**Methane Modeling—Predicting the Inflow
of Methane Gas into Coal Mines**

**Quarterly Technical Progress Report
for the Period**

January 2, 1981 - March 31, 1981

MASTER

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April 15, 1981**

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Prepared for the

**U. S. Department of Energy
under Contract DE-AC22-80PC30123**

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Abstract

This first quarterly technical progress report summarizes contract activities related to literature review, selection of mathematical model components, and development of one-dimensional numerical models for predicting methane flows into coal mines. Progress statements for each of these tasks are presented as separate attachments. The plan is that each attachment will be appended in successive technical progress reports and will ultimately form separate sections of a final report and user manual with relatively little modification.

Salient features of technical progress for the first quarter are the following.

I. Computer-assisted literature searches have been completed for several strategies designed to cover different aspects of the model development and evaluation program. Some strategy refinement and additional searches are required. Ultimately a comprehensive bibliography will have been compiled and evaluated.

II. Basic mathematical components that are sufficient for the development of a first numerical model for water and methane flows to coal mines have been identified. This initial set of components is a basis for the collection and analysis of refinements to provide more realistic accounts of the complex factors affecting coal-bed methane during mining and degasification.

III. A set of basic partial differential equations for flow of water and gas in a horizontal, homogeneous coal seam has been formulated in terms of pressure, pore saturation, and adsorbed gas variables and presented in normalized form for numerical solution. Equation sets corresponding to alternative choices of dependent variables will be formulated and compared with this initial set.

IV. Computer subroutines have been modified and assembled to implement one-dimensional, nonsteady, two-phase flow models. These programs implement numerical, finite-difference, method-of-lines algorithms in a format that facilitates substitution of mathematical components and equation sets. Initial runs with this software package have illustrated the superiority of a particular space-discretization scheme and provide data for comparison of grid and permeability weighting schemes.

Literature Review

Computer-Assisted Searches

The literature review was initiated by utilizing the DIALOG Information Retrieval Service from Lockheed Information Services. Eight data bases were reviewed during the first search, including

- 1) NTIS (File 6). Abstracted information of government-sponsored research, development, and engineering plus analyses prepared by federal agencies, their contractors, or grantees. Material includes both hard and soft sciences.
- 2) COMPENDEX (File 8). A machine-readable version of the Engineering Index (Monthly/Annual) providing abstracted information from the world's significant engineering and technological literature. This includes publications of engineering societies and organizations, papers from proceedings of conferences, and selected government reports and books.
- 3) INSPEC (Files 12 and 13). A machine-readable version of Physics Abstracts, Electrical and Electronics Abstracts, and Computer and Control Abstracts. Journal papers, conference proceedings, technical books, patents, and university theses are abstracted and utilized in this data base.
- 4) Comprehensive Dissertation Abstracts (File 35). A definitive subject, title, and author guide to virtually all American dissertations accepted at an

accredited institution since 1861. In addition, a large number of Canadian and overseas dissertations are included.

- 5) SSIE Current Research (File 65). A data base of both government and privately funded scientific research projects either currently in progress or initiated and completed during the most recent two years.
- 6) GPO Monthly Catalog (File 66). A machine-readable version of the Monthly Catalog of U. S. Government Publications containing records of reports, studies, fact sheets, maps, handbooks, and conference proceedings issued by all U. S. Federal Government agencies.
- 7) GEOREF (File 89). A geoscience data base including serials, books, conferences, dissertations, technical reports, and geologic maps from the U. S. and the world.

Strategy for Coal-Bed Methane Search

Strategy for the first search directed towards gas and water emissions to coal mines consisted of combining three topics, each topic containing numerous descriptors. Titles, abstracts, keywords and descriptors for each reference in the data base were scanned, and a reference was selected if a match was found with one or more descriptions from each of the three topics. The initial strategy had the following composition.

Mine or Mining

and

Ventilation, Methane, Firedamp, Fire Damp, Mine Water
Mine Gas, Water, or Gas

and

Mathematical Model, Simulation, Computer Model,
Computer Models, Modeling, or Modelling

This search resulted in 157 titles with their respective abstracts. Of these, only 15 titles were directly applicable to the current project. This indicated a need for refinement and change in the search strategy. The first search had over-emphasized mine ventilation, especially in combination with mathematical and computer models. Although the final results of this project should be applicable to ventilation design and models, the usefulness of these ventilation articles at this time is limited. Therefore, second and third search strategies were formulated. These searches were designed to emphasize

1. Methane and water emissions and coal degasification.
2. Fluid flow through porous media and its modeling.

Initial results of these two searches indicate a much higher percentage of pertinent articles (30% to 50%). Details and evaluation of these two searches will be reported in the next technical report.

Strategy for Search of Numerical and Computational Methods

The first strategy consisted of a review of the Science Citation Index for articles that referenced the following three papers.

- i. Peaceman, D. W. and H. H. Rachford, Jr., The numerical solution of parabolic and elliptic differential equations, J. Soc. Indust. Appl. Math., 3 (1955), 28-41.
- ii. Douglas, J., Jr. and B. F. Jones, On predictor-corrector methods for non-linear parabolic differential equations, J. Soc. Indust. Appl. Math., 11 (1963), 195-204.
- iii. Crank, J. and P. Nicolson, A practical method for numerical evaluation of solutions of partial differential equations of the heat-conduction type, Proc. Cam. Phil. Soc., 43 (1947), 50-67.

These papers were chosen on the basis of the type of equations (parabolic) being considered in this study. These papers have also served as a starting point for many extensions and novel methods which should be identified by the search.

Because the Science Citation Index surveys the references of articles appearing in a number of domestic and foreign technical journals, the above strategy resulted in the isolation of 147 papers, of which 24 were pertinent.

A second pass was made through six different data bases with a list of key words and authors taken from the first search. Papers written by the authors or that contained the key words in the title or abstract were specified for output. Of the 252 references obtained, a number of duplications occurred and 39 were considered to be useful.

A final pass will be made to seek papers that deal with the method-of-lines procedure. This is the basic technique being employed in the present study to treat the evolutionary character of the solution scheme. Also, some surveying of current issues of relevant journals defined by the above searches and not presently included in the data bases will be done.

Basic Equation Sets

Pressure-Saturation Equations - Homogeneous Horizontal Seam

A mathematical model for gas-water flow in coal beds can be formulated by using equations for two-phase, horizontal Darcy flow in porous media. To represent the constituents that enter these expressions, the water is assumed to be incompressible and the gas is taken to be ideal. Also, the coal bed is assumed to have constant porosity and relative permeabilities that can be stated in a parametric form. Finally, the coal-gas sorption process is described by a simple kinetic model.

For one-dimensional linear flow in terms of the primary variables, the equations are

$$\frac{\partial}{\partial X} \left[K \frac{k_{rw}}{\mu_w} \frac{\partial P}{\partial X} \right] = \phi \frac{\partial S_w}{\partial \tau}$$

$$\frac{\partial}{\partial X} \left[C_g P K \frac{k_{rg}}{\mu_g} \frac{\partial P}{\partial X} \right] = \phi C_g \frac{\partial (S_g P)}{\partial \tau} + \frac{\partial N}{\partial \tau}$$

$$\frac{\partial N}{\partial \tau} = -\beta (N - N_e)$$

in which K is the absolute permeability, k_{rw} and k_{rg} are saturation-dependent relative permeabilities for water and gas, and μ_w and μ_g are the corresponding viscosities. The porosity is

denoted by ϕ , the gas constant by C_g , and kinetic constants by β and N_e . The dependent variables are P , the pressure of both phases assuming no capillary pressure; S_w and S_g , the saturations of water and gas; and N , the mass of adsorbed gas per unit volume.

To express the equations in dimensionless form, the independent variables X and τ are normalized to a boundary value X_B and a time constant τ_0 using

$$X = \bar{X}/\bar{X}_B$$

$$t = \tau/\tau_0$$

where

$$\tau_0 = \frac{\phi S_{go} \bar{X}_B^2 \mu_g}{K P_0}$$

with P_0 representing the gas pressure at time zero and S_{go} denoting an initial value of gas saturation. The dependent variables can then be normalized as

$$p = P/P_0$$

$$s = S_g/S_{go}$$

$$n_A = N/N_0$$

for

$$N_0 = C_g P_0 \phi S_{go}.$$

The resulting form is

$$\frac{\partial}{\partial X} \left[k_{rw} \frac{\partial P}{\partial X} \right] = - v \frac{\partial s}{\partial t}$$

$$\frac{\partial}{\partial X} \left[p k_{rg} \frac{\partial p}{\partial X} \right] = \frac{\partial}{\partial t} (s p) + \frac{\partial n_A}{\partial t}$$

$$\frac{\partial n_A}{\partial t} = -\beta (n_A - n_e)$$

wherein v is the ratio of the water to gas viscosity and the water saturation has been eliminated by using the assumption that the saturations sum to unity.

For radial flow in one dimension, the normalized equations are

$$\frac{1}{r} \frac{\partial}{\partial r} \left[r k_{rw} \frac{\partial p}{\partial r} \right] = - v \frac{\partial s}{\partial t}$$

$$\frac{1}{r} \frac{\partial}{\partial r} \left[p r k_{rg} \frac{\partial p}{\partial r} \right] = \frac{\partial}{\partial t} (s p) + \frac{\partial n_A}{\partial t}$$

$$\frac{\partial n_A}{\partial t} = -\beta (n_A - n_E).$$

These equations are to be solved subject to initial and boundary conditions on the variables p and s . The initial conditions are the values of pressure and saturation at time zero for all values of the space variable. The boundary conditions describe the type of problem being solved. For example, for an infinite seam,

$$\frac{\partial p}{\partial X} = 0, \quad \frac{\partial s}{\partial X} = 0$$

at some point X located at a large distance from the mine face. At $X = 0$, specifying constant pressure for all time specifies mine-face pressure regulation.

Relative Permeability

General Relations

When more than a single mobile fluid phase is present, the absolute permeability of a porous medium is modified by a relative permeability for each phase. In general, relative permeabilities are a function of the relative fraction of the pore structure occupied by each fluid phase. Although for some simulations it might be desirable—and appropriate data might exist—to specify relative-permeability functions for a particular geological unit, it is also necessary to have a more general description for relative-permeability functions for cases when specific values are not available. A modified version of a set of relations described by Corey (1954) provides a general description of relative permeabilities as functions of an effective saturation:

$$s = [S_w - S_{wc}] / [1 - S_{wc} - S_{gr}]$$

where S_w is the saturation of the wetting phase (fraction of the pore volume occupied by water), S_{wc} is the irreducible (or connate) water saturation, and S_{gr} is the residual gas saturation. In general, $S_g (= 1 - S_w)$ is the saturation of the non-wetting phase (methane).

The Corey relations for the relative permeabilities of the wetting phase (water), k_{rw} , and of the nonwetting phase (methane), k_{rg} , are

$$k_{rw} = k_{rw}(S_{gr}) s^4$$

$$k_{rg} = k_{rg}(S_{wc}) [1 - s]^2 [1 - s^2]$$

where the scaling factors corresponding to the relative water permeability at residual gas saturation, $k_{rw}(S_{gr})$, and the relative gas permeability at connate water, $k_{rg}(S_{wc})$, are nominally one.

The modified Corey relations can be derived from a generalized form of the Kozeny-Carmen equations [Wyllie and Gardner, 1959]

$$k_{rw} = s^2 \int_0^s ds/P_c^2 \bigg/ \int_0^1 ds/P_c^2$$

$$k_{rg} = (1 - s)^2 \int_s^1 ds/P_c^2 \bigg/ \int_0^1 ds/P_c^2$$

on the basis of a linear relation between s and P_c^{-2} where P_c is the capillary pressure.

The functional form of the Core relation is illustrated in Figure II.2-1 for the particular set of parameters,

$$k_{rw}(S_{gr}) = k_{rg}(S_{wc}) = 1, S_{wc} = 0.3.$$

Tab II.2-3

Capillary Pressure

General Relations

In addition to being able to prescribe specific relations for capillary pressure for a particular geological unit, it is also desirable to have recourse to more general relations for cases when appropriate data are not available. An equation presented by Leverett (1941) factors capillary pressure into a general function of the saturation of the wetting phase and a prefactor related to the absolute permeability, k , and the porosity, ϕ , of the porous medium, the surface tension, γ , of the wetting phase; and a tortuosity parameter, T , characteristic of the pore network (Wyllie and Garner, 1959; Scheidegger, 1957). Specifically,

$$\begin{aligned} P_C &= (\gamma/T) (\phi/5k)^{1/2} f(s) \\ &= (155/T) (\phi/k)^{1/2} f(s) \end{aligned}$$

where the second equation is specifically for P_C in psi, permeability in millidarcies, and porosity as pore volume fraction. The tortuosity is defined as the ratio of the length of a capillary to the length of the porous medium. As noted in the discussion of relative permeabilities, the Corey relations are consistent with $f(s) = s^{-1/2}$. This Leverett-Corey relation for the capillary pressure is illustrated in Figure II.2-1 for the same set of parameters used to illustrate the relative-permeability relations with the additional values $k = 10$ md, $\phi = 0.03$ and $T = 2$.

Gas Sorption

General Relations

In addition to being present as a free gas in the coal pores and fracture network and as a dissolved species in the pore water, methane is also stored or retained in coal by a sorption process usually identified as physical adsorption of the gas onto internal coal surfaces. Of the models available for adsorption, the simplest theory by Langmuir for monolayer adsorption appears to be appropriate for most coal seam environments. In this case, adsorption isotherms, which determine the volume of adsorbed gas, V_E , in equilibrium with a free gas at pressure, P , can be defined in terms of two parameters as

$$V_E = P V_L [P_L + P]^{-1}$$

where V_L is the volume of gas contained in a molecular monolayer covering the internal surfaces and P_L is an effective pressure related to the average time gas molecules spend on the surface (de Boer, 1953). In general the adsorption isotherm, and therefore the parameters V_L and P_L , depend on temperature, water content, porosity, and rank (chemical structure) of the coal.

It is generally thought that transport of gas and water over large distances in coal is due to flow of these fluids through the coal fracture network and that these flows can be described mathematically by the equations for multiphase flows in porous media. When the gas pressure in the fracture network changes as a result of fluid flows, the volume of adsorbed gas in

adjacent parts of the coal matrix is no longer in equilibrium with the free gas. For surfaces that bound the fracture network, gas is adsorbed or desorbed sufficiently rapidly that equilibrium conditions can be considered to be established instantaneously. However, for internal surfaces away from the fracture network, longer times are required for the movement of gas molecules required to obtain equilibrium.

The movement of gas molecules between internal surfaces and the fracture network may be controlled by surface diffusion over the internal surfaces, by bulk diffusion of gas molecules through the coal matrix, or by transport of gas molecules through capillaries in the pore structure. The transport of molecules in the capillaries can be treated as a diffusion problem. Consequently, depending upon specific assumptions concerning the distribution of internal "source" surfaces, fracture network "sink" surfaces, and intervening transportation paths, variants of the diffusion equation are obtained to describe the time-dependent transition of gas molecules between a free gas state in the fracture network and the adsorbed state on the internal surfaces.

The simplest mathematical equation that takes into account the principal physical features of the sorption process is

$$\frac{\partial V_A}{\partial t} = - \frac{1}{\tau_A} [V_A(X,t) - V_E(P)]$$

where the volume of gas adsorbed, V_A , can be a function of time and position and the equilibrium adsorbed gas volume, V_E , is a function of free-gas pressure, which is itself a function of time and position. The characteristic sorption time, τ_A , can be expressed in terms of a characteristic average transportation distance between sorption and fracture-network surfaces, a , and a diffusion constant, D , as

$$\tau_A \doteq a^2/D$$

The diffusion constant depends on the transport mechanism. For example, for transport through capillaries the diffusion constant is a function of capillary diameter, temperature, and adsorption time.

Software for One-Dimensional Models

General Approach

The general approach used here to obtain computer solutions for a set of one-dimensional-time, dependent partial differential equations is similar to that described by Sincovec and Madsen (1975) in which a subroutine is used to transform a set of partial differential equations into a set of ordinary differential equations (ODE's) by discretizing the space variable and then a robust time integrator is used to solve the set of ODE's. In addition to the general time-integrator and space-discretizer routines, the computer software package for the one-dimensional numerical model consists of problem-specific routines to define components in the partial differential equations, to update algebraic quantities at selected time steps, and to provide specific values for parameters and normalized variables, and a main executive program to schedule the various routines and handle input/output functions. At some cost in program size and speed, this approach effectively isolates the code that defines a specific problem and thereby facilitates changes in the basic set of differential equations, boundary conditions, and functional forms of parameters.

Time-Integrator Routine

The time-integrator routine is essentially the EPISODE package [Byrne and Hindmarsh, 1975; Hindmarsh and Byrne, 1975] which incorporates several variable time-step algorithms and has been designed to solve a variety of stiff and nonstiff sets of ordinary differential equations. The June 24, 1975, version of EPISODE (available from the Argonne Code Center, Argonne National Laboratory) was modified in several ways for the present application.

Entry to EPISODE is through the routine DRIVE. Two arguments have been added to the formal parameters list for DRIVE such that the calling statement is now

```
CALL DRIVE (N, TO, HO, YO, TOUT, EPS, IERROR, MF, INDEXO,  
            IEQNDIM, EQUATE)
```

where the new parameters are

IEQNDIM, which indicates the number of space dimensions with 0 meaning a set of ordinary differential equations, and

EQUATE, which is an external user-supplied routine that defines the set of differential equations to be solved.

When IEQNDIM = 0, subroutine EQUATE is called directly by DRIVE, whereas when IEQNDIM = 1 or 2, DRIVE calls the space-discretizer routine which in turn makes calls to EQUATE.

The range of the formal parameter INDEX which is used on input to DRIVE to specify the type of call has been extended

to include the value 4, which indicates that a user supplied routine PUPDATE is to be called at each time interval. This option permits a "continuous" updating of parameters such as would be required to accomodate time-dependent boundary conditions.

In addition, all dimensioned variables in the EPISODE package have been collected into separate labelled common blocks to permit efficient changing of the maximum problem size by simply redimensioning the common blocks in the executive main program.

The formal parameter list and required structure of routines EQUATE AND PUPDATE and the format of the labelled common blocks for variable dimensions are described in the listing for the modified EDISODE package.

Space-Discretizer Routine — One-Space Dimension

A subroutine, PDEØNE, to transform a set of one-dimensional partial differential equations into a set of ordinary differential equations by discretizing the space variable was developed by using a structure similar to that described by Sincovec and Madsen (1975). The subroutine is formatted to be called from the modified version of EPISODE. It has two entries selected by the input formal parameter INIT. The entry corresponding to INIT = 1 sets up the space grid according to user-specified spacing options, calculates and stores coefficients for the finite-difference scheme, and determines initial values for the dependent variables by calls to the user-supplied routine identified with EQUATE.

Three alternative methods for producing the finite-difference equations are coded in PDEØNE, all based on a point-centered grid. The first method is a variable-order Taylor series method with which direct substitutions are made for the first and second derivatives in the partial differential equations. The second and third methods are derived from a single space integration of the partial differential equations. The second method is identical to the one described by Sincovec and Madsen (1975) and uses a first-order central difference scheme for the first derivatives, with block boundaries defined as the midpoints between nodes. The third method uses second-order differences for the first derivatives and determines block and effective endpoint boundaries from the requirement that finite difference expressions be equal to exact expressions for

fluxes at block and endpoint boundaries under conditions of constant flux.

The entry corresponding to $INIT = 0$ is the usual entry for calls from EPISODE but contains a further option to specify the type of weighting to be given to the transport coefficients; that is, the type of permeability weighting. Options include specifying the permeability at a block boundary to be the series flow weighted average from adjacent blocks, to be equal to the permeability in the upstream or downstream block, to be equal to the maximum or minimum permeability in the adjacent blocks, or to be discontinuous between the constant values in adjacent blocks.

Initial runs show the superiority of the third discretization algorithm for the type of boundary conditions applied to the present nonsteady-flow problem. Furthermore, the need for upstream weighting is also encountered for special conditions.

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