An interactive graphics approach to the simulation was emphasized to facilitate the use of the model in urban planning and environmental control planning. This became part of an even larger system which allowed the assessment of regional development projects from the point of view of economic, social, and environmental impact [58-60].

Radiation transfer equation

The air pollution models which have been described have dealt with macroscopic advection and diffusion processes in the atmosphere. Other atmospheric processes are important in studying the interaction between the use of energy and the environment. One of the most fundamental is that of radiation scattering in the atmosphere, which may be described by the radiative transfer equation [61]. This equation is an integro-differential equation whose solution is important in computer modeling in such diverse areas as the effect of an increase in atmospheric dust on climatic cooling or that of carbon dioxide on climatic warming, the effect of change in ozone content of the atmosphere on the ultraviolet radiation reaching the biosphere, the photovoltaic harvesting of solar energy, and the remote sensing of earth resources. The large number of variables involved in any of these simulations has, in turn, generated requirements for numerical methods of solving the radiative transfer equation which not only yield accurate approximations to the solution, but which require as little computer time as possible for any particular combination of values of parameters defining a given calculation. Over the past decade, in the studies which are briefly described, the amount of computer time required for many of these calculations has been decreased by several orders of magnitude, while at the same time the numerical solutions have become more accurate. The work on decreasing the computer time was motivated by the scientific significance of the problems and has taken place because of improved methods of solving the equations arising from the spherical harmonics approximation [62] to the radiative transfer equation. As a result of this work, the validity of the use of this method for calculations not only of the radiation flux but also for the intensity of radiation has been established.

A good reference point for reviewing progress in this area is the work on Mie atmospheres, that is, atmospheres in which it is assumed that spherical particles are present which are large compared to the wavelengths of interest (Mie scattering [63]). In this case, if the intensity of the radiation is expressed in terms of a Fourier series, then tens to hundreds of terms may be required in order to represent the process of scattering. In [64], Dave and Gazdag developed the method of "successive scattering," an iterative method of determining from the radiative transfer equation the coefficients in the Fourier expansion of the intensity. This technique was successfully applied to the problem of calculating the polarization of the radiation emerging from an atmosphere containing aerosols [65], and, possibly for the first time, reliable results of multiple scattering calculations involving Mie scattering were presented. See also [66].

A much more extensive application of the method was made in the study of the possibility of the inadvertent modification of the earth's climate [67]. Papers by Braslau and Dave [68, 69] presented quantitative calculations of the effect of aerosols on the solar energy absorbed, reflected, and transmitted in atmospheric models which were intended to simulate conditions in which carbon dioxide and differing amounts of suspended particulate matter (aerosols) are present in the atmosphere. The discussion of [67] makes clear the importance of such radiative properties of the atmosphere on changes of the heat balance of the earth which potentially may bring changes of great consequence to man by changing patterns in precipitation and the circulation of the atmosphere.

It was necessary to restrict these very extensive calculations to cloud-free atmospheric models because of the computational times involved. The concentration of aerosols (nonabsorbing and partly absorbing), ozone, and water vapor were specified for a large number of layers of varying thicknesses up to an altitude of 45 km. Average mid-latitude summer conditions were used, and different amounts, types, and height distributions of aerosols were used in different models. The results are too extensive to adequately summarize here; however, it was noted that an increase in the atmospheric dust may lead to cooling or heating depending upon the scattering and absorbing characteristics of the aerosol substance and upon the location of dust within the atmosphere. It must be concluded that the explanation for the change in the mean temperature of the surface is much more complex than can be explained on this basis alone, and, while these effects are important, more complex models must be used [70].

These computational results and tools were also utilized in a study of urban atmospheres in which aerosol

concentrations were primarily due to emissions from process industries and fossil fuel consumption [71], *i.e.*, models in which the aerosol refractive index, the particle size, and the vertical distribution were varied. The results obtained showed that the absorbing aerosols in the amounts associated with the anthropogenic polluting source do play a significant role in the absorption of shortwave radiation in the boundary layer of the earth.

This work also was forced *not* to consider the effect of clouds because of the computational time required. The development and implementation of an alternative computational method was required in order to include the effect of clouds in these studies.

- *Spherical harmonics methods*

While the spherical harmonics method was first suggested for solving the radiative transfer equation [61], the necessity to use high-order approximations and the numerical problems encountered in optically thick media made the method unattractive for many years. However, it was successfully applied to obtain approximate solutions of the neutron transport equation in which the phase functions were more isotropic, and it was possible to use low-order approximations. It was in connection with this particular problem that Canosa and Penafiel [72] were led to the development of a new parallel shooting method for the solution of the two-point boundary value problem for a system of linear ordinary differential equations. This system was generated by the spherical harmonics method as applied to the neutron transport problem (or the radiative transfer problem). By the use of finite difference approximations, these equations are reduced to an algebraic problem in block form. Using a significant generalization of earlier work by Conte [73] and Godunov [74], numerical instabilities are eliminated by performing linear transformations of the matrices of the problem. The contribution of Canosa and Penafiel was to develop a method which was both computationally efficient *and* stable against the growth of roundoff error. The details of the method are given in [72], and further refinements and extensions given in [75] and [76]. Sample calculations showed that the method was about 370 times faster than the iterative method previously used, and also an order of magnitude more accurate. In [77], Dave extended the earlier studies, which considered only the azimuth-independent component of the intensity, to the case in which the azimuth-dependent components are computed. It was established in a most definitive manner that spherical harmonics methods could be used for intensity calculations as well as for the calculations of the flux as carried out in earlier papers [78]. Thus, the basis was laid for the use of this method in new application areas.

- *Ozone*

The presence of ozone in the earth's atmosphere is essential for the protection of the biosphere from the harmful effects of ultraviolet radiation received from the sun. It has been believed that a small perturbation in the natural balance of the ozone layer can possibly lead to some harmful consequences. The possibility that a fleet of supersonic transport planes could significantly decrease the ozone content of the earth's atmosphere was, therefore, a major area of concern in the early 1970s when the development of large numbers of such planes was under consideration [80].

While an earlier study by Cutchis [79] had considered only an atmospheric model with a vertical distribution of ozone as observed under average mid-latitude summer conditions, the study by Halpern *et al.* [80] considered a variety of models ranging from one with ozone but no dust or clouds to several models with climatic cloud cover and high concentrations of aerosols. The spectral distribution of the solar energy received at the ground was shown to be affected strongly and variably by the atmospheric aerosol and clouds. Further, even when the ozone content is held constant, life in the biosphere is subjected to considerably smaller doses of ultraviolet and visible radiations than those computed from atmospheric models with Rayleigh scattering only. The necessity of carrying out comprehensive radiation transfer studies was thus established.

The further discovery that the diffusion of fluorochlorocarbons could lead to the generation of trace substances through the tropopause, which could, in turn, significantly reduce the ozone content of the atmosphere, indicated the desirability of even more detailed calculations. Results of additional calculations for six different vertical distributions of ozone were presented in [81].

- *Solar cells*

For ground-based applications of photovoltaic solar cells, not only the cost and physical properties of the cell but also the variability of the atmosphere must be considered in the evaluation of the design of any system utilizing these cells. For any given location of such a system from which optimum performance is desired, knowledge of the spectral, angular, diurnal, and day-to-day variations of the direct solar radiation and diffuse sky radiation received by an arbitrarily oriented surface is required. The cost, complexity, and lack of reliability of any instrumentation system which could experimentally obtain the data required for the evaluation of the performance of the cell suggests the desirability of using computer models, not only for the simulation of the response of the cell itself, but also for the characteristics of the solar energy incident upon the cell.

Initial models incorporated standard but relatively crude approximations [82]. More sophisticated studies [83–85] demonstrated clearly the need to include sky radiation and ground-reflected radiation contributions in any meaningful evaluation of the response of solar cells under different atmospheric conditions. For a solar cell lying horizontally, and for atmospheric models with aerosol particles which are mildly absorbing and with a stratus cloud layer, more than 99.9 percent of the photocurrent generated is due to diffuse sky radiation when the solar zenith angles exceed 60 degrees.

In [86], it was shown that the commonly used isotropic-distribution approximation for the sky radiation used for converting the diffuse component value for a horizontal plate to that for a tilted plate systematically underestimates the diffuse energy contribution. This emphasized the need for even more detailed calculations of atmospheric models which would predict the intensity of the diffuse radiation emerging in the terrestrial atmosphere. In [83], calculations are reported for five different models of the mid-latitude summer, cloud-free, terrestrial atmosphere which show both the direct solar radiation and the diffuse sky radiation. In all, about 35–40 million datapoints were obtained from which information could be derived about the spectral, directional, altitudinal, and solar position dependence of the solar energy, taking into account all orders of scattering within the atmosphere. These calculations were made feasible only through the increased efficiency of the numerical methods described in preceding sections and the availability of fast computers with large memory and direct-access capability. An immediate application of the results was made to calculations for a tilted plate [87].

Other uses of these data sets for studies of solar cells were suggested in [83]. Dave [88–90] has also utilized these data sets for some initial studies in remote sensing. Importantly, these studies all demonstrated the necessity of more knowledge of atmospheric conditions if the results of remote measurements are to be fully utilized. For future satellites, with more sophisticated scanners, even more detailed studies will undoubtedly be required.

- *The SVD method*

While the studies described above established the effectiveness of the method of Canoda, Penafiel, and Dave, a basic limitation exists because of the use of a finite difference approximation to the derivative appearing in the radiative transfer equation. It is necessary to divide even a homogeneous layer of the atmosphere into subintervals of small optical thickness in order to obtain an accurate solution. In such a layer, however, the spherical harmonics approximation is determined by differential equations with constant coefficients, and an analytical solution to these equations may be written down almost immediately. The evaluation of this solution, on the other hand, presents considerable numerical difficulties because of both scaling problems and the apparent necessity to determine the eigenvectors and eigenvalues of a matrix dependent upon the original coefficients. These difficulties have in the past (see Gelbard [91]) prevented the use of this method. In some very recent work, Karp, Greenstadt, and Fillmore [92] have shown how these numerical difficulties may be overcome using methods which involve the singular value decomposition (SVD) of a matrix. By the use of these methods, the amount of calculation will then be independent of the optical thickness of any particular layer of the atmosphere and will depend linearly on the number of layers of the atmosphere. This scaling can be contrasted to the earlier method which depended linearly on the number of subintervals, which was, in turn, determined by the optical thickness of each layer.

Complete details of this method are given in [92]. Comparisons of this method with earlier methods have been very favorable. For example, with a 15-year atmosphere having a total optical thickness of 1.061 and for an approximation of order 59, the new SVD method takes only 1/3 the computer time and conserves flux to 10 digits more than the earlier method used by IBM workers. While the basis for comparison of the computational efficiency with other methods is less exact because of the desire to use a uniform measure, the results indicate that the SVD method is markedly superior. Additional comparisons were reported in [93] and established that relatively low orders of approximation could be used when computing net fluxes even for optically thick atmospheres. It is quite probable that the accuracy and decreased computational time afforded by the SVD method will make feasible new areas of study in the next decade.

Plasma physics

Controlled thermonuclear fusion has offered the prospect of almost unlimited energy without the environmental problems associated with fossil or fission fueled generators. This process depends upon the possibility of extracting energy from a thermonuclear reaction in which very light nuclei such as hydrogen and helium fuse together in a process that also releases energy. This reaction requires the overcoming of electrostatic repulsive forces, which keep the particles apart, by creating a plasma (a gas whose particles are at least partly charged) at a sufficiently high temperature and sufficient density to overcome these electrostatic forces. If the plasma can be confined long enough to obtain energy from the reaction, then a basis for a practical source of power will exist.

However, some of the early intuitive and simple theoretical ideas about plasma confinement proved to be in error, and extensive theoretical and experimental investigations of the behavior of the plasma under differing conditions were initiated. An analysis [94] of the magnitude of the computational problem posed by a three-dimensional particle code showed the impracticality of such detailed calculations at that time (1971), and these calculations remain among the largest now carried out. In order to understand the nature of the computer requirements imposed, a series of studies was initiated.

These initially focused on particle methods used to simulate plasma oscillations [95], but a study [96] of the damping of the oscillations led to a detailed consideration of the numerical solution of the linearized Vlasov-Poisson system for cutoff equilibrium distributions. Very importantly, it was shown in [97] that a finite difference Eulerian model can solve Vlasov's equation accurately during the time necessary to follow the physical phenomena of interest. However, a particularly interesting aspect of the calculations is the approximate recurrence of the initial state, which is illustrated in Fig. 1. While this phenomenon had been observed previously, it had been thought by some to be of physical origin. In this paper, the origin was recognized to be strictly numerical in nature, and in a subsequent paper [98], this question was explored in detail. It was shown that the recurrence was due to the finite velocity resolution of the numerical methods used and did not originate from beaming instabilities (growing modes) within the model itself. Physical results obtained in that paper were later observed by Jacob and Hirschfield in laboratory experiments [99].

- *Accurate Space Derivative method*

The need for accurate numerical solutions to problems in plasma physics led to the development of the Accurate Space Derivative (ASD) method by Gazdag [100, 101]. Briefly, this method of solution of partial differential equations approximates that solution by means of a Taylor series expansion in one of the independent variables, for example, time. The order p of the highest derivative appearing is the order of the ASD method. The time derivatives are computed by differentiating the differential equation. The derivatives with respect to the other variables are computed by using finite Fourier transform methods and may be evaluated in a very accurate manner, essentially limited only by the accuracy to which a function may be defined over a finite set of mesh points. Extensive calculations using the method have established the overall high accuracy of the method even for systems with nonperiodic boundary conditions. Analysis has shown the method to be stable at least for $p = 3, 4, 7$, and 8.

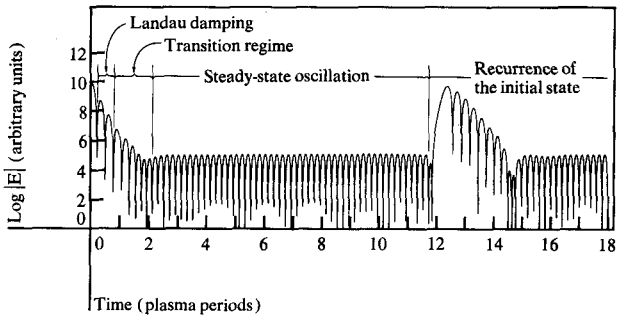

Figure 1 Electric field *versus* time, showing the recurrence of the initial state.

An evident difficulty in the method can be the complicated form for the higher-order time derivatives. Consequently, more computer time than is desirable may be required in particular cases. Several methods analogous to predictor corrector methods for ordinary differential equations and requiring only values for the first-order time derivative were investigated [102], and it was found that methods could be devised which offered an attractive computational alternative to the original method, but yet remained accurate. This method has subsequently been applied successfully in other areas, notably that of wave equation migration in seismic data analysis [103].

The significant advances in the computational state of the art in plasma calculations were demonstrated by some calculations carried out in 1975 and reported in [104, 105]. In this work, unambiguous and quantitative agreement was achieved between theory, the model calculations, and the experiments on frequency shifts reported by Vidmar, Malmberg, and Starke [106]. These authors found that the frequency shift was mainly determined by the initial damping of the wave amplitude, and that this damping for large amplitudes was larger than the linear Landau rate. The calculations by IBM established the precise scaling law, namely, that the initial damping grows linearly with the square of the initial wave amplitude—a result established before the experimental results were obtained [106].

Coal gasification

Coal is probably the only fossil fuel which is likely to remain in abundant supply through the end of this century. Once the dominant commercial fuel, its use has declined because of both convenience and environmental considerations. However, significant studies are now underway which consider coal as a potential source of synthetic oil and gas, and computer modeling of the

processes involved is being extensively employed, although the lack of some physical data inhibits the full use of such models.

The modeling of the coal gasification process which has been carried out by IBM scientists has considered a moving-bed gasifier, one in which the solids stream moves slowly downward through the reactor while the gas stream flows upward. Coal is added at the top of the reactor and ash (and/or clinker or molten slag) is removed from the bottom. A mixture of steam and oxygen or air is fed to the bottom of the reactor to provide some of the reactants for the combustion and gasification of the coal. The reactor model is developed from the principles of conservation of mass, energy, and momentum and is comprised of a system of nonlinear differential equations together with appropriate boundary conditions. Not only are the equations nonlinear, but they are "stiff," that is, they are characterized by large ratios between the magnitudes of some of their eigenvalues, which may be as large as 500 in cases of interest, and significant numerical difficulties may be encountered as a consequence.

IBM workers have developed two different models. The first [107–109] involves a one-dimensional steady-state model which exhibits a full range of physical and chemical effects in the reactor. Collocation techniques based on the use of splines were used to solve the equations, and convergence was obtained for a series of test problems, including data taken from operating units in a commercial plant.

Another model of the gasifier was a "plug flow" version in which there is no backmixing in the gasifier. In [110] it was shown that the simulation model could successfully match actual operating data taken from a Lurgi gasifier at Westfield, Scotland. Comparisons were also made for ash (Lurgi), clinker, and slagging gasifiers.

Energy conservation

The desire to minimize the use of energy for heating and cooling its buildings has led to the development of optimization programs for this purpose. These programs incorporated models ("load programs") for the building and involved the solution of a constrained optimization problem formulated to minimize the total heating and cooling cost. This approach was applied to the use of a heat pump within a building [111], and while successful, demonstrated that the real difficulty was in the development of approximations which were both sufficiently accurate as well as computationally realistic.

One of the more significant computational problems involved in the use of the optimization program in any study, however, is the proper utilization of weather data. For example, these data could be represented by hourly measurements of nine or more variables over periods of time up to ten years. While it is possible that such information might be utilized for a single calculation, it would be extremely expensive to use it repetitively as might be required for optimization calculations. In [112], methods were investigated which by use of a computer program called a weather data filter would generate a small set of weather data which would adequately represent the larger data set. These filters generally preserve one or more statistical properties of the original weather data, such as means and extremes, and construct a small number of "weather days" to represent some longer period of time. Thermal loads are then computed for these weather days and scaled to predict annual thermal loads.

Through the use of grouping techniques for the weather data, a weather filter was constructed and two experiments carried out. In both experiments, the error generated by the use of the filter was less than 1% as measured by the results of using unfiltered data, and the computations required only about 6% of the time [112]. In a subsequent paper [113], Silverman and Low developed a new method to construct this filter, which was much less expensive to compute and was based on quadratic programming techniques.

Studies [114, 115] have been carried out using these techniques for optimizing the size of windows which should be used in an energy efficient building. These studies used approximations for the direct and diffuse radiation intensity which were derived from indirect measurements and estimations. The second paper [115] described new calculations based upon the use of Dave's data sets for solar radiation [83] described in a previous section as well as a more sophisticated model for estimating the amount of natural light received in the perimeter zone of a building. In studies of buildings both in Los Angeles and Tucson, it was shown that a significant potential for energy savings existed if the contribution of natural light to required illumination were accounted for. While the optimizations were over window size, it was clear that the visible transmission coefficient and shading coefficients could have been used as the parameters, and thereby left the architect with more freedom for his design.

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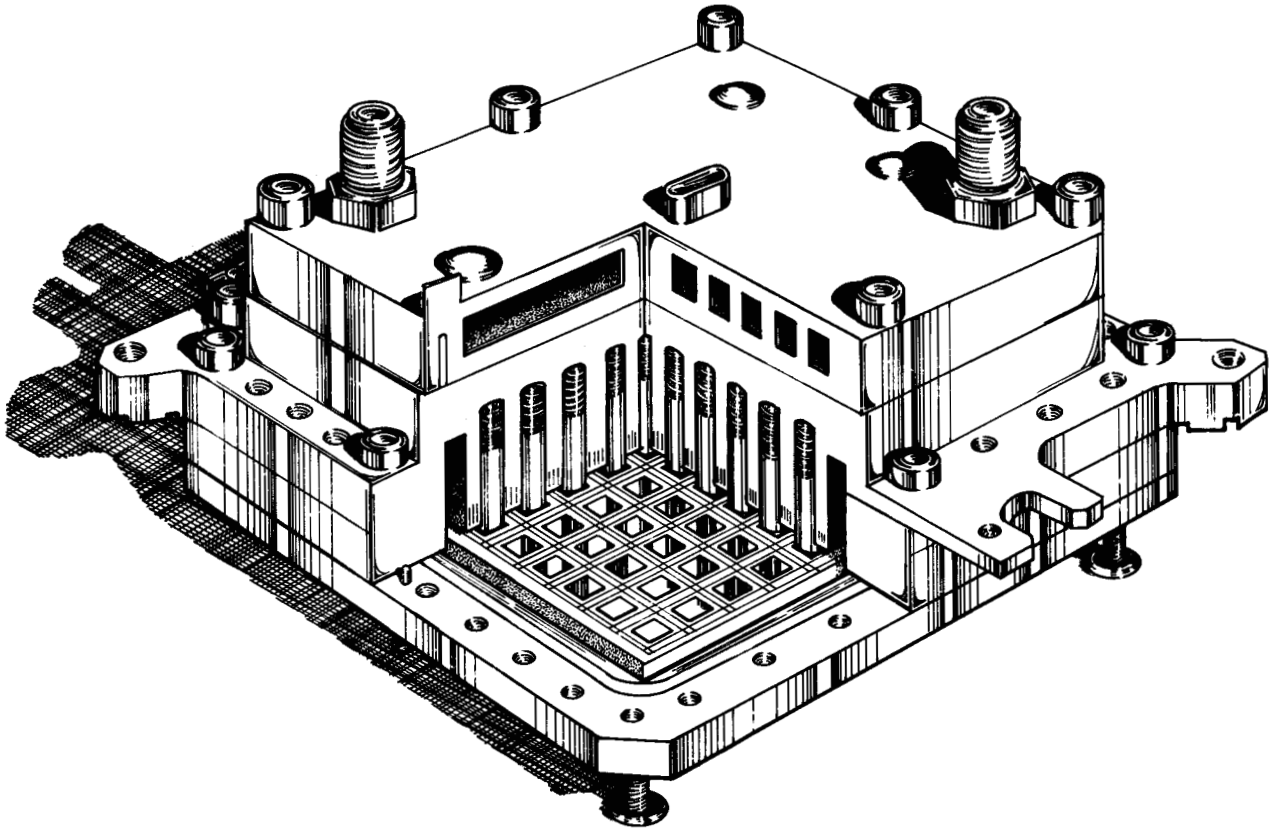
Component Development and Manufacturing Technology



Thermal conduction module

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