Appendix A

付録A　地下水流動シミュレーション法

APPENDIX A

Numerical Simulation Technology for Subsurface Fluid Flow

A.1 Introduction

The numerical simulation techniques for subsurface fluid flow problems have been widely studied in several related fields, such as petroleum, geothermal, mining and civil engineerings, water resources field, agricultural field, and so on.

Current technological developments in numerical techniques and computer hardwares/softwares have made us solve the fluid flow equations on a large domain of space and time under realistic conditions. In many fields, successful applications have been made for evaluating reserves of fluids, explaining fluid behavior in the past and present, and for predicting the future performance.

In this Appendix, the numerical simulation techniques are described on a 2-phase, 3-dimension general purpose simulator, GWS3D2P, originally developed by Hiroyuki TOSAKA of Tokyo University.

A.2 Basic Equations of 2-Phase Subsurface Fluid Flow

The basic governing relationship for the flow through porous media was obtained in the middle of 19th century, and it is known as Darcy's law which has the form of pressure diffusivity equation. Today, Darcy's law is recognized applicable to general geological media such as soil, rock and rock fractures, when the flow is thought to be laminar.

The subsurface fluid system can be modeled as a system comprising of two phases, air and water. The flow of two immiscible fluids through porous media is generally described by employing the extended form of Darcy's law and mass balance equations as,

$$\nabla \cdot \frac{K k_{rw}}{\mu_w B_w} \nabla (P_w - \gamma_w \nabla D) - q_w = \frac{\partial}{\partial t} \left(\frac{\phi S_w}{B_w} \right) \quad \cdots\cdots (A.1)$$

$$\nabla \cdot \frac{K k_{rg}}{\mu_g B_g} \nabla (P_g - \gamma_g \nabla D) - q_g = \frac{\partial}{\partial t} \left(\frac{\phi S_g}{B_g} \right) \quad \cdots\cdots (A.2)$$

where, $\nabla = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right)$:Laplace's differential operator,

P_w and P_g :phase pressure of water and gas respectively,

μ_w and μ_g :viscosities of water and gas, respectively,

r_w and r_g :column density of water and gas, respectively,

B_w and B_g :formation volume factors of water and gas, respectively,

k_{rw} and k_{rg} :effective permeabilities of water and gas, respectively,

S_w and S_g :saturation of water and gas, respectively,

q_w and q_g :production/injection rate of water and gas, respectively,

ϕ :porosity of porous media,

and D :depth of points.

Supplementarily, we have a constraint relationship between Sw and Sg as

$$Sw+Sg=1 \qquad \cdots\cdots (A.3)$$

and one for phase pressures as

$$Pw=Pg-Pc \qquad \cdots\cdots (A.4)$$

where, Pc is the capillary pressure explained later.

The fluid and rock properties listed above are usually dependent upon pressure or saturation if isothermal condition is assumed.

Substituting Sg and Pw in eqs. (A.1) and (A.2) using eqs(A.3) and (A.4), we finally have two equations consisting of unknown pressure Pg and unknown saturation Sw for each spatial point.

For practical purposes, it is necessary to use numerical technique to solve basic equations giving proper initaial and boundary conditions and rock/fluid properties.

In the following sections, points of numerical treatment are witten based upon the simulator GWS3D2P.

A.3 Discretization and Geological Setting

Discretization of Space and Time

To approximate the domain that the differential equations are defined and solved, Finite Difference Method(FDM) is applied. The entire portion of objective three dimensional spatial domain is discretized into a number of rectangular parallel-piped gridblocks, and for each gridblock, the fully implicit FDM expansion of the basic equations in terms of pressure and water saturation is done. The time domain is also divided into proper finite time difference. If the objective space is discretized into N finite gridblocks, we have 2xN unknowns in 2xN equations, therefore, it is solvable under proper condition. Fig. A-1 shows

the typical grid system used in the simulation. To treat irregular outer boundary shape in field-scale problems, which is usually a tracing line of surrounding watersheds, the grid system can be taken as shown in Fig. A-2.

Geological Setting

In numerical simulation, required geological data to describe the objective field structure are depth and thickness of each discretized gridblocks. Their distributions prescribe the surface topography and subsurface structure as shown in Fig. A-3. To keep precision of finite difference approximation in case of inclined, thickness-varying and permeability-varying formation, proper averaging and correction methods are used as explained in the later section A. 4.

A. 4 Treatment of Rock Parameters

Porosity

For simulation purpose, a effective porosity, which is defined as the ratio of block pore volume having pressure communication and block bulk volume, is used. Note that whenever "porosity" is referred to, it is the "effective" one without exceptions.

It is treated as a pressure dependent property with the form

$$\phi=\phi_{ref}\{1+C_r(P-P_{ref})\} \quad \text{(A. 5)}$$

where, ϕ_{ref} is the porosity at reference pressure P_{ref}, and C_r is the rock compressibility which corresponds to the rate of expansion of rock pore or fractures with the unit increase of fluid pressure. For wide field

problem where it is thought to have no significant effect on the flow, rock compressibility can be set at 0.0.

Permeability

The rock permeability, K, is treated as one of inherent physical constants of rock. It is usually treated as an independent parameter of pressure and saturation, but is treated dependent on flow direction to model anisotropic rock media. In general, the interblock permeability of neighboring gridblocks $\overline{K}$ with different permeability and thickness is calculated by harmonic averaging as

$$\overline{KH} = \frac{L_1 + L_2}{L_1 / (K_1 H_1) + L_2 / (K_2 H_2)} \quad \cdots\cdots (A.6)$$

where, K_1 and K_2 are permeabilities of two neighboring gridblocks, L_1 and L_2 are their lengths in one of discretized coordinates, and, H_1 and H_2 are thicknesses of respective gridblocks. For the flow between gridblocks with different depth points, above permeability value is corrected further as

$$\overline{KH}_{cor} = \overline{KH} \frac{0.25 (L_1 + L_2)^2}{0.25 (L_1 + L_2)^2 + (Z_1 - Z_2)^2} \quad \cdots\cdots (A.7)$$

Fig. A-4 shows schematically the averaging and correction process.

For special cases, non-neighboring connections can be defined to model faulted combination of gridblocks as shown in Fig. A-5.

Relative permeability

The relative permeabilites for water and gas are nonlinear functions

of water saturation. The typical curves measured for core samples in the laboratory are shown in Fig. A-6.

For practical simulation purpose, relative permeability curves on core samples is not valid and should be modified. The reason is that the relative permeability may be direction-dependent for the system with high contrast of densities. In such system, gravitational segregation of phases have to be considered and, at least, three different relative permeability curves should be used for horizontal, upward and downward directions.

Capillary Pressure

The capillary pressure in the porous media is defined by the difference of pressures of both sides of phase interface. In the laboratory, it is measured as a function of wetting phase saturation. The typical curve is shown in Fig. A-7.

In the simulation using large gridblocks, it should not be used directly as was noted for relative permeability. It should be used in a pseudofunction form, by which gravitatinal segregation of phases can be modeled.

A.5 *Treatment of Fluids Parameters*

Formation Volume Factor

Assuming isothermal condition, density of the fluid is treated as a function of phase pressure. To treat it in the mass balance equation, the notation of Formation Volume Factor(FVF, denoted as Bw or Bg in the basic equations) is used by defining

$$B = V / V_o \quad \text{.....(A.8)}$$

where, V is the fluid volume at arbitrary pressure P, and Vo is that at the standard temperature and pressure. Using this, density is expressed as

$$\rho = \rho_s / B \quad \text{.....(A.9)}$$

where, ρ is the fluid density at arbitrary pressure P, and ρ_s is the density of fluid at standard temperature and pressure.

For the air which is strongly compressible, the formation volume factor decreases nonlinearly as pressure increases. The water formation volume factor is around 1.0 at atomospheric pressure and decreases almost linearly with the slope of the order of about $10^{-5}atm^{-1}$. The water and air FVFs are shown in Fig.A-8(a) and A-9(a), respectively.

Viscosity

Under isothemal condition, viscosity of fluid varies as pressure changes. The water viscosity is almost constant in the pressure range of our interest. The gas viscosity increases as its density increases with the pressure. The typical curves for water and air viscosities are presented in Fig.A-8(b) and A-9(b), respectively.

A.6 Treatment of Boundary and Initial Conditions

Boundary Conditions

The external boundaries to be specified for a 3-dimensional hydrological problem are side, bottom, and upper ones.

The side boundary of wide areal problem is usually set on the watershed line surrounding the objective region, and is treated as no-flow boundary (Dirichlet boundary condition). But practically, as there may some water spills through river or subsurface openings to the external groundwater system, constant pressure boundary or constant influx boundary is required for proper modeling. Constant pressure boundary is realized by giving unrealistically large pore volume, i.e.,porosity, to the gridblock which should keep constant pressure, while constant influx boundary can be set by allocating a constant rate well to the objective gridblock.

The bottom bondary is, usually with few exceptions, a closed boundary set at sufficiently deep underground.

The upper boundary is the atomosphere that has almost constant pressure value. In the application of 2-phase simulation technique, the top layer is a air-saturated layer with the pressure at atomospheric value of the region and the water saturation at almost 0.0. To maintain constant pressure at the top layer at any simulation stage, permeabilities and porosities of the gridblocks of the top layer are set at very large values.

The well boundary condition, i.e., inner boundary condition, plays an important role when evaluating the areal fluid flow behavior including some pumping/injecting wells. Wells are specified on the gridblock basis. Considering the practical well operations, they are classified as bottomhole pressure specified wells and total rate specified wells. For the former, bottomhole pressure is specified and the rate of each productive block is calculated using analytical method. For the latter, total well rate is given and the production/injection rate of each gridblock is calculated based upon similar method as above.

To treat rainfall in hydrological simulation, it is necessary to all ocate some amount of rain in mm/day for all of the surface gridblocks.

Conveniently it is realized utilizing the same treatment as rate-specified, multiple-perforation horizontal well. In groundwater simulation, the input rainfall is usaully the downward filtration rate which is calculated by subtracting river flow rate and evaporated rate from total rainfall. The surface and river flows, which are characterized as much faster flows compared with subsurface flow, are not directly treated.

Initial Conditions

Initial distributions of pressure(usually air pressure) and saturation(usually water saturation) are set simultaneously for all of the domain modelled. The initialization process usually requires the following two steps.

In the first step, the distribution of free water level over the objective region is estimated by utilizing field measurements and geological occurences/knowledges. Using this, the pressure distribution is determined hydrostatically according to the depth of gridblock from the free water surface. For the gridblock above the free water level whose pores are filled with dominant air and irreducible trace of water, pressure is set at atomospheric one. The saturation value of the gridblock is also calculated by considering the relative position of the depth of the gridblock to the free water level.

In the second step of initialization, dynamic condition is checked by initiating simulation run for proper period of time. The distributions of pressure and saturation set in the first step may change dynamically to its final equilibrium condition as the time is proceeded. The hydrological condition that we seek for as the starting point may be found elsewhere in this process if the first step initialization is something good. If there are much field information about free graundwater level and seepages, it is useful for determining the desirable starting condition.

A.7 Solution Procedures and Features of GWS3D2P

Solution Procedures

The basic equations are solved simultaneously for gas pressure Pg and water saturation Sw of each discretized gridblock by the fully implicit FDM, which is, nominally, unconditionally stable. The FDM expansion of the basic equations results in a matrix equation having tridiagonal structure for 1-D problem, pentadiagonal one for2-D problem, or heptadiagonal one for 3-D problem, respectively. Such structured sparse matrix equation can be solved by using conventional direct or iterative matrix solvers. The truncated conjugate residual algorithm, called ORTHOMIN method, preconditioned by the Nested Factorization, is used for the matrix solution in GWS3D2P.

The Nonlinearity associated with saturation functions and fluid compressibility is overcome by the Newton-Raphson iterative procedure.

The flow chart of the simulator is shown in Fig. A.10.

Features of GWS3D2P

The features of the numerical simulator GWS3D2P used in this study can be briefly summarized as follows.

- Compressible and immiscible two fluids, such as water-air, water-oil or oil-gas, can be dealt with.
- Cartesian and cylindrical coordinate systems can be used.
- Fully implicit Finite Difference Method(FDM) is used to solve basic equations.
- Non-linearity is treated by Newton-Raphson iterative procedure.
- Linear matrix equations system is solved by Preconditioned Conjugate Residual(PCR) algorithm.
- Irregular Geometry of external boundary can be set.
- Block permeability can be set directionally for each of 6 surfaces

of a rectangular parallel-piped grid. Relative permeability can also be set in 6 directions

- Production/injection wells can be treated by specifying either bottomhole pressure or total rate. Wells operating for multiple layers, or penetrating horizontally, can be set.
- Rainfalls to all of the surface gridblocks can be allocated by utilizing horizontal well option.
- Faulted connections among diferent geological formations can be set through special FAULT option for non-neiboring connections.
- Artificially boundaries arising from underground caverns such as tunnels in mines, or large underground caverns, can be properly set into the numerical model time by time.
- A Special technique to reduce the CPU time required for large-scale field problems can be used.

Conventional FDM Gridding

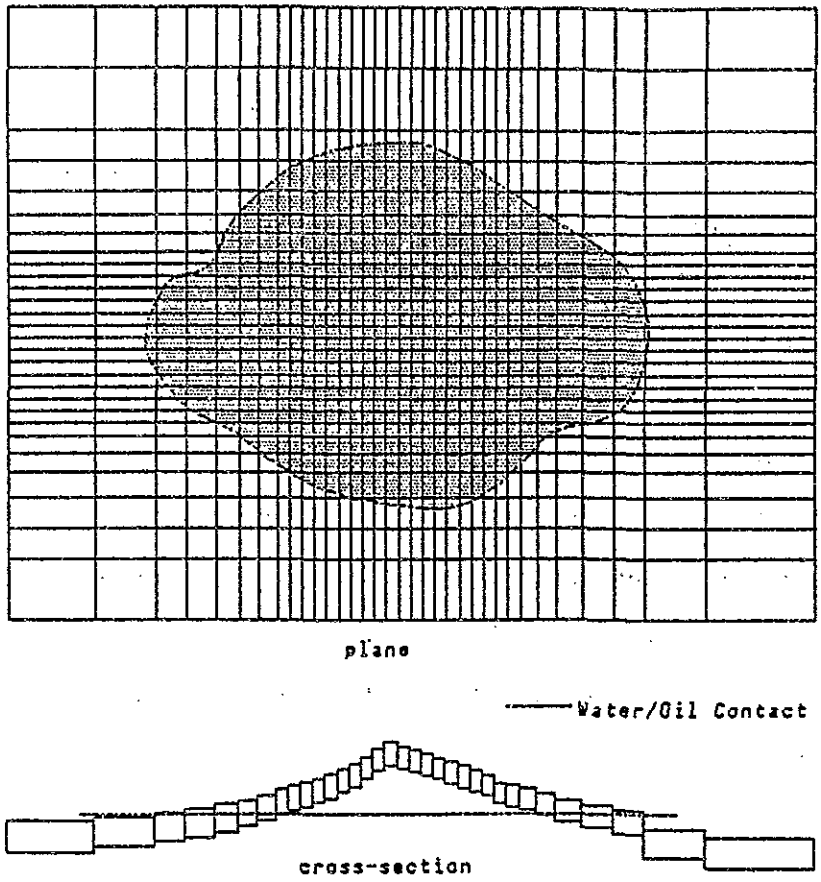


Fig. A-1 A Typical FDM Gridding

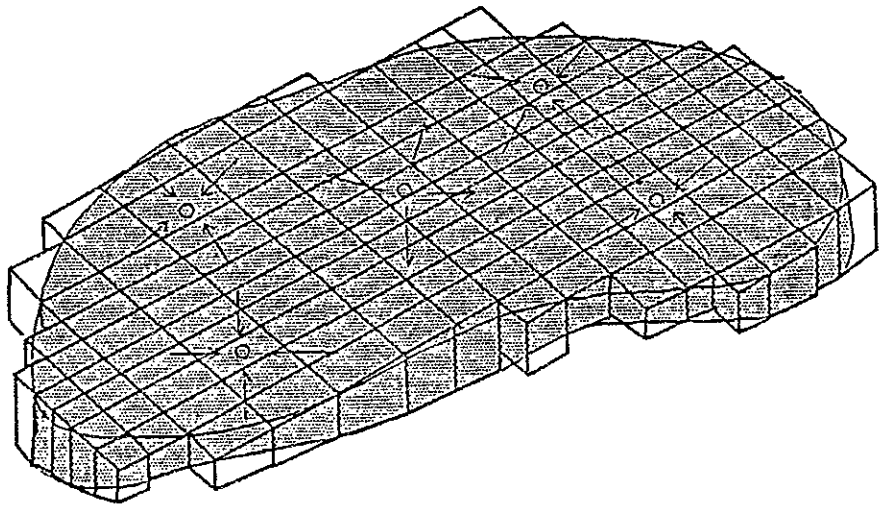


Fig. A-2 Gridding for Irregular Boundary Shape

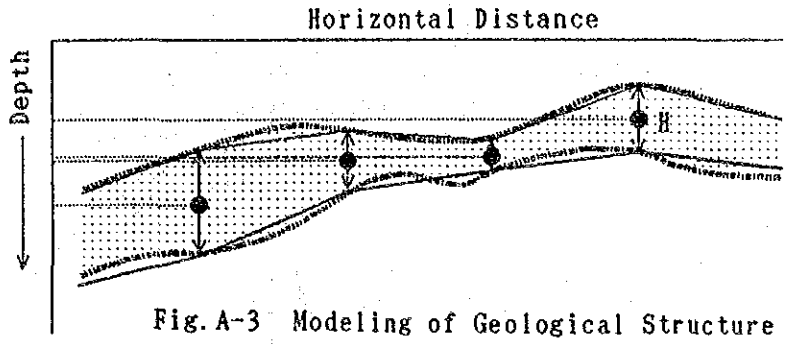
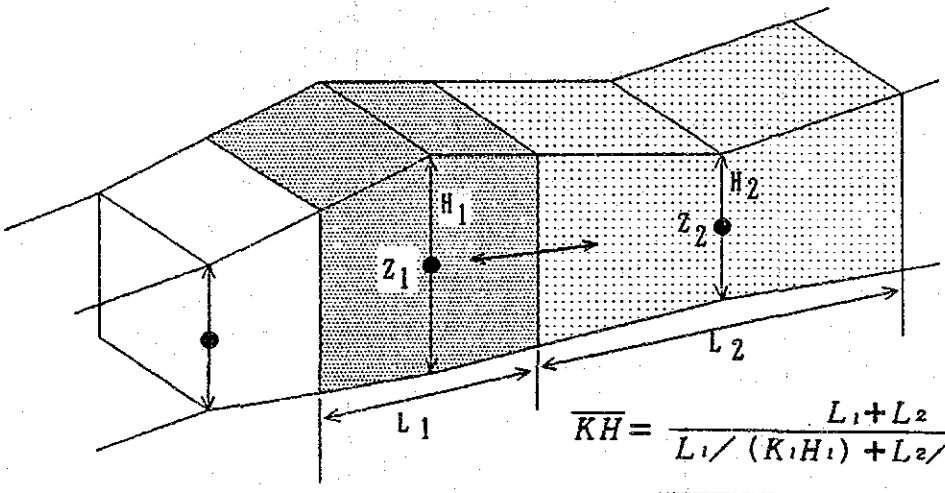


Fig. A-3 Modeling of Geological Structure



$$\overline{KH} = \frac{L_1 + L_2}{L_1 / (K_1 H_1) + L_2 / (K_2 H_2)}$$

$$\overline{KH}_{cor} = \overline{KH} \sqrt{\frac{0.25 (L_1 + L_2)^2}{0.25 (L_1 + L_2)^2 + (Z_1 - Z_2)^2}}$$

Fig. A-4 Calculation of Interblock Permeability

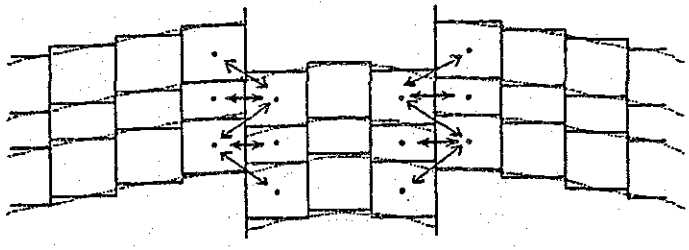


Fig. A-5 Non-neighboring Connections around Faults

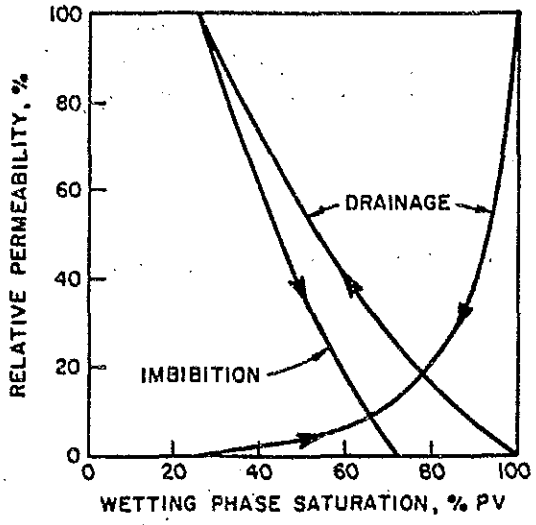


Fig. A-6 Typical Relative Permeability Curves

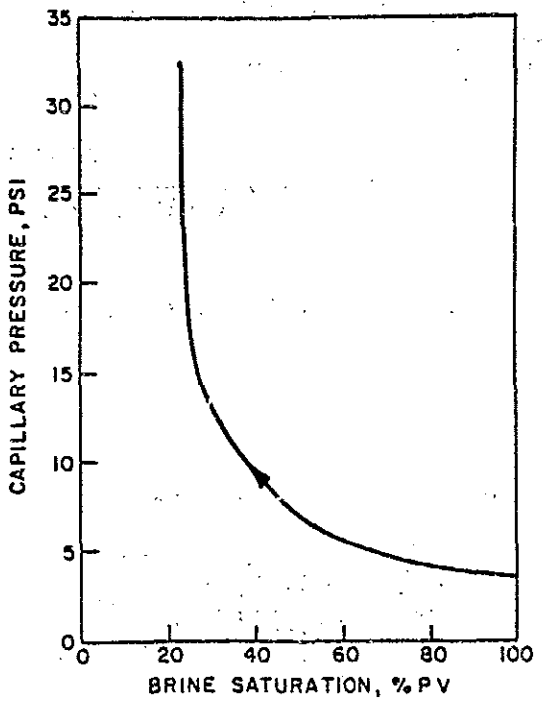
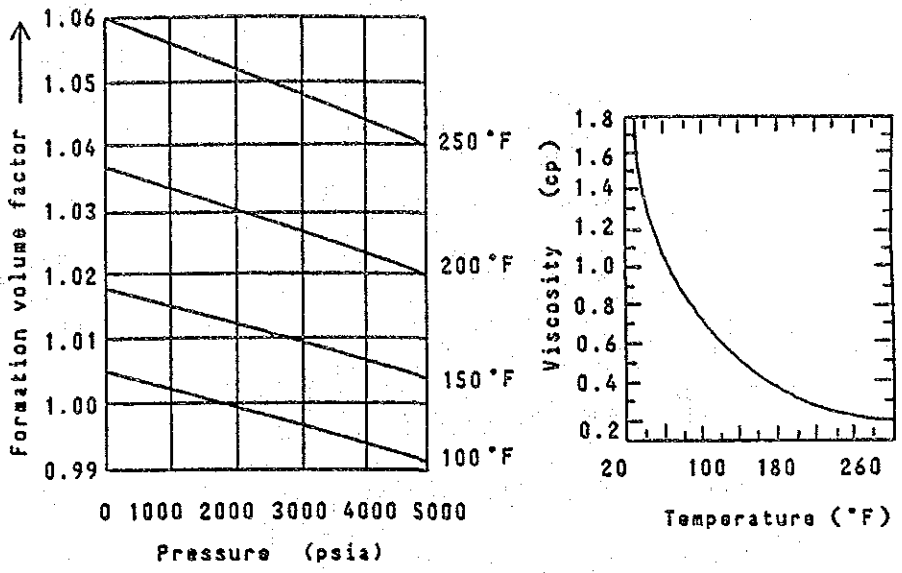


Fig. A-7 Typical Capillary Pressure Curve



(a) Formation volume factor of water

(b) Change in viscosity of water along temperature

[from Properties of Petroleum Reservoir Fluids by Emil J. Burcik.]

[from Frick, T.C. ed.: Petroleum Production Handbook.]

Fig. A-8 Water Properties

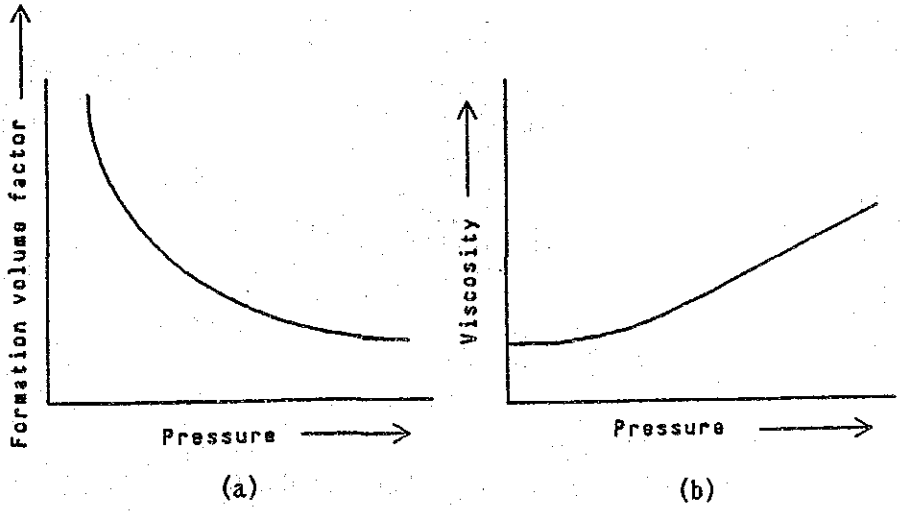


Fig. A-9 General Tendency of Gas Properties

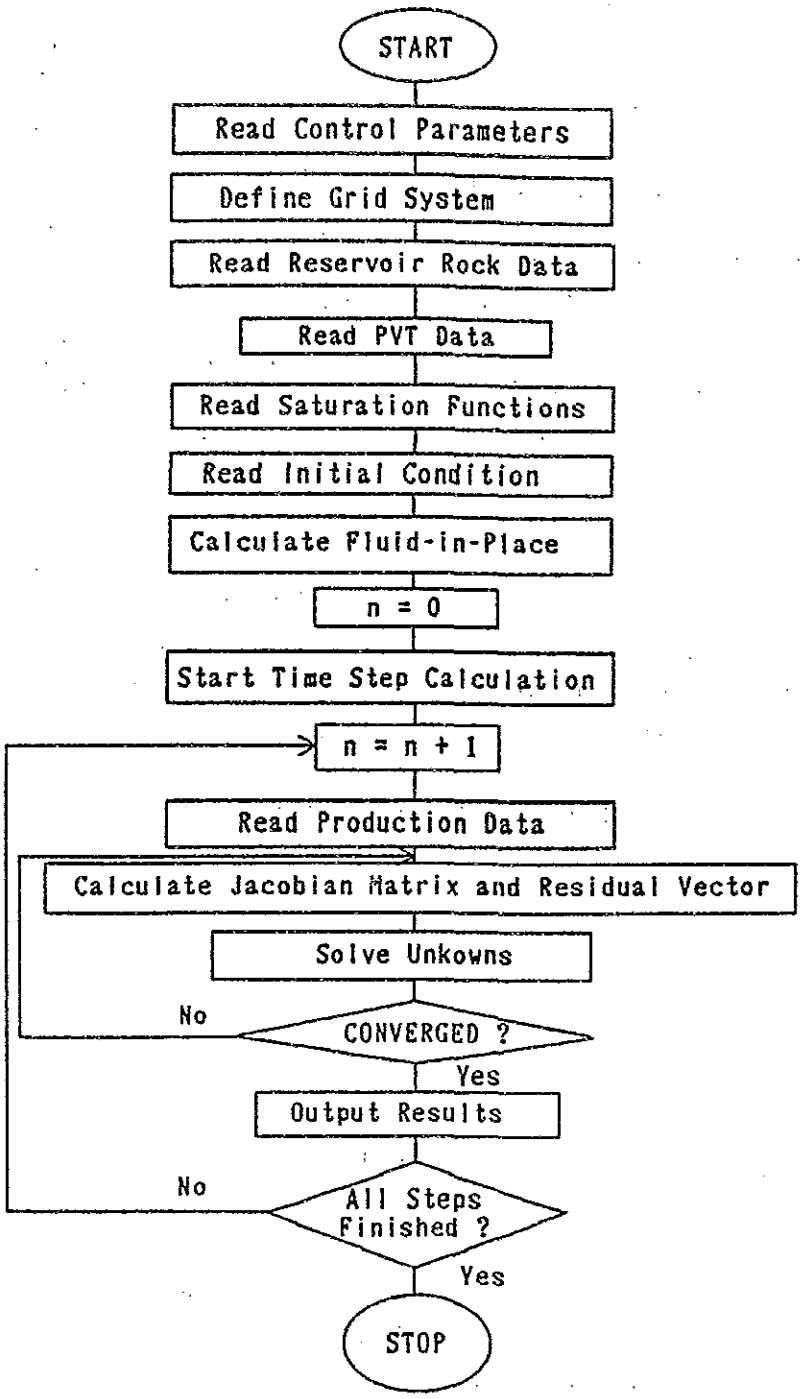


Fig. A-10 A Flow Chart of GWS3D2P