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Advances in G E O P H Y S I C S

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SEISMIC WAVE PROPAGATION IN LATERALLY HETEROGENEOUS ANELASTIC MEDIA: THEORY AND APPLICATIONS TO SEISMIC ZONATION

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1. INTRODUCTION

The guidelines of the International Decade for Natural Disaster Reduction (ID-NDR, sponsored by United Nations), for the drawing up of precatastrophe plans of action, have led to the consolidation of the idea that zoning can and must be used as a means of prevention in areas that have not yet been hit by a disaster but are potentially prone to it. The urgency for improving earthquake risk assessment and risk management is clearly pointed out in the monograph on seismic zonation edited by Hays *et al.* (1998). Optimization of the techniques aimed at the prevention will be one of the basic themes of the development of seismic zoning in the 21st century.

The first scientific and technical methods developed for zoning were deterministic and based on the observation that damage distribution is often correlated to the spatial distribution and the physical properties of the underlying terrain and rocks. The 1970s saw the beginning of the construction of probabilistic seismic zoning maps on a national, regional, and urban (microzoning) scale. In the 1990s these instruments for the mitigation of seismic hazard were coming to prevail over deterministic cartography.

The most controversial question regarding definition of standards to be used in the evaluation of seismic hazard may be formulated as follows: should probabilistic or deterministic criteria and methods be used? Because probabilistic and deterministic approaches play mutually supportive roles in earthquake risk mitigation, at

the current level of development in the modeling of seismogenesis and of seismic wave propagation, the best policy for the future is to combine the advantages offered by both methods, using integrated approaches (e.g., Reiter, 1990). In this way, among others, we have the main advantage of making possible the extension of seismic zoning to long periods; a period band up to now almost totally ignored by all methods, but which is acquiring continuously increasing importance, due to the widespread existence in the built environment of special objects, with relatively long free periods.

Studies carried out following strong earthquakes (e.g., 1985 Michoacan; 1995 Kobe) proved to be important sources of basic knowledge and have acted as catalysts for the use of zoning in seismic risk management. The impetus for this has come essentially from politicians and administrators particularly interested in rapid reconstruction, according to criteria which reduce the probability of a repetition of disasters. These postearthquake studies have led to the conclusion that the destruction caused by an earthquake is the result of the interaction of three complex systems: (1) the solid Earth system, made up of (a) seismic source, (b) propagation of the seismic waves, and (c) geometry and physical conditions of the local geology; (2) the anthropic system, whose most important feature in this context is the quality of constructions (buildings, bridges, dams, pipelines, etc.); and (3) the social, economic, and political system, which governs the use and development of a settlement before it is struck by an earthquake.

Results have shown that in an area of human development it is now technically possible to identify zones in which the heaviest damage can be predicted. A first-order zoning can be carried out at regional scale, based on the knowledge of the average properties of seismic sources and structural models. Microzonations are possible as well, provided that very detailed information about the source, path, and local site conditions are available.

Seismic zoning can use scientific data bases, integrated in an expert system, by means of which it is possible to identify the safest and most suitable areas for urban development, taking into account the complex interaction between the solid Earth system, the environmental system, and the social, economic, and political system. It is also possible to define the seismic input that is going to affect a given building. The construction of an integrated expert system will make it possible to tackle the problem at its widest level of generality and to maintain the dynamic updating of zoning models, dictated by the acquisition of new data and the development of new model-building methods.

With the acquired knowledge, a drastic change is required in the orientation of zoning that must no longer be considered a postdisaster activity. It is necessary to proceed to predisaster surveys that can be usefully employed to mitigate the effects of the next earthquake, using all available technologies. As clearly indicated by the 1994 Northridge, California, and 1995 Kobe, Japan, events, we cannot confine ourselves to using what has been learned from a catastrophe solely in the area in

which it took place. We must be able to take preventive steps, extending results obtained in a scientifically acceptable way, to areas in which no direct experience has yet been gained. An opportunity is offered in this direction by the scientific community's ability to make realistic simulations of the behavior of the solid Earth system through the computation of increasingly realistic synthetic seismograms with a broad frequency content.

The contribution of seismology to knowledge of the Earth's interior dramatically improved starting in the 1960s, when good quality instrumental data became available, and computers allowed for fast processing. From the analysis of good quality seismograms it became evident that large lateral heterogeneities are not confined to the transition areas between oceans and continents, or just to the surficial geology, but characterize the whole structure of the Earth with the possible exception of the outer core.

Seismic waves can be represented as elastic perturbations propagating within a medium, originated by a transient disequilibrium in the stress field. The properties of seismic waves are ruled by the physics of elastic bodies, and are studied using the formalisms of elastodynamic theory.

It is necessary, therefore, to incorporate the effects of lateral heterogeneities in the direct modeling of the wavefield in order to retrieve a correct image of the heterogeneity itself and consequently to understand the geodynamics of the studied portion of the Earth.

Macroseismic observations made corresponding to the destructive events of the past 100 years or so have clearly evidenced the strong influence of near-surface geological and topographical conditions on damage distribution. Because most anthropic areas (e.g., megacities) are settled in relation to sedimentary basins such as river valleys, a realistic definition of the seismic input that takes into account site response has become one of the most relevant tasks in seismic engineering analysis.

An additional reason to extend modeling techniques to laterally heterogeneous structures is connected with the seismic hazard assessment. Using the available geological and geotechnical information, a low-cost parametric analysis can be performed to estimate the groundshaking site response. The theoretical approach, based on computer codes and developed from a detailed knowledge of the seismic source process and the propagation of seismic waves in heterogeneous media, can simulate the ground motion associated with a given earthquake scenario.

2. THE SEISMIC WAVEFIELD

Seismic waves can be represented as elastic perturbations propagating within a medium, originated by a transient disequilibrium in the stress field. In the study of elastic bodies, to take into account macroscopic phenomena, it is assumed that the

medium is a *continuum*, i.e., that the matter is distributed continuously in space. Therefore it is possible to define the mathematical functions that describe the fields associated with displacement, stress, and deformation. Furthermore, being interested in the motion of the considered elastic body, the Lagrangian description is used, where the motion of each particle is analyzed in space and time, and the vector field $\mathbf{u}(\mathbf{x}, t)$, associated with the displacement, is defined at any point of the body.

2.1. Equations of Motion and Constitutive Relations

Considering the balance of forces, including inertia, body forces and surface forces acting on a cubic element within the continuum, and applying Newton's law, we obtain the system of equations of motion

$$\begin{aligned}\rho \frac{\partial^2 u_x}{\partial t^2} &= \rho X + \frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{yx}}{\partial y} + \frac{\partial \sigma_{zx}}{\partial z} \\ \rho \frac{\partial^2 u_y}{\partial t^2} &= \rho Y + \frac{\partial \sigma_{xy}}{\partial x} + \frac{\partial \sigma_{yy}}{\partial y} + \frac{\partial \sigma_{zy}}{\partial z} \\ \rho \frac{\partial^2 u_z}{\partial t^2} &= \rho Z + \frac{\partial \sigma_{xz}}{\partial x} + \frac{\partial \sigma_{yz}}{\partial y} + \frac{\partial \sigma_{zz}}{\partial z},\end{aligned}\tag{1}$$

where a Cartesian coordinate system (x, y, z) is adopted. $\sigma_{ij}(\mathbf{x}, t)$ ($i = x, y, z; j = x, y, z$) indicates the second-order stress tensor, ρ is the density of the material, and X, Y, Z are the components of body forces for a unit mass.

Deformations, indicated by the second-order tensor $e_{kl}(\mathbf{x}, t)$ ($k = x, y, z; l = x, y, z$), if assumed infinitesimal, can be written as a function of displacements

$$\begin{aligned}e_{xx} + e_{yy} + e_{zz} &= \frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} + \frac{\partial u_z}{\partial z} \\ e_{xy} = e_{yx} &= \frac{1}{2} \left(\frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x} \right) \quad e_{yz} = e_{zy} = \frac{1}{2} \left(\frac{\partial u_z}{\partial y} + \frac{\partial u_y}{\partial z} \right) \\ e_{xz} = e_{zx} &= \frac{1}{2} \left(\frac{\partial u_z}{\partial x} + \frac{\partial u_x}{\partial z} \right).\end{aligned}\tag{2}$$

In general, the relation between stress and deformation can take a very complex form since it has to include the effects of parameters like pressure, temperature, and the amount and variability of stress. Nevertheless, considering small deformations and stresses of short duration (conditions mostly satisfied in ground motion estimation problems), we can assume that the solid behaves linearly and the constitutive relation linking stresses and deformation becomes *Hooke's law*

$$\sigma_{ij} = C_{ijkl} e_{kl},\tag{3}$$

where the convention of repeated indices is used; C_{ijkl} is a fourth-order symmetric tensor, whose 81 elements are the elastic moduli. If the solid is isotropic (as mostly occurs for the Earth), the components of the tensor C_{ijkl} assume the same value for all the axes, and (3), using the Kronecker delta δ_{ij} , becomes

$$\sigma_{ij} = \lambda \delta_{ij} e_{kk} + \mu (e_{ij} + e_{ji}) + \nu (e_{ij} - e_{ji}), \quad (3a)$$

where λ , μ , and ν are scalar quantities (Jeffreys and Jeffreys, 1950). Because e_{ij} is a symmetric tensor, (3a) can be rewritten as

$$\sigma_{ij} = \lambda e_{kk} \delta_{ij} + 2\mu e_{ij} \quad (4)$$

and the quantities λ and μ are called *Lamé parameters*.

Using relations (3) and (4), Eq. (1) becomes a linear system of three differential equations with three unknowns: the three components of the displacement vector, whose coefficients depend upon the elastic parameters of the material. It is not possible to find the analytic solution for this system of equations; therefore it is necessary to add further approximations, chosen according to the adopted resolving method. Two ways can be followed. In the first one an exact definition of the medium is given, and a direct *numerical* integration technique is used to solve the set of differential equations. The second way implies that exact *analytical* techniques are applied to an approximated model of the medium that may have the elastic parameters varying along one or more directions of heterogeneity. In the following we introduce the analytical solution valid for a flat layered half-space that constitutes the base of knowledge for the treatment we will develop for models with lateral discontinuities.

2.2. Equations of Elastic Motion for a Halfspace with Vertical Heterogeneities

Let us consider a halfspace in a system of Cartesian coordinates with the vertical z axis positive downward and the free surface, where vertical stresses (σ_{xz} , σ_{yz} , σ_{zz}) are null, is defined by the plane $z = 0$ (Fig. 1).

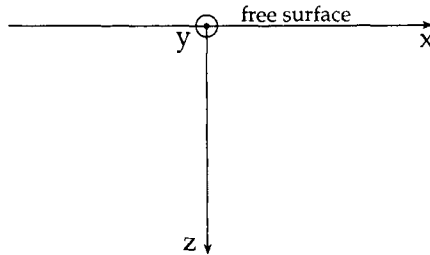


FIG. 1. Adopted reference system for a vertically heterogeneous halfspace.

Let us assume that λ , μ , and ρ are piecewise continuous functions of z , and that body wave velocities, $\alpha = \sqrt{\frac{\lambda+2\mu}{\rho}}$ and $\beta = \sqrt{\frac{\mu}{\rho}}$, assume their largest value, α_H and β_H , when $z > H$, remaining constant for greater depths.

If the elastic parameters depend only upon the vertical coordinate, using (1), relations (3) and (4) become

$$\begin{aligned}
 \rho \frac{\partial^2 u_x}{\partial t^2} &= \rho X + (\lambda + 2\mu) \frac{\partial^2 u_x}{\partial x^2} + (\lambda + \mu) \frac{\partial^2 u_y}{\partial x \partial y} + (\lambda + \mu) \frac{\partial^2 u_z}{\partial x \partial z} \\
 &\quad + \mu \frac{\partial^2 u_x}{\partial y^2} + \mu \frac{\partial^2 u_x}{\partial z^2} + \frac{\partial \mu}{\partial z} \frac{\partial u_x}{\partial z} + \frac{\partial \mu}{\partial z} \frac{\partial u_z}{\partial x} \\
 \rho \frac{\partial^2 u_y}{\partial t^2} &= \rho Y + (\lambda + 2\mu) \frac{\partial^2 u_y}{\partial y^2} + (\lambda + \mu) \frac{\partial^2 u_x}{\partial x \partial y} + (\lambda + \mu) \frac{\partial^2 u_z}{\partial y \partial z} \\
 &\quad + \mu \frac{\partial^2 u_y}{\partial x^2} + \mu \frac{\partial^2 u_y}{\partial z^2} + \frac{\partial \mu}{\partial z} \frac{\partial u_y}{\partial z} + \frac{\partial \mu}{\partial z} \frac{\partial u_z}{\partial y} \\
 \rho \frac{\partial^2 u_z}{\partial t^2} &= \rho Z + (\lambda + 2\mu) \frac{\partial^2 u_z}{\partial z^2} + (\lambda + \mu) \frac{\partial^2 u_x}{\partial x \partial z} + (\lambda + \mu) \frac{\partial^2 u_y}{\partial y \partial z} \\
 &\quad + \mu \frac{\partial^2 u_z}{\partial x^2} + \mu \frac{\partial^2 u_z}{\partial y^2} + \frac{\partial \lambda}{\partial z} \left(\frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} + \frac{\partial u_z}{\partial z} \right) + 2 \frac{\partial \mu}{\partial z} \frac{\partial u_z}{\partial z}.
 \end{aligned} \tag{5}$$

The boundary conditions that must be satisfied when solving (5) are the free surface condition at $z = 0$

$$\begin{aligned}
 \sigma_{zz} &= (\lambda + 2\mu) \frac{\partial u_z}{\partial z} + \lambda \left(\frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} \right) = 0 \\
 \sigma_{zx} &= \mu \left(\frac{\partial u_x}{\partial z} + \frac{\partial u_z}{\partial x} \right) = 0 \\
 \sigma_{zy} &= \mu \left(\frac{\partial u_y}{\partial z} + \frac{\partial u_z}{\partial y} \right) = 0,
 \end{aligned} \tag{6}$$

and the continuity condition for the displacement and stress components u_x , u_y , u_z , σ_{zx} , σ_{zy} , σ_{zz} all along the vertical axis, including the points where λ , μ , and ρ are eventually discontinuous.

The complete solution of Eq. (5) can be represented in an integral form. At large distances from the source, compared with the wavelength, the main part of the solution is given by Rayleigh and Love modes (see e.g., Levshin (1973) and Aki and Richards (1980)).

Neglecting the body forces, we can consider solutions of (5) having the form of plane harmonic waves propagating along the positive x axis

$$\mathbf{u}(\mathbf{x}, t) = \mathbf{F}(z) e^{i(\omega t - kx)}, \tag{7}$$

where k is the wavenumber connected with the phase velocity c , i.e., $k = \omega/c$, and ω is the angular frequency.

Let us consider the case $c < \beta_H$. Using (7), Eq. (5) becomes

$$\begin{aligned} \omega^2 \rho F_x - k^2(\lambda + 2\mu)F_x - ik(\lambda + \mu)\frac{\partial F_z}{\partial z} - ik\frac{\partial \mu}{\partial z}F_z + \frac{\partial}{\partial z}\left(\mu\frac{\partial F_z}{\partial z}\right) &= 0 \\ \omega^2 \rho F_y - k^2\mu F_y + \frac{\partial}{\partial z}\left(\mu\frac{\partial F_y}{\partial z}\right) &= 0 \quad (8) \\ \omega^2 \rho F_z - k^2\mu F_z - ik(\lambda + \mu)\frac{\partial F_x}{\partial z} - ik\frac{\partial \lambda}{\partial z}F_x + \frac{\partial}{\partial z}\left[(\lambda + 2\mu)\frac{\partial F_z}{\partial z}\right] &= 0. \end{aligned}$$

We have to solve two independent eigenvalue problems for the three components of the vector $\mathbf{F} = (F_x, F_y, F_z)$. The first one describes the motion in the plane (x, z) , i.e., P-SV waves. It has the form

$$\begin{aligned} \frac{\partial}{\partial z}\left[\mu\frac{\partial F_x}{\partial z} - ik\mu F_z\right] - ik\lambda\frac{\partial F_z}{\partial z} + F_x[\omega^2 \rho - k^2(\lambda + 2\mu)] &= 0 \\ \frac{\partial}{\partial z}\left[(\lambda + 2\mu)\frac{\partial F_z}{\partial z} - ik\lambda F_x\right] - ik\mu\frac{\partial F_x}{\partial z} + F_z(\omega^2 \rho - k^2\mu) &= 0 \end{aligned} \quad (9)$$

and must be solved with the free surface boundary condition at $z = 0$

$$\begin{aligned} \sigma_{zz} &= (\lambda + 2\mu)\frac{\partial F_z}{\partial z} - ik\lambda F_x = 0 \\ \sigma_{zx} &= \mu\left(\frac{\partial F_x}{\partial z} - ikF_z\right) = 0. \end{aligned} \quad (10)$$

The second eigenvalue problem describes the case when the particle motion is limited to the y -axis and determines phase velocity and amplitude of SH waves. It has the form

$$\frac{\partial}{\partial z}\left(\mu\frac{\partial F_y}{\partial z}\right) + F_y(\omega^2 \rho - k^2\mu) = 0 \quad (11)$$

and must be solved with the boundary condition

$$\sigma_{zy} = \mu\frac{\partial F_y}{\partial z} = 0, \quad (12)$$

when $z = 0$.

2.3. Multimodal Method (SH and P-SV Waves) in a Layered Halfspace

Let us now assume that the vertical heterogeneity in the halfspace is modeled with a series of $N-1$ homogeneous flat layers, parallel to the free surface, overlying a homogeneous halfspace (see Fig. 2). Let ρ_m , α_m , β_m , and d_m , respectively, be the density, P-wave and S-wave velocities, and the thickness of the m th layer.

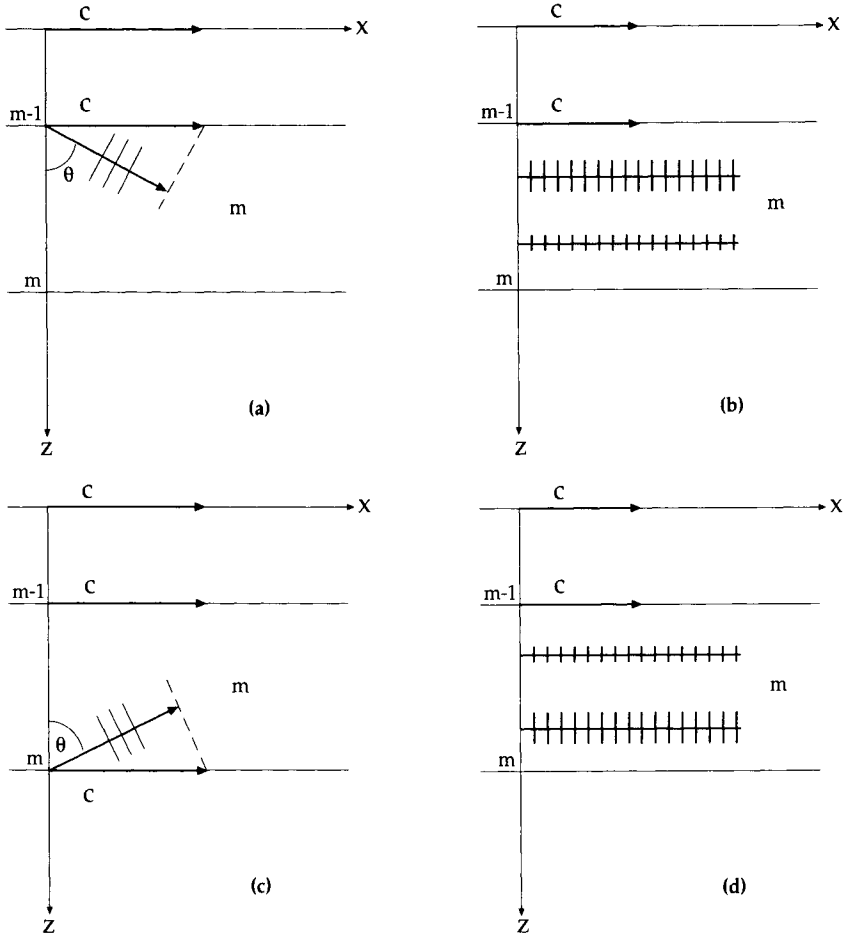


FIG. 2. For the adopted reference system the term in v' of Eq. (14) represents a plane wave whose direction of propagation makes an angle $\cot^{-1} r_{\beta m}$ with the $+z$ direction when $r_{\beta m}$ is real (a), and a wave propagating in the $+x$ direction with amplitude diminishing exponentially in the $+z$ direction when $r_{\beta m}$ is imaginary (b). Similarly, the term in v'' represents a plane wave making the same angle with the direction $-z$ when $r_{\beta m}$ is real (c), and a wave propagating in the $+x$ direction with amplitude increasing in the $+z$ direction when $r_{\beta m}$ is imaginary (d).

Furthermore, let us define

$$r_{\alpha m} = \begin{cases} \sqrt{\left(\frac{c}{\alpha_m}\right)^2 - 1} & \text{if } c > \alpha_m \\ -i\sqrt{1 - \left(\frac{c}{\alpha_m}\right)^2} & \text{if } c < \alpha_m \end{cases} \quad r_{\beta m} = \begin{cases} \sqrt{\left(\frac{c}{\beta_m}\right)^2 - 1} & \text{if } c > \beta_m \\ -i\sqrt{1 - \left(\frac{c}{\beta_m}\right)^2} & \text{if } c < \beta_m \end{cases} \quad (13)$$

2.3.1. Love Modes

For Love modes, the periodic solutions of the elastic equations of motion for the m th layer are

$$\begin{aligned} u_x &= u_z = 0 \\ u_y &= (v'_m e^{-ikr_{\beta m} z} + v''_m e^{+ikr_{\beta m} z}) e^{i(\omega t - kx)} \end{aligned} \quad (14)$$

and the associated stress component is

$$\sigma_{zy} = \mu \frac{\partial u_y}{\partial z} = ik\mu r_{\beta m} (-v'_m e^{-ikr_{\beta m} z} + v''_m e^{+ikr_{\beta m} z}) e^{i(\omega t - kx)}, \quad (15)$$

where v'_m and v''_m are constants. Given the sign conventions adopted, the term in v' represents a plane wave whose direction of propagation makes an angle $\cot^{-1} r_{\beta m}$ with the $+z$ direction when $r_{\beta m}$ is real, and a wave propagating in the $+x$ direction with amplitude diminishing exponentially in the $+z$ direction when $r_{\beta m}$ is imaginary. Similarly, the term in v'' represents a plane wave making the same angle with the direction $-z$ when $r_{\beta m}$ is real and a wave propagating in the $+x$ direction with amplitude increasing in the $+z$ direction when $r_{\beta m}$ is imaginary (Fig. 2).

For Love modes the boundary conditions that must be satisfied at any interface are the continuity of the transverse component of displacement, u_y , and the continuity of the tangential component of stress, σ_{zy} . Then we can use the Thomson–Haskell method and its modifications (e.g., Schwab and Knopoff, 1972; Florsch *et al.*, 1991) to efficiently compute the multimodal dispersion of surface waves and therefore synthetic seismograms in anelastic media.

Let us consider the m th layer and interface $(m - 1)$, where we set the origin of the coordinate system. It is convenient to use $\frac{\dot{u}_y}{c} = ik u_y$ instead of displacement, u_y , so that we deal with nondimensional quantities.

At the interface $(m - 1)$ we have

$$\begin{aligned} \left(\frac{\dot{u}_y}{c} \right)_{m-1} &= ik(v'_m + v''_m) \\ (\sigma_{zy})_{m-1} &= ik\mu_m r_{\beta m} (v''_m - v'_m), \end{aligned} \quad (16)$$

while at the m th interface we have

$$\begin{aligned} \left(\frac{\dot{u}_y}{c} \right)_m &= ik(v'_m + v''_m) \cos Q_m - k(v''_m - v'_m) \sin Q_m \\ (\sigma_{zy})_m &= -k\mu_m r_{\beta m} (v''_m + v'_m) \sin Q_m + ik\mu_m r_{\beta m} (v''_m - v'_m) \cos Q_m, \end{aligned} \quad (17)$$

where we define $Q_m = kr_{\beta m} d_m$ and we drop the time-dependent term $e^{i\omega t}$.

Eliminating the quantities v'_m and v''_m in Eqs. (16) and (17) we obtain

$$\begin{aligned} \left(\frac{\dot{u}_y}{c}\right)_m &= \left(\frac{\dot{u}_y}{c}\right)_{m-1} \cos Q_m + i(\sigma_{zy})_{m-1}(\mu_m r_{\beta_m})^{-1} \sin Q_m \\ (\sigma_{zy})_m &= \left(\frac{\dot{u}_y}{c}\right)_{m-1} i\mu_m r_{\beta_m} \sin Q_m + (\sigma_{zy})_{m-1} \cos Q_m. \end{aligned} \quad (18)$$

Introducing the layer matrix

$$a_m = \begin{bmatrix} \cos Q_m & \frac{i \sin Q_m}{\mu_m r_{\beta_m}} \\ i\mu_m r_{\beta_m} \sin Q_m & \cos Q_m \end{bmatrix}, \quad (19)$$

Eq. (18) can be rewritten in the matrix form

$$\begin{bmatrix} \left(\frac{\dot{u}_y}{c}\right)_m \\ (\sigma_{zy})_m \end{bmatrix} = a_m \begin{bmatrix} \left(\frac{\dot{u}_y}{c}\right)_{m-1} \\ (\sigma_{zy})_{m-1} \end{bmatrix}. \quad (20)$$

Subsequently substituting m with values between $(N - 1)$ and 0 we have that

$$\begin{bmatrix} \left(\frac{\dot{u}_y}{c}\right)_{N-1} \\ (\sigma_{zy})_{N-1} \end{bmatrix} = A \begin{bmatrix} \left(\frac{\dot{u}_y}{c}\right)_0 \\ (\sigma_{zy})_0 \end{bmatrix} \quad (21)$$

$$A = a_{N-1} a_{N-2} \cdots a_2 a_1,$$

where A is a 2×2 matrix.

If we now use (16) with $m = N$, and remembering that the boundary conditions of surface waves and the free surface implies that $v''_N = 0$ and $(\sigma_{zy})_0 = 0$, we have that

$$A_{21} + \mu_N r_{\beta_N} A_{11} = 0. \quad (22)$$

The left-hand side of Eq. (22) is the *dispersion function* for Love modes (SH waves), where A_{21} and A_{11} are elements of the matrix A . The couples (ω, c) for which the dispersion function is equal to zero are its roots and represent the eigenvalues of the problem. Eigenvalues, according to the number of zeroes of the corresponding eigenfunctions, $u_y(z, \omega, c)$ and $\sigma_{zy}(z, \omega, c)$, can be subdivided in the dispersion curve of the fundamental mode (which has no nodal planes), of the first higher mode (having one nodal plane), of the second higher mode and so on. Once the phase velocity c is determined, we can compute analytically the group velocity using the implicit functions theory (Schwab and Knopoff, 1972), and the eigenfunctions (Florsch *et al.*, 1991).

2.3.2. Rayleigh Modes

For P-SV waves, periodic solutions of the elastic equation of motion for the m th layer may be found by combining dilatational and rotational wave solutions

$$\begin{aligned}\Delta_m &= \frac{\partial u_x}{\partial z} + \frac{\partial u_z}{\partial x} = (\Delta'_m e^{-ikr_{\alpha m} z} + \Delta''_m e^{+ikr_{\alpha m} z}) e^{i(\omega t - kx)} \\ \delta_m &= \frac{1}{2} \left[\frac{\partial u_x}{\partial z} - \frac{\partial u_z}{\partial x} \right] = (\delta'_m e^{-ikr_{\beta m} z} + \delta''_m e^{+ikr_{\beta m} z}) e^{i(\omega t - kx)},\end{aligned}\quad (23)$$

where Δ'_m , Δ''_m , δ'_m , and δ''_m are constants. Given the sign conventions adopted, the term in Δ'_m represents a plane wave whose direction of propagation makes an angle $\cot^{-1} r_{\alpha m}$ with the $+z$ direction when $r_{\alpha m}$ is real, and a wave propagating in the $+x$ direction with amplitude diminishing exponentially in the $+z$ direction when $r_{\alpha m}$ is imaginary. Similarly, the term in Δ''_m represents a plane wave making the same angle with the direction $-z$ when $r_{\alpha m}$ is real and a wave propagating in the $+x$ direction with amplitude increasing in the $+z$ direction when $r_{\alpha m}$ is imaginary (e.g., see Fig. 2). The same considerations can be applied to the terms in δ'_m and δ''_m , substituting $r_{\alpha m}$ with $r_{\beta m}$. Dropping the term $\exp[i(\omega t - kx)]$, the displacements and associated stress components corresponding to the dilatation and rotation, given by Eq. (23), can be written as

$$u_x = -\frac{\alpha_m^2}{\omega^2} \left(\frac{\partial \Delta_m}{\partial x} \right) - 2\frac{\beta_m^2}{\omega^2} \left(\frac{\partial \delta_m}{\partial z} \right) \quad (24)$$

$$u_z = -\frac{\alpha_m^2}{\omega^2} \left(\frac{\partial \Delta_m}{\partial z} \right) + 2\frac{\beta_m^2}{\omega^2} \left(\frac{\partial \delta_m}{\partial x} \right) \quad (25)$$

$$\sigma_{zz} = \rho_m \left\{ \alpha_m^2 \Delta_m + 2\beta_m^2 \left[\frac{\alpha_m^2}{\omega^2} \left(\frac{\partial^2 \Delta_m}{\partial x^2} \right) + 2\frac{\beta_m^2}{\omega^2} \left(\frac{\partial^2 \delta_m}{\partial z^2} \right) \right] \right\} \quad (26)$$

$$\sigma_{zx} = 2\beta_m^2 \rho_m \left\{ -\frac{\alpha_m^2}{\omega^2} \left(\frac{\partial^2 \Delta_m}{\partial x \partial z} \right) + \frac{\beta_m^2}{\omega^2} \left[\left(\frac{\partial^2 \delta_m}{\partial x^2} \right) - \left(\frac{\partial^2 \delta_m}{\partial z^2} \right) \right] \right\}. \quad (27)$$

For Rayleigh waves the boundary conditions that must be satisfied at any interface are the continuity of the displacement and stress components given in Eqs. (24–27).

As we did for Love modes, iterating over the interfaces we can build up the dispersion function, whose roots are the eigenvalues associated with the Rayleigh wave modes (P-SV waves). This is the procedure at the base of the modern and efficient methods for the computation of multimodal dispersion in anelastic media (e.g., Schwab and Knopoff, 1972; Schwab *et al.*, 1984; Panza, 1985).

2.3.3. Modes Radiated by Point Sources in Anelastic Media

The source is introduced in the medium representing the fault, which is supposed to be planar, as a discontinuity in the displacement and shear stress fields, with respect to the fault plane. On the contrary, normal stresses are supposed to be continuous across the fault plane. Maruyama (1963) and Burridge and Knopoff (1964) demonstrated with the representation theorem the rigorous equivalence of the effects between a faulted medium with a discontinuity in the displacements and shear stress fields, and an unfaulted medium where proper body forces are applied.

Following the procedure proposed by Kausel and Schwab (1973), we assume that periods and wavelengths which we are interested in are large compared with the rise time and the dimensions of the source. Therefore the source function, describing the discontinuity of the displacement across the fault, can be approximated with a step function in time and a point source in space. Furthermore, if the normal stress is continuous across the fault, then for the representation theorem the equivalent body force in an unfaulted medium is a double-couple with null total moment. With this assumption, the eigenvalues and eigenfunctions of the problem having been determined, we can write the expression of the displacement with varying time, i.e., the synthetic seismogram, for the three components of motion. The asymptotic expression of the Fourier transform (hereafter called FT) of the displacement $\mathbf{U} = (U_x, U_y, U_z)$, at a distance r from the source, can be written as $\mathbf{U} = \sum_{m=1}^{\infty} {}^m\mathbf{U}$, where m is the mode index and

$$\begin{aligned} {}^m U_x(r, z, \omega) &= \frac{e^{-i(3/4)\pi}}{\sqrt{2\pi}} \left[\chi_R(h_s, \varphi) S(\omega) \frac{\sqrt{k_R} e^{-ik_R r - \omega r C_{2R}}}{\sqrt{r}} \frac{\epsilon_0 u_x(z, \omega)}{2C_R v_{gR} I_{1R}} \right]_m \\ {}^m U_y(r, z, \omega) &= \frac{e^{-i(3/4)\pi}}{\sqrt{2\pi}} \left[\chi_L(h_s, \varphi) S(\omega) \frac{\sqrt{k_L} e^{-ik_L r - \omega r C_{2L}}}{\sqrt{r}} \frac{u_y(z, \omega)}{2C_L v_{gL} I_{1L}} \right]_m \\ {}^m U_z(r, z, \omega) &= {}^m U_x(r, z, \omega) e^{-i(\pi/2)} \epsilon_0^{-1}. \end{aligned} \quad (28)$$

The suffixes R and L refer to quantities associated with Rayleigh and Love modes, respectively.

In Eq. (28), $S(\omega) = |S(\omega)| \exp[i \arg(S(\omega))]$ is the FT of the source time function, while $\chi(h_s, \varphi)$ represents the azimuthal dependence of the excitation factor (Ben-Menhaem and Harkrider, 1964)

$$\begin{aligned} \chi_R(h_s, \varphi) &= d_0 + i(d_{1R} \sin \varphi + d_{2R} \cos \varphi) + d_{3R} \sin 2\varphi + d_{4R} \cos 2\varphi \\ \chi_L(h_s, \varphi) &= i(d_{1L} \sin \varphi + d_{2L} \cos \varphi) + d_{3L} \sin 2\varphi + d_{4L} \cos 2\varphi \end{aligned} \quad (29)$$

with

$$\begin{aligned}
 d_0 &= \frac{1}{2} B(h_s) \sin \lambda \sin 2\delta \\
 d_{1R} &= -C(h_s) \sin \lambda \cos 2\delta \\
 d_{2R} &= -C(h_s) \cos \lambda \cos \delta \\
 d_{3R} &= A(h_s) \cos \lambda \sin \delta \\
 d_{4R} &= -\frac{1}{2} A(h_s) \sin \lambda \sin 2\delta \\
 d_{1L} &= G(h_s) \cos \lambda \sin \delta \\
 d_{2L} &= -G(h_s) \sin \lambda \cos 2\delta \\
 d_{3L} &= \frac{1}{2} V(h_s) \sin \lambda \sin 2\delta \\
 d_{4L} &= V(h_s) \cos \lambda \sin \delta,
 \end{aligned} \tag{30}$$

where φ is the angle between the strike of the fault and the direction obtained connecting the epicenter with the station, measured anticlockwise; h_s is the focal depth; δ is the dip angle; and λ is the rake angle (see Fig. 3). The functions of h_s that appear in (30) depend on the values assumed by the eigenfunctions at the

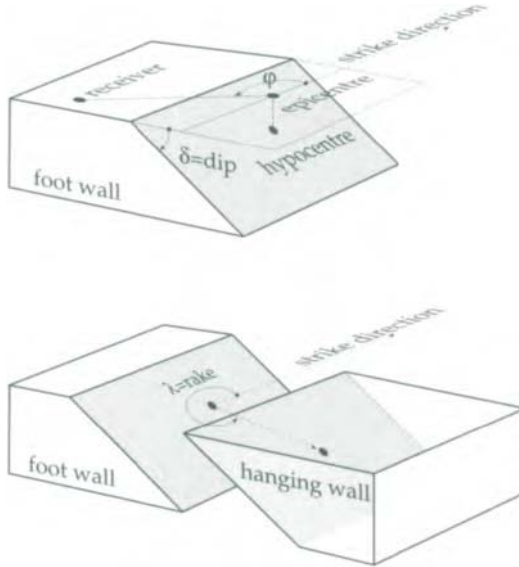


FIG. 3. Angle conventions used for the source system.

hypocenter

$$\begin{aligned}
 A(h_s) &= -\frac{u_x^*(h_s)}{u_z(0)} \\
 B(h_s) &= -\left(3 - 4\frac{\beta^2(h_s)}{\alpha^2(h_s)}\right)\frac{u_x^*(h_s)}{u_z(0)} - \frac{2}{\rho(h_s)\alpha^2(h_s)}\frac{\sigma_{zz}^*(h_s)}{\dot{u}_z(0)/c} \\
 C(h_s) &= -\frac{1}{\mu(h_s)}\frac{\sigma_{zx}(h_s)}{\dot{u}_z(0)/c} \\
 G(h_s) &= -\frac{1}{\mu(h_s)}\frac{\sigma_{zy}^*(h_s)}{\dot{u}_y(0)/c} \\
 V(h_s) &= \frac{\dot{u}_y(h_s)}{\dot{u}_y(0)} = \frac{u_y(h_s)}{u_y(0)},
 \end{aligned} \tag{31}$$

where the asterisk * indicates the imaginary part of a complex quantity, i.e., u_x^* , σ_{zz}^* , and σ_{zy}^* are real quantities.

The quantity I_1 in (28) are the *energy integrals* defined as

$$\begin{aligned}
 I_{1L} &= \int_0^\infty \rho(z)(u_y(z)/u_y(0))^2 dz \\
 I_{1R} &= \int_0^\infty \rho(z)[y_1^2(z) + y_3^2(z)] dz,
 \end{aligned} \tag{32}$$

where

$$\begin{aligned}
 y_1 &= \frac{u_z(z)}{u_z(0)} \\
 y_3 &= -i\frac{u_x(z)}{u_z(0)} = \frac{u_x^*(z)}{u_z(0)}.
 \end{aligned} \tag{33}$$

In Eq. (28), v_g is the group velocity that can be calculated analytically from the phase velocity

$$v_g = \frac{c}{1 - (\omega/c)(\partial c/\partial \omega)}, \tag{34}$$

while C_2 indicates the phase attenuation and expresses the effect due to anelasticity. C_2 can be calculated analytically using variational techniques (e.g., Takeuchi and Saito, 1972; Aki and Richards, 1980).

For Love modes one has (Florsch *et al.*, 1991)

$$C_{2L} = \frac{\int_0^\infty \mu B_1 B_2 \left[\frac{1}{\mu^2} \left(\frac{\sigma_{zy}^*}{\dot{u}_y(0)/c} \right)^2 + \left(\frac{u_y}{u_y(0)} \right)^2 \right] dz}{c \int_0^\infty \mu \left(\frac{u_y}{u_y(0)} \right)^2 dz}, \tag{35}$$

where c is the phase velocity in the perfectly elastic case, while B_1 and B_2 are, respectively, the S-wave velocity and the S-wave phase attenuation that are related to the complex body-wave velocity (Schwab and Knopoff, 1972)

$$\frac{1}{\beta} = \frac{1}{\beta_1 + i\beta_2} = \frac{1}{B_1} - iB_2. \quad (36)$$

For Rayleigh modes one has (Panza, 1985)

$$C_{2R} = \frac{Im(I_{4R})}{2\omega k I_{3R}}, \quad (37)$$

where k is the wavenumber in the perfectly elastic case and the integrals I_{3R} and I_{4R} are defined as

$$I_{3R} = \int_0^\infty \left\{ \left[(\lambda + 2\mu) - \frac{\lambda^2}{(\lambda + 2\mu)} \right] y_3^2 - \frac{1}{k} \left[y_1 y_4 - \frac{\lambda}{(\lambda + 2\mu)} \right] y_2 y_3 \right\} dz \quad (38)$$

$$\begin{aligned} I_{4R} = \int_0^\infty \left\{ \delta(\lambda + 2\mu) \left[\frac{1}{(\lambda + 2\mu)^2} (y_2^2 - 2k y_2 y_3) \right. \right. \\ \left. \left. + k^2 \left(1 + \frac{\lambda^2}{(\lambda + 2\mu)^2} \right) y_3^2 \right] + \delta\mu \frac{y_4^2}{\mu^2} \right. \\ \left. + \delta\lambda \left[\frac{2k}{(\lambda + 2\mu)} (y_2 y_3 - k\lambda y_3^2) \right] \right\} dz, \end{aligned} \quad (39)$$

where

$$\begin{aligned} y_2 &= \frac{\sigma_{zz}(z)}{u_z(0)} = -\frac{k\sigma_{zz}^*(z)}{\dot{u}_z(0)/c} \\ y_4 &= -i \frac{\sigma_{zx}(z)}{u_z(0)} = \frac{k\sigma_{zx}(z)}{\dot{u}_z(0)/c} \end{aligned} \quad (40)$$

and y_1 and y_3 are defined in (33). The variational quantities in (39) are

$$\begin{aligned} \delta(\lambda + 2\mu) &= \rho(\alpha_1^2 - \alpha_2^2 - \bar{\alpha}^2) + i2\rho\alpha_1\alpha_2 \\ \delta\mu &= \rho(\beta_1^2 - \beta_2^2 - \bar{\beta}^2) + i2\rho\beta_1\beta_2 \\ \delta\lambda &= \rho \left[(\alpha_1^2 - \alpha_2^2 - \bar{\alpha}^2) - 2(\beta_1^2 - \beta_2^2 - \bar{\beta}^2) \right] (\alpha_1^2 - \alpha_2^2 - \bar{\alpha}^2) \\ &\quad + i2\rho(\alpha_1\alpha_2 - 2\beta_1\beta_2), \end{aligned} \quad (41)$$

where $\bar{\alpha}$ and $\bar{\beta}$ are the P-wave and S-wave velocities in the perfectly elastic case,

while for anelastic media one has (analogously to (36) for S-waves)

$$\frac{1}{\alpha} = \frac{1}{\alpha_1 + i\alpha_2} = \frac{1}{A_1} - iA_2, \quad (42)$$

where A_1 and A_2 are, respectively, the P-wave velocity and the P-wave phase attenuation.

The synthetic seismogram can be obtained with three significant digits using the FT of (28) as long as the condition $kr > 10$ is satisfied (Panza *et al.*, 1973), and a realistic kinematic model of a finite fault can easily be adopted (e.g., Panza and Suhadolc, 1987; Saraò *et al.*, 1998) in conjunction with the modal summation technique. The fault of finite length is modeled as a series of point sources on a defined grid, placed along the faultplane, with appropriate spacing. The seismogram is computed by summing the time series radiated by the single point-sources with the appropriate time-shifts that are defined by the rupture process. The resultant time series show the great influence that directivity and the distribution of energy release in time may have on the synthesized ground motion.

3. ALGORITHMS FOR Laterally HETEROGENEOUS MEDIA

Linear system (1) is composed of three partial differential equations, with parameters that are dependent on the spatial variables, for which it is not always possible to find an exact analytical solution. We can distinguish between two main classes of methods that can be used to solve the system of Eqs. (1), i.e., analytical and numerical methods. It is not easy to choose which method is the best: advantages and disadvantages are related to the final goal and usually a compromise is necessary. Technically speaking, the choice depends on the ratio between the wavelength of the seismic signal and the dimensions of the lateral heterogeneities. For instance, if one wants to study the response of a complex sedimentary basin, it can be worth using a numerical approach. On the other hand, analytical methods may be certainly preferred when dealing with models with dimensions several orders of magnitude larger than the representative wavelengths of the computed signal, because of limitations in the dimensions of the model that affect numerical techniques. To make use of the advantages of each method, analytical and numerical approaches can be combined in the so-called hybrid techniques. Typically the analytical solution is applied to the regional model characterizing the path from the source to the local area of interest, and the numerical solution is applied to model the local site conditions.

In Sections 3.1–3.5 we describe the methods summarized in the scheme of Fig. 4. (Methods based upon Alsop's approach are considered in Section 4.) For hybrid techniques, in the following we concentrate just on the approach based on the modal summation technique and a finite difference scheme. The so-called Boundary Integral Equations (BIE) share elements of both subdivisions.

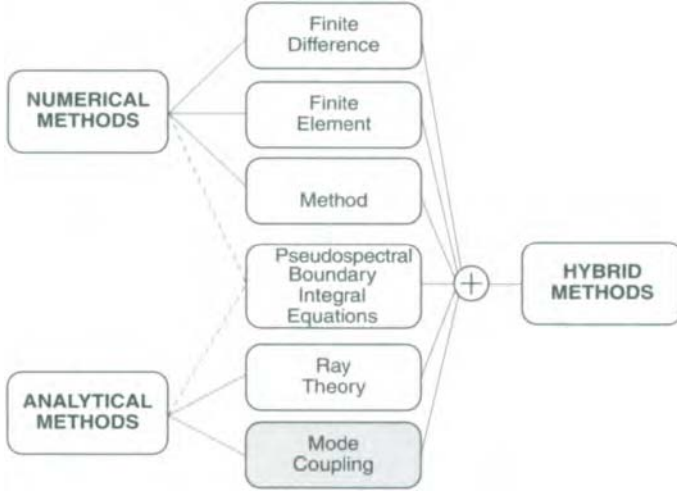


FIG. 4. Schematic diagram showing the techniques for the synthetic seismogram calculation in laterally heterogeneous media. The mode couplings techniques will be further expanded.

3.1. Numerical Methods

3.1.1. Finite Difference

The core of this technique is the substitution, in the wave equation, of the differential operators with finite difference operators defined by the Taylor expansion

$$u(x \pm h) = u(x) \pm \frac{du}{dx}h + \frac{1}{2} \frac{d^2u}{dx^2}(h)^2 \pm o(h^3). \quad (43)$$

In such a way the continuum is approximated by a regular grid of points.

For instance, we can define the operators of forward difference, D_+ , central difference, D_0 , and backward difference, D_- , that can substitute the initial first-order differential operator

$$Du(x) = \frac{du}{dx} \rightarrow \begin{cases} D_+u(x) = \frac{u(x+h) - u(x)}{h} \\ D_0u(x) = \frac{u(x+h) - u(x-h)}{2h} \\ D_-u(x) = \frac{u(x) - u(x-h)}{h} \end{cases} \quad (44)$$

Truncation errors have a dominant term proportional to h , h^2 , and h (first, second, and first order), respectively. With a proper linear combination of the operators defined in (44) we can find the expressions for substitution of the second derivative operator, and of the operator D , to higher-order accuracy by including additional

terms. We can extend the same considerations to temporal and spatial derivatives with respect to any spatial coordinate.

In the following general considerations we consider the example of the 1-D SH motion equation, assuming that the elastic parameters vary only along the x coordinate

$$\rho(x) \frac{\partial^2 u_y}{\partial t^2} = \frac{\partial}{\partial x} \left[\mu(x) \frac{\partial u_y}{\partial x} \right]. \quad (45)$$

To avoid the evaluation of partial derivatives with respect to μ , we can rewrite (45) using a velocity-stress formulation

$$\begin{aligned} \frac{\partial \dot{u}_y}{\partial t} &= \frac{1}{\rho(x)} \frac{\partial \sigma_{xy}}{\partial x} \\ \frac{\partial \sigma_{xy}}{\partial t} &= \mu(x) \frac{\partial \dot{u}_y}{\partial x}. \end{aligned} \quad (46)$$

Let us sample the plane (x, t) in the locations $(l\Delta t, m\Delta x)$, where l and m are integer numbers. To determine stress and velocity in the point $(m\Delta x)$ at a given instant of time $((l+1)\Delta t)$, we can approximate the system (46) by D_0 operator in space, i.e., using the values of σ_{xy} and $\dot{u}_y$ at three space-adjacent points $((m-1)\Delta x, m\Delta x, (m+1)\Delta x)$, and by D_+ operator in time

$$\begin{aligned} \frac{(\dot{u}_y)_m^{l+1} - (\dot{u}_y)_m^l}{\Delta t} &= \frac{1}{\rho_m} \frac{(\sigma_{xy})_{m+1}^l - (\sigma_{xy})_{m-1}^l}{2\Delta x} \\ \frac{(\sigma_{xy})_m^{l+1} - (\sigma_{xy})_m^l}{\Delta t} &= \mu_m \frac{(\dot{u}_y)_{m+1}^l - (\dot{u}_y)_{m-1}^l}{2\Delta x}. \end{aligned} \quad (47)$$

This system must be iterated in space and time (Aki and Richards, 1980), satisfying the proper boundary conditions. Because the truncation error, ε , grows exponentially with increasing time, the stability of the system, $1/\varepsilon$, tends to zero, making the scheme adopted in (47) always unstable. If a D_0 operator is adopted also for the time derivative, the resulting scheme is a conditionally stable one, i.e., the integration step in time must satisfy the relation

$$\Delta t < \frac{\Delta x}{\beta}, \quad (48)$$

where the boundary in the time step corresponds to the physical condition that information cannot propagate across the mesh faster than the velocity $\Delta x/\Delta t$. The stability condition (48) can be extended to a homogeneous medium with N spatial dimensions simply by dividing the right-hand side of (48) by $\sqrt{N}$. One of the most important topics for any practical application of a stable finite difference scheme, explicit in time, to a laterally varying medium, is to find the proper combination of Δx and Δt .

As for the stability criteria, the accuracy control of the adopted scheme, i.e., the rate of convergence of the numerical phase and group velocities to the correct ones, the so-called numerical dispersion, can be derived. For example, in the case of the 1-D central difference scheme for time and space which leads to condition (48), it can be demonstrated (e.g., Aki and Richards, 1980) that the accuracy of modeling the signal dispersion (grid dispersion) requires that at least 10 grid points are defined per wavelength

$$\Delta x < \frac{c}{10\omega} \quad (49)$$

Condition (49) significantly limits the spatial extension of the structural model. Given that both (48) and (49) must be simultaneously satisfied, the lowest phase velocity drives the choice of Δx , while the highest phase velocity determines the time sampling Δt , that, due to computational limitations, is generally chosen as close as possible to the highest allowed value. Therefore the numerical error introduced varies with time.

The application of finite difference schemes to some dynamical problems described by partial differential equations may result implicit in time approaches, where the solution is obtained by solving a linear set of equations. The characteristic of such solutions is that their stability does not have to satisfy a given condition (unconditionally stable), but often no gain in accuracy is provided unless a mixed scheme is adopted.

A possibility for improving the overall accuracy of an explicit finite difference scheme is to adopt the so-called staggered grids, where the fields, velocity and stress in the case of Eq. (46), are defined on separate grids shifted in space (Madariaga, 1976). Another approach leads to the adoption of higher-order operators (compared to (44)) for the spatial derivatives (e.g., Levander, 1988) that use more information, by means of the Taylor series, than that coming from the nearest neighbor grid points.

Among the advantages of the methods based on finite-differences schemes are the easy creation of computer codes and the possibility for treating media with spatially varying parameters compared with the signal wavelength. The drawback of the method is the requirement of huge computer CPU time and memory.

3.1.2. Hybrid Method Mode Summation–Finite Difference

Fäh *et al.* (1993a,b) developed a hybrid method that combines the modal summation technique, valid for laterally homogeneous anelastic media (see Sec. 2.3), with finite difference, and optimizes the advantages of both methods. Wave propagation is treated by means of the modal summation technique from the source to the vicinity of the local, heterogeneous anelastic structure that we may want to model in detail; the particular case in which the source is located beneath the

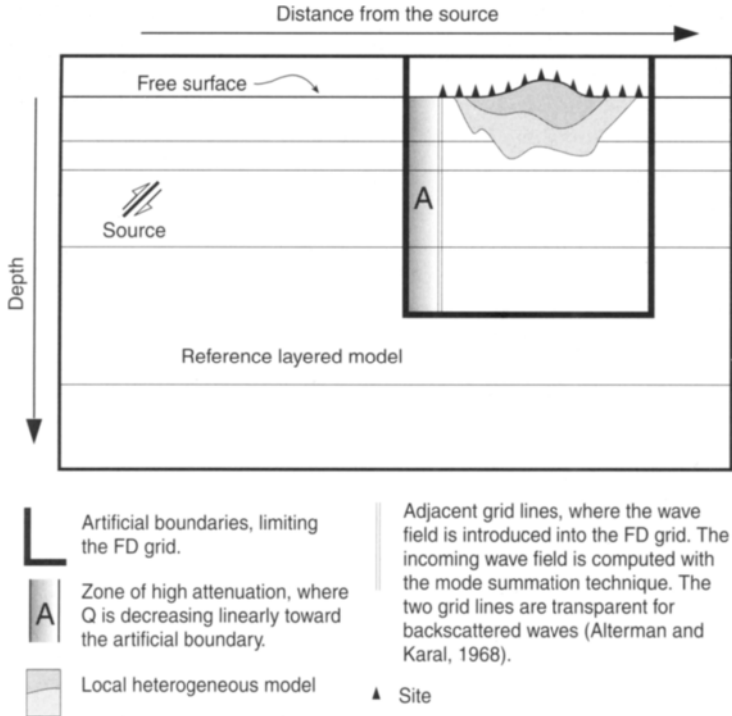


FIG. 5. Schematic diagram of the hybrid (modal summation and finite difference) method.

receiver can be studied with the classical propagator-matrix techniques (e.g., Haskell, 1962). A laterally homogeneous anelastic structural model is adopted, which represents the average crustal properties of the region. The generated wave-field is then introduced in the grid that defines the heterogeneous area, and it is propagated according to the finite-differences scheme (see Fig. 5). A more realistic modelling of wave propagation in the regional structure can be obtained using extension of the modal summation technique to laterally heterogeneous media described in Section 4.

With this approach, source, path, and site effects are all taken into account, and it is therefore possible to carry out a detailed study of the wavefield that propagates at large distances from the epicenter. This hybrid approach has been successfully applied, for the purpose of seismic microzoning, in several urban areas like Mexico City, Rome (Fäh and Panza, 1994), Benevento (Fäh and Suhadolc, 1995; Marrara and Suhadolc, 1998), Naples (Nunziata *et al.*, 1995), and Catania (Romanelli *et al.*, 1998a,b) in the framework of the IUGS-UNESCO-IGCP Project 414 (Panza *et al.*, 1999b).

3.1.3. Pseudospectral Method

The pseudospectral, or Fourier, method employs directly, like the finite-difference methods, the discrete form of Eq. (1): the computation domain is represented by a grid in space and an explicit scheme is adopted in the time domain. The wavefield at future time steps is calculated using the information of the current and previous time steps; if a second-order finite-difference integration scheme is used, one has

$$(\dot{u}_y)_m^{l+1} = (\dot{u}_y)_m^{l-1} + (\ddot{u}_y)_m^l \Delta t, \quad (50)$$

where the same notation of Eq. (47) is adopted. In scheme (50) the time step has to be chosen in order to keep the dispersion error to an acceptable level. A criterion similar to (48) has to be adopted for a 2-D scheme

$$\Delta t < 0.2 \frac{\Delta x}{v_{max}}. \quad (51)$$

The spatial derivatives that appear in Eq. (1) are analytically evaluated in the wavenumber domain, after FT, by means of orthogonal functions (e.g., Chebyshev polynomials, Fourier series; the proper choice depends on the periodicity of the problem). For example, the simplified Eq. (46) become

$$\begin{aligned} \frac{\partial \dot{\tilde{u}}_y}{\partial t} &= \frac{1}{\rho(x)} \frac{\partial \tilde{\sigma}_{xy}}{\partial x} \\ \frac{\partial \tilde{\sigma}_{xy}}{\partial t} &= \mu(x) \frac{\partial \dot{\tilde{u}}_y}{\partial x}, \end{aligned} \quad (52)$$

where the notation

$$\tilde{g}(x, k, t) = \int_{-\infty}^{\infty} g(x, y, t) e^{-iky} dy \quad (53)$$

is adopted, and k is the wavenumber for the y variable. For each value of k , Eq. (52) can be solved in the wavenumber domain. In the actual calculations, k has to be discretized and such an operation is correctly done only by assuming that the source-medium configuration is periodic along the y -axis. If the periodicity length is L , one has that $k = n\Delta k$ where $\Delta k = 2\pi/L$ and n is an integer. The sum over the wavenumbers can be truncated at $N\Delta k$, where N is defined as

$$N \geq 1.1 \frac{L}{\lambda_{min}} \quad (54)$$

and λ_{min} is the minimum wavelength associated to the model. Once the k components of the displacement are calculated, they can be converted to the physical

domain applying a discrete inverse FT

$$u_y(x, y_d, t) = \frac{1}{L} \sum_{k=-N\Delta k}^{N\Delta k} u_y(x, k, t) e^{iky_d}, \quad (55)$$

where y_d is the source-receiver distance.

Approximation of the spatial derivatives is infinitely accurate for periodic functions with a limited bandwidth and with spatial cutoff wavenumbers smaller than the cutoff wavenumbers of the grid, whose total dimension has to be sufficiently large to avoid space-aliasing problems (Kosloff *et al.*, 1984). Considerations valid for the choice of the grid dimension are similar to those made for the finite-difference techniques when the reflections from the domain boundaries have to be avoided. Use of Cartesian grids with insufficient number of points per wavelength can lead to the diffraction of spurious waves from the staircase approximation of the interfaces between the layers present in the model. This problem can be solved using curved grids that conform to the geometry of the actual interfaces; in such a way the local density of the grid points can be varied according to the velocity of each single layer (Nielsen *et al.*, 1995). Other numerical techniques that have been developed for optimization of the pseudospectral methods (e.g., inclusion of the anelasticity and nonlinearity effects), are revised by Fumura and Takenaka (1996).

Comparing the efficiency of the pseudospectral method with finite difference or finite element, it appears that for a given final accuracy fewer grid points are required per wavelength (about one-fourth), but more computations are necessary at each grid point (Fornberg, 1987; Kosloff *et al.*, 1984). In general we can state that the pseudospectral method is more efficient when implemented on fast computers and when not requiring a large amount of memory.

3.1.4. Finite Element

The finite element method can be applied to models where the geological irregularities are placed between two flat layered media, separated by vertical interfaces (Fig. 6).

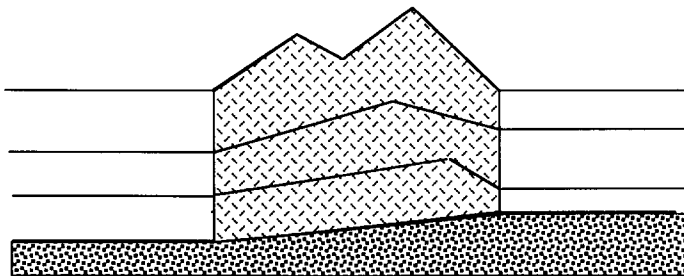


FIG. 6. Typical structural model for finite element method.

The classic procedure (Lysmer and Drake, 1972) implies a stationary analysis with finite elements of the irregular area. Special boundary conditions simulate the presence of the two layered halfspaces at each side. In the first step of the procedure the model is subdivided into a finite number of plane elements with proper values of the elastic parameters. Accuracy of the analysis depends on the detail of the mesh: as a general rule each element should not extend more than one-tenth of the wavelength of the S-wave associated with it. The elements are connected in a discrete number of nodal points. The basic assumptions are: (1) the displacements of the nodal points define the displacement field of the whole structure, and (2) all the external forces and the forces between the elements are transmitted through the nodal points.

As a consequence, the displacement field and the forces acting on the structure can be represented by two column vectors, each with dimensions equal to the number of nodal points for Love modes, and twice as big for Rayleigh modes.

For Love modes, the equations of motion can be written in the matrix form

$$\{M\}\{\ddot{u}_y\} + \{K\}\{u_y\} = \{Q\}, \quad (56)$$

where the matrices M and K are the mass and the force matrix, respectively, and contain information relative to (a) the elastic parameters of the model, (b) the excitation of one of the regular structures due to the seismic source, and (c) the boundary conditions. Equation (56) forms a system of second-order differential equations with constant coefficients, and can be solved with several numerical techniques.

The finite element technique is affected by the same kind of limitations described for finite difference: for complicated models it requires huge amounts of CPU time and memory. On the other hand, being a flexible method, it is a very good choice for seismic engineering studies such as the analysis of soil-structure interaction (Wolf and Song, 1996).

3.2. Boundary Integral Equations (BIE)

In this method the equations of motion are written in the integral form

$$\varphi(x) = f(x) + \int_a^x K(x, t)\varphi(t) dt, \quad (57)$$

(named Volterra equation of the second type) where $\varphi(x)$ is the unknown function and $K(x, t)$, called “kernel,” and $f(x)$ are known functions. An integral equation associates the unknown function not only with its values in the neighboring points but in a whole region. The boundary conditions are contained within the equation, through the values assumed by the kernel, rather than applied at the end of the solution procedure.

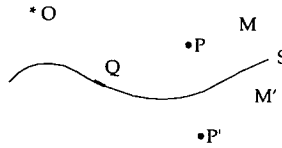


FIG. 7. Starting configuration of the BIE method.

To describe this approach in the field of seismology we follow Bouchon and Coutant (1994), and we consider SH-waves in the simple configuration shown in Fig. 7.

The source of the elastic perturbation is placed at point O of medium M , and it generates at point P a direct wavefield $V_0(P)$. The wavefield diffracted in medium M' from interface S , separating M and M' , can be described as a radiation generated by secondary sources distributed along the interface. Therefore the wavefield in P can be described as

$$V(P) = V_0(P) + \int_S \sigma(Q) G(P, Q) dQ, \quad (58)$$

where $\sigma(Q)$ is a density function of the source that represents the force of the wavefield diffracted from point Q , and $G(P, Q)$ is the wavefield generated in P by a unit source placed in Q (it is also known as the *Green function*).

Analogously, the diffracted wavefield in P' is

$$V'(P') = \int_S \sigma'(Q) G'(P', Q) dQ, \quad (59)$$

where G' is the Green function of M' .

The next step in obtaining a numerical solution is the discretization of the surface integral, approximating the surface S with N elements of area ΔS_i , for which the source density functions are assumed constant. Supposing that P and P' are lying, at the same point Q , on the two sides of the interface, Eqs. (58) and (59) become

$$\begin{aligned} V(Q_j) &= V_0(Q_j) + \sum_{i=1}^N \sigma_i \int_{\Delta S_i} G(Q_j, Q) dQ \\ V'(Q_j) &= \sum_{i=1}^N \sigma'_i \int_{\Delta S_i} G'(Q_j, Q) dQ. \end{aligned} \quad (60)$$

The continuity condition across the interface of displacements $V(Q_j) = V'(Q_j)$, and of stresses $T(Q_j) = T'(Q_j)$, leads to a system of $2N$ equations with $2N$ unknowns represented by the source density functions. To solve the integrals of (60) we need the expression for the Green functions. Usually the discrete wavenumber method is adopted (Bouchon and Aki, 1977), supposing that the medium is periodic and avoiding the occurrence of mathematical and numerical singularities

often associated with pure BIE techniques. For instance, in the frequency domain the Green function, when considering SH-waves, can be written as (Bouchon and Aki, 1977)

$$G'(Q_j, Q) = \frac{1}{2i\rho\beta^2 L} \sum_{n=-M}^M \frac{\exp(-i\gamma_n|z_j - z_Q|) \exp(-ik_n|x_j - x_Q|)}{\gamma_n}, \quad (61)$$

where (x_j, z_j) and (x_Q, z_Q) are the coordinates of Q_j and Q , respectively, ρ is the density of the medium, β is the shear wave velocity, L is the length of the medium periodicity, and M is an integer big enough to guarantee the convergence of the series, and

$$\begin{aligned} k_n &= \frac{2\pi}{nL} \\ \gamma_n &= \left(\frac{\omega^2}{\beta^2} - k_n^2 \right), \text{Im}(\gamma_n) \leq 0. \end{aligned} \quad (62)$$

When surface S degenerates into a plane, the Green functions are those of a stratified medium and can be computed analytically using the formalism described in Sect. 2.3.

The BIE method has several advantages with respect to the so-called domain techniques (finite difference and finite element), since it requires the discretization of a surface rather than of a volume, but it is limited to relatively simpler models than those treatable by numerical techniques. Solution of the equation system (60) becomes heavy in terms of computational time when many irregular surfaces are present in the model. The BIE method has been successfully applied in seismology to the study of wave propagation in irregular media (Bouchon and Coutant, 1994), and its variants (e.g., Boundary Element Methods) are used in engineering analysis (Maier *et al.*, 1991).

3.3. Analytical Methods

Among the methods that attempt to solve equations of motion in flat laterally heterogeneous media with numerical techniques applied to analytical solutions, we can distinguish two main complementary classes: methods based on ray theory and methods based on mode coupling.

Ray methods are based on the principles of classic geometrical optics. The synthetic signal is built up as a superposition of rays, reflected and transmitted according to the Snell law. The modal approaches, that will be more extensively analyzed, share the idea that the unknown wavefields are built up as a superposition of the normal modes characteristic of the medium. The choice between the two physical representations of the wavefield depends upon the kind of data that one wants to model. It depends on whether one is interested in the dispersive features

of the complete signal or in the study of the arrival times of some early phases. The number of rays necessary to model the late arrivals in one seismogram becomes huge and difficult to handle. Furthermore, at long periods, ray theory can no longer be applied, being rigorously defined at infinite frequency, and problems arise for peculiar transition zones, known as caustics. On the other hand, the number of modes necessary to describe adequately the first arrivals in a seismogram could be too large to be efficiently handled. The duality between rays (P-SV, SH-waves) and modes (Rayleigh, Love) is evident also from the formal point of view: Marquering (1996) has shown that any of the two representations can be written as the FT of the other.

3.4. Ray Theory

Ray theory is based on a hypothesis (ansatz) of the form of the solution of the elastic equations of motion (Babich, 1956)

$$\mathbf{u}(\mathbf{x}, \omega) = \mathbf{A}(\mathbf{x}, \mathbf{x}_0, \omega) \frac{e^{i\omega\theta(\mathbf{x}, \mathbf{x}_0)}}{\sqrt{J(\mathbf{x}, \mathbf{x}_0)}}, \quad (63)$$

where $\theta(\mathbf{x}, \mathbf{x}_0)$ is called phase, and represents the time necessary for the wave to travel from point $\mathbf{x}_0$ to point $\mathbf{x}$, and J is the geometrical decay of the wave-fronts.

Expression (63) does not contain any approximation since $\mathbf{A}$ is a generic function of $\mathbf{x}$ and ω . To obtain the approximation of the classic ray theory we have to expand the amplitude vector in a series of inverse powers of ω

$$\mathbf{A}(\mathbf{x}, \mathbf{x}_0, \omega) = S(\omega) \sum_{i=0}^{\infty} \mathbf{A}_i(\mathbf{x}, \mathbf{x}_0) \omega^{-i}, \quad (64)$$

where $S(\omega)$ is the FT of the source time function. If we consider only the first term in (64), then (63) becomes

$$\mathbf{u}(\mathbf{x}, \omega) = S(\omega) \mathbf{A}_0(\mathbf{x}, \mathbf{x}_0) \frac{e^{i\omega\theta(\mathbf{x}, \mathbf{x}_0)}}{\sqrt{J(\mathbf{x}, \mathbf{x}_0)}} \quad (65)$$

and represents an approximation of the solution of the wave equation valid only at high frequencies, when the higher terms can be neglected in (65). Furthermore, we assume that the terms $\mathbf{A}_0$, J , and θ in (65) are smoothly varying functions of the spatial coordinates. In such a way (65) becomes a form of the solution suitable for computation of a synthetic seismogram, since its FT can very easily be computed.

Introducing (65) in the equations of motion, we obtain an independent set of solutions that, for SH-waves, can be written as (Cerveny, 1987)

$$\begin{aligned} (\nabla\theta)^2 &= \frac{1}{\beta} \\ \mathbf{A}_0 \cdot (\nabla\theta) &= 0, \end{aligned} \tag{66}$$

also called the eikonal equation.

We define the surface $\theta(\mathbf{x}) = \text{const}$ as a wavefront. The slowness vector, $\mathbf{p} = \nabla\theta$, is normal to the wavefront and has modulus $1/\beta$: its trajectory describes a ray. The horizontal component of p is analogous to the phase velocity c , equal to $\sin\theta/\beta$ (see Fig. 2), for the mode with horizontal wavenumber $k = \omega/c$. Given an initial wavefront $t_0 = \theta(\mathbf{x}, \mathbf{x}_0)$, the rays and the following wavefronts can be computed using (66) with so-called *ray tracing*. As in geometrical optics, an alternative to the above mentioned approach, based on Huygens principle, is represented by a variational formulation corresponding to the Fermat principle: the ray corresponds to the trajectory between two given points for which the travel time is minimum.

Expression (65) can become unstable or singular under certain conditions, for instance, in the vicinity of a caustic, where ray theory predicts an infinite amplitude. Furthermore, classic ray theory is extremely sensitive to small local perturbations of the velocity field, because of the crucial assumption of infinite frequency in (65). The so-called spectral methods furnish a partial solution to these problems, keeping intact the physical meaning of ray theory. In a spectral method, the wavefield is not computed using (65) directly, but rather by a sum of ray beams having the form of (65). Among the spectral methods, the most popular is the WKBJ method (acronym for G. Wentzel, H. Kramers, L. Brillouin, and H. Jeffreys), where the source is represented as a sum of Snell waves, each one propagating independently from the other ones. The seismogram is then calculated summing all the propagated waves (Chapman, 1978).

Recently, advances in ray theory have been obtained applying the ray perturbation theory. In this way the techniques known as paraxial rays and Gaussian beams have been developed (Farra and Madariaga, 1987; Madariaga, 1989). The ray perturbation theory is used for evaluation of ray amplitude and for solving iteratively ray tracing problems. The most important perturbations are those related to the initial and final values of the position and propagation velocity. Ray perturbation theory also computes the trajectories of paraxial rays that propagate in the neighborhood of a reference ray. The study of paraxial rays simplifies computation of geometrical spreading and facilitates better following of the rays crossing a curved interface.

In summary, the fundamental limitations of the techniques based on ray theory are connected with the dimensions of the heterogeneities that must be much

larger than the dominating wavelength of the considered waves. Advantages with respect to numerical techniques are that models whose lateral dimensions are several orders of magnitude larger than representative wavelengths of the computed signal can be considered. Furthermore, ray theory can easily separate the different phases that contribute to the wavefield, since one can follow, using an intuitive physical approach, the way energy associated with seismic waves propagates through the medium. With these considerations, one can understand the importance of ray theory for seismic tomography studies based on body wave arrivals, bearing in mind the difficulty of recognizing the phases in the synthesized seismogram (a feasible operation only when travel times are reliable).

3.5. Mode Coupling

Whenever the source-receiver configuration is like the one shown in Fig. 5, surface waves (fundamental and first few higher modes) represent the longest and strongest portion of a seismic signal generated from an earthquake. These waves constitute the dominant part of the seismogram and thus supply the data with the most favorable signal/noise ratio. Therefore analysis of surface waves is crucial for gaining knowledge of the elastic and anelastic properties of the areas crossed by the waves (Snieder, 1986; Nolet, 1990; Du *et al.*, 1998), and for seismic hazard studies, with engineering implications (see Sect. 5).

Surface waves cannot be modelled easily with methods based on ray theory, because of computational problems: it is not a theoretical limitation but a practical one. There is no doubt that the modal summation is the most suitable technique for modeling the dominant part of seismic ground motion. The key point of the technique is the description of the wavefield as a linear combination of given base functions: the normal modes characteristic of the medium. In the case of the Earth, the modal summation technique is an exact method, since for a finite body the normal modes form a complete set. If we approximate the Earth with a flat layered halfspace, the completeness of normal modes is no longer satisfied, since they are associated only with the discrete part of the wavefield spectrum. Nevertheless this limitation can be overcome or controlled using several procedures described in Sects. 3.5.1–3.5.3 and 4.

Extension of the modal summation technique, described in Section 2.3, to laterally heterogeneous media can be performed following different procedures. The choice of the most suitable procedure must take into account the geometry and physical properties of the medium.

In the following, the term “intracoupling” refers to the coupling of a mode with itself, while “intercoupling” indicates the coupling of a mode with another one (Snieder, 1986).

3.5.1. WKBJ Method

The main assumption of WKBJ method, widely used in seismology (Woodhouse, 1974), is that the lateral variations of the elastic parameters are *regular* (compared to the wavelength). Once this hypothesis is satisfied, we can assume that the energy carried by each mode in a given structure is neither reflected nor transmitted to other modes. In other words, modes are not coupled; each mode propagates with a wavenumber driven by the local structure. The amplitude is not changed, while phase perturbations are computed by averaging the whole source-receiver path, neglecting the horizontal position of the heterogeneities.

Let us assume that the solution of Eq. (11), associated with the m th mode, is ${}^m u_y^0$. Asymptotic expression of the perturbed mode at point x , due to regular lateral variations, can be written as

$${}^m u_y(x) = {}^m u_y^0(x) \exp[i({}^m \delta k)x], \quad (67)$$

where

$${}^m \delta k(x) = \int_0^\infty \left(\frac{\partial({}^m k)}{\partial \rho} \delta \rho + \frac{\partial({}^m k)}{\partial \alpha} \delta \alpha + \frac{\partial({}^m k)}{\partial \beta} \delta \beta \right) dz \quad (68)$$

and $\delta \rho$, $\delta \alpha$, and $\delta \beta$ are the perturbations of the elastic parameters, at point x , with respect to the reference model.

The total wavefield computed at a distance r from the source can be written as the sum of the contributions of each single mode

$$u_y(r) = \sum_{m=1}^{\infty} {}^m u_y^0(r) \exp[i({}^m \overline{\delta k})x], \quad (69)$$

where

$${}^m \overline{\delta k} = \frac{1}{r} \int_0^r {}^m \delta k(x) dx. \quad (70)$$

Expanding the term $\exp[i({}^m \delta k)x]$, expression (69) can be seen as an infinite sum of multiple intracoupling terms.

The WKBJ method has been used for large-scale inversions (Nolet *et al.*, 1986), but in some cases it can be unrealistic, as true phase perturbations must depend upon the position of the heterogeneities along the path (Marquering, 1996). In spite of this limitation, including amplitude variations of the seismogram in the formalism facilitates performing an efficient fully analytical waveform inversion scheme (Du and Panza, 1999) at a regional scale.

3.5.2. The Born Approximation

Let us relate the perturbations of the elastic parameters of the laterally heterogeneous medium to the unperturbed medium as follows

$$\begin{cases} \rho(x, z) = \rho_0(z) + \varepsilon \delta \rho(x, z) \\ \alpha(x, z) = \alpha_0(z) + \varepsilon \delta \alpha(x, z) \\ \beta(x, z) = \beta_0(z) + \varepsilon \delta \beta(x, z) \end{cases} \quad (71)$$

The transmitted wavefield can then be written as follows

$$\mathbf{u} = \mathbf{u}_0 + \varepsilon \delta \mathbf{u}(\delta \rho, \delta \alpha, \delta \beta) + o(\varepsilon^2). \quad (72)$$

Perturbation of the wavefield in (72) can be written as a function of the so-called “scattering matrix” that describes the coupling between modes (Snieder, 1986). If we assume normal incidence and that the lateral variations exist only along the x direction, there are no conversions between Love and Rayleigh modes both in the transmitted and in the reflected wavefields.

If the perturbations are weak, i.e., if in (71) ε is small enough, then the contributions due to multiple scattering can be neglected. In the Born approximation only the mode coupling of the first order is considered: the total contribution is given by the unperturbed mode plus a term that describes the coupling between modes, due to lateral heterogeneity. If the intercouplings are neglected, the Born approximation coincides with the WKB method (Marquering, 1996). The main limit of the Born approximation is that it can correctly treat only small perturbations of the wavefield.

3.5.3. Invariant Imbedding Technique (IIT)

Kennett (1984) developed a representation of the mode coupling where the wave equation is expressed by a set of first-order coupled differential equations. The complete wavefield in a laterally heterogeneous medium is written as a properly weighted superposition of the modes of a reference model. This method has been extended to tridimensionally heterogeneous media by Bostock (1992). In these techniques, named IIT, the effects due to lateral heterogeneity along the source-receiver path are described by coupling mode coefficients, c_i in (73) and (74), that depend on the local structures.

The unperturbed displacement can be written as (Marquering and Snieder, 1995)

$${}^m u_y^0(r, z) = \sum_{i=1}^N c_i^0(r) \phi_i^0(z) \frac{e^{ik_i r}}{\sqrt{k r}}, \quad (73)$$

where $c_i^0(r)$ is the modal coefficient, constant for laterally homogeneous media, relative to the i th mode.

The modal coefficients, that are complex, can be defined for the transmitted and reflected wavefield from the heterogeneity $c_i^+(r)$, $c_i^-(r)$. If the heterogeneity is limited in space, the coefficients can be defined by transmission and reflection matrices (analogous to the scattering matrix) linking the incoming modes with the modes outgoing from the heterogeneity (transmitted and reflected).

The mode at the receiver is given by the sum of the unperturbed mode and the effects due to multiple couplings (forward and backward). If reflections and the intercouplings are neglected, the IIT method coincides with the WKB method. Neglecting the reflections and second-order couplings makes IIT coincident with the Born approximation (Marquering and Snieder, 1995).

The limitation of this method is the considerable computational effort necessary to solve the complete problem. To overcome this, several techniques have been developed, based on the IIT method. Among them we mention here the Matrix Exponent Approximation (MEA) (Marquering and Snieder, 1995), where the reflection matrix is neglected and the transmission coefficient can be written as

$$c_i^+(r) = c_i^0 + \sum_{m=1}^N M_{im} c_m^0 + \sum_{m=1}^N \sum_{k=1}^N M_{im} M_{mk} c_k^0 + \dots, \quad (74)$$

where the first term represents the unperturbed term, excited at the source and propagated to the receiver. The second term represents all the first-order couplings with the i th mode. The third term in (74) is the contribution to the i th mode of the k th mode coupled with the m th and represents the second-order coupling. The MEA method is a powerful tool for computation of the arrivals associated mainly with body waves, but it is computationally expensive whenever the investigated media are characterized by strong lateral discontinuities.

A technique quite similar to IIT has been developed by Odom (1986) and by Maupin (1988). In their formulation the base functions appearing in (73) are those relative to the local structure and therefore depend on the horizontal coordinate.

4. ANALYTICAL COMPUTATION OF THE MODE COUPLING COEFFICIENTS

In Section 3 we described several methods that can be used to extend the modal summation technique to laterally heterogeneous media. These techniques share the idea that the unknown wavefield generated by the lateral heterogeneities is written as a linear combination of base functions representing the normal modes (Love and Rayleigh) of the considered structure, therefore the problem reduces to the computation of the coefficients of this expansion.

If we consider a heterogeneous medium made of two layered quarterspaces in welded contact, the traditional method (Alsop, 1966; McGarr and Alsop, 1967) assumes that at a given frequency the set of eigenfunctions is complete for each

of the two quarterspaces. If this condition is satisfied, then the unknowns of the problem, i.e., the transmission and reflection coefficients, can be computed assuming the proper continuity conditions at the vertical interface. There are two problems with this approach: (1) at a given frequency the discrete spectrum of the eigenfunctions is not complete and the continuous spectrum should be included, and this requires the cumbersome computation of branch-line integrals; and (2) expansion in series of the base functions can be carried out for a finite number of terms, so that a control over the approximations introduced becomes necessary.

In a modal approach alternative to the original Alsop's method, the coupling coefficients for the modes transmitted and reflected at the vertical interface are computed, and the outgoing (inhomogeneous) surface waves are obtained as a superposition of homogeneous and inhomogeneous waves using Snell's law at each section (supposed infinite) of the vertical interface (Alsop *et al.*, 1974). The main objection to this approach is that the horizontal boundary conditions are no longer satisfied and therefore some diffracted waves, near the vertical interface, are not properly taken into account. Nevertheless it is possible to estimate the severity of the approximation introduced by checking the energy balance between the incoming and the outgoing wavefields.

In this Section, starting from the original formulation by Gregersen and Alsop (1974), we describe the analytical solution of the problem associated with SH waves. The results shown include the effect of topography (Romanelli *et al.*, 1996). For the P-SV problem, the analytical solution is given by Vaccari *et al.* (1989) for poissonian media, and extended to non-poissonian media by Romanelli *et al.* (1997).

The basic model treated in this Section consists of two layered quarterspaces in welded contact, but the formalism can be extended to any laterally heterogeneous structure using a series of 1-D layered structures in welded contact at the vertical interfaces. In Sect. 5 this approach will be used to model the wavefield in sedimentary basins.

4.1. Coupling Coefficients for Love Modes

Let us consider a mode of medium I, incident on the vertical interface between medium I and medium II as shown in Fig. 8. We consider normal incidence at the vertical interface, but the case of oblique incidence can be treated as well.

The wavefield associated with the incoming mode can be described by the stress-displacement vector defined as

$$\mathbf{A}_I = (u_{xI}, u_{yI}, u_{zI}, \sigma_{xxI}, \sigma_{yxI}, \sigma_{zxI}), \quad (75)$$

where $\mathbf{u}_I = (u_{xI}, u_{yI}, u_{zI})$ is the displacement vector and $\sigma_{i x I} (i = x, y, z)$ are the three components of the stress acting on the vertical interface defined by the equation $x = 0$.

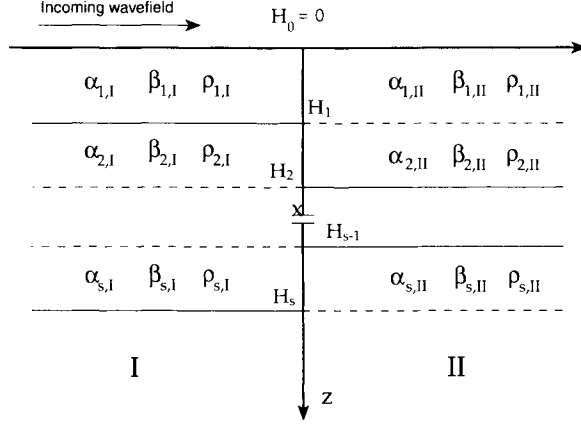


FIG. 8. 2-D model. Dashed lines represent the fictitious interfaces introduced to line up the layers of the two quarterspaces.

Similarly we can define the stress-displacement vector associated with a mode belonging to medium *II*

$$\mathbf{A}_{II} = (u_{xII}, u_{yII}, u_{zII}, \sigma_{xxII}, \sigma_{yxII}, \sigma_{zxII}). \quad (76)$$

The projection of vector (75) on vector (76) can be defined as follows (Herrera, 1964)

$$\begin{aligned} \langle \mathbf{A}_I, \mathbf{A}_{II} \rangle = & \frac{1}{2i} \int_0^\infty [u_{xI} \bar{\sigma}_{xxII} + u_{yI} \bar{\sigma}_{yxII} + u_{zI} \bar{\sigma}_{zxII} \\ & + -\bar{u}_{xII} \sigma_{xxI} - \bar{u}_{yII} \sigma_{yxI} - \bar{u}_{zII} \sigma_{zxI}] dz, \end{aligned} \quad (77)$$

where (here and in the following) the bar denotes the complex conjugation operator. This scalar product fully describes the orthogonality relation for the considered eigenfunction sets. Actually, if vectors $\mathbf{A}^{(n)}$ and $\mathbf{A}^{(m)}$ represent two modes (*n* and *m*) of the same medium at the same frequency, then if $n \neq m$ $\langle \mathbf{A}^{(n)}, \mathbf{A}^{(m)} \rangle = 0$, while if $n = m$ (Alsop, 1966)

$$\langle \mathbf{A}^{(m)}, \mathbf{A}^{(m)} \rangle = \pm \frac{1}{\omega} E, \quad (78)$$

where *E* is proportional to the energy flux carried by the incoming mode crossing the vertical interface. The sign in (78) is chosen according to the propagation direction: (+) for transmitted and (−) for reflected waves.

The stress-displacement vectors associated with transmitted and reflected modes, indicated as

$$\mathbf{A}_T = (u_{xT}, u_{yT}, u_{zT}, \sigma_{xxT}, \sigma_{yxT}, \sigma_{zxT}) \quad (79)$$

$$\mathbf{A}_R = (u_{xR}, u_{yR}, u_{zR}, \sigma_{xxR}, \sigma_{yxR}, \sigma_{zxR}) \quad (80)$$

can be regarded as a superposition of propagating modes of medium II and medium I, respectively. In each horizontal section the displacement, due to a Love mode, can be written as (see Eq. 14)

$$u_y(x, z, t) = [A_s \cos(kr_{\beta_s} z) + B_s \sin(kr_{\beta_s} z)]e^{i(\omega t - kx)}, \quad (81)$$

where A_s and B_s are the layer constants and

$$r_{\beta_s} = \begin{cases} \sqrt{\frac{c^2}{\beta_s^2} - 1} & \text{if } c > \beta_s \\ -i\sqrt{1 - \frac{c^2}{\beta_s^2}} & \text{if } c < \beta_s, \end{cases} \quad (82)$$

where c is the phase velocity and β_s is the S-wave velocity in section s . Therefore, in each horizontal section a Love mode can be considered as a superposition of SH-waves incident on the vertical interface with an angle

$$\theta_s = \cos^{-1} \left(\frac{\beta_s}{c} \right). \quad (83)$$

From (83) we can see that, according to the values of c , which for a given mode and a given frequency are the same for all the sections, and according to the S-wave velocity, which generally varies with varying sections, the resulting SH-waves in each section can be homogeneous (θ_s real) or inhomogeneous (θ_s imaginary). Now the transmission and reflection coefficients can be computed in each horizontal section using Snell's law, which is valid for an infinite surface of contact. For a homogeneous SH-wave with unitary amplitude the coefficients are (Aki and Richards, 1980)

$$\begin{aligned} b_s &= \frac{2\rho_{s,I}\beta_{s,I} \cos \theta_{s,I}}{\rho_{s,I}\beta_{s,I} \cos \theta_{s,I} + \rho_{s,II}\beta_{s,II} \cos \theta_{s,II}} \\ a_s &= \frac{\rho_{s,I}\beta_{s,I} \cos \theta_{s,I} - \rho_{s,II}\beta_{s,II} \cos \theta_{s,II}}{\rho_{s,I}\beta_{s,I} \cos \theta_{s,I} + \rho_{s,II}\beta_{s,II} \cos \theta_{s,II}}, \end{aligned} \quad (84)$$

where θ_I and θ_{II} are the angles of incidence and refraction, respectively. Iterating the procedure for each horizontal section we can define vectors (79) and (80). The procedure is approximated, since the horizontal boundary conditions are no longer satisfied and not all the diffracted waves are included in the computations. In Sect. 4.2.1 we shall describe a method that allows us to estimate the level of the approximation introduced.

The transmission coupling coefficient, i.e., the quantity that describes how the amplitude of mode m' in medium II is excited by the incoming mode m of medium

I is (Vaccari *et al.*, 1989)

$$\gamma_T^{(m,m')} = \frac{\langle \mathbf{A}_T^{(m)}, \mathbf{A}_{II}^{(m')} \rangle}{\langle \mathbf{A}_I^{(m)}, \mathbf{A}_I^{(m)} \rangle^{1/2} \langle \mathbf{A}_{II}^{(m')}, \mathbf{A}_{II}^{(m')} \rangle^{1/2}}. \quad (85)$$

If we prefer to consider an incoming mode with unit surface amplitude we need to define a normalization coefficient, and the following quantity must be used

$$\Gamma_T^{(m,m')} = \gamma_T^{(m,m')} \frac{\langle \mathbf{A}_I^{(m)}, \mathbf{A}_I^{(m)} \rangle^{1/2}}{\langle \mathbf{A}_{II}^{(m')}, \mathbf{A}_{II}^{(m')} \rangle^{1/2}} = \frac{\langle \mathbf{A}_T^{(m)}, \mathbf{A}_{II}^{(m')} \rangle}{\langle \mathbf{A}_{II}^{(m')}, \mathbf{A}_{II}^{(m')} \rangle}. \quad (86)$$

The reflection coupling coefficient can be defined as

$$\gamma_R^{(m,m')} = \frac{\langle \mathbf{A}_R^{(m)}, \mathbf{A}_I^{(m')} \rangle}{\langle \mathbf{A}_I^{(m)}, \mathbf{A}_I^{(m)} \rangle^{1/2} \langle \mathbf{A}_{II}^{(m')}, \mathbf{A}_{II}^{(m')} \rangle^{1/2}}, \quad (87)$$

while if we consider an incoming mode with unit surface amplitude

$$\Gamma_R^{(m,m')} = \gamma_R^{(m,m')} \frac{\langle \mathbf{A}_{II}^{(m')}, \mathbf{A}_{II}^{(m')} \rangle^{1/2}}{\langle \mathbf{A}_I^{(m)}, \mathbf{A}_I^{(m)} \rangle^{1/2}} = \frac{\langle \mathbf{A}_R^{(m)}, \mathbf{A}_I^{(m')} \rangle}{\langle \mathbf{A}_I^{(m)}, \mathbf{A}_I^{(m)} \rangle}. \quad (88)$$

From (88), and considering the orthogonality relations holding at a fixed frequency (Romanelli *et al.*, 1996), it can be shown that the only non-zero reflection coefficients are those relative to the coupling of homologous modes, i.e., the in-tracoupling coefficients.

For Love waves, vectors (75), (76), and (79) are

$$\mathbf{A}_I = (0, u_{yI}, 0, 0, \sigma_{yxI}, 0) \quad (89)$$

$$\mathbf{A}_{II} = (0, u_{yII}, 0, 0, \sigma_{yII}, 0) \quad (90)$$

$$\mathbf{A}_T = (0, u_{yT}, 0, 0, \sigma_{yT}, 0) \quad (91)$$

since in the case of normal incidence there is no conversion of SH-waves into P-SV waves. The scalar product (77) becomes

$$\langle \mathbf{A}_I, \mathbf{A}_{II} \rangle = \frac{1}{2i} \int_0^\infty [u_{yI} \bar{\sigma}_{yII} - \bar{u}_{yII} \sigma_{yI}] dz. \quad (92)$$

Remembering that

$$\sigma_{yx} = \mu \frac{du_y}{dx} = -ik\mu u_y \quad (93)$$

the two products in the denominator of (85) can be written as

$$\langle \mathbf{A}_I^{(m)}, \mathbf{A}_I^{(m)} \rangle = k_I^{(m)} \int_0^\infty \mu_I (u_{yI}^{(m)})^2 dz = \omega v_{gI}^{(m)} I_{II}^{(m)} \quad (94)$$

$$\langle \mathbf{A}_{II}^{(m')}, \mathbf{A}_{II}^{(m')} \rangle = k_{II}^{(m')} \int_0^\infty \mu_{II} (u_{yII}^{(m')})^2 dz = \omega v_{gII}^{(m')} I_{III}^{(m')}, \quad (95)$$

where I_1 and v_g are, respectively, the energy integral and the group velocity of the Love mode at angular frequency ω . These two spectral quantities, defined by Eqs. (32) and (34) in Sect. 2.3.1, can be quickly and accurately computed using the algorithms already available for the case of a layered halfspace.

The numerator of (85) is given by

$$\langle \mathbf{A}_T^{(m)}, \mathbf{A}_{II}^{(m')} \rangle = \frac{(k_T^{(m)} + k_{II}^{(m')})}{2} \int_0^\infty \mu_{II} (u_{yT}^{(m)} u_{yII}^{(m')}) dz. \quad (96)$$

If we introduce in the two quarterspaces some horizontal interfaces so that the layer thickness is the same at the two sides of the vertical interface (see Fig. 8), expression (96) can be written as

$$\sum_{s=0}^{S-1} \mu_{s,II} b_s^{(m)} \int_{H_s}^{H_{s+1}} (u_{yI}^{(m)} u_{yII}^{(m')}) dz + \mu_{S,II} b_S^{(m)} \int_{H_S}^\infty (u_{yI}^{(m)} u_{yII}^{(m')}) dz, \quad (97)$$

where coefficients b_s are defined in (84). From (97) we can see that the integrals, that must be computed in each horizontal section, are

$$\int_0^{d_s} (u_{yI}^{(m)} u_{yII}^{(m')}) dz \quad d_s = H_{s+1} - H_s \quad (98)$$

and using (81), for instance when $c > \beta_{sI}$ and $c > \beta_{sII}$ (98) becomes

$$\begin{aligned} & \int_0^{d_s} (\cos(k_I r_{\beta Is} z) \cos(k_{II} r_{\beta IIs} z)) dz + w_1 \int_0^{d_s} (\cos(k_I r_{\beta Is} z) \sin(k_{II} r_{\beta IIs} z)) dz \\ & + w_2 \int_0^{d_s} (\sin(k_I r_{\beta Is} z) \cos(k_{II} r_{\beta IIs} z)) dz + w_3 \int_0^{d_s} (\sin(k_I r_{\beta Is} z) \sin(k_{II} r_{\beta IIs} z)) dz, \end{aligned} \quad (99)$$

where w_i are constants, and the analytical solution is immediately available. When dealing with inhomogeneous waves on both sides of the vertical interface, expression (99) is still valid but the hyperbolic functions must be used instead of the corresponding trigonometric ones. When the integrals must be computed over the depth occupied by one of the terminating homogeneous halfspaces, their argument involves decaying exponential functions. For instance, if $\alpha_{sII} < \beta_{sII} < c$, the integrals assume the form

$$\int_0^{d_s} (e^{-ik_I r_{\beta Is} z} \cos(k_{II} r_{\beta IIs} z)) dz \text{ or } \int_0^{d_s} (e^{-ik_I r_{\beta Is} z} \sin(k_{II} r_{\beta IIs} z)) dz. \quad (100)$$

Finally, when the two terminating homogeneous halfspaces are in contact, the integral is

$$\int_0^\infty (e^{-ik_I r_{\beta Is} z} e^{-ik_{II} r_{\beta IIs} z}) dz. \quad (101)$$

4.1.1. Energy Conservation

The condition of welded contact between medium I and medium II implies that the energy flux (incident, transmitted, and reflected) across the vertical interface must be preserved

$$\langle \mathbf{A}_I, \mathbf{A}_I \rangle = \langle \mathbf{A}_R, \mathbf{A}_R \rangle + \langle \mathbf{A}_T, \mathbf{A}_T \rangle. \quad (102)$$

The continuity conditions at the vertical interface are, for displacement and stress components

$$\begin{aligned} \mathbf{u}_I + \mathbf{u}_R &= \mathbf{u}_T \\ \sigma_{xiI} + \sigma_{xiR} &= \sigma_{xiT} \quad (i = x, y, z) \end{aligned} \quad (103)$$

or, introducing the stress-displacement vector

$$\mathbf{A}_T = \mathbf{A}_R + \mathbf{A}_I. \quad (104)$$

Equation (104) can be written as

$$\langle \mathbf{A}_T, \mathbf{A}_T \rangle = \langle \mathbf{A}_R + \mathbf{A}_I, \mathbf{A}_R + \mathbf{A}_I \rangle \quad (105)$$

and using the orthogonality relations we obtain

$$\langle \mathbf{A}_T, \mathbf{A}_T \rangle = \langle \mathbf{A}_I, \mathbf{A}_I \rangle + 2Re\langle \mathbf{A}_I, \mathbf{A}_R \rangle - \langle \mathbf{A}_R, \mathbf{A}_R \rangle = \langle \mathbf{A}_I, \mathbf{A}_I \rangle - \langle \mathbf{A}_R, \mathbf{A}_R \rangle, \quad (106)$$

which is exactly Eq. (102).

The transmitted vector, for the whole set of outgoing modes, can be written as

$$\langle \mathbf{A}_T, \mathbf{A}_T \rangle = \sum_{m'=0}^{\infty} \langle \mathbf{A}_T^{(m')}, \mathbf{A}_T^{(m')} \rangle. \quad (107)$$

Defining column vector, $B_{m,m'}$, as the vector whose elements are the transmission coefficients for each single section, defined by relation (84) for the incoming mode m , we can write

$$\langle \mathbf{A}_T, \mathbf{A}_T \rangle = \sum_{m'=0}^{\infty} \sum_{m=0}^{\infty} B_{m,m'}^2 \langle \mathbf{A}_I^{(m)}, \mathbf{A}_I^{(m)} \rangle = \sum_{m'=0}^{\infty} \sum_{m=0}^{\infty} B_{m,m'}^2. \quad (108)$$

Likewise, for the reflected vector, from (106) we obtain

$$\sum_{m'=0}^{\infty} \sum_{m=0}^{\infty} B_{m,m'}^2 + \sum_{m'=0}^{\infty} \sum_{m=0}^{\infty} A_{m,m'}^2 = 1, \quad (109)$$

which corresponds to the condition of unitary scattering matrix as defined by Vaccari *et al.* (1989). If we consider a single incident mode m of unitary amplitude, expression (109) can be written as

$$\sum_{m'=0}^{\infty} (\gamma_T^{(m,m')})^2 + \sum_{m'=0}^{\infty} (\gamma_R^{m,m'})^2 = 1, \quad (110)$$

where γ refers to the coupling energy with transmitted and reflected modes. Equation (110) is the fundamental relation to estimate the approximation introduced by neglecting diffracted body waves.

4.1.2. Numerical Examples

To test the validity of the analytical algorithm, the transmission and reflection coupling coefficients are computed for a medium defined by the two layered lithospheric models shown in Fig. 9, in welded contact.

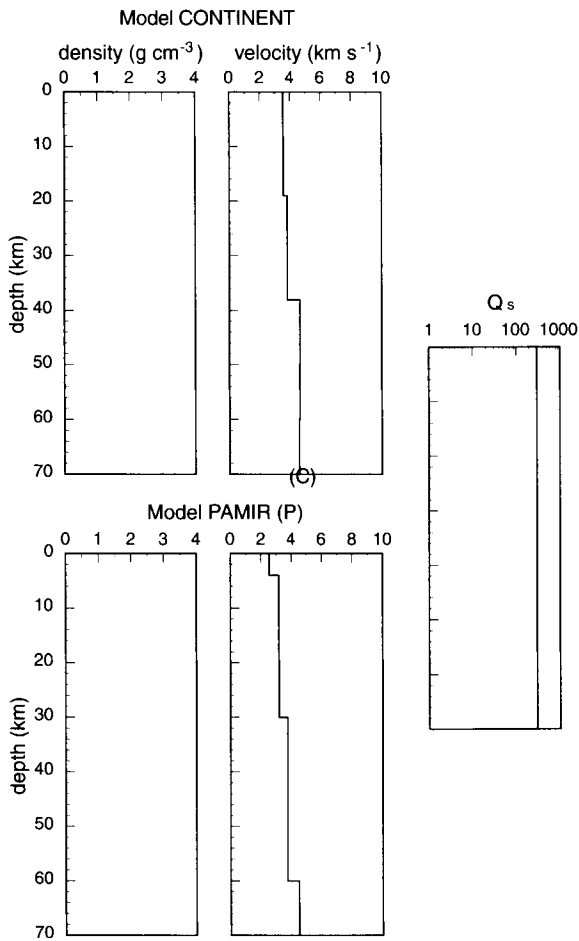


FIG. 9. Elastic and anelastic parameters of model C and model P. Thick lines represent S-wave velocities; Q_s is the quality factor common to both structures.

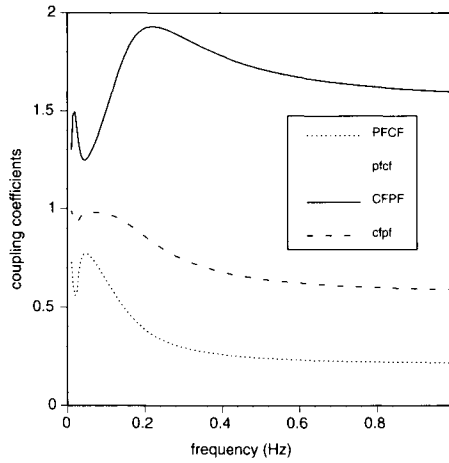


FIG. 10. Coupling coefficients for CFPF and PFCF. The dashed and the thin lines indicate the coefficients defined by Eq. (85).

For the sake of simplicity, in the following figures the models CONTINENT and PAMIR (Levshin, 1985) will be called model C and model P, while the fundamental mode and the higher modes are indicated, respectively, as F, 1, 2, etc. Therefore, the fundamental mode of model C is named CF, the first higher mode of model P is named P1, and so on. Each coupling coefficient is associated with a four-character acronym: the first two characters identify the incoming mode, the last two identify the outgoing mode. With this convention, the coupling between the fundamental mode of model C (incident) and the fundamental mode of model P (outgoing) is indicated with CFPF. The corresponding coupling energy is identified by the same acronym, written in lowercase letters.

In Fig. 10 the intracoupling coefficients (85) and (86) are shown for the incident fundamental mode, in both directions (CFPF and PFCF). The two curves corresponding to coefficient (85) overlap almost perfectly. Actually, since the coupling energy for two modes belonging to two different structures is the square of coefficient (85), Fig. 10 demonstrates that in this case the reversibility theorem for the scattering matrix (Vaccari *et al.*, 1989) is satisfied for the whole set of frequencies considered.

In Figs. 11 and 12 it is shown how the energy carried by one incident mode of model C is redistributed within several outgoing modes of model P. In Fig. 11 the coupling energies, i.e., the square of coefficient (85), are shown for the incident fundamental mode, while in Fig. 12 we consider the incidence of the first higher mode. In both figures, the curves indicated as SUM T represent the sum of the transmitted energy for five outgoing modes, while the curves marked as SUM include the reflected energy. From Figs. 11 and 12 we can see that the amount

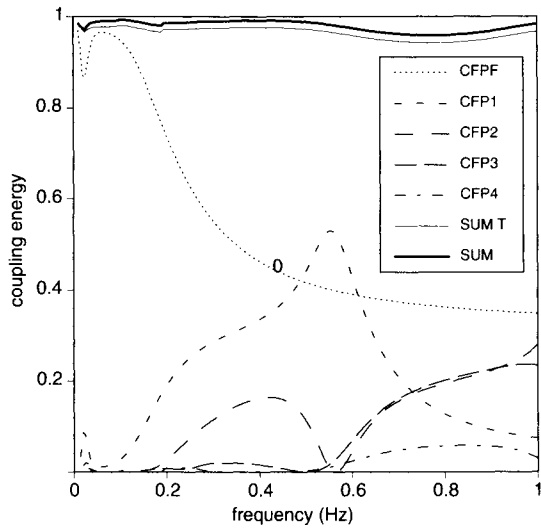


FIG. 11. Transmission of energy from incident fundamental mode of model C to first five modes of model P. SUM T and SUM are the curves describing the outgoing energy, without and with the inclusion of reflected energy.

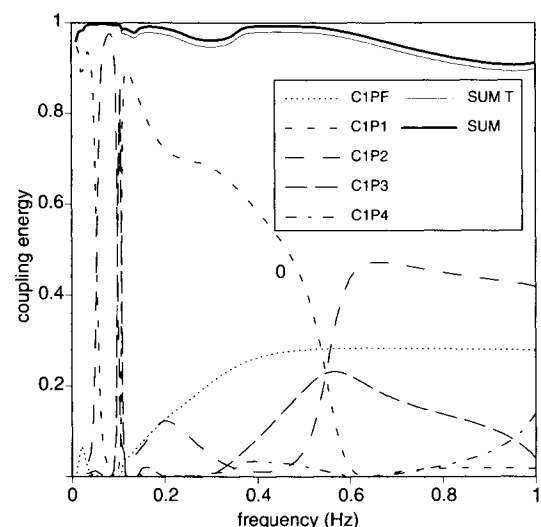


FIG. 12. Transmission of energy from incident first higher mode of model C to first five modes of model P. SUM T and SUM are the curves obtained summing the outgoing energy, without and with the inclusion of reflected energy.

of energy neglected corresponds, in the worst case, to 5 and 9% of the incident energy, respectively.

Numerical tests performed with models C and P suggest that, in order to obtain accuracy of three significant digits in the calculated signal (i.e., graphical accuracy), the maximum amount of scattered energy that can be neglected is of the order of 5%. Thus, the results shown in Fig. 12 indicate that when the first higher mode of model C is considered, the couplings with modes with order number higher than five have to be included in the computations if a graphically accurate seismogram is needed. This is an easy task to perform when only two models are considered, due to the high efficiency of the computations. In Sect. 4.3 the results, obtained considering more than 100 incoming modes each coupled with more than 100 outgoing modes, are shown. It has to be mentioned, however, that the resulting intracouplings and intercouplings are strongly dependent on the physical difference of the models adopted and on the frequency that is considered. The more similar the two models are, they will be felt by the wavetrain, i.e., for wavelengths greater than the dimension of the heterogeneity, nearer to 1 will be the computed intracoupling energy.

In Fig. 13 we show the coupling energy for the case of reflection, i.e., the square of the coefficients (Eq. 87), for the first five incident modes of model C. Only the intracoupling coefficients are shown, since for the reflected wavefield the intercouplings are all zero.

In order to assess the importance of topography in wave propagation we consider the model shown in Fig. 14. The two layered structures differ only for the thickness of the uppermost layer.

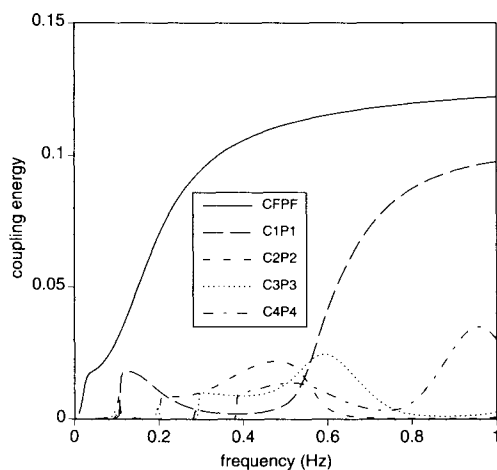


FIG. 13. Reflection of energy for the first five modes incident from model C.

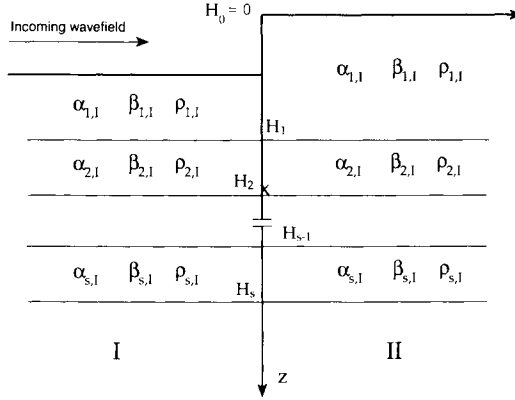


FIG. 14. 2-D model with a topographic step.

The variability of thickness ($H_0 - H_1$) of the uppermost layer of medium II defines a variable topographic step that is assumed positive when the thickness is larger in medium II, and negative in the opposite case. In Fig. 15 we show the coupling energy (for three different steps: 1, 5, and 10 km) of the fundamental mode of model C (medium I in Fig. 14) with the fundamental mode (FF;1, FF;5, and FF;10) and with the first higher mode (F1;1, F1;5, and F1;10) of medium II. The higher the step is, the larger the difference between the obtained coupling energy

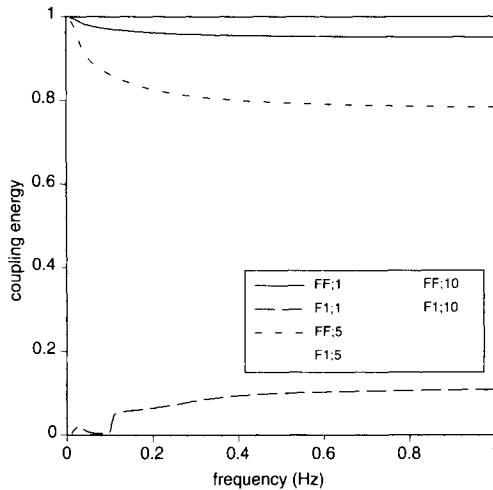


FIG. 15. Coupling energy for incident fundamental mode of medium I and first two outgoing modes of medium II (for the model see Fig. 14). The third parameter in the legend is the thickness of the topographic step, expressed in km.

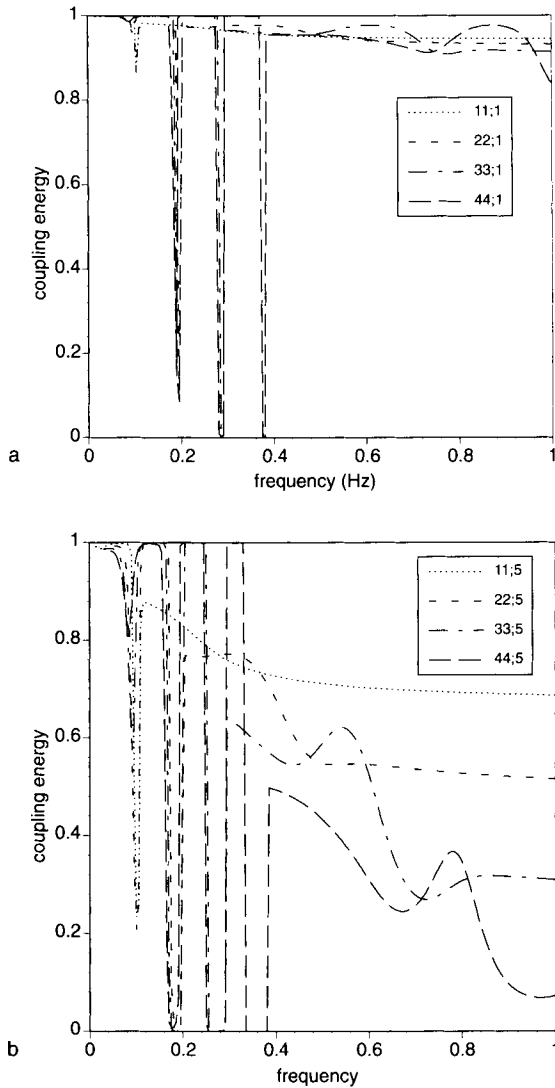


FIG. 16. Transmission of energy for the intracoupling of the first four higher modes: (a) topographic step of 1 km; (b) topographic step of 5 km.

and the values characterizing the absence of the step (1 for intracouplings and 0 for intercouplings).

In Fig. 16 we show the intracoupling energies for the first four higher modes and for topographic steps of 1 or 5 km. The minima in the coupling value become wider and deeper as the height of the topographic step increases.

4.2. Coupling Coefficient for Rayleigh Modes

For Rayleigh modes the formulation is similar to the one discussed in Sect. 4.1, and the basic definitions (75–80) and (85–88) are identical; the stress-displacement vectors in medium I and medium II and their scalar product can be written as

$$\mathbf{A}_I = (u_{xI}, 0, u_{zI}, \sigma_{xxI}, 0, \sigma_{zxI}) \quad (111)$$

$$\mathbf{A}_{II} = (u_{xII}, 0, u_{zII}, \sigma_{xxII}, 0, \sigma_{zxII}) \quad (112)$$

$$\langle \mathbf{A}_I, \mathbf{A}_{II} \rangle = \frac{1}{2i} \int_0^\infty [u_{xI} \bar{\sigma}_{xxII} + u_{zI} \bar{\sigma}_{zxII} - \bar{u}_{xII} \sigma_{xxI} - \bar{u}_{zII} \sigma_{zxI}] dz. \quad (113)$$

The problem of the analytical computation of transmission and reflection coupling coefficients has been solved by Vaccari *et al.* (1989) who computed the transmission and reflection coefficients at each section of the vertical interface (analogous to (84)) using Nafe (1957) expressions, which are valid only for Poissonian media ($\alpha/\beta = \sqrt{3}$). This assumption in several cases can be highly unrealistic, for instance, in sedimentary basins or geothermal regions (Stümpel *et al.*, 1984; Vaccari and Panza, 1993) where the ratio α/β can vary from 1.5 to approximately 5 (in the sediments) and from 1.7 to 1.9 (in the lower crust and upper mantle of geothermal areas).

The computation of coefficients can be extended to non-poissonian media by modifying in the scalar product (113) the equations of stresses. The component of the stress tensor involved is

$$\sigma_{xx} = \begin{cases} \mu \left(3 \frac{\partial u_x}{\partial x} + \frac{\partial u_z}{\partial z} \right) & \text{Poissonian media} \\ \lambda \left(\frac{\partial u_x}{\partial x} + \frac{\partial u_z}{\partial z} \right) + 2\mu \frac{\partial u_x}{\partial x} & \text{Non-Poissonian media} \end{cases} \quad (114a)$$

$$\quad (114b)$$

Therefore, by substituting (114b) into (113) we can compute the coefficients (85–88) for non-poissonian media (non-poissonian formulation).

4.2.1. Computation of Coupling Coefficients in Non-Poissonian Media

The transmission coupling coefficients have been computed for a 2-D structural model, M0, made up of the two lithospheric models C and P (see Figs. 8 and 9). Keeping α fixed, the β values have been modified in order to consider the two models M1 and M2, with ratios $\alpha/\beta = 1.5$ and 2.0, respectively. In the following, the fundamental mode is indicated by F, the poissonian formulations by P, and the non-poissonian formulations by NP. In the figures, each coupling coefficient is associated with an acronym of seven or eight characters: the first two refer to the incident mode, the next two to the outgoing mode, the fifth and sixth indicate the model, and the last one (or two) is connected with the formulation employed. As

an example, coupling between the fundamental mode of model C (incoming) with the fundamental mode of model P (outgoing) for $\alpha/\beta = 2.0$, using the poissonian formulation is identified by CFPFM2*P*. The corresponding coupling energy is indicated by the same acronym, written with lowercase letters.

In Fig. 17 we show the intracoupling energies and the intracoupling transmission coefficients, respectively, given by Eqs. (85) and (86) when $m = m'$, for the fundamental mode of models M0, M1, and M2, computed using formulations *P* and *NP*. The percentage difference in the values of Γ_T obtained with the two formulations is shown in Fig. 18. For model M0, which can be considered quasi-poissonian, the two results are in very good agreement; therefore M0 can be used as a reference model.

If we apply formulation *P* to model M2, both coupling energy and Γ_T are underestimated in the whole frequency range considered, because of the small value of the Lamé parameter λ adopted in the computations. This leads to low values for σ_{xx} and consequently for $\langle \mathbf{A}_T, \mathbf{A}_{II} \rangle$. On the contrary, if we apply formulation *P* to model M1, both coupling energy and Γ_T are overestimated. Furthermore, using the formulation *P* the computed coupling energy becomes larger than 1 for frequencies below 0.3 Hz, violating Vaccari *et al.*'s (1989) theorem of energy conservation. Therefore formulation *P* cannot be used when α/β differs noticeably from $\sqrt{3}$.

Figure 19 shows the reflection coupling energy and the reflection coupling coefficient, respectively, given by Eqs. (87) and (88), for the incident fundamental mode of models M1 and M2. The percentage difference of Γ_R for models M0, M1, and M2 is given in Fig. 20.

The higher the mode index is, the stronger the frequency dependence, but we can say that, in the considered frequency range, the percentage difference is generally smaller than the one computed for the fundamental mode. For instance, the maximum percentage difference for the first higher mode is about 2%. When considering high-frequency signals, the error introduced by using formulation *P* for non-poissonian media can be significant. This error increases when dealing with a sequence of 1-D models in welded contact, since at each vertical interface a value of Γ must be computed and the final result contains their product (see Sect. 4.3). Based on the computation of the coupling coefficients, Gregersen and Vaccari (1993) and Vaccari and Gregersen (1998) have given a simple physical explanation of the propagation and attenuation of Lg waves seen as a superposition of Love and Rayleigh modes (Knopoff *et al.*, 1973; Panza and Calcagnile, 1975).

4.3. Synthetic Seismograms in Laterally Heterogeneous Anelastic Media

Once the coupling coefficients have been computed for Love and Rayleigh modes, following the algorithm developed in Sects. 4.1 and 4.2, it is possible to

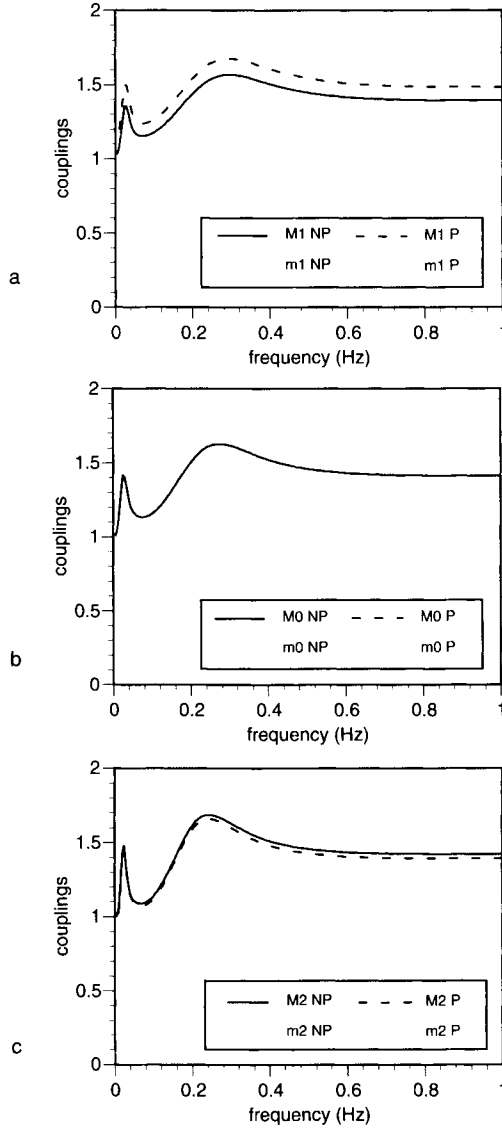


FIG. 17. Transmission coupling coefficients (M) and coupling energies (m) for incident fundamental mode of model C and outgoing fundamental mode of model P. NP and P indicate the non-poissonian and the poissonian formulations, respectively. Structural models: (a) Model 1; (b) Model 0; (c) Model 2.

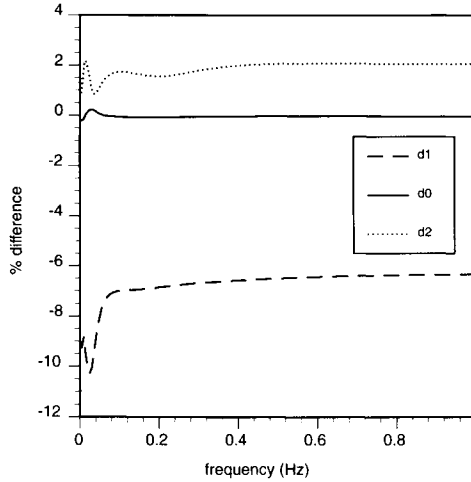


FIG. 18. Percentage difference between the transmission coupling coefficients computed with formulations *NP* and *P* for the fundamental mode. *d0*, *d1*, and *d2* indicate the percentage differences calculated using the structural models *M0*, *M1*, and *M2* respectively.

compute the synthetic seismograms for a laterally heterogeneous medium like the one shown in Fig. 8.

The expression that describes the displacement due to Love and Rayleigh wave modes propagating in a layered halfspace (28) has been generalized to laterally heterogeneous structures by Levshin (1985), who applied ray theory to surface waves.

Asymptotic expression of the FT of the transverse component of displacement, ${}^m U_y$, associated with the incoming Love mode m and transmitted into the mode m' , at a distance r from the source can be written as

$$\begin{aligned}
 {}^{m,m'} U_y(r, z, \omega) &= \frac{\exp(-i3\pi/4)}{\sqrt{8\pi}} \left[\frac{\chi_L(h_s, \varphi) S(\omega)}{c_L \sqrt{v_{gL} I_{1L}}} \right]_m \\
 &\times \left[\frac{\exp[-i(k_L d + k'_L d') - \omega(dC_{2L} + d'C'_{2L})]}{\sqrt{d/k_L + d'/k'_L}} \gamma_{\tau_L}^{(m,m')} \right]_{mm'} \\
 &\times \left[\frac{u_y(z, \omega)}{\sqrt{v_{gL} I_{1L}}} \right]_{m'},
 \end{aligned} \tag{115}$$

where the subscript L refers to Love modes, prime-indexed quantities are related to medium II (the medium with the receiver) and those without index refer to medium I (the medium with the source), and d and d' indicate the distances traveled in medium I and II , respectively. Expression (115) represents the contribution of

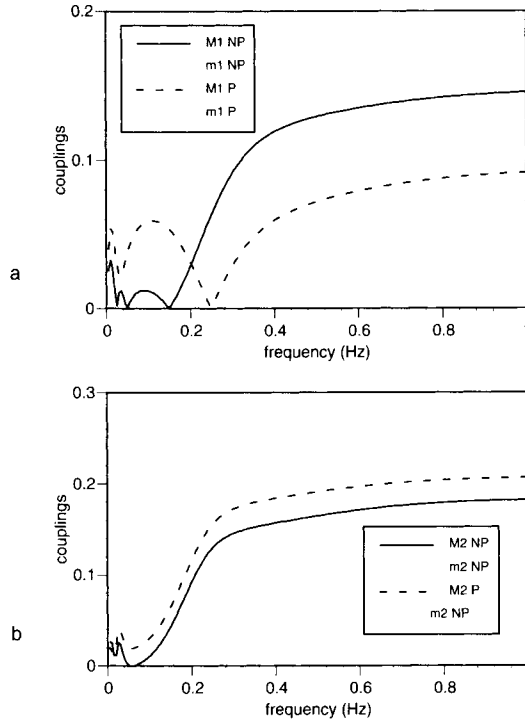


FIG. 19. Reflection coupling coefficients (M) and coupling energies (m) for incident fundamental mode of model C and fundamental mode of model P. NP and P indicate the non-poissonian and the poissonian formulations, respectively. Structural models: (a) M1; (b) M2.

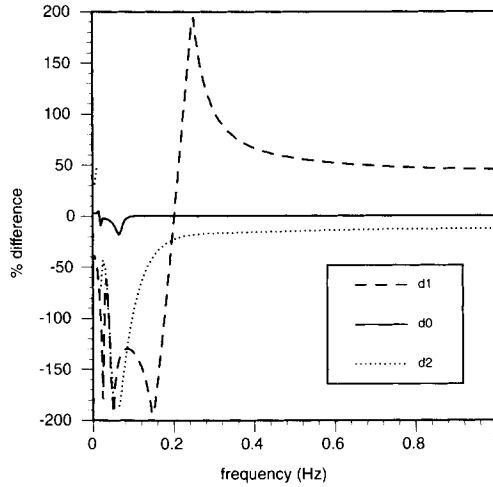


FIG. 20. Percentage difference between the reflection coupling coefficients computed with formulations NP and P for the fundamental mode. $d0$, $d1$, and $d2$ indicate the percentage differences calculated using the structural models M0, M1, and M2, respectively.

one single mode m generated by a point-source placed in medium I , transmitted across the vertical interface and recorded as mode m' in medium II at a distance $r = d + d'$. If medium I and medium II are equal, (115) reduces exactly to the second expression of (28), valid for a layered halfspace.

If we consider a model composed of N one-dimensional structures in welded contact, separated by vertical interfaces, (115) becomes

$$\begin{aligned}
 {}^{m,m'}U_y(r, z, \omega) &= \frac{\exp(-i3\pi/4)}{\sqrt{8\pi}} \left[\frac{\chi_L(h_s, \varphi)S(\omega)}{c_L \sqrt{v_{gL} I_{1L}}} \right]_m \\
 &\times \left[\frac{\exp[-i(\sum_{j=1}^N k_L^j d_j) - \omega(\sum_{j=1}^N d_j C_{2j})]}{\sqrt{\sum_{j=1}^N d_j / k_L^j}} \prod_{j=1}^{N-1} \gamma_{TL}^j \right] \\
 &\times \left[\frac{u_y(z, \omega)}{\sqrt{v_{gL} I_{1L}}} \right]_{m'}, \quad (116)
 \end{aligned}$$

where mode m is in the first structure and mode m' is in the last one.

The expressions analogous to (115) associated with the FT of the radial (U_x) and vertical (U_z) components are

$$\begin{aligned}
 {}^{m,m'}U_x(r, z, \omega) &= \frac{\exp(-3i\pi/4)}{\sqrt{8\pi}} \left[\frac{\chi_R(h_s, \varphi)S(\omega)}{c_R \sqrt{v_{gR} I_{1R}}} \right]_m \\
 &\times \left[\frac{\exp[-i(k_R d + k'_R d') - \omega(d C_{2R} + d' C'_{2R})]}{\sqrt{d/k_R + d'/k'_R}} \gamma_{TR}^{(m,m')} \right]_{mm'} \quad (117)
 \end{aligned}$$

$${}^{m,m'}U_z(r, z, \omega) = {}^{m,m'}U_x(r, z, \omega) \exp(-i\pi/2)(\epsilon_0 |_{m'})^{-1}, \quad (118)$$

where subscript R refers to Rayleigh modes. Using expressions (115–118) it is very easy to extend the existing, highly efficient mode summation computer codes (Panza, 1985; Florsch *et al.*, 1991) to laterally heterogeneous media.

In the following figures we show some examples of synthetic seismograms calculated for a laterally heterogeneous structural model that is assembled starting from models C and P, used in Sect. 4.2 (see Fig. 9). The source-receiver distance is 100 km and the vertical interface between the two media is placed right at the middle of the path. An instantaneous point-source is placed at the depth of 10 km, with a scalar seismic moment of 10^{13} Nm. The orientation of the double-couple of forces is defined as follows: strike-receiver angle = 60° , dip = 90° , rake = 180° . The cut-off frequency for the computations is 1 Hz.

In Fig. 21 the seismograms are shown for the three components of displacement, grouped for the four structural models: models C and P and 2-D models CP and PC. For each group there are four rows according to the number of incoming

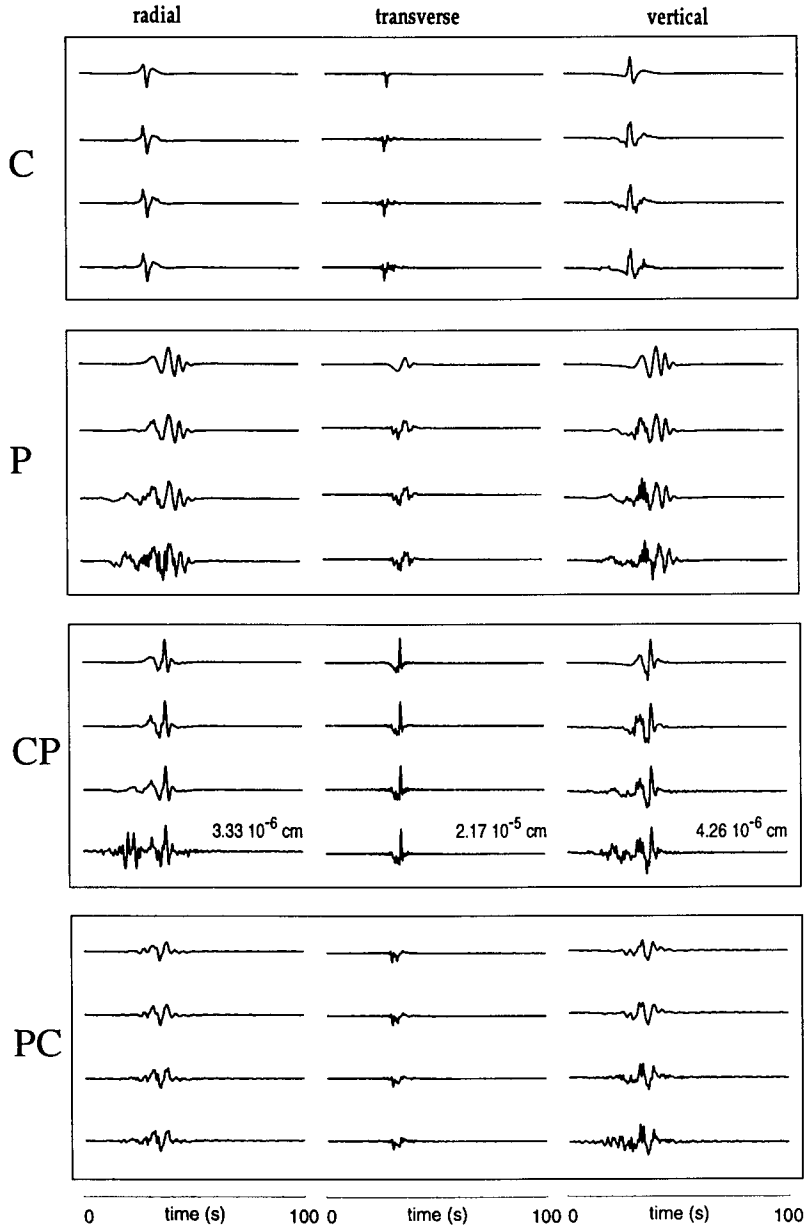


FIG. 21. Synthetic seismograms for the three components of displacement, grouped for the four structural models: models C and P and 2-D models CP and PC. For each group four rows are shown, according to the number of incoming modes: the first row is for the fundamental mode, the second row is for the first 5 incoming modes, the third row is for the first 10 modes, and the fourth row is for 110 incoming modes. For each component of motion the seismograms are normalized to the maximum amplitude associated with the signal computed for 2-D model CP summing 110 modes.

modes: the first row is for the fundamental mode, the second row is for the first 5 incoming modes, the third row is for the first 10 modes, and the fourth row is for 110 incoming modes. For each component of motion the seismograms are normalized to the maximum amplitude associated with the signal computed for 2-D model CP summing 110 modes.

Arrival times of the wavetrains propagating in the laterally heterogeneous structure are a kind of average of the arrival times characteristic of the two 1-D models. Peak amplitude of the signals computed for model CP is always larger than the peak value obtained in the laterally homogeneous media. Looking at the waveforms obtained for the laterally heterogeneous anelastic models CP and PC, it appears that the transverse component is controlled more by the model where the source is placed. For radial and vertical components, the model where the receiver is placed seems to have greater importance. A possible interpretation is that the ellipticity factor, ϵ_0 , could be more relevant than the radiation pattern, χ_R , for P-SV motion (see expressions (116–118)). In the general case, the relative position of the source and of the receiver with respect to the vertical interface can play a more fundamental role.

In Fig. 21, the difference between the signal shown in the last row of the CP-radial component of motion (and, to a minor extent, of the CP-vertical component) and the corresponding signals, obtained summing modes with lower order numbers, is bigger than in the other cases. This can be explained by the fact that, in the P-SV motion problem for the CP case, the intercoupling energy for the higher modes becomes significant, making the amplitude of the early phases, with higher frequency content, comparable to that of the later dominant arrivals associated with lower order modes (see Fig. 22).

The described methodology can be applied to improvement of the existing laterally variable models at a regional scale (Du *et al.*, 1998), as well as to study of the site response of local heterogeneous models (see Sect. 5.2.2).

5. DETERMINISTIC SEISMIC HAZARD ASSESSMENT: FROM SEISMIC ZONATION TO SITE RESPONSE ESTIMATION

Strong earthquakes such as the 1985 Michoacan and the 1995 Kobe have acted as catalysts for the use of zoning in seismic risk management. Politicians and administrators are more and more interested in rapid reconstruction according to criteria which reduce the probability of a repetition of disasters. In an anthropic area it is now technically possible to identify zones in which the heaviest damage can be predicted. A first-order zoning can be carried out at regional scale, based on the knowledge of the average properties of seismic sources and on structural models. Microzonations are possible as well, provided that detailed information about the source, path, and local site conditions are available.

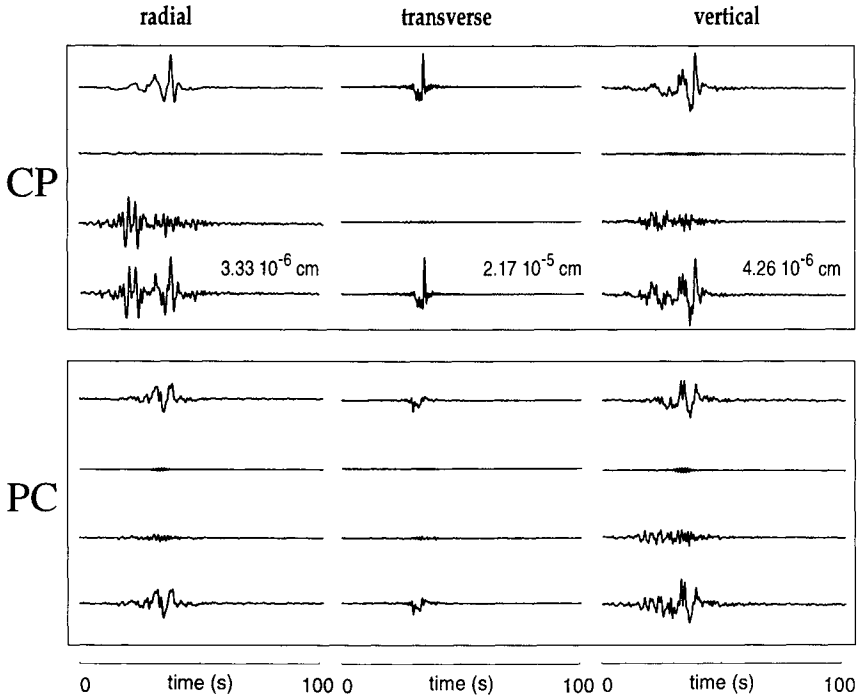


FIG. 22. Synthetic seismograms for the three components of displacement, grouped for the 2-D structural models CP and PC. For each group four rows are shown, according to the number of incoming modes and the considered couplings: first and last rows are for the first 10 incoming modes and 110 incoming modes, respectively (same as Fig. 21); second and third rows are for 10–110 incoming modes, excluding and including cross-couplings, respectively. For each component of motion the seismograms are normalized to the maximum amplitude associated with the signal computed for the 2-D model CP summing 110 modes.

A drastic change is required in the orientation of zoning that must be a predisaster activity performed to mitigate the effects of the next earthquake, using all available technologies. The events in Los Angeles (1994) and Kobe (1995) clearly show that we must be able to take preventive steps, extending, in a scientifically acceptable way, the obtained results to areas in which no direct experience has yet been gained. Seismic zoning can use scientific data banks, integrated in an expert system, by means of which it is possible not only to identify the safest and most suitable areas for urban development, but also to define the seismic input that is going to affect a given building. Examples of this capability, closely linked to the ability to calculate realistic synthetic seismograms, are given in Sects. 5.1 and 5.2.

5.1. Deterministic Seismic Zoning: Regional Scale

The procedure for deterministic seismic zoning developed by Costa *et al.* (1992, 1993) and subsequently widely applied (Orozova-Stanishkova *et al.*, 1996; Alvarez *et al.*, 1999; Aoudia *et al.*, 2000; Bus *et al.*, 2000; Markušić *et al.*, 2000; Radulian *et al.*, 2000; Živčić *et al.*, 2000) represents one of the new and most advanced approaches. It can be used also as a starting point for the development of an integrated approach that will combine the advantages of the probabilistic and deterministic methods, thus minimizing their respective drawbacks. This approach addresses some issues largely neglected in probabilistic hazard analysis, namely, how crustal properties affect attenuation: ground motion parameters are not derived from overly simplified attenuation functions, but rather from synthetic time histories.

Starting from the available information on the Earth's structure, seismic sources, and the level of seismicity of the investigated area, it is possible to estimate maximum ground acceleration, velocity, and displacement (AMAX, VMAX, and DMAX, respectively) or any other parameter relevant to seismic engineering, which can be extracted from the computed theoretical signals. This procedure allows us to obtain a realistic estimate of the seismic hazard in those areas for which scarce (or no) historical or instrumental information is available and to perform the relevant parametric analyses.

Synthetic seismograms can be constructed to model ground motion at sites of interest, using knowledge of the physical process of earthquake generation and wave propagation in realistic media. The signals are efficiently generated by the modal summation technique (see Sect. 2), so it becomes possible to perform detailed parametric analyses at reasonable costs. For instance, different source and structural models can be taken into account to create a wide range of possible scenarios from which to extract essential information for decision making.

In first-order zoning, average structural models are defined, representing the lithospheric properties at a regional scale. Synthetic seismograms are computed, taking into account the effects of lateral heterogeneities in a rough way: if the source-receiver path crosses one or more boundaries between adjacent structural models, the signal is computed assuming the model of the receiver as representative of the whole path. This is justified by the results shown in Fig. 21, where the signals obtained for the laterally heterogeneous medium look more similar to the signals computed in the receiver structural model than to those computed using the structural model containing the source.

The flowchart of the procedure is shown in Fig. 23. The first problem to tackle in the definition of seismic sources is the handling of seismicity data. Basically, what is needed is an evenly spaced distribution of the maximum magnitude over the territory; but the data available from earthquake catalogues are widely scattered.

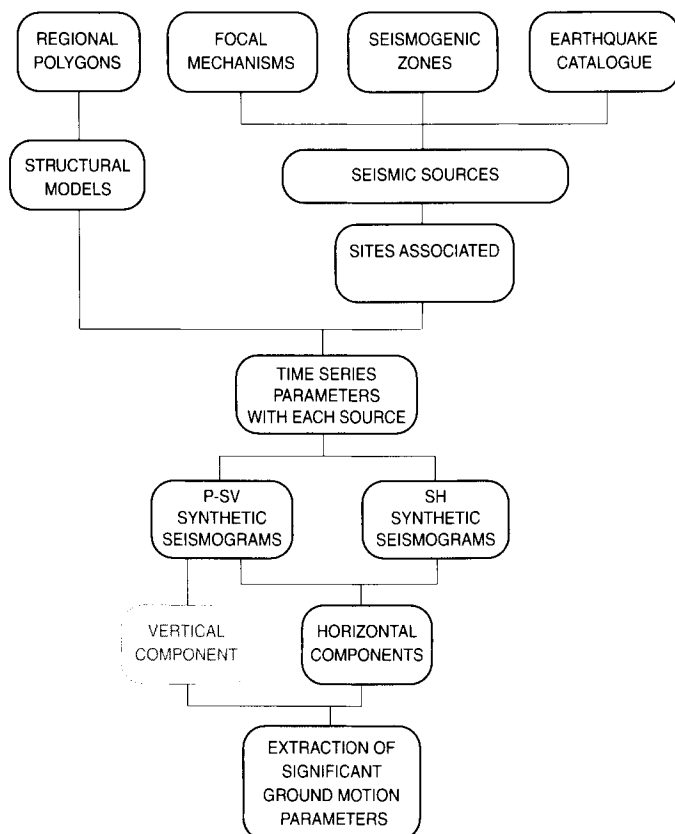


FIG. 23. Flowchart of the deterministic procedure for seismic hazard assessment at regional scale. The vertical component is routinely not used.

Furthermore, earthquake catalogues are both incomplete and affected by errors, so a smoothed distribution is preferable (Panza *et al.*, 1990).

The smoothing procedure is shown in Fig. 24. The punctual distribution of epicenters given in Fig. 24a is discretized into cells (Fig. 24b) and the maximum magnitude of the events pertinent to each cell is retained. In the case where the earthquake catalogue contains different estimates of magnitude (e.g., magnitude computed from body waves, from surface waves, or from macroseismic intensity), the maximum between them is considered. It is then convenient to represent the data graphically, and symbols are associated with magnitude ranges (Fig. 24c). In most cases, the smoothing obtained by considering just the discretized cells is not enough. A centered smoothing window is then considered so that earthquake magnitudes are analyzed not only in the central cell but also in the neighboring ones. The idea of a constant magnitude within each seismogenic area (choosing

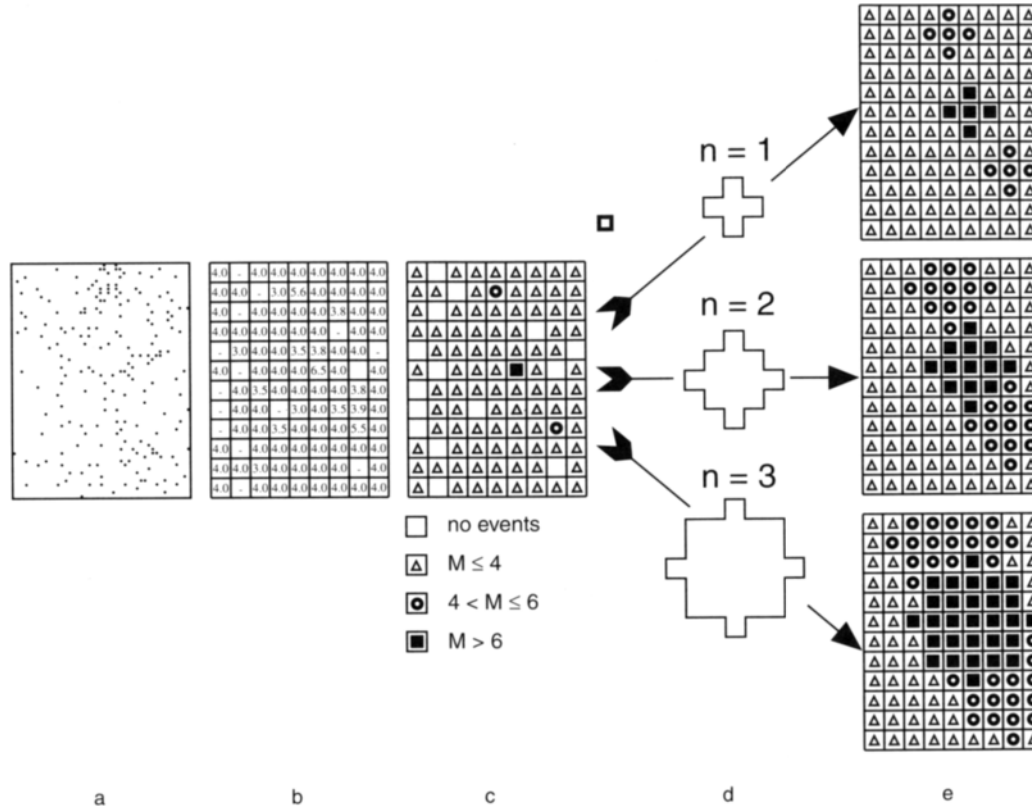


FIG. 24. Discretization and smoothing of seismicity. (a) Distribution of epicenters; (b) definition of cells and choice of the maximum magnitude; (c) graphic representation; (d) smoothing windows of radius $n = 1$, $n = 2$, $n = 3$; (e) smoothed distribution of magnitude.

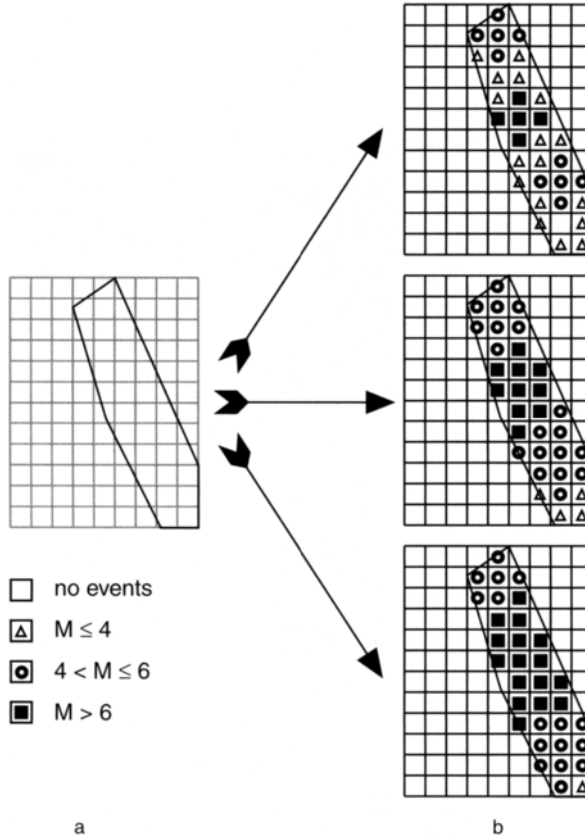


FIG. 25. (a) Seismogenic zone and (b) its intersection with the smoothed data shown in Fig. 24(e).

the maximum available value) has been shown to be a poor choice, since for the larger seismogenic areas it leads to an overestimation of the seismicity. Three possible smoothing windows are shown in Fig. 24d. Their radius is expressed in terms of number of cells n . In the example, the values $n = 1$, $n = 2$, and $n = 3$ are considered. By applying those windows to the distribution in Fig. 24c, the results of Fig. 24e are obtained. At first glance, it appears that distribution of the maximum magnitude given by the window with $n = 3$ is quite exaggerated with respect to the starting data of Fig. 24c. Its intersection with a hypothetic seismogenic area (shown in Fig. 25a), however, gives quite a reasonable distribution (Fig. 25b), which allows us to account for errors in the location of the source and for its extension in space. The smoothing corresponding to radius $n = 3$ (smoothing 1) is chosen to produce deterministic maps of hazard, while the smoothing $n = 1$, applied only to the strongest shocks (smoothing 2), is employed to derive empirical

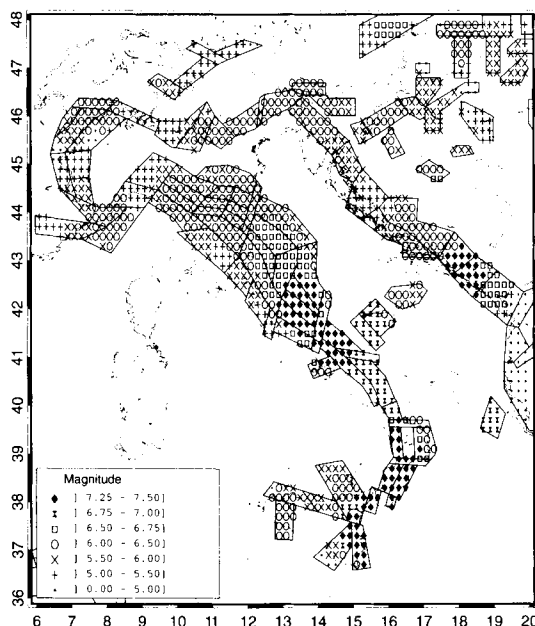


FIG. 26. Smoothed magnitude distribution for the cells belonging to the seismogenic zones defined by GNDT (Corsanego *et al.*, 1997) and updated by A.A.V.V. (2000).

relations between ground motion parameters and observed intensities. In Figs. 24 and 25, symbols are used only to improve readability. In the actual smoothing procedure magnitudes are not divided into classes.

For definition of the seismic sources that generate the synthetic seismograms, only the cells located within a seismogenic area are retained. The map shown in Fig. 26 is the result of the application of smoothing 1 to the NT4.1 earthquake catalogue (Camassi and Stucchi, 1996).

The focal mechanisms of the seismic source placed at the center of each cell are defined as the *best* double-couple, corresponding to the arithmetic average of the tensor elements of the available mechanisms in the relevant seismogenic zone. This simple procedure appears to be reasonable when the mechanisms on average are similar, and this condition should always be checked for each seismogenic area.

Once the structures and the sources have been defined, sites are considered on a grid ($0.2^\circ \times 0.2^\circ$) that covers the whole territory. The synthetic signals are computed for an upper frequency content of 1 Hz, and the scaled point-source approximation (Gusev, 1983) is still acceptable. This is fully justified by practical considerations, as several-story buildings have a peak response in the frequency range below 1 Hz (Manos and Demosthenous, 1992), and by the fact that modern seismic design approaches and technologies, such as seismic isolation, tend to

lower the free oscillation frequencies of buildings. As a rule of thumb (in Italian legislation) the resonance period (in seconds) of a building can be expressed as $0.1H/B^{0.5}$, where H is the height and B is the maximum lateral extension, in meters. When shorter periods are considered, it is no longer possible to neglect the finite dimensions of the faults and the rupturing process at the source.

To reduce the number of computed seismograms, the source-receiver distance is kept below an upper threshold, which is taken to be a function of the magnitude associated with the source. The maximum source-receiver distance has been set equal to 25, 50, and 90 km, respectively, for $M < 6$, $6 \leq M < 7$, and $M \geq 7$. All seismograms are computed for a hypocentral depth which is a function of magnitude (10 km for $M < 7$, 15 km for $M \geq 7$), but it is also possible to assign to each source an average depth determined from analysis of the available catalogues. Keeping the hypocentral depth fixed (for classes of magnitude) and shallow is important due to the large errors generally affecting hypocentral depth reported in the earthquake catalogues and due to the fact that strong ground motion is mainly controlled by shallow sources (Vaccari *et al.*, 1990), with the spectacular exception of the Vrancea region (Radulian *et al.*, 2000) as seen in Figs. 32–34.

Synthetic seismograms for P-SV-waves (radial and vertical components) and SH-waves (transverse component) are originally computed for a seismic moment of 10^{-7} Nm. The amplitudes are then properly scaled according to the smoothed magnitude associated with the cell of the source. For the moment-magnitude relation, we have chosen that given by Kanamori (1977). The finiteness of the source is accounted for by scaling the spectrum using the spectral scaling law proposed by Gusev (1983) as reported in Aki (1987). At each site, the horizontal components are first rotated to a reference system common to the whole territory (North–South and East–West directions) and then the vector sum is computed.

Among the parameters representative of strong ground motion we have focused our attention on maximum ground acceleration, velocity, and displacement (AMAX, VMAX, and DMAX). In computing the complete time series we are not limited to this choice, and it is possible to consider integral quantities that can be of interest in earthquake engineering or engineering seismology (Uang and Bertero, 1990; Decanini and Mollaioli, 1998).

The Fourier spectra of displacements and velocities show that an upper frequency limit of 1 Hz is sufficient to take into account the dominant part of seismic waves, while this is definitely not true for accelerations (Panza *et al.*, 1999a). On the other hand, the required knowledge about seismic sources and lateral heterogeneities, which might justify the choice of a higher frequency limit in the computations, is not usually available at the scale of the areas generally considered in the zoning.

For accelerations, deterministic results may be extended to frequencies higher than 1 Hz by using design response spectra, for instance, Eurocode 8 (EC8, 1993), which define the normalized elastic acceleration response spectrum of the ground motion, for 5% critical damping. In general, this operation should be made taking

into account the soil type. If the regional structural models used are all of type A, as defined in EC8, we can immediately determine the Design Ground Acceleration (DGA) (Panza *et al.*, 1996).

5.1.1. Seismic Zoning of Italy

The NT4.1 file prepared by Gruppo Nazionale per la Difesa dai Terremoti (GNDT) (Camassi and Stucchi, 1996) is used for the definition of seismicity. The smoothed magnitude distribution for cells belonging to the seismogenic zones defined by GNDT (Corsanego *et al.*, 1997) is given in Fig. 26. The focal mechanisms associated with each seismogenic zone are obtained from a collection of data gathered by Suhadolc (1990) and Suhadolc *et al.* (1992). DGA, VMAX, and DMAX maps are shown in Figs. 27, 28, and 29, respectively. In Figs. 30 and 31 the periods associated with VMAX and DMAX are shown. In some regions such as Central Italy around latitude 42°N , long periods in the range between 20 and 30 s dominate.

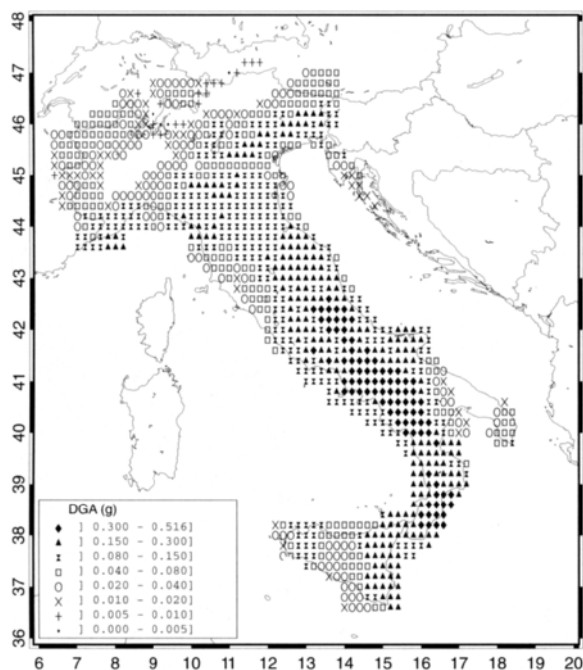


FIG. 27. Distribution of DGA, obtained as a result of deterministic zonation extended to high frequencies using the design spectra of EC8 for soil A. Similar maps can be readily constructed using other design spectra. Units: $1g = 980 \text{ cm/s}^2$.

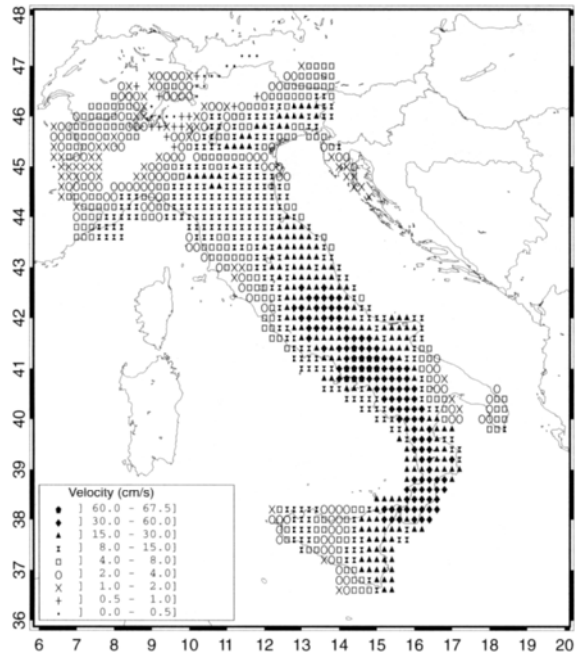


FIG. 28. Horizontal VMAX distribution, obtained as a result of deterministic zonation.

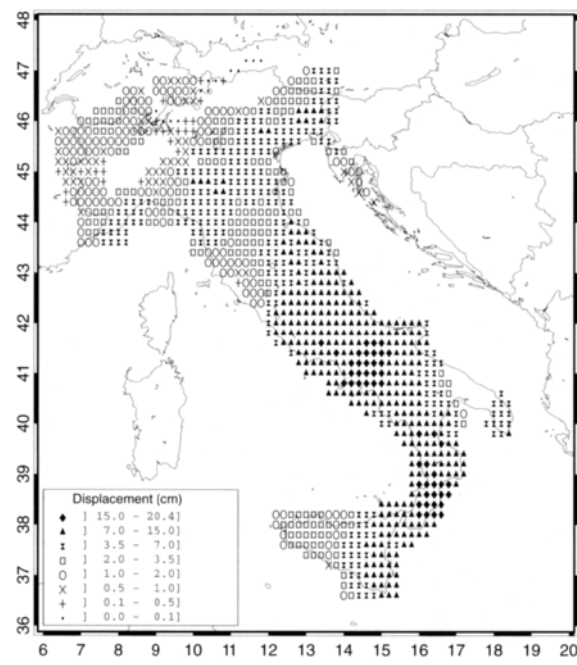


FIG. 29. Horizontal DMAX distribution, obtained as a result of deterministic zonation.

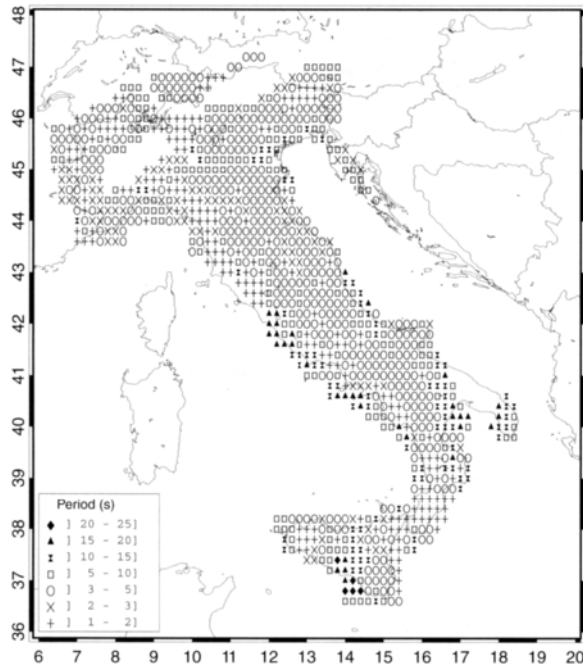


FIG. 30. Period in seconds of the maximum of VMAX at each site.

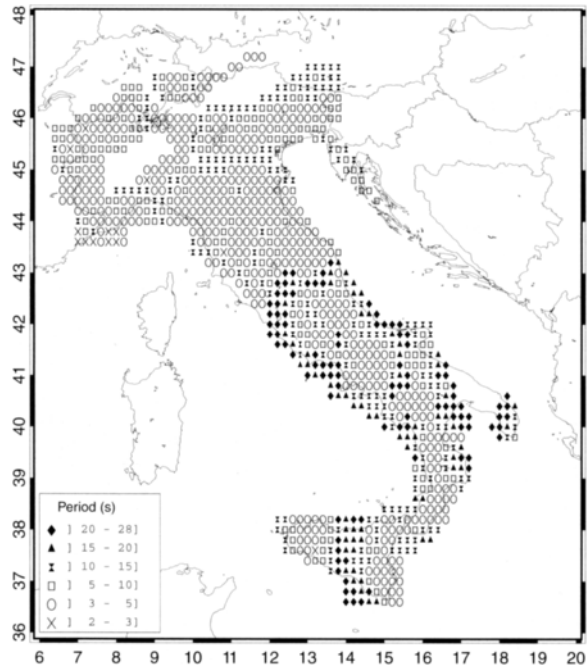


FIG. 31. Period in seconds of the maximum of DMAX at each site.

They are related to signals generated by strong earthquakes occurring at large distances from the site (about 90 km), while the magnitude of the closer events, which are responsible for the higher frequencies (between 2 and 5 s in our computations), is not big enough to let these frequencies dominate the ground motion scenario.

Results of the deterministic procedure are particularly suitable for civil engineers as seismic input for the design of special buildings. In fact, the relevance of the displacements at periods on the order of 10 s or so is a key issue for seismic isolation and in general for lifelines with large linear dimensions, such as bridges and pipelines, where differential motion plays a relevant role in their stability (Monti *et al.*, 1996).

Deterministic modelling can be used to derive correlations between the maximum-felt macroseismic intensity, I , and DMAX, VMAX, and DGA. This possibility is particularly relevant for countries with a long seismological history since it facilitates the engineering use of historical events that are quantified only in terms of macroseismic intensity. Smoothing 2 is applied to the procedure described in Figs. 24 and 25, assuming $n = 1$ for events with magnitude larger than 6.75 (Panza *et al.*, 1997, 1999a). In this way only the source dimension is accounted for, and the mislocation errors that possibly affect the historical catalogues are neglected, since the same error is present in the observations as well. Using (1) the map of maximum macroseismic intensity felt in Italy, made by Istituto Nazionale di Geofisica (ING) (Boschi *et al.*, 1995), and (2) the set of maximum intensity felt in every municipal land, compiled jointly by ING, SSN, and GNDT (ISG) (Molin *et al.*, 1996), Panza *et al.* (1997, 1999a) obtained two sets of regressions from which the intervals shown in Tables 1 and 2 can be defined.

5.1.2. Zoning of the Circum Pannonian Region

The results summarized in this section have been obtained using the framework of the international project EC-COPERNICUS "Quantitative seismic zoning of the

TABLE 1 CONVERSION TABLE BETWEEN MACROSEISMIC INTENSITY AND GROUND MOTION PARAMETERS, DMAX, VMAX, DGA, USING ING INTENSITY DATA

Intensity	DMAX (cm)	VMAX (cm/s)	DGA (g)
V	0.1–0.5	0.5–1.0	0.005–0.01
VI	0.5–1.0	1.0–2.0	0.01–0.02
VII	1.0–2.0	2.0–4.0	0.02–0.04
VIII	2.0–3.5	4.0–8.0	0.04–0.08
IX	3.5–7.0	8.0–15.0	0.08–0.15
X	7.0–15.0	15.0–30.0	0.15–0.30
XI	15.0–30.0	30.0–60.0	0.30–0.60

TABLE II CONVERSION TABLE BETWEEN MACROSEISMIC INTENSITY AND
GROUND MOTION PARAMETERS, DMAX, VMAX, DGA, USING ISG
INTENSITY DATA

Intensity	DMAX (cm)	VMAX (cm/s)	DGA (g)
VI	1.0–1.5	1.0–2.0	0.01–0.025
VII	1.5–3.0	2.0–5.0	0.025–0.05
VIII	3.0–6.0	5.0–11.0	0.05–0.1
IX	6.0–13.0	11.0–25.0	0.1–0.2
X	13.0–26.0	25.0–56.0	0.2–0.4

Circum-Pannonian region (QSEZ-CIPAR)” and the NATO Linkage Grant “Earthquake hazard associated to the Vrancea region seismicity” and are described in the special issue of Pure and Applied Geophysics: Seismic Hazard of the Circum-Pannonian Region (A.A.V.V., 2000). Details about the definition of the structural models and source characteristics are given in Orozova-Stanishkova *et al.* (1996), Radulian *et al.* (2000), Bus *et al.* (2000), Markušić *et al.* (2000), and Živčić *et al.* (2000).

The main effort has been to harmonize Eastern and Western Europe in terms of seismic safety compliance. Standard deterministic procedure described in Sect. 5.1 has been applied, with the exception of the strong events occurring at intermediate-depth in the Vrancea (Romania) region. To handle this case, response spectra especially determined for Romanian intermediate-depth earthquakes (Lungu *et al.*, 1996) have been considered instead of EC8, and the computations have been performed over Romanian, North-Eastern Croatian, and Hungarian territory, and elsewhere within a circle of 350 km radius, centered on the Vrancea epicenter cell. The hypocentral depth of the intermediate-depth events is 90 km for magnitudes less than 7.4, and 150 km for the larger ones. In Figs. 32, 33, and 34 we show maps of peak values of horizontal motion (DMAX, VMAX, and DGA) for the European countries that have been involved in this major effort for mitigating seismic hazard.

Peak values for DGA, VMAX, and DMAX, and pertinent periods associated with displacements, T(D), and velocities, T(V), obtained with the deterministic approach at the sites where nuclear power plants are located (Fig. 35), are summarized in Table 3. The values obtained at Cernavoda, Kozloduy, and Paks are due to the intermediate-depth Vrancea events.

5.1.3. Validation of the Synthetic Models against Independent Observations

Quantitative validation of the deterministic results has been made using the observed accelerograms recorded during the Irpinia earthquake on 23 November 1980 ($M = 6.9$, Camassi and Stucchi, 1996) and the Friuli earthquake on 6 May 1976 ($M = 6.5$, Camassi and Stucchi, 1996). The source rupturing process of

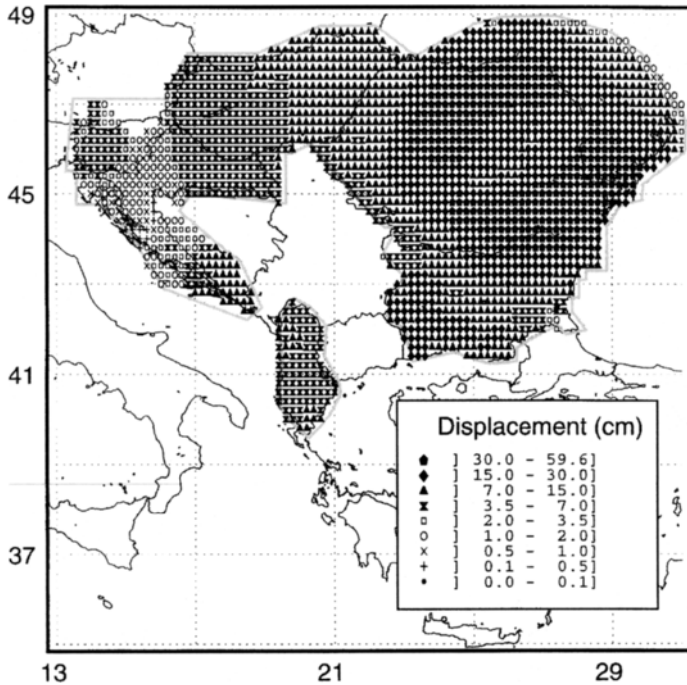


FIG. 32. Maximum displacements. Shallow seismicity has been considered, limiting computations to epicentral distances shorter than 90 km. In the case of Vrancea intermediate-depth events, computations have been performed over the Romanian, North-Eastern Croatian, and Hungarian territory and elsewhere within a circle of 350 km radius, centered on Vrancea epicenter cell. The hypocentral depth is 90 km for magnitude less than 7.4, and 150 km for larger events. The thick gray outline defines the polygons where computations have been performed.

the Irpinia event is very complex (Bernard and Zollo, 1989) and the dimension of the source has been estimated to be on the order of several tens of kilometers. Nevertheless, it seems that the signal recorded at the station of Sturno is mostly due to a single subevent that occurred rather close to the station itself, while the energy contributions coming from other parts of the source seem less important (Vaccari *et al.*, 1990). With the cut-off frequency at 1 Hz, the horizontal accelerations recorded at Sturno have been lowpass-filtered to be compared with the computed signals for the Irpinia region. The example shown in Fig. 36a refers to the NS component, but the same considerations can be applied to the EW component of motion. The early phases and the AMAX of the recorded signal (upper trace) and the synthetic one computed in the point-source approximation (middle trace) are in good agreement. The later part of the observed recording is more complicated and this is mostly related to the complexity of the source, which is deliberately

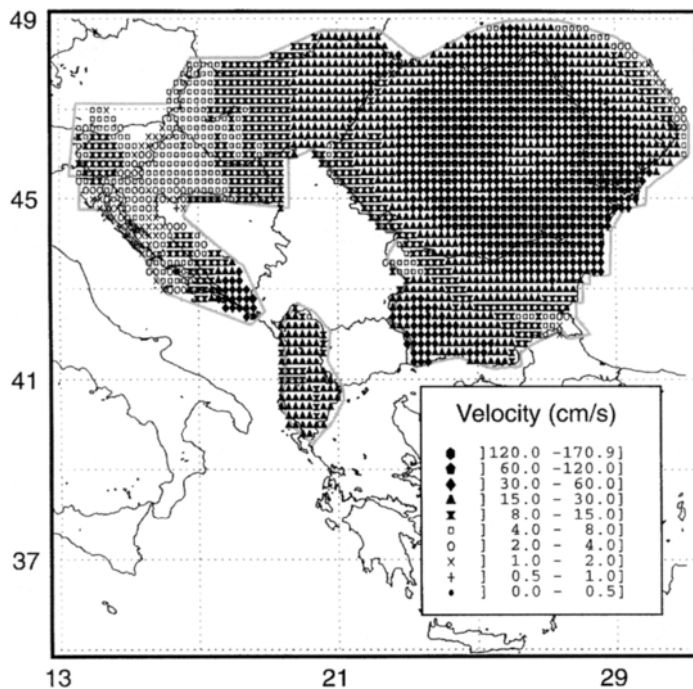


FIG. 33. Same as in Fig. 32, but for maximum velocities.

neglected in the computation of the synthetic signal, to be used in the zoning. The lower trace is shown as an example of modeling of the source complexity. It is the result of a superposition of four subevents, each one modeled with the middle trace properly weighted and shifted in time according to the model by Vaccari *et al.* (1990).

The same approach has been used for comparison of the NS component recorded at Tolmezzo during the Friuli (1976) earthquake (Fig. 36b, upper trace) and two synthetic signals obtained for that area (middle and lower traces). In the case of the Tolmezzo record of the Friuli event, the point-source approximation seems to be satisfactory even for an event with $M_s = 6.1$. Quite good agreement has been obtained using a similar procedure by Moldoveanu and Panza (1999) for Vrancea events. The zonation map of Italy proved the prediction capabilities of peak values in the Umbria-Marche region (Central Italy), where a long sequence of events occurred, starting in September 26, 1997, with the largest shock being of magnitude 6.1 (NEIC). The peak of horizontal acceleration, lowpass-filtered at 1Hz, predicted with the modeling, is 70 cm/s^2 , and the observed one is 44 cm/s^2 . The agreement is improved for peak velocities: about 20 cm/s both for synthetic and for observed time series (obtained by integration of the recorded acceleration).

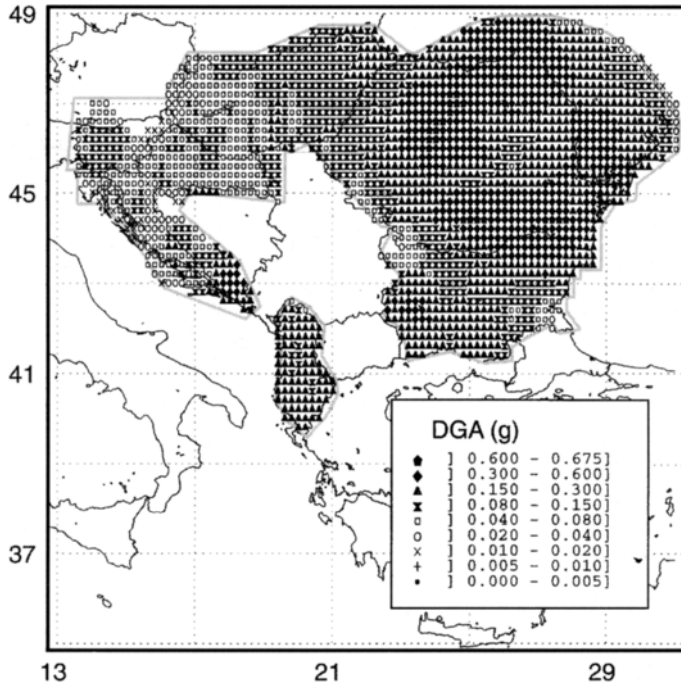


FIG. 34. DGA based on the European Building Code EC8 for shallow events and on response spectra especially determined for the Romanian intermediate-depth earthquakes in the case of Vrancea intermediate-depth events.

5.2. Deterministic Seismic Zoning: Subregional and Urban Scale

One of the basic problems associated with the study of seismic hazard is determining the seismic ground motion, at a given site, from an earthquake with a given magnitude or moment and epicentral distance from the site. The ideal



FIG. 35. Nuclear power plants location.

TABLE III MODELLED GROUND SHAKING FOR THE NUCLEAR POWER PLANTS OF FIG. 35

Site Name	DMAX (cm)	T(DMAX) (s)	VMAX (cm/s)	T(VMAX) (s)	DGA (g)
Cernavoda	35	11.0	91	1.5	0.32
Kozloduy	9	18.0	15	4.0	0.10
Krsko	1	4.5	3	4.5	0.04
Paks	6	3.5	8	3.5	0.07

solution for such a problem could be to use a database of recorded strong motions and to group those accelerograms that have similar source, path, and site effects. In practice, however, such a database is not available. Actually, the number of recorded signals is relatively low and the installation of local arrays in each zone with a high level of seismicity is too expensive an operation, requiring a long time interval to gather statistically significant data sets. An alternative method is based on computer codes, developed from knowledge of the seismic source process and the propagation of seismic waves, that can simulate the ground motion associated with a given earthquake scenario. Synthetic signals can then be produced immediately at a very low cost/benefit ratio, to be used as seismic input in subsequent engineering analysis.

Once the gross features of the seismic hazard are defined, and the parametric analyses have been performed, a more detailed modeling of the ground motion can be carried out for sites of specific interest. Such a detailed analysis should take into account the source characteristics, the path, and the local geological and geotechnical conditions. This deterministic modeling goes well beyond the conventional deterministic approach taken in hazard analyses—in which only a simple wave attenuation relation is invoked—in that it includes full waveform modeling.

It is not possible to refine the results obtained with first-order zoning by simply assuming a higher cutoff frequency (>1 Hz) in the computation of synthetic seismograms. A more detailed zoning requires better knowledge of the seismogenic process in the region. Furthermore, to model wave propagation in greater detail the structural model used in the computation of synthetic seismograms must take into account lateral heterogeneities. Detailed numerical simulations play an important role in the estimation of ground motion in regions of complex geology. They can provide synthetic signals for areas where recordings are absent. Numerical simulations are, therefore, useful for the design of earthquake-resistant structures, in particular when seismic isolation techniques are applied. In fact, the number of available strong motion recordings containing reliable information at periods of a few seconds is very small and will not increase very rapidly, since strong earthquakes in densely instrumented areas are rare events.

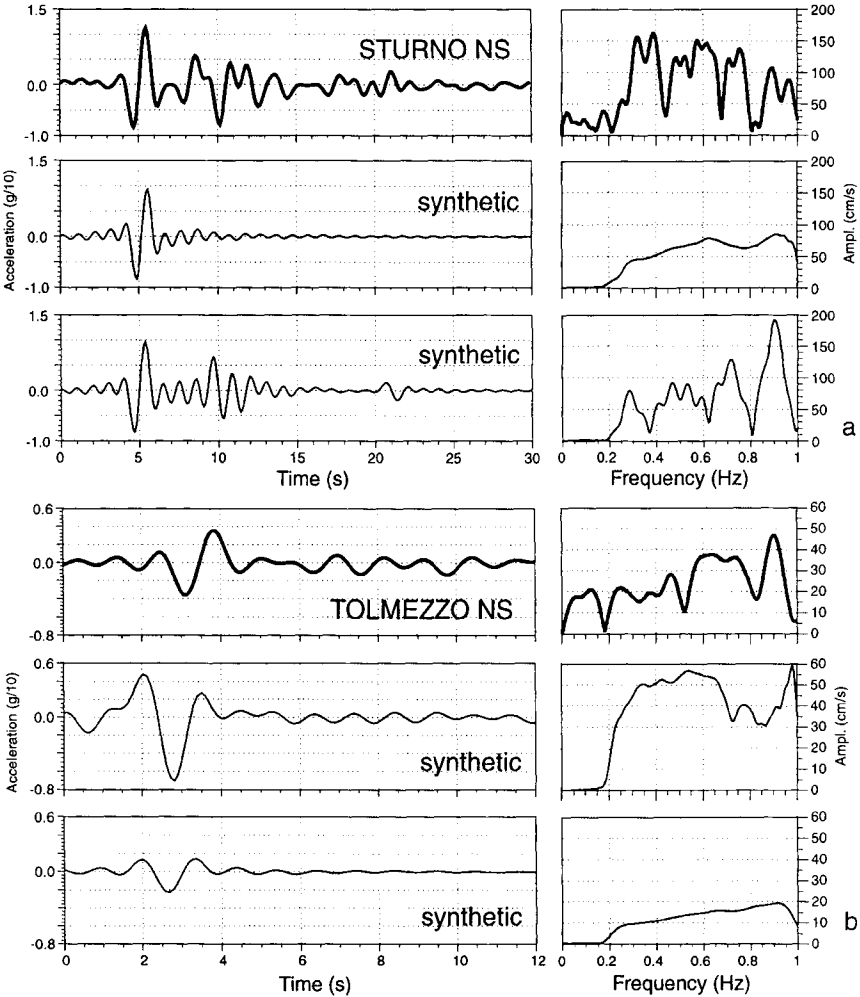


FIG. 36. (a) Comparison of NS component of acceleration recorded at Sturmo, filtered with a cut-off frequency of 1 Hz (top trace), and two synthetic seismograms computed at the closest grid point, in the point-source approximation (middle trace), and for a complex source (bottom trace), with spectral amplitude. (b) Comparison of NS component of acceleration recorded at Tolmezzo, filtered with a cut-off frequency of 1 Hz (top trace) and two synthetic signals computed at the grid point closest to the station (middle and bottom trace), with spectral amplitude.

5.2.1. Local Site Response

One of the most important factors influencing spatial variability of ground motion is the site response. The local amplification, or deamplification, effects can dominate the ground shaking response whenever lateral heterogeneities, such as

surface topographical features or soft-sedimentary basins, are present in the vicinity of a site.

Topographical site effects have not been studied extensively, but their importance is confirmed both by instrumental evidence (Géli *et al.*, 1988; Bard, 1997) and by numerical simulations (Pedersen *et al.*, 1988; Chávez-García *et al.*, 1996). Although there is no general quantitative agreement between theory and observation, a valid qualitative conclusion is that the seismic ground motion is amplified on mountain tops, i.e., over *convex* topographies, with respect to the valley bottoms (Bard, 1997). Numerical simulations have shown (Géli *et al.*, 1988) that the amplification patterns are strongly dependent on the incidence angle, the nature of the incoming wavefield, and the sharpness of the topography. Focusing the diffracted seismic energy may explain the fact that the greater amplifications occur at those wavelengths that are comparable with the horizontal dimension of the topographical feature (Bard, 1997).

A simpler physical explanation for local amplification of ground motion, due to soft surface layering, is the trapping of seismic energy, due to the impedance contrast between soft surface soils and the underlying bedrock. Moreover, the relatively simple onset of vertical resonances can be transformed into a complex pattern of resonances, strongly dependent on the characteristics of the subsurface topography of the sedimentary deposits.

Macroseismic observations made of the destructive events of the twentieth century have clearly shown the strong influence of near-surface geological and topographical conditions on damage distribution. Most anthropic areas (e.g., megacities) are settled in relation to sedimentary basins (e.g., river valleys); therefore a realistic definition of the seismic input that takes into account site response has become one of the most relevant tasks in seismic engineering analysis. In the last decade, a huge amount of literature has been dedicated to estimation of the site effects, and a practical definition of the site effect, that combines the purposes of the engineering and seismological communities, is proposed by Field (1996): “the unique behavior of a site, relative to other sites, that persists given all (or most) of the potential sources of earthquake ground motion in the region.” Such a definition implicitly reveals the difficulties connected with the correct site response estimation, i.e., identification of the different ingredients involved in the resulting ground motion signal: source, path (including the presence of lateral heterogeneities), and local soil effect including its possible nonlinear behavior. The nonlinear effects will not be treated in the following; we just mention that the assumption of linearity between stress and strain can be no longer valid for accelerations larger than 0.1–0.3 g, quite important values from the seismic engineering point of view (Beresnev and Wen, 1996). In fact, due to nonlinearity the actual shear wave velocity decreases with increasing stress, and hysteresis leads to energy loss at any deformation cycle. As a consequence, the resonance of surficial layers can be shifted to lower frequencies, and this can lead to a lower amplification of ground motion at higher frequencies.

The experimental approach to estimation of the site response is based on the measure of ground motion at different sites. This implies the recording, with a network of instruments, of multiple seismic sources. If a network of I sites has recorded J events, the amplitude spectrum, O , of the j th event recorded at the i th site is usually represented as (Field and Jacob, 1995)

$$O_{ij}(\omega) = E_j(\omega) \cdot P_{ij}(\omega) \cdot S_i(\omega) \quad (119)$$

where E is the source term, P is the path term, and S is the site-effect term. The most traditional techniques for estimation of the S term are based on computation of the ratio between the spectrum of the signal (or a portion of it) at the sedimentary site and the spectrum of a reference signal, preferably recorded at a nearby bedrock site (Borcherdt, 1970). Andrews (1986) recasted the traditional method into a generalized-inverse problem by solving for all the site-effect and source terms simultaneously. However, quite often a signal recorded on bedrock is not available close to the investigated sites, so that directional effects due to the source could become relevant. Some techniques have been proposed that are non-reference-site dependent: for example, Boatwright *et al.* (1991) proposed a parameterized source and path inversion scheme based on assumptions regarding the source-spectra, frequency and distance attenuation laws, etc.

An alternative approach is based on the spectral ratio between the horizontal and vertical components of motion. This method was originally applied by Langston (1979) for crustal and upper mantle studies and it is based on the assumption that propagation of the vertical component of motion (in general only S-waves are considered) is minimally perturbed by the surficial layers, and therefore, it can be used to remove source and path effects from the horizontal components. Lermo and Chávez-García (1993) applied the same technique at higher frequencies for the site response estimation in Mexico city. Similarly, Nakamura's (1989) method is based on computation of the spectral ratio between horizontal (usually the square root of the product between the spectra of the NS and EW components is used) and vertical components obtained from seismic noise (microtremors). Theoretical investigations (e.g., Lachet and Bard, 1994; Dravinski *et al.*, 1996) and experimental studies (e.g., Field and Jacob, 1995; Field, 1996) have shown that Nakamura's method can reveal the fundamental resonant frequency of a site but that it is usually not able to give the correct amplification level. Furthermore, Nakamura's (1989) assumptions seem questionable since several studies (e.g., Lachet and Bard, 1994; Konno and Ohmachi, 1998) have demonstrated that the horizontal to vertical ratio is strictly correlated with the polarization of Rayleigh waves.

Table 4 summarizes schematically the most frequently used techniques for the empirical estimation of site effects. These techniques supply reliable information about the site response to noninterfering seismic phases; they are not always adequate in most real cases when the seismic sequel is formed by several

TABLE IV SUMMARY OF THE MOST FREQUENTLY USED TECHNIQUES FOR THE EMPIRICAL ESTIMATION OF THE SITE RESPONSE

Technique	Earthquake (E) or microtremors (M)	Reference site (R) or not (NR)	Example reference
Sediment/bedrock (S/B)	E	R	Borcherdt (1970)
Generalized inversion scheme	E	R	Andrews (1986)
Parametrized source and path inversion	E	NR	Boatwright <i>et al.</i> (1991)
Coda waves analysis	E	NR	Philips and Aki (1986)
Horizontal/vertical (H/V) (receiver function)	E	NR	Lermo and Chávez-García (1993)
Sediment/bedrock (S/B)	M	R	Yamanaka <i>et al.</i> (1993)
Horizontal/vertical (H/V)	M	NR	Nakamura (1989)
Array analysis	M	NR	Malagnini <i>et al.</i> (1993)

interfering waves. For each technique the signal type used (i.e., earthquakes or ambient noise signals), its characteristic (i.e., if it is a reference site-dependent technique or not), and a bibliographic reference are given. For a more comprehensive comparison of the various empirical techniques the reader is referred to Bard (1997).

An alternative to the experimental approach to site response estimation is based on computer codes, developed from detailed knowledge of the seismic source process and the propagation of seismic waves. This approach can simulate the ground motion associated with a given earthquake scenario. In such a way, using available geological and geotechnical information, a low-cost parametric analysis can be performed, since the installation of site arrays in each zone with a high level of seismicity is too expensive an operation.

In principle all techniques presented in Sect. 3 could be used for the theoretical estimation of the site response, each one being more or less suited according to the problem to be solved. For example, it has been shown that boundary techniques (Dravinski *et al.*, 1996), and domain techniques (Coutel and Mora, 1998) can be used to test the reliability of empirical techniques, as well as to study the dependence of the site response on source and path parameters. Progress in computational techniques has allowed extension of numerical analysis to 3-D structural models by using domain methods such as finite difference methods (e.g., Olsen and Archuleta, 1996; Graves, 1998). These techniques could be useful in areas

characterized by severe subsurface topography and by embedded extended faults (e.g., the Los Angeles basin), in order to study the 3-D diffraction effects and the 3-D ground motion amplifications. However, computational demands limit the application of 3-D techniques to periods greater than 1 s and to seismic velocities larger than 1 km/s; the corresponding minimum wavelength is on the order of 1 km, which represents the limit of the spatial resolution of such modeling.

5.2.2. Examples of Ground Motion Scenarios

In the following we consider two examples of the application of deterministic techniques for seismic hazard assessment at a subregional and urban scale, showing results for the Catania (Sicily) area, where the mode coupling analytical technique (see Sect. 4) is used, and for city of Rome, where the modal summation-finite difference hybrid method (see Sect. 3.1.3) is used. These results are produced in the framework of the IUGS-UNESCO-IGCP Project 414 (Panza *et al.*, 1999b).

5.2.2.1. Site response estimation in the Catania (Sicily) area. A realistic definition of the seismic input for the Catania area is obtained using the modeling techniques, described in Sect. 4, that allow us to create a database of synthetic signals which can be used for the study of the local response in a set of selected sites located within the Catania area.

The main task is to define a scenario corresponding to an earthquake of the same size as the destructive event that occurred on January 11, 1693. From analysis of the felt intensities (up to XI) it has been possible to estimate a magnitude ranging from 7.0 to 7.8 (e.g., Boschi *et al.*, 1995; Decanini *et al.*, 1993).

It is very difficult to determine the source characteristics for such a historical event, as the macroseismic data are the only available information. The poor control over hypocentral coordinates does not permit use of the macroseismic data for inversion of the source mechanism, but with these data it is possible to perform an analysis to test the validity of the source mechanism models that can be formulated on the basis of seismotectonics. The observed intensities can be converted into accelerations, velocities, or displacements (e.g., Decanini *et al.*, 1995; Panza *et al.*, 1997, 1999a) and they can be compared with the synthetic data. Applying such a procedure to the 1693 event (Romanelli *et al.*, 1998a,b), good agreement with the macroseismic data is obtained for a seismic source located on the Northern Segment of the off-shore Hyblean fault, which is considered the most important seismogenic structure of the zone.

Because our attention focuses on the lateral variations of the model, to minimize the number of free parameters we account for source finiteness by properly weighting the point source spectrum using the scaling laws of Gusev (1983), as reported in Aki (1987). We have chosen these curves for several reasons: compared to ω^{-2} spectra (e.g., Joyner, 1984; Houston and Kanamori, 1986), Gusev curves, that are

based on solid statistical analysis of experimental data, are more conservative in the range from 2 to 0.1 s, they often provide a corner frequency that allows us to fit the observed amplitudes with the synthetic seismograms (e.g., Vaccari, 1995; Moldoveanu and Panza, 1999).

The focal mechanism parameters of the source, located approximately in the center (latitude: 37.44° ; longitude: 15.23°) of the Northern Segment of the Hyblean fault, are strike = 352° , dip = 80° , rake = 270° , focal depth = 10 km, and seismic moment = $3.5 \cdot 10^{19}$ Nm.

For definition of the model, we use the geotechnical information collected within GNDT (GNDT, 1997): a simplified geotechnical zonation map and a set of five detailed geotechnical cross sections. Because our method can be applied to both rough and detailed laterally heterogeneous models, we first employ the simplified map, to analyze effects of the gross features of geotechnical zonation on ground motion. As a second step, in order to test the usefulness of the simplified models, we consider a detailed version of one of the simplified cross sections.

In Fig. 37 the simplified geotechnical zonation map for the Catania area, together with the 13 cross sections considered in the analysis, are shown. Along each section, a set of sites is considered and the site locations are chosen both in the proximity of the boreholes and at the edges of the section. The laterally varying models associated with each cross section are built up by putting in welded contact (from 2 to 4) different 1-D local models: the regional model, assigned to Eastern Sicily (Costa *et al.*, 1993), is chosen as the bedrock model and the geotechnical information related with the selected boreholes are used for definition of the local models. Synthetic signals are calculated with the modal summation technique for laterally heterogeneous models (see Sect. 4), with a cut-off frequency of 10 Hz. The map shown in Fig. 37 defines the borders between the local models, i.e., the distances between the vertical interfaces separating the different 1-D models. In Fig. 37 the velocity time series calculated, for the transverse component of motion, corresponding to all sites, are shown. Their spectra show that most of the energy is present for frequencies below 4 Hz. Each record is 20 s long and is normalized to the peak velocity value, VMAX, for the entire region. The largest computed values of VMAX are consistent with the reported macroseismic intensity value, XI (Tables 1 and 2). Figure 37 shows how the source and propagation effects can combine a big variety of signals; if laterally heterogeneous models and azimuthal dependencies are included in the analysis, the parameters describing the ground motion are strongly site dependent.

For section S10 (dot-dashed line in Fig. 37), detailed geotechnical information is available (GNDT, 1997), and we examine it with the purpose of comparing the results obtained using a simplified laterally heterogeneous model with those obtained for a realistic model of a geological cross section.

The detailed laterally heterogeneous model used for calculation of the synthetic seismograms along S10 is built up using 48 local models in welded

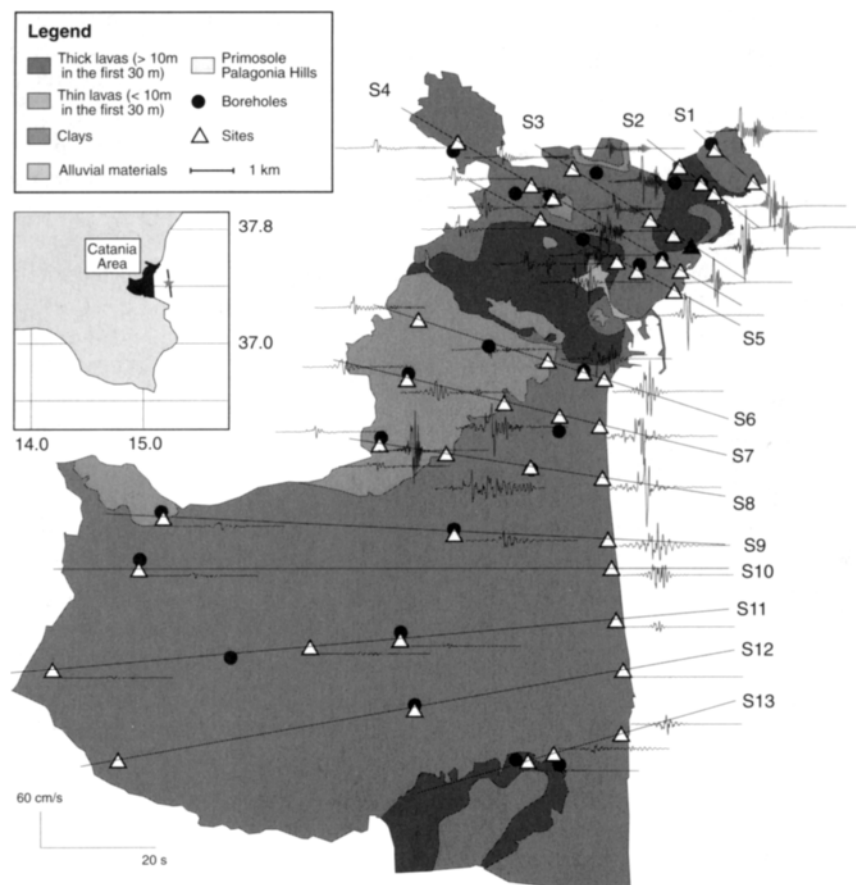


FIG. 37. Simplified geotechnical zonation map for the Catania area and the first 20 s of the velocities time series, calculated at the sites. Each signal is scaled to the maximum value of VMAX (63 cm/s) over the entire area (black triangle) (modified from Romanelli and Vaccari, 1999).

contact, for a total extension of approximately 13 km. The geological cross section and its detailed model are shown in Fig. 38, together with the elastic parameters of each geotechnical unit; the Q values vary in the range from 40 to 300, depending upon the unit considered. The source is buried in the regional bedrock model.

The results shown by Somerville (1996), who supplies the ground motions for a magnitude 7.0 earthquake on the northern Hayward fault, and the spectral analysis of the signals shown in Fig. 37, indicate that a reasonable upper frequency limit in the calculations can be 4 Hz.

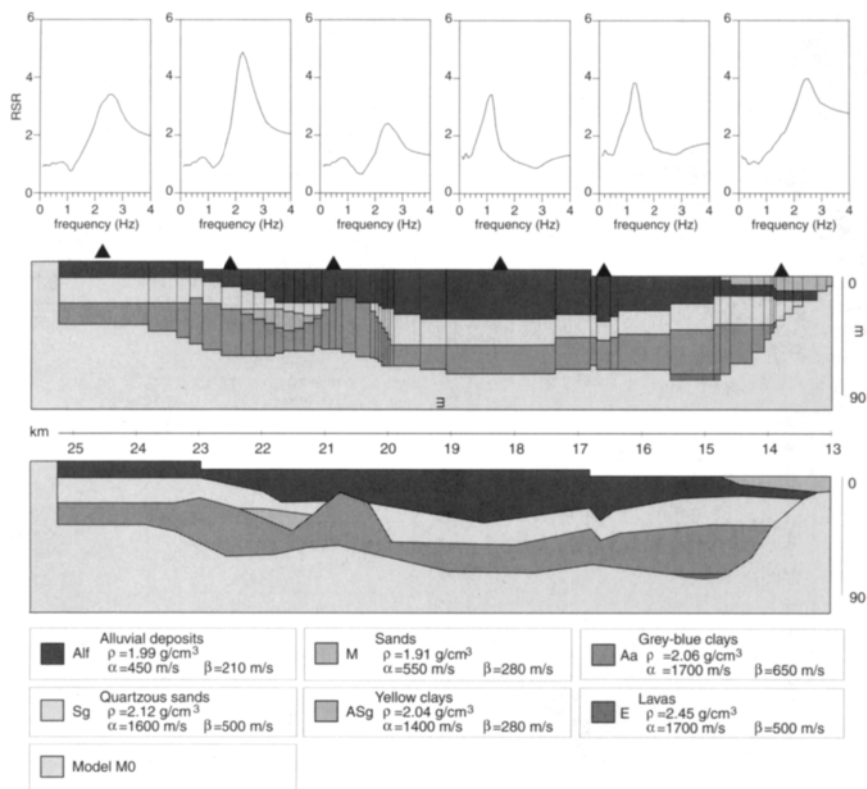


FIG. 38. Cross-section (bottom) and corresponding model for section S10. The distance along the section is measured in km from the source, while the vertical scale is in m. Six selected RSR, are shown (modified from Romanelli and Vaccari, 1999).

The signals are calculated for a set of sites, one for each local model, along the section; in Fig. 38 a set of selected signals is shown for the transverse component of motion. We give an estimation of the local response at a given site, evaluating the response spectra ratio (RSR) corresponding to the laterally varying model and to the bedrock model.

Figure 39 shows the variation of the RSR (SH motion) along the profile: (a) shows the RSR at four selected frequencies (0.2, 0.5, 1.0, and 2.5 Hz) obtained using the signals calculated with a strike-section angle equal to 80° ; (b) is obtained for a value of the strike-section angle equal to 180° , that corresponds to a maximum of the SH radiation pattern in the direction of the cross-section. As expected, at low frequencies (0.2–0.5 Hz) the ratios are approximately 1 along all the section, but at higher frequencies the wavelengths are comparable to the

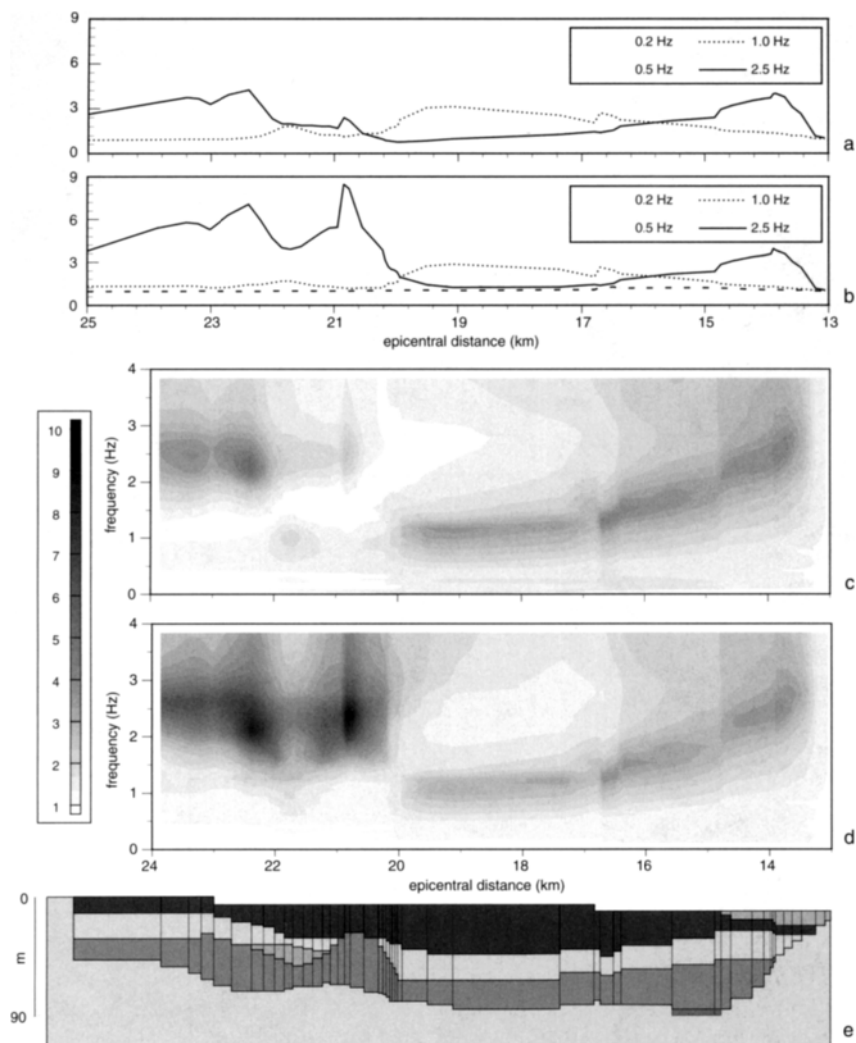


FIG. 39. (a) RSR at four selected frequencies (0.2, 0.5, 1.0, and 2.5 Hz) versus epicentral distance, for the transverse component of motion; strike-section angle is equal to 80° . (b) Same as (a) but the strike-section angle is equal to 180° . (c) RSR versus epicentral distance and versus frequency; strike-section angle is equal to 80° . (d) Same as (c) but the strike-section angle is equal to 180° (modified from Romanelli and Vaccari, 1999). (e) Model for S10.

dimensions of the lateral heterogeneities, and the local effects become important. The shape of the curves corresponding to 2.5 Hz seems to resemble the subsurface topography of the Alf and Aa layers, respectively. In Fig. 39c and d the RSR versus the epicentral distance and frequency are shown for strike-section angles equal to 80° and 180° , respectively. For the first part of the section (up to an epicentral distance of approximately 20 km) the amplification patterns are practically the same, but in the remaining part the amplification levels change significantly. This example shows that the interference between the seismic waves and the lateral heterogeneities is azimuthally dependent and may therefore be responsible for different responses in the same site (e.g., Field, 1996; Riepl *et al.*, 1998). Such a result sends a warning against the general use of the schematic representation used in Eq. (119) and of the validity of determinations of local soil effects made with very popular methods that do not consider the realistic propagation and interference of seismic waves.

Results obtained using the detailed model for section S10 can easily be compared with those from the simplified model. A set of 48 synthetic signals is calculated along S10, using the simplified laterally heterogeneous model shown in Fig. 40a, at the same epicentral distances used for computation of the signals for the detailed model. These signals have been lowpass-filtered with a cut-off frequency of 4 Hz. In Fig. 40b–c the RSR are shown, versus epicentral distance and versus frequency, for the strike-section angle equal to 80° : (b) shows the results corresponding to the detailed section (same as Fig. 39c), while (c) shows the results obtained using the simplified model. The RSR corresponding to the simplified model has a very sharp discontinuity close to the beginning of the local model at an epicentral distance of 13 km. This discontinuity is responsible for the excitation of high-frequency diffracted waves that are rapidly decaying with increasing distance from the boundary. Away from the boundary, the pattern assumes a relatively simple shape: the greater amplifications are obtained at a frequency of approximately 1.5 Hz, that is the value of the fundamental resonant frequency for the stack of local layers shown in the left part of Fig. 40a. The results summarized in Fig. 40 show that the extension of punctual information to extended sections, i.e., the adoption of simplified models, could lead to misleading conclusions concerning the seismic response of sedimentary basins.

Therefore, accurate estimation of the site effects in complicated geometries requires a parametric study that takes into account the complex combination of the source and propagation parameters.

The RSR, obtained using the synthetic signals calculated for the P-SV motion along the detailed section S10, are shown versus epicentral distance and frequency in Fig. 41. The strike-section angle is 80° , a value that, for the given focal mechanism, corresponds approximately to a maximum in the radiation pattern for the P-SV waves. For epicentral distances less than about 20 km the pattern of the resonance frequencies, shown in Fig. 41a (radial component), is in good agreement

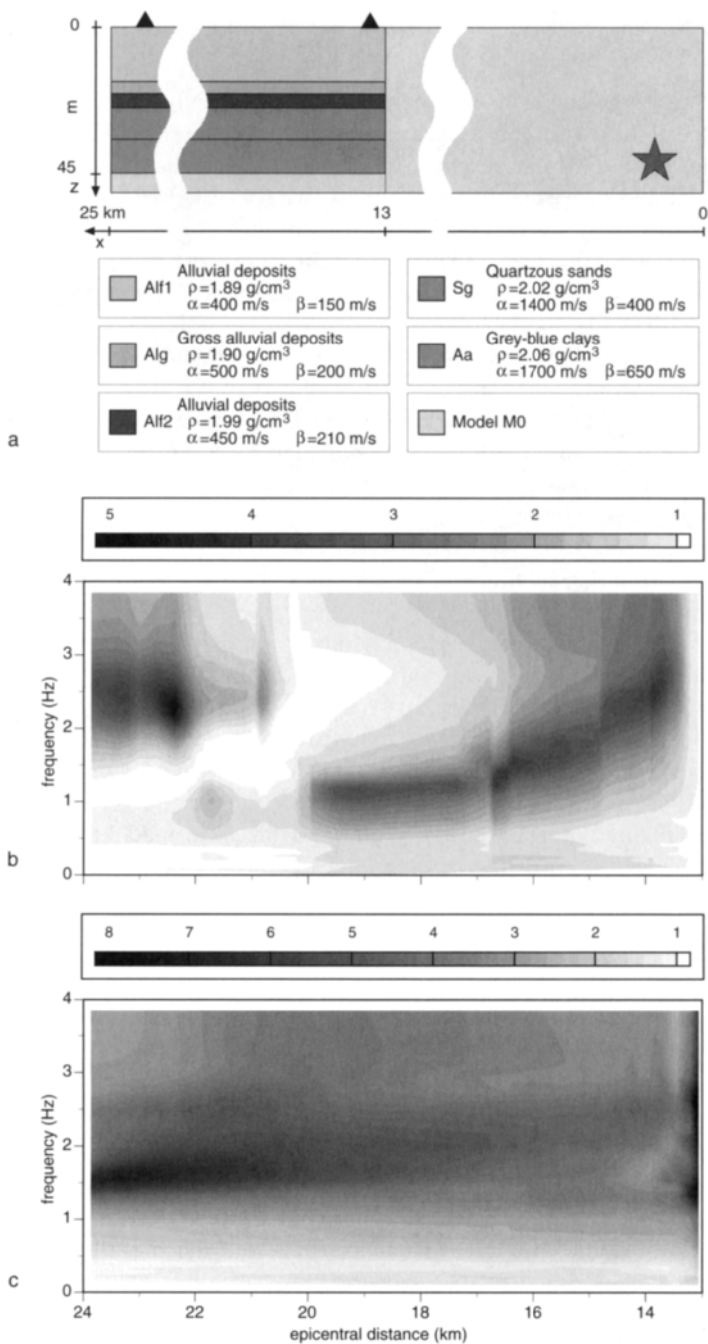


FIG. 40. (a) Simplified model of S10 constructed from the geotechnical map shown in Fig. 37. Comparison of the RSR obtained for the detailed (b) and for the simplified (c) laterally heterogeneous models of section S10. The RSR are plotted versus the epicentral distance and versus frequency for the strike-section angle equal to 80° . The gray scales are different in the two cases.

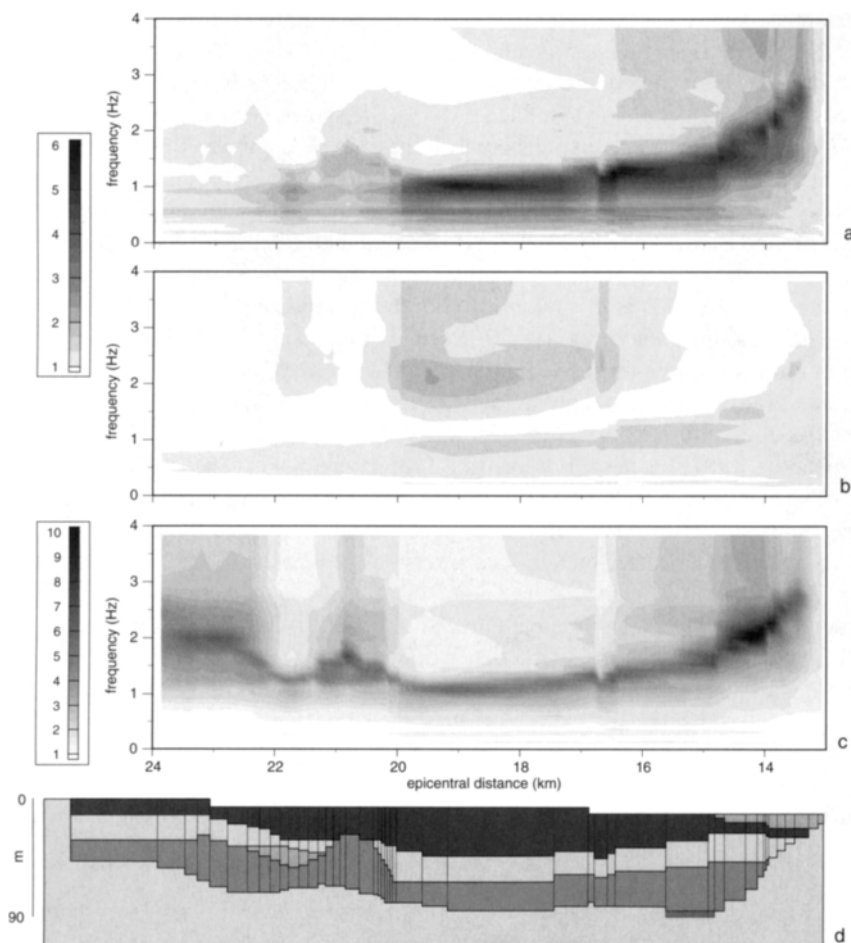


FIG. 41. (a) RSR for the radial component of motion versus epicentral distance and frequency; (b) RSRs for the vertical component of motion versus epicentral distance and frequency; (c) H/V RSR versus epicentral distance and frequency. Strike-section angle equal to 80° (modified from Romanelli and Vaccari, 1999). (d) Model of S10. The gray scale in (c) is different from the ones in (a) and (b).

with the pattern visible in Fig. 39c and d. Figure 41b shows that, in this case, the vertical component of motion is not affected significantly by the local geological conditions.

The fact that the vertical component of motion is free from near surface influences is one of the original assumptions (Nakamura, 1989) of the horizontal-to-vertical spectral ratio technique (H/V RSR) for the estimation of the site response. The main advantage of this technique is its independence from the

reference-site. If earthquake recordings are used, the H/V technique is usually called the receiver function technique (Lermo and Chávez-García, 1993), while if ambient noise recordings are considered it is known as Nakamura's technique (Nakamura, 1989). In Fig. 41c the H/V RSR are shown versus epicentral distance and frequency. The calculations confirm the empirical conclusions that the resonance patterns are very well correlated with surface geology, but the absolute level of amplification cannot be straightforwardly determined (Theodulidis *et al.*, 1996; Lachet and Bard, 1994). The H/V RSR obtained for the bedrock model (not shown) has a simple pattern, with a practically constant value of the resonance frequency along the path. This is in agreement with the theoretical explanation concerning the physical meaning of the H/V RSR: the vertical component of Rayleigh wave motion has a minimum or vanishes, according to the vertical velocity contrast, around the S-wave resonance frequency, and the H/V RSR is a sort of mapping of the ellipticity curve of Rayleigh wave modes (e.g., Panza, 1985; Panza and Suhadolc, 1987; Lachet and Bard, 1994; Konno and Ohmachi, 1998).

The synthetic signals database assembled for the Catania area, which can easily be expanded to other earthquake scenarios, can be used as seismic input in subsequent engineering analyses, at a very low cost/benefit ratio. For estimation of the destructive potential of some of the signals calculated for the simplified models (e.g., Fig. 37), some parameters, obtained from their (a) direct analysis, (b) integration in the time or frequency domain, and (c) the structural (elastic and anelastic) response, have been investigated by Decanini *et al.* (1999). On the basis of the parameters characterizing earthquake destructive power, derived from available strong motion records, the results show that the synthetic signals provide an energy response which is typical of accelerograms recorded on intermediate-firm soil, at a distance from the causative fault between 12 and 30 km, and with a magnitude between 6.5 and 7.1.

5.2.2.2. Microzoning of Rome. A large quantity of descriptions of earthquakes that have been felt in Rome is available (Ambrosini *et al.*, 1986; Molin *et al.*, 1986; Basili *et al.*, 1987). Use of the hybrid method described in Sect. 3.2.2 allows us to give a simple and natural explanation of the damage distribution observed as a consequence of the the January 13, 1915, Fucino earthquake—one of the strongest events to have occurred in Italy during this century (Intensity XI on the Mercalli-Cancani-Sieberg, MCS, scale). The well-documented distribution of damage in Rome, caused by the Fucino earthquake, is successfully compared by Fäh *et al.* (1993b, 1995) with the results of a series of different numerical simulations, using AMAX and the so-called total energy of acceleration, W (Jennings, 1983), which is proportional to the Arias Intensity (Arias, 1970).

High relative AMAXs are obtained where the impedance of surficial sediments is small, whereas relative AMAXs are low where volcanic rocks are thick, and this is in good agreement with the observed damage distribution. An even better correlation with the observed damage is obtained considering the relative W . An

additional important result of Fäh *et al.* (1993b) is the demonstration that sharp variations in the spatial distribution of spectral ratios can be due to polarization of P-SV waves into the radial component, a resonance effect similar to the one described in Sect. 5.2.2.1 for the H/V RSR, even when the geometry of the different sedimentary layers is relatively regular. This is quite a logical explanation of the often observed concentration of damage in very small, scattered zones, and it is easier to accept than the often invoked presence of unlikely abrupt variations in the geotechnical properties of the subsoil. Similar results have been obtained by Marrara and Suhadolc (1998) in a case study at Thessaloniki.

The good correlation between AMAX, W , and the damage statistics makes it possible to extend zoning to the entire city of Rome, thus providing a basis for prediction of the expected damage from future strong events.

In addition to the Central Apennines, whose earthquakes caused maximum intensity VII–VIII (MCS) in Rome and may generate significant perturbations at long periods (Figs. 30 and 31), the most important seismogenic zone (Fig. 42) the earthquakes of which can cause structural damage in Rome are the Alban Hills (observed maximum MCS in Rome VI–VII) (Molin *et al.*, 1986). Therefore, Fäh *et al.* (1995) used the sources shown in Fig. 42: (1) the epicenter of the January 13, 1915,

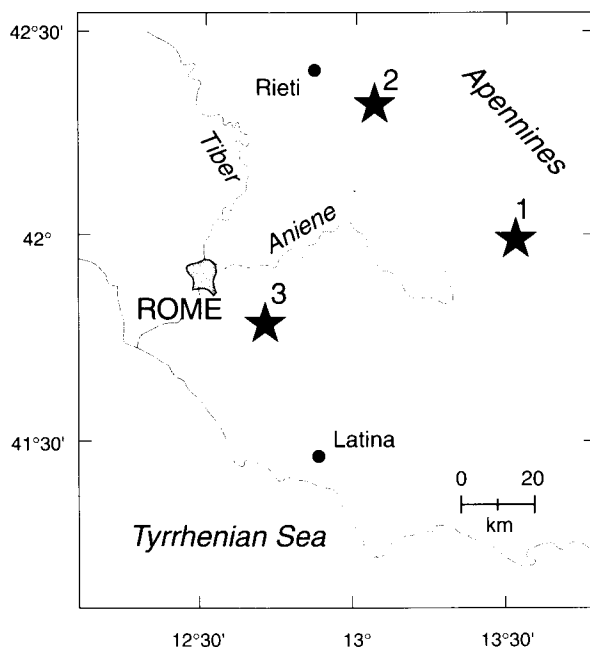


FIG. 42. Epicenter locations of the events considered in the numerical simulations used for micro-zoning. The source positions are: (1) the epicenter of the January 13, 1915, Fucino earthquake, (2) the Carseolani Mountains, and (3) the Alban Hills (after Fäh *et al.*, 1995).

Fucino earthquake, (2) the Carseolani Mountains where, from the study of pattern recognition (Caputo *et al.*, 1980), a strong earthquake is expected to occur, and (3) the Alban Hills. The source mechanisms assigned to these earthquakes are the mechanism of the Fucino earthquake (Gasparini *et al.*, 1985) for event 1 and 2, and the mechanism of an earthquake in the Alban Hills (Amato *et al.*, 1984) for event 3.

Fäh *et al.* (1995) consider the RSR computed along the profiles of Fig. 43, and using the results obtained from the modeling of the Fucino event, they define the six zones shown in Fig. 44: zone 1 includes the edges of the Tiber river, zone 2

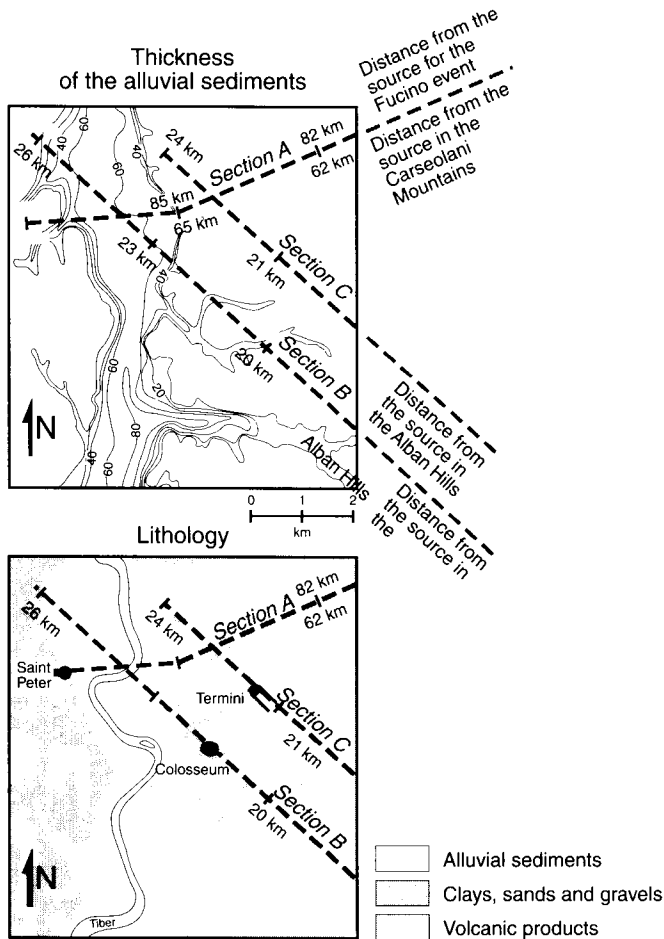


FIG. 43. Lithology and thickness of the alluvial sediments in Rome (Ventriglia, 1971; Funicello *et al.*, 1987; Feroci *et al.*, 1990). The dashed lines indicate positions of the cross sections, for which numerical modeling is performed (after Fäh *et al.*, 1995).

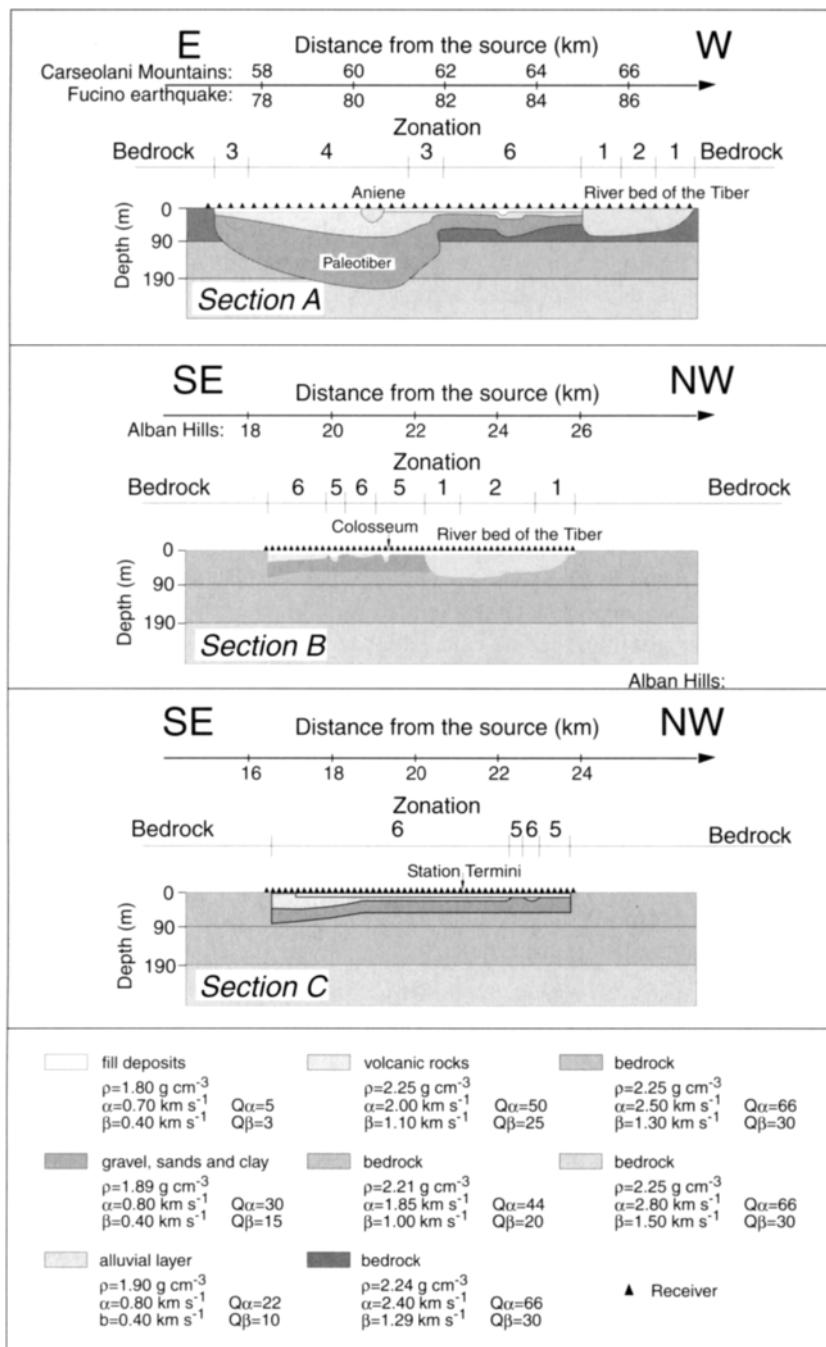


FIG. 44. Two-dimensional models corresponding to the dashed lines shown in Fig. 43. Only the part near to the surface is shown, where the laterally varying model deviates from the horizontally layered bedrock reference models. The microzonation, identified by numbers from 1 to 6, is described in the text (after Fäh *et al.*, 1995).

extends over the central part of the alluvial basin of the Tiber, zone 3 includes the edges of the Paleotiber basin, and zone 4 extends over the central part of the Paleotiber basin. Zones 5 and 6 include areas located outside the large basins of the Tiber and Paleotiber where we distinguish between areas without (zone 5) and with (zone 6) a layer of volcanic rocks close to the surface. Some of these zones can also be recognized in the sections considered in relation to the events located in the Carseolani Mountains and the Alban Hills (Fig. 44). The RSR have been computed for all the sites located in each of the six zones, for all two-dimensional models, shown in Fig. 44, and for all three events, located in Fig. 42. From these values the average and the maximum RSR (shown in Fig. 45) for zero and 5% damping of the oscillator, are determined for each given zone.

Whenever possible, the spectral characteristics defined in Fig. 45 have been assigned to areas located outside the profiles, but characterized by a lithological setting close to one of the six zones identified (see Fig. 44). In such a way, the zoning performed along the three sections has been extended to larger areas using the information available on geological and geotechnical conditions. The result of such tentative extrapolation is shown in Fig. 46.

Given that in Rome the DGA calculated for a bedrock model is about 0.1 g (see Fig. 27), the absolute response spectra that one should expect in the six zones of Fig. 46) is shown in Fig. 47. We may assume that the DGA expected in each zone can be obtained by dividing the largest spectral value by 2.5 (as is the case for EC8 design spectrum). Therefore in Rome the largest estimated DGA is about 0.2 g. Using the correlation between DGA and intensity given in Tables 1 and 2 the intensity is either X or IX, respectively. The intensity due to the 1915 Fucino earthquake (90 km from Rome, $M = 7.3$ in catalogue NT4.1) is VIII. The conservative values we obtain are due to the smoothing of magnitude (smoothing 1, described in Sect. 5.1) and to the geometry of the seismogenic zones, which permits us to account for possible stronger events that might occur closer to the city. Actually, after the smoothing procedure, a magnitude as large as the one of the Fucino event is associated with a source 45 km from Rome. On the other hand, if we want to compare our modeling with the observations, applying smoothing 2 (Sect. 5.1.1), the DGA reduces to 0.10 g. From Tables 1 and 2, the corresponding intensity is either IX or VIII, respectively; well compatible with observations (Molin *et al.*, 1986).

Thus, in the absence of instrumental data, and without having to wait for a strong earthquake to occur, a realistic numerical simulation of the ground motion has been used for microzonation of Rome. The highest values of the spectral amplification are observed at the edges of the sedimentary basin of the Tiber, and strong amplifications are observed in the Tiber river bed. This is caused by the large amplitudes and long duration of the ground motion due to (1) low impedance of the alluvial sediments, (2) resonance effects, and (3) excitation of local surface waves.

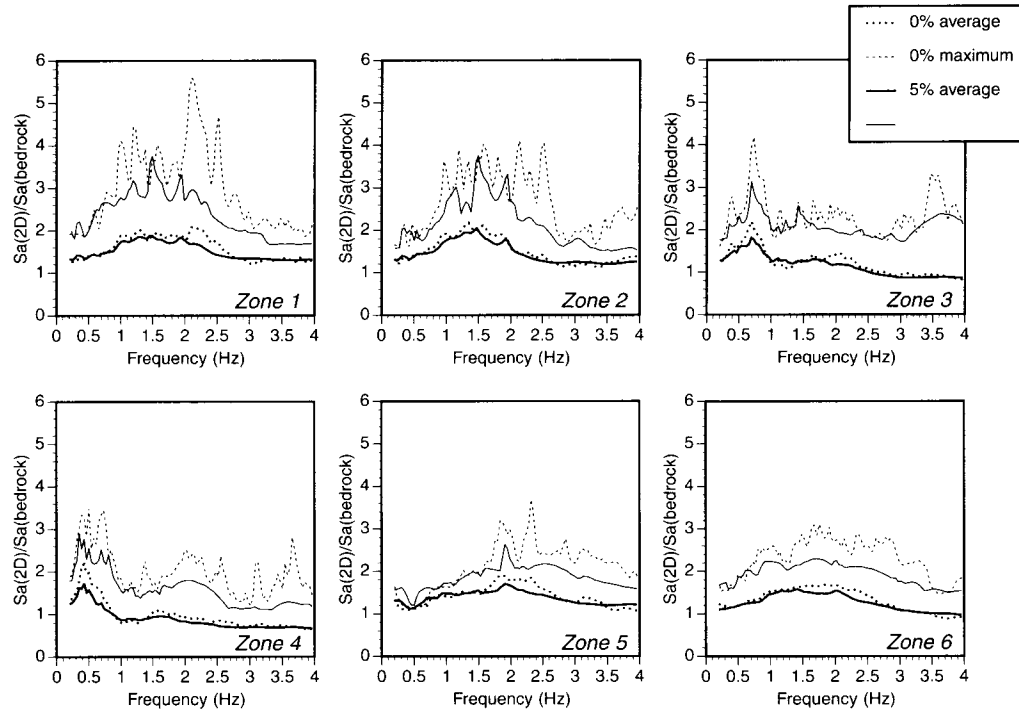


FIG. 45. Maximum and average RSR for the zones defined in Fig. 44, for zero damping and 5% damping (after Fäh *et al.*, 1995).

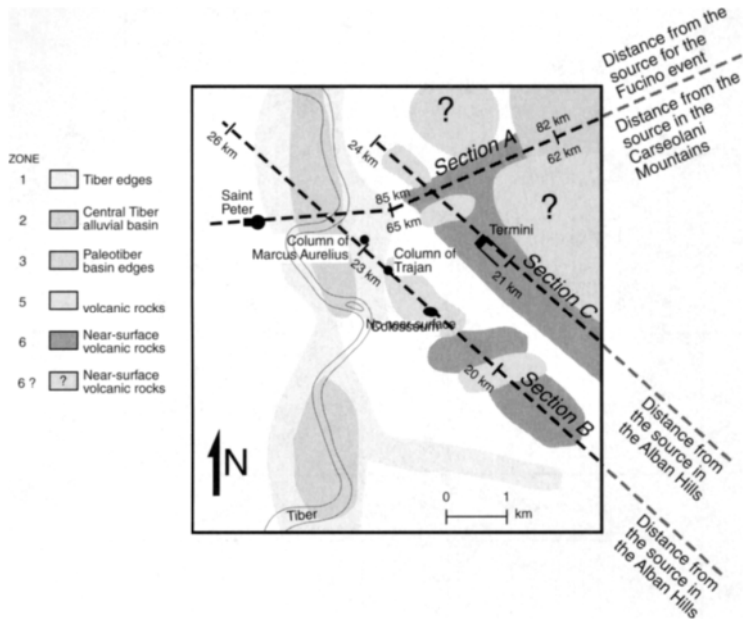


FIG. 46. Microzonation for the city of Rome.

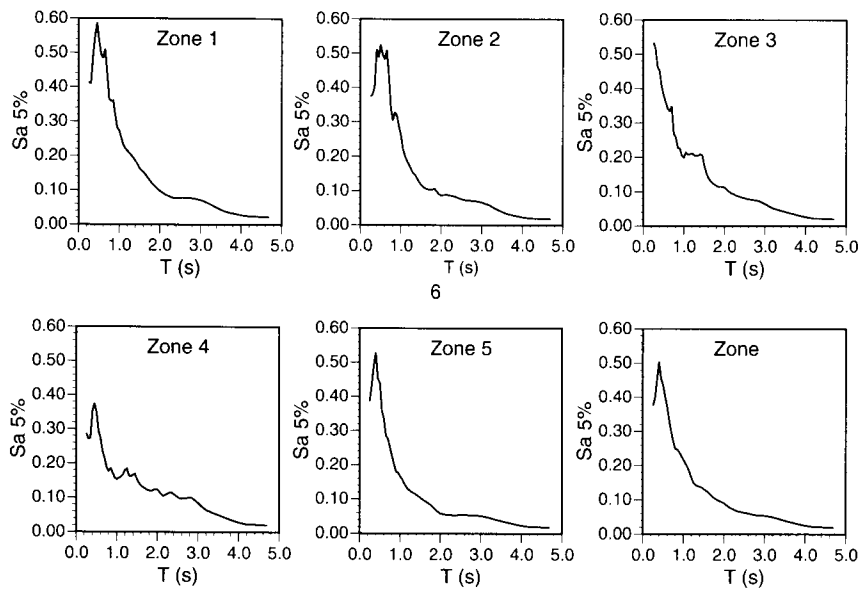


FIG. 47. Spectral accelerations (5% damping) in units of g for the 6 zones shown in Fig. 44.

The presence of near-surface rigid volcanic rocks is therefore not sufficient to classify a location as a *hard-rock site*, since the existence of an underlying sedimentary complex can cause amplifications due to resonance effects. Reliable zonation requires knowledge of both the thickness of the surficial layer and the deeper parts of the structure, down to the real bedrock. This is especially important in volcanic areas, where volcanic flows often cover alluvial basins.

6. SUMMARY AND CONCLUSIONS

Traditional deterministic methods for seismic zoning can lead to only a kind of *postevent* zoning whose validity cannot easily be extrapolated in time and to different regions and which, therefore, must be considered obsolete.

The ability to estimate accurately seismic hazard at very low probability of exceedance may be important in protecting special objects in the built environment against rare earthquakes. The deterministic approach, based upon the assumption that several earthquakes can occur within a predefined seismic zone, represents a conservative definition of seismic hazard for *preevent* localized planning for disaster mitigation, over a broad range of periods.

Computation of realistic synthetic seismograms, using methods that take into account source, propagation, and site effects, and utilizing the huge amount of available geological, geophysical, and geotechnical data, goes well beyond the conventional deterministic approach and gives a powerful and economically valid scientific tool for seismic zonation and microzonation.

The definition of realistic seismic input can be obtained from computation of a wide set of time histories and spectral information, corresponding to possible seismotectonic scenarios for different source and structural models. Such a data set can be fruitfully used by civil engineers in the design of new seismo-resistant constructions and in the reinforcement of the existing built environment, and can therefore provide a particularly powerful tool for the prevention aspects of Civil Defense. The possibility of modeling broad-band seismic input is a useful tool for engineering design and for the retrofitting of special objects, with relatively long free periods, and is acquiring continuously increasing importance, due to the widespread existence, in the built environment, of special objects.

The procedure is scientifically and economically valid for immediate action, since there is no need to wait for a strong earthquake to occur. First-order zonations can be made at regional scale, considering average structural models and a set of sources with damaging potential distributed within the identified seismogenic areas. Seismic microzonations of urban areas can be performed even more accurately when the required geotechnical data are available, so that local site effects can be soundly modeled.

A practical definition of site effect, that accounts for both the seismological and engineering point of view, is the one given by Field (1996): "the unique behaviour of a site, relative to other sites, that persists given all (or most) of the potential sources of earthquake ground motion in the region." This definition implicitly indicates the difficulties connected with a correct estimate (or prediction) of the site effect. These are the determination and separation of the other factors contributing to the seismic signal: source effect, path effect (including lateral heterogeneity), and possible (but not considered here) nonlinear soil response. The theoretical site response estimations that we performed using different types of seismic motion and different techniques, confirm that the identification of the behavior of a site with a set of resonant frequencies could be a very difficult task, especially when the amplification is azimuthally dependent. Furthermore, our results show that the extension of discrete information for limited areas to extended source, i.e., the adoption of simplified models, could lead to misleading conclusions concerning the seismic response of sedimentary basins. The results suggest that, in order to perform an accurate estimate of the site effects in complicated geometries, it is necessary to make a parametric study that takes into account the complex combination of the source and propagation parameters.

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TERRESTRIAL SEQUESTRATION OF CO₂: AN ASSESSMENT OF RESEARCH NEEDS

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1. INTRODUCTION

National and international concern is rising about the possible effects of greenhouse gases on the climate. Currently, the burning of fossil fuels provides about 85% of the world's energy. In the United States, approximately 90% of anthropogenic greenhouse gas emissions are due to energy production, most of which result from burning fossil fuels. Although the development of more efficient and alternative energy systems will lead to reduced greenhouse gas emissions, it is

inevitable that the burning of fossil fuels will continue to provide a considerable proportion of the nation's energy well into the next century. With that in mind, one strategy for reducing greenhouse gas emissions into the atmosphere is to capture carbon dioxide from the products of fossil fuel burning and sequester it below the earth's surface, either on land or in the oceans. The period of geological sequestration should be for a minimum of 50–100 years, and 1000 years would be better.

This paper addresses geoscience issues associated with terrestrial sequestration of carbon dioxide. The primary venues being considered for terrestrial sequestration are active or depleted oil and gas reservoirs, deep saline aquifers, and underground coal beds. Creation of large underground cavities is another possibility, but this solution is thought to be prohibitively expensive. The technology exists for removing carbon dioxide from flue gases and injecting it into the earth. In the petroleum industry, for example, CO₂ is regularly injected into reservoirs for enhanced oil recovery and used for hydraulic fracture. In Norway, CO₂ has been injected into saline aquifers for disposal, and natural gas is regularly stored underground.

Although the considerable experience of the oil industry in CO₂ injection and gas storage is relevant, issues arise in long-term sequestration that are different from those associated with energy extraction or seasonal storage. Examples include the following questions:

- Did production of hydrocarbon reservoirs degrade the properties that made the reservoirs desirable?
- How will CO₂ interact chemically and mechanically with fluids present in the reservoirs (brine, oil)?
- Under what conditions will CO₂ displace existing fluids?
- How will CO₂ react with existing rock?
- Can rock–fluid–CO₂ -interactions be assessed at the temperatures and time scales (hundreds to thousands of years) of interest?

Other issues common to both hydrocarbon retrieval and CO₂ sequestration concern uncertainties about the response of geological reservoirs over long time periods in complicated mechanical, hydrological, and chemical environments. For example, what rock types and material properties (permeability, porosity, connectivity, and current level of saturation) make a good reservoir? Can reservoir properties be identified remotely by geophysical techniques such as seismic, electromagnetic, or others? Can these techniques identify rapid-flow pathways that could compromise the integrity of the reservoir or make effective utilization of pore space difficult? Although the oil industry has considerable experience with hydrocarbon reservoirs, much less is known about the geologic, thermal, and fluid properties of deep aquifers.

There is little question that terrestrial sequestration of CO₂ is possible. But determining whether it is an effective strategy to reduce greenhouse gases in the

atmosphere will require careful consideration of economic issues, including the cost of removing and collecting gases from fuel byproducts, transportation of the gas to sequestration sites, and compression for injection. Furthermore, the efficiency of injection and the safety and integrity of containment will depend largely on the scientific understanding of the hydrological, mechanical, and chemical behavior of the reservoir.

We begin with a brief review of major characteristics of reservoir structures and lithologies as a guide to reservoir selection for CO₂ disposal. The remainder of the chapter focuses on existing experience and uncertainties in reservoir characterization and response to CO₂ injection and long-term containment of sequestration sites. The associated sections are organized according to the disciplinary points of view of geochemistry, geomechanics, geohydrology, and geophysics—although an effective debate on questions of interest would require interaction among them. Within each disciplinary division, the sections address concerns relating to reservoir characterization, changes during injection, and long-term containment and integrity.

1.1. Geologic Setting of Reservoirs

Oil and gas reservoirs and aquifers share some common geometric elements. Generally, both are tabular bodies in which the fluid flow is constrained by upper and lower less-permeable lithologies. Typically, such barriers are presumed to be formed by shale. Faults may cut both reservoirs and aquifers with variable and often unpredictable effects on fluid flow. Aquifers typically have large lateral extents; hydrocarbon reservoirs tend to be restricted. Lateral, low-permeability barriers may be caused by facies changes or by faults that inhibit flow across them. The latter is illustrated by the southern boundary of the Anadarko Basin, Oklahoma, where the fault contact places sedimentary against crystalline rocks and acts as a seal to fluid migration (Al-Shaieb *et al.*, 1994). Hydrocarbon reservoirs vary from a few meters to thousands of meters thick and range in aerial extent from a few kilometers to over 100 square kilometers. Small reservoirs may contain only one producing well, but large fields may contain hundreds of wells.

Although reservoirs can be classified according to whether the fluid-trapping mechanism is structural or stratigraphic (Fig. 1), they are more commonly distinguished by dominant lithology: clastics and carbonates (Tables 1 and 2). Fractured reservoirs are generally treated as a third class (Nelson, 1985; Roehl and Choquette, 1985; Coalson *et al.*, 1989).

Clastic reservoirs are found in sandstones, siltstones, and shales, often with interlayered sequences of each, such as in the Powder River Basin, Wyoming (Surdam, 1997). The sandstones and siltstones generally have a granular, quartz framework that may be poorly consolidated or cemented by quartz, clays, or

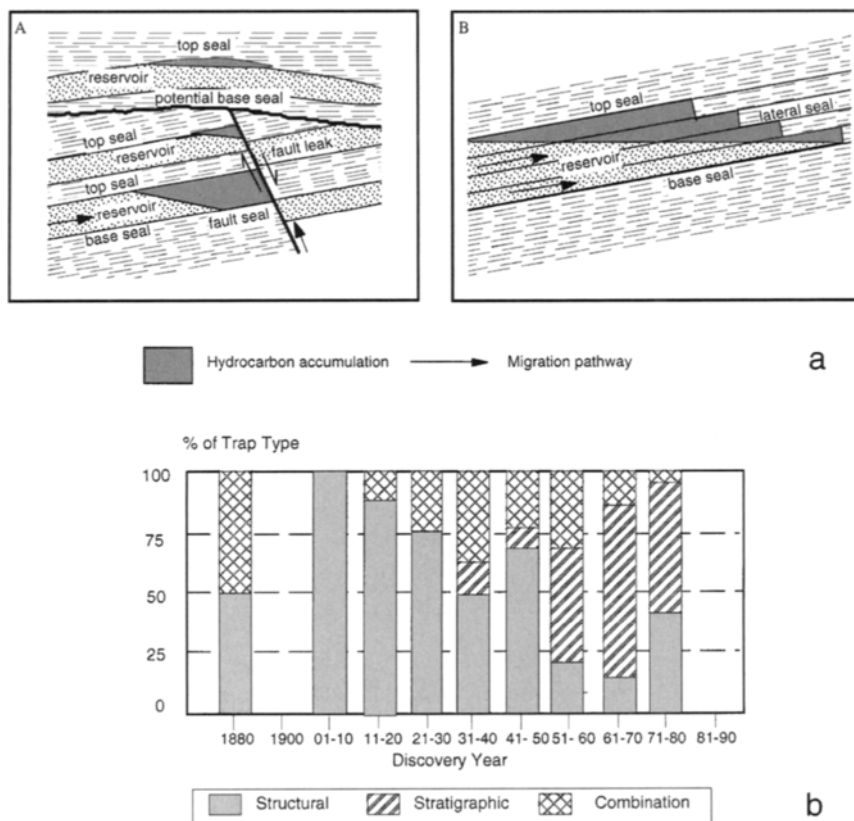


FIG. 1. (a) Major elements of (A) structural and (B) stratigraphic traps (from Biddle and Wielchowsky, 1994). (b) Relative distribution of structural, stratigraphic, and combination petroleum fields for the Rocky Mountain region through 1980. The 155 fields are for sandstone reservoirs that produced more than ten million barrel equivalents of petroleum. The change in relative percentage with time reflects a shift from surface structure recognition to the development of new seismic techniques for subsurface exploration (from Coalson *et al.*, 1989).

carbonates. Porosities and permeabilities are determined to a large degree by the depositional environment and, thus, tend to be relatively homogeneous over wide areas, at least compared to other environments. This element of predictability has made them attractive for hydrocarbon production and for water aquifers. Porosity and permeability, however, vary widely from reservoir to reservoir. For example, within the Rocky Mountain region the Muddy “J” Sandstone in the Denver Basin, Colorado, has porosities from 8 to 12% and permeabilities from 0.05 to 0.005 md, while the Muddy Sandstone in the Bell Creek Field, Montana, has porosities from 6 to 26% and permeabilities from 0.1 to 13,000 md (Coalson *et al.*, 1989).

TABLE 1 CHARACTERISTICS OF SELECTED CLASTIC RESERVOIRS

Field	Location	Producing horizon	Nature of trap	Average depth (m)	Thickness (m)	Areal extent (sq. km)	Porosity (%) (avg.—max.)	Permeability (md) (avg.—max.)	Fractures
Bell Creek	Powder River Basin, Montana	Muddy Sandstone	Stratigraphic	1372	7	29.2	28–36	2250–13,000	Associated with vertical faults
Hawk Point	Powder River Basin, Wyoming	Minnelusa "B" Sandstone	Stratigraphic	3459	9	2	13–18	30–144	Negligible
Lexington	Anadarko Basin, Kansas	Morrow "A" Sandstone	Stratigraphic	1683	3–12	4	15–27	275–2000	Limited, healed vertical
Luckey Ditch	Southern Moxa Arch, Wyoming/Utah	Dakota Sandstone	Structural/stratigraphic	4420	3–11	51.8	14–23	60–713	Insignificant
Painter Reservoir	Thrust Belt, Wyoming	Nugget Sandstone	Structural: thrust belt	2950	255–285	9	12–21	9–1450	Abundant vertical, open or gouge filled
Rangely	Piceance Basin, Colorado	Weber Sandstone	Structural	981	84	77	12–25	2–250	Extensive; provide permeability
Spindle	Denver Basin, Colorado	Terry Sandstone member, Pierre Shale	Stratigraphic	370	6	256	14–19	2–17	Insignificant
Wattenberg	Denver Basin, Colorado	Muddy "J" Sandstone	Stratigraphic	2316	6	2535	8–12	0.005–0.05	Insignificant
Weld Draw	Powder River Basin, Wyoming	Teapot Sandstone member, Mesaverde Fm.	Stratigraphic	2067	5	453	14–20	4–17	Insignificant
West Lindrith	San Juan Basin, New Mexico	Dakota Sandstone	Stratigraphic	2225	12	25.2	8–18	0.05–2.5	Assisted permeability some members

Note: Data selected and compiled by J. M. Logan from Coalson *et al.* (1989) and Nelson (1994).

TABLE II CHARACTERISTICS OF SELECTED CARBONATE RESERVOIRS

Field	Location	Producing horizon	Lithology	Nature of trap	Average depth (m)	Thickness (m)	Areal extent (sq. km)	Porosity (%) (avg.—max.)	Permeability (md) (avg.—max.)	Fractures
Belle River Mills (converted to gas storage, 1965)	Michigan Basin, Michigan	Guelph Formation	Dolomite	Stratigraphic	762	131	1	10–30	8–1000	Non-tectonic
Chatom	Gulf of Mexico coastal plain, Arkansas	Smackover Formation	Dolomite	Stratigraphic; structural	4900	0–9	13	25–35	63–200	Minor, generally calcite healed
Fairway	Texas	James Reef Formation	Limestone	Stratigraphic; structural	2900	30	115	11 avg.	3–27	Sparse
Little Knife	Williston Basin, North Dakota	Mission Canyon Formation	Dolomite; calcitic dolomite	Stratigraphic; structural	3000	7–33	96	14–27	30–167	Common; widely spaced; vertical hairline
Mt. Everette; South Reeding	Anadarko Basin, Oklahoma	Hunton group	Limestone; dolomite	Stratigraphic	2401	15	5	8–20	93–560	Locally important; high angle, open or calcite filled
North Bridgeport	Illinois Basin, Illinois	St. Genevieve Formation	Limestone; dolomite	Stratigraphic; structural	490	5–12	4.4	20–40	240–9500	Moderate in dolomite; few in limestone
Puckett	Central Basin Platform, Texas	Ellenburger Formation	Dolomite	Structural	4115	0.3–45	68	3–12	30–169	Tectonic and solution collapse
Seminole Southeast	Permian Basin Texas	Strawn Formation	Limestone	Stratigraphic	3292	4	6	13–18	29–80	Vertical; hairline to solution enlarged
Sunniland	South Florida Basin, Florida	Sunniland Formation	Limestone; dolomite	Stratigraphic; structural	3540		9	18–30	65–1000	Negligible
West Cat Canyon	Santa Maria Valley, California	Monterey Formation	Dolomite; siltstones; shales	Structural	1190	175	10	12 avg	186 avg.	Numerous

Note: Data selected and compiled by J. M. Logan from Roehl and Choquette (1985) and Nelson (1994).

Carbonate reservoirs include those that are primarily composed of dolomite such as the Williston, North Dakota, and the Central Basin Platform of Texas; dolomite and limestone such as the Anadarko Basin; chalks such as in the North Sea; and limestone reefs such as those found in the Michigan Basin (Roehl and Choquette, 1985). In contrast to clastics, the properties of carbonate reservoirs more often reflect facies variations and early diagenetic changes. Because the latter are often spatially and temporally variable, reservoir properties are relatively heterogeneous. Although carbonate reservoirs often have high porosity, the permeability can be low and, even more importantly, often unpredictable within a given formation. Approximately 60% of the recoverable oil in the world resides in carbonates (Oil and Gas Journal, 1983).

Fractured reservoirs occur in all types of lithologies: limestone in Kirkuk, Iraq (one of the largest fields in the world), schist in the Wilmington Field of California, Devonian shale in a gas-producing reservoir in the Big Sandy Field in Kentucky and West Virginia, sandstones in California, and granite in Kansas (Nelson, 1985). In some fields, fractures enhance the permeability but in others, they provide the essential porosity and permeability. For example, in the Big Sandy Field, the shales have low to negligible intrinsic porosity and permeability, and the fractures provide all transport avenues. On the other hand, in the Sprayberry Field of Texas, the reservoir siltstone has an average porosity of 8% and a permeability of 0.29 to 0.50 md, but abundant fractures increase the total permeability to 16 md or higher (Hubbert and Willis, 1955). The disadvantage of fractured reservoirs is the low storage capacity of the fracture-bounded blocks and the low recovery of fluids from them. Commonly, fractures cause the flow to be strongly anisotropic because of either their preferred orientation or their response to the *in situ* stress field. Frequently, the presence and importance of fractures to reservoir development are discovered only indirectly by significant discrepancies between the results of pressure-decay tests in exploratory wells and predictions by means of single- and double-porosity theoretical models.

Most reservoirs do not consist of a single complex but are made up of several isolated compartments. The existence of these compartments for millions of years indicates a measure of stability to tectonic and diagenetic processes. Some reservoir compartments retain extreme over- or underpressure (Fig. 2, see color insert). This suggests very low permeability of their bounding seals and a number of pressure-controlling processes, including compaction, volume-increasing organic and inorganic reactions and phase transitions, and thermal expansion. Some compartments are extremely large (basin scale) and therefore represent great holding capacity (Ortoleva, 1994a, 1998, and Ortoleva *et al.*, 1995). Underpressured compartments appear to be particularly attractive for the purposes of CO₂ sequestration. Breaching of their seals would tend to draw in fluids from the environment rather than expel them.

1.2. Differentiating Characteristics of Coal Reservoirs

Another possible subsurface candidate for the sequestration of CO₂ is an underground coal deposit. As in other reservoirs, gas is stored in pores and fractures and is dissolved in formation water. However, in coal beds, most of the methane, other light hydrocarbons, and carbon dioxide are primarily held in the adsorbed state on the internal surface of the coal micropores (Bell and Rakop, 1986), most probably as a monolayer. These micropores constitute a large surface area on the order of 1 million sq. ft/lbm (205 m²/t; McElhiney *et al.*, 1989) that enables a much greater amount of methane (or CO₂) to be stored than can be accommodated in the compressed state or dissolved in formation water. For example, Bell and Rakop (1986) observed that the Mary Lee coal group in the Black Warrior Basin in Alabama had an average gas content of 400 scf/ton (11.3 m³/t) at pressures just less than hydrostatic pressure. The equivalent amount of compressed gas would require a coal porosity of 66%. Therefore, coal beds can store three to seven times the amount of methane that can be held in conventional reservoirs at conventional depths and pressures (McElhiney *et al.*, 1989). Redistribution, drainage, and recharge of methane in coal are controlled by ubiquitous fracture systems referred to as cleats. The cleat-transport properties are determined not only by *in situ* stress states, but also by considerable shrinkage of coal following the release of methane.

Research into the adsorption/desorption of methane, CO₂ and other gases has been performed by several researchers (Anderson *et al.*, 1966; McCulloch *et al.*, 1975; Lee, 1982; Ruppel *et al.*, 1974; Bell and Rakop, 1986; McElhiney *et al.*, 1989). The amount of gas content of a coal bed (which conversely may be the amount of gas that can be readsorbed after dewatering and methane release) will depend on moisture content, thermal maturity (rank), coal quality, and reservoir pressures (Ayers and Kelso, 1989). Kim (1977) showed that the quantity of adsorbed methane and the density of coal grew with increasing coal rank, i.e., from high-volatile bituminous to anthracite. The gas content of coal also varies with regional formation pressure (McElhiney *et al.*, 1989), pressure-gradient, inorganic (ash) content, moisture content (Joubert *et al.*, 1973; Yalcin and Durucan, 1991), temperature, and the wettability of coal (Bell and Rakop, 1986).

2. GEOHYDROLOGY

2.1. Introduction and Experience in CO₂ Enhanced Oil Recovery

Primary aspects of CO₂ sequestration in geologic formations include the geohydrologic characterization, injection behavior, and long-term containment of supercritical CO₂ for storage in aquifers and reservoirs. A supercritical fluid has some of the properties of a liquid (e.g., density) and a gas (e.g., low viscosity), and is

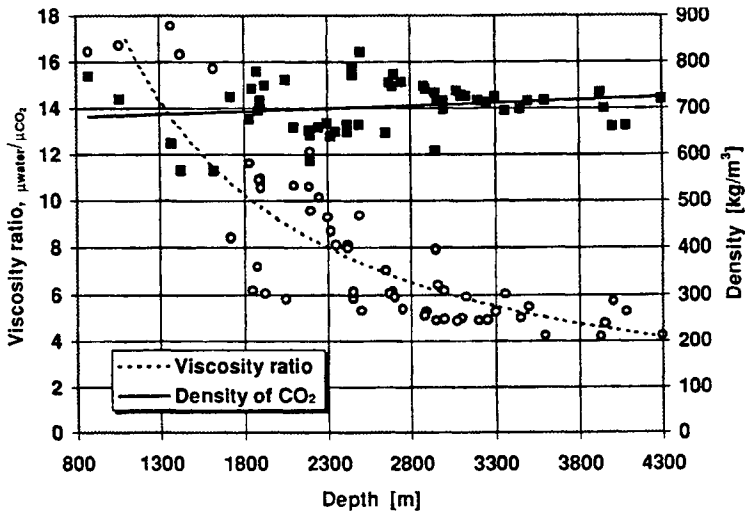


FIG. 3. Viscosity and density ratios between water and CO₂ for 63 different North Sea formations, illustrating the low viscosity of supercritical CO₂ and higher density (from Lindeberg and van der Meer, 1996).

not miscible with water. Therefore, the properties of supercritical CO₂, including density, viscosity and miscibility, have a profound effect on its behavior in candidate aquifers saturated with water and in oil and gas reservoirs containing water as well as other fluids. For example, the supercritical CO₂ phase injected in an aquifer below approximately 800 m will exist as a separate phase that is less dense than water and will rise from an injection point and gravity segregate along the top of the aquifer (Fig. 3).

The following deliberations focus on the geohydrologic characterization, injection behavior, and long-term containment of supercritical CO₂ for storage in aquifers and reservoirs. The section will emphasize the physics of fluid flow in heterogeneous formations. Important ties of geohydrologic processes to the geochemical (e.g., formation of carbonate minerals) or geomechanical (e.g., fracturing) behaviors of the systems will be discussed later. In addition to process-based research in geochemistry, geomechanics, and the physics of flow, site-specific data from reservoirs or aquifers will be required to flesh out numerous important issues concerning CO₂ sequestration. Thus, case studies will be an important element of future research.

Early industrial practices for sequestering CO₂ in geological formations are based on many years of proven experience injecting supercritical CO₂ for enhanced oil recovery (EOR) (Orr and Taber, 1984; Blunt *et al.*, 1993). As of January 1998, about 179,000 barrels/day (28,460 m³/day) of oil were recovered using CO₂ injection in about 66 projects (Moritis and Guntis, 1998). Typically, it takes 4–10 MCF

of CO₂ to recover a barrel of oil (17 Mcf = 1 ton of CO₂). Most of the CO₂ is being injected in West Texas, where several large pipelines bring CO₂ from natural occurrences in New Mexico and Colorado to the Permian Basin fields. The current capacity of major pipelines is about 1.25 Bcf/day (35.4 Mm³) or about 20,000 tons/day of carbon—about 0.6% of the U.S. daily carbon emissions in 1990 due to fossil fuel burning. By replacing existing CO₂ injections, which are essentially all natural CO₂, with CO₂ now being emitted to the atmosphere there would be a measurable but modest effect on overall CO₂ emissions. Since some production of CO₂ with the oil is inevitable, most projects reinject significant quantities of CO₂ over a project's life. The fraction of CO₂ retained in an oil field after a project is complete can vary considerably, but it is certainly a significant portion of the CO₂ purchased for injection.

The efficiency of a CO₂ enhanced oil-recovery flood depends strongly on the equilibrium phase behavior of mixtures of CO₂ with the oil (Blunt *et al.*, 1993; Orr *et al.*, 1995). When the CO₂ is dense enough, it is a solvent for some hydrocarbons in the oil. As the injected CO₂ flows through the reservoir rock, components in the oil are extracted into the CO₂, and some of the CO₂ dissolves in the oil and water that is inevitably present. If the pressure is high enough, the partitioning of hydrocarbons into the CO₂—coupled to the flow at different velocities of CO₂-rich and oil-rich phases—can create mixtures that pass close to the critical locus for the CO₂/hydrocarbon mixtures. Mathematical analysis (similar to that applied in chromatography theory) has proved that essentially 100% of the oil present in a one-dimensional porous medium can be displaced (in the absence of dispersive mixing) if the pressure exceeds the so-called “minimum miscibility pressure” (MMP), which depends on the composition of the oil and the temperature (Orr *et al.*, 1995; Wang and Orr, 1998). The MMP is the pressure at which CO₂ readily dissolves in the oil and the interfacial tension between oil and CO₂ becomes small. Real displacements always include some dispersion, but even then, it is theoretically possible to displace more than 90% of the oil in the zone swept by CO₂ if the pressure exceeds the MMP (Fig. 4). Efficiencies in the field are significantly lower, especially when a reservoir has strong heterogeneities or is heavily fractured. When paths of high permeability or fractured rock connect injectors and producers, significant channeling and cycling of CO₂ from injection to production wells may occur (Tchelepi and Orr, 1994). This leads to an undesirable, early breakthrough of injected CO₂ and large amounts of unwanted CO₂ production.

Injection of CO₂ for enhanced oil recovery is equally applicable in sandstone and in carbonate reservoirs. A primary consideration is whether the reservoir is deep enough so the pressure is above the MMP for the oil at the reservoir temperature. (Of course, this is not an issue for CO₂ sequestration.) If the pressure has been lowered in the reservoir (e.g., by depletion), it may be possible to raise the pressure again by water injection, for example, as long as there is not a large gas cap or aquifer. CO₂ is attractive for injection into relatively low-permeability reservoirs because the low CO₂ viscosity allows pumping at a greater volumetric rate than water. In

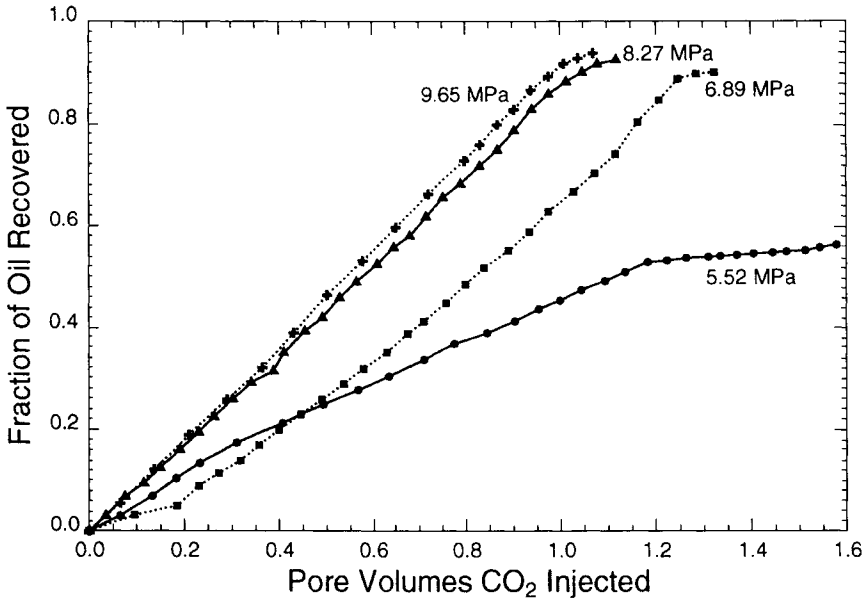


FIG. 4. Recovery of oil by CO₂ injection in an ideal flow setting. Displacement efficiency increases with displacement pressure when a Permian Basin crude oil is displaced by CO₂ in a nearly one-dimensional flow setting (a long tube packed with small glass beads). More than 90% of the oil is displaced by the CO₂ when the pressure exceeds about 7 MPa, the MMP for this oil at the displacement temperature of 32°C (from Orr *et al.*, 1983).

order for the use of CO₂ for EOR to be economic, the reservoir must be large enough to justify the cost of pipeline, injection well, and CO₂ separation facilities.

2.2. Reservoir Identification and Characterization

Injection of CO₂ for storage in reservoirs or aquifers is not inherently different from water (secondary recovery) or EOR injection in oil reservoirs. Primary flow characterization issues include preinjection fluid pressure and composition as well as thickness and permeability that determine the rate of injection, pressure buildup at the injection well, and changes in the stress field. Equally important are porosity and reservoir/aquifer volume, permeability heterogeneity affecting what fraction of the aquifer can be reached by injected CO₂ and how far the injected CO₂ propagates, and the location and character of faults and fracture systems. Although existing methods can be used to investigate many of these site-characterization questions, the currently achievable resolution appears to be inadequate.

The characterization problem will differ with reservoir and aquifer type. Oil and gas reservoirs will be much better characterized than aquifers. Reservoirs have a

record of production history, well tests, and seismic and other geophysical data, as well as many existing holes that can be used for additional characterization activities. On the other hand, aquifers can provide significantly more space for storage. A potential optimal solution is a well-characterized reservoir overlying a large aquifer. Characterization information from the reservoir could be projected into the surrounding (underlying) aquifer. Since reservoirs have already demonstrated long-term integrity, the underlying aquifers should also have this property.

One of the most important geohydrologic issues is the identification of candidate subsurface reservoirs and aquifers. What characteristics, especially geological characteristics, define the best candidates for CO₂ storage? Is it, for example, depth, lithology, or proximity to CO₂ generators? A detailed answer to this question depends on the research outlined in this paper, especially in geochemistry and geomechanics, but there are two clear factors: depth and the nature of the pressure confinement. The deeper the reservoir or aquifer, the higher the pressure and the larger the mass of CO₂ stored per unit volume (at the cost of the compression of CO₂, which will generate more CO₂ if fossil fuel is used to drive the compression). Whatever the depth, underpressurized reservoirs and aquifers provide additional incremental storage capacity for injected fluids. Underpressures can be statically maintained by seals (Demming, 1994; Bradley and Powley, 1994; Ortoleva *et al.*, 1995; see Section 4: Geomechanics), transient dynamic hydrologic processes (Bredehoeft and Hanshaw, 1968; Neuzil, 1995), or simply topographically driven flow systems (Toth, 1962; Neuzil, 1995). Distinguishing among these possibilities will be important for assessing long-term confinement.

2.3. Injection

Geohydrologic issues associated with CO₂ injection start at the wellhead and then move with the injected fluid as it migrates into the aquifer or reservoir until it finds a storage place in the pore space as a separate fluid, dissolved in water, or until it is converted into a mineral. Two fundamental questions must be answered: (1) How far does the CO₂ travel? and (2) What happens to it when it gets there, particularly when viewed on the scale of hundreds of years?

Whichever form—fluid, dissolved, or precipitate—storage will take place in the primary, intergranular porosity, i.e., the spaces between the grains. The numerical value of the primary porosity represents the proportion of a volume occupied by this space. It can vary from a small percentage in deeply buried and diagenetically altered sandstone to almost 50% in shallow, unconsolidated sand. The porosity is determined by the depositional environment (e.g., as it affects sorting) and subsequent diagenesis and compaction, as described further in the Geochemistry and Geomechanics sections of this chapter. The organization of the pore space also determines the permeability, which controls the movement of fluids. Primary

porosity is usually viewed as a tortuous network of larger pore bodies connected by narrower pore throats (Fig. 5, see color insert). Most of the storage volume is in the pore bodies. Pore throats play the major role in permeability since they determine pore-space connectivity.

Diagenetic precipitation or solution of minerals in the pore space has, more or less, a linear effect on storage (e.g., volume of rock dissolved or precipitated equals volume of storage gained or lost, respectively). However, the precipitation or solution of minerals in the pore throats results in strongly nonlinear changes of permeability. Both precipitation and solution are possible in the presence of dissolved CO₂, depending on the chemistry and minerals present.

A major geohydrologic issue is the natural spatial variability or heterogeneity of permeability, porosity, and other rock properties (Gelhar, 1993; Dagan and Neuman, 1997). In homogeneous rock (e.g., Berea sandstone), permeability ranges over two orders of magnitude, while seven orders of magnitude is not uncommon in typical heterogeneous sandstones (Fig. 6, see color insert). Carbonates show more spatial variation of properties, and fractured systems are often even more heterogeneous. Because of the depositional, diagenetic, and stress history, natural heterogeneity is usually geometrically organized, such as in layers, and can be described using geostatistical and geological models. With geometrically organized heterogeneities, zones of flow and high permeability create preferential flow paths or channels if the heterogeneities are sufficiently correlated in layers or other structures. As a result, not all portions of an aquifer or reservoir are accessible to injected fluids, which can diminish the volume of CO₂ that can be stored.

Permeability and porosity will change with time and space as a consequence of CO₂ injection and storage (or prior oil or gas production), for both geochemical and geomechanical reasons. Usually, the result will be a reduction of permeability and porosity, making transport and storage of CO₂ more difficult. Because of the presence of different minerals on the pore scale and because of larger scale heterogeneities on the aquifer/reservoir scale, precipitation and dissolution may occur simultaneously in adjacent portions of the pore space or aquifer/reservoir.

Injection of CO₂ into reservoirs or aquifers presents several special flow problems, many of which have already been addressed by the community using CO₂ for EOR. Because CO₂ has relatively low viscosity (a few hundredths of a centipoise) no matter what the injection conditions, hydrodynamically unstable displacement will occur. In a homogeneous porous medium, displacement of a viscous fluid by a less viscous one leads to "viscous fingering" in which fingers of low viscosity fluid penetrate the high viscosity fluid rather than displacing it uniformly (Homsy, 1987; Fig. 7, see color insert). It is now known, however, that in many if not most oil reservoirs and aquifers, the distribution of permeability dominates the formation of viscous fingers (Tchelepi *et al.*, 1993; Tchelepi and Orr, 1994). The low viscosity CO₂ easily finds the preferential flow paths. In effect, the permeability distribution creates the paths in which fingers develop. This situation is often

called “channeling.” Thus, permeability heterogeneity can reduce substantially the fraction of a reservoir or aquifer that can be swept by the injected CO₂ in a reasonable time (Fig. 8). In an EOR application, adequate characterization of the spatial distribution of permeability within an oil reservoir is important to predicting CO₂ flood performance or sweep efficiency. CO₂ is usually lighter than oil and always less dense than water, so gravity segregation of the injected CO₂ also contributes to reduced sweep efficiency (Tchelepi and Orr, 1994).

In a water-filled aquifer, supercritical CO₂ will be displacing an immiscible water phase. Even in the absence of viscosity or gravity effects, displacement will be inefficient because of capillary effects caused by the relatively high interfacial tension between CO₂ and water. The water usually is more wetting, and the CO₂ displacement will prefer larger pore spaces. This is the same space preferred by single-phase viscous flow and by viscous fingers of CO₂ displacing water. Capillarity amplifies the effects of heterogeneity, with CO₂ bypassing large volumes of tighter rock, further reducing sweep efficiency.

Viscous, gravity, and capillary forces act together in a heterogeneous rock to create channels of preferred flow in higher-permeability materials with large bypassed zones in between. Since the objective is to sequester CO₂ rather than use it to drive oil, sweep efficiency may not be an important issue: it matters less where the CO₂ goes as long as there is sufficient volume available at reasonable injection pressure and the CO₂ stays in the reservoir or aquifer. If fluid is not being withdrawn from the aquifer (to create volume, for example), then cycling of CO₂ through high-permeability flow paths is less important. As discussed later, it only appears to be an issue when chemistry is considered and may even be advantageous for delivering large amounts of CO₂ far from the well.

Transport of CO₂ along the preferred flow paths will be relatively quick, especially when the paths are composed of open fractures, with a much slower transfer of CO₂ from these paths to the surrounding bypassed zones. If the material around the preferred flow paths is composed of much finer pores, supercritical CO₂ will have difficulty penetrating the tighter porous rock matrix where storage will take place, especially because capillary forces may limit penetration. If the CO₂ is dissolved in the aqueous phase it will enter the surrounding rock by diffusion (if the permeability contrast is not large) and by cross-flow. In any event, the time scales for chemical reactions will be completely different in the fast paths and the bypassed zones because the supply of reactants will be controlled by different processes. The large-scale kinetics of interaction between the fast paths and bypassed zones will be determined by their contrasting properties, configuration, and relative size and frequency. Only in this sense does it appear that the details of heterogeneity and preferred flow become important. Ideally, the chemistry might be arranged such that precipitation of carbonates occurs in the bypassed zones, while transport is maintained or even enhanced by dissolution along the preferred flow paths.

Fractured porous rock represents a special case of heterogeneity, with an interaction potential between matrix rock and fractures depending on the size distributions of the matrix blocks and fracture apertures, and the fracture connectivity. Storage in the fractures themselves is often negligible. The conceptual view of this process requires the consideration of large rock volumes in order to invoke continuum concepts like porosity. In the standard “double porosity” model of naturally fractured systems, all large-scale flow is assumed to take place in the fracture network, while the matrix blocks provide the storage. Communication between the two is due to local cross-flow, caused by pressure gradients between the isolated matrix blocks and the surrounding fractures or, in the case of dissolved CO₂, by diffusion. The next most sophisticated model assumes that there is also some net flow through the matrix blocks. This “double permeability model” is appropriate when the permeability contrast between matrix and fractures is small. These multiple porosity models fail, however, when the number density of fractures drops and the continuum hypothesis is no longer valid. Discrete fracture models are then used if the geometry of the fracture network is represented explicitly. The difficulty with this approach lies in determining the location, connectivity, and properties of the fractures that are parallel characterization issues in geomechanics and geophysics. Natural fracture porosity could move significant amounts of CO₂ from an injection site to storage locations in matrix blocks far away. Single-phase flow in fractured systems is not well understood if alterations of fracture geometry and connectivity by stress or chemistry are considered, and much less is known about multiphase flow in fractures, such as would occur with supercritical CO₂ displacing water.

CO₂ could also be injected into shallower aquifers and reservoirs (Fig. 9, see color insert). Depending on the salinity, significant amounts of CO₂ can be dissolved in water—enough to increase its density by as much as several percent (Bachu *et al.*, 1996). However, viscosity would effectively be unchanged. One major disadvantage of this option is the much larger volumes of fluid that would need to be injected to store the same amount of CO₂. Following injection in an aquifer, the pore space would continue to be saturated with water. The resulting single fluid phase flow would be determined by the permeability of the aquifer and the composition, temperature, and pressure of the water as it affects viscosity and density. There would be no viscous fingering. Preferred flow paths and bypassed zones would still be issues, but would be determined by the permeability heterogeneity with no contributions from viscous fingering or capillarity. Density gradients would continue to be significant and produce a tendency for water to segregate by gravity along the bottom of the aquifer. If the bottom were sloped, then a dense plume of CO₂-saturated water would tend to move deeper into the subsurface. This same principle is used to support one of the ocean-disposal options for CO₂, and could limit the need for an overlying seal in aquifers.

Mathematical modeling of CO₂ injection performance for all kinds of reservoirs (including coal) must consider cross-coupling of geochemistry, geomechanics,

flow, and transport—this will be referred to as RTM (reaction, transport, mechanics) modeling. Over the last 30 years, considerable effort has been expended to build and improve flow and transport models of oil recovery CO₂ flood performance at the reservoir scale. Although these models often ignore chemistry and mechanics, many issues of these models also apply to the CO₂ storage problem. This experience suggests three essential components for accurate field-scale predictions for CO₂ storage in aquifers and reservoirs:

1. Accurate representation of capillary pressure behavior and phase equilibria of CO₂/hydrocarbon/water systems with an equation of state to determine local displacement efficiency
2. Accurate description of the spatial distribution of permeability (which strongly influences the fraction of the reservoir or aquifer swept). The difficulty in acquiring detailed reservoir description data is often the limiting factor in reservoir EOR performance predictions. Careful use of geostatistical descriptions can help but cannot eliminate problems because of sparse sampling of reservoir properties.
3. Flow simulations performed on a computational grid fine enough to resolve heterogeneities and any gravity segregation that occur. The computational costs associated with very fine grids have induced considerable research on ways to compute average properties that can be used on a coarser grid, with limited success for multiphase flow.

The foregoing components should be part of an RTM modeling approach simulating the movement of CO₂ away from the injection points to storage locations, where mineral trapping might occur. Coupled modeling also creates the opportunity to address related questions:

- How do the natural aquifer/reservoir heterogeneities influence the location and nature of mineral trapping?
- Do the mineral-trapping reactions plug the preferred flow paths, especially fractures?
- Or, as plugging occurs, does CO₂ injection drive the formation pressure to the threshold for fracturing?

2.4. Long-Term Containment, Monitoring, and Integrity of Seals

Gravity segregation will bring supercritical CO₂ upward until it meets a seal at the top of the aquifer or reservoir. Not much is known about the long-term integrity of seals, even in oil and gas reservoirs. In general, seals have much lower strength than the rock they overlie, and it is not clear how they will react to the changing stress and chemical conditions that follow CO₂ injection (see Geochemistry and Geomechanics sections). By definition, no seal is perfect; they all leak. It is only a matter of time. Trapped oil and gas reserves prove that the time can

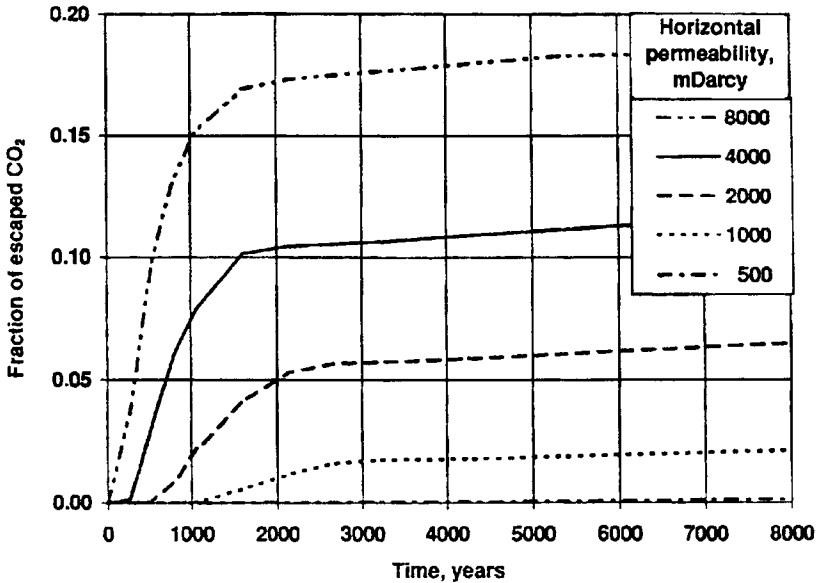


FIG. 10. Simulated CO₂ escape curves from a large but finite, horizontal, homogeneous aquifer. The boundary is 8000 m from the injection well. The CO₂ accumulates under the seal and slowly migrates under gravity toward the boundary, where it escapes. The rate of escape depends strongly on the horizontal permeability. There is no fingering in this simulation (from Lindeberg and van der Meer, 1996).

be very long indeed, but the many dry reservoirs that leaked off long before they were drilled demonstrate that leakage is the rule. Slow leakage of CO₂ to adjacent, overlying formations may be of no consequence, particularly if those formations are other deep saline aquifers. Slow leakage that returns CO₂ to the atmosphere is unacceptable because it defeats the purpose of disposal. Catastrophic leakage is unacceptable. What is needed is systematic investigations of what constitutes a good seal ("trap"), on one hand, and seal failure modes, on the other, over the time scales of interest for CO₂ sequestration (Fig. 10). The Geochemistry and Geomechanics sections review these issues. However, one aspect that those sections do not treat is sealing mechanisms. A pressure seal blocks all pore fluid movements over "substantial intervals of geologic time" (Neuzil, 1995). A capillary seal functions by a wetting fluid preferentially occupying the fine-grained pore space of the seal (e.g., shale), thus preventing the movement of a nonwetting fluid (Revil *et al.*, 1998). Of importance is the absence of methods for evaluating the sealing potential of aquifers (for example, significant under- or overpressures or anomalous water chemistry). This raises additional characterization issues for aquifers and reiterates the need for site-specific data and case studies.

Monitoring of injection and long-term integrity will involve a combination of monitoring wells completed in the storage reservoir or aquifer and in overlying

units. Monitoring will have to rely heavily on geophysical techniques. In abandoned oil and gas reservoirs, other wells can be used to monitor performance, but in aquifers, the number of monitoring wells will be limited. Conventional monitoring of injection pressures will be essential, while samples of fluid composition would help track the progress and nature of the displacement. Seals are usually inferred by observing large differences in pressures (Bradley and Powley, 1994) or chemistry across strata. During and after injection, additional holes could be drilled and cores extracted to track the progress of mineral trapping.

2.5. Issues of CO₂ Disposal in Coal Beds

A potentially attractive option for CO₂ sequestration is coal beds. CO₂ would be injected into buried and fractured coal seams, bounded by lower-permeability sediments. Coal has a greater affinity for CO₂ than for methane (CH₄). This adsorption is a self-stabilizing (antifingering) process and mitigates the effects of preferred flow paths caused by heterogeneity and fractures (called cleats in coal), resulting in high sweep efficiencies. Thus, CO₂ is stored efficiently within the coal seam, with breakthrough occurring only after filling most of this storage. Since storage is likely to take place at depths shallower than those for supercritical CO₂ injection, it is important that the probability for release to the surface be low. Therefore, a critical element is the integrity of the confining beds bounding the coal seam. In spite of some apparent advantages, CO₂ sequestration in coal beds entails several major uncertainties. These include the fundamentals of desorption and adsorption processes (CH₄ vs CO₂), wettability, moisture content, temperature, the geometry and characteristics of the fracture network, the flow through the network, and the effects of changing stress on all of these.

Desorption of the gas from the coal is controlled by the hydrostatic head of the aquifer (McElhiney *et al.*, 1989), but also appears to vary nonlinearly with pressure. By dewatering the coal seams, the pressure is reduced and methane is desorbed from the coal. After desorption, the methane diffuses through the coal into the cleat system and flows to the production well. For example, Bumb and McKee (1988) found that a 70% reduction in external pressures was required before 25% of the absorbed methane was released from the Mary Lee coal group in the Warrior Basin, Alabama.

If coal-bed methane reservoirs have been reflooded with water after production, it becomes important to understand the effect of coal wettability to CO₂ and other reservoir fluids on coal-seam permeability and relative permeability. Satisfactory history matches for water and gas flow in coal-reservoir simulations appear to suggest that it is acceptable to treat coal as water-wet. However, on the field scale, a coal seam is made up of coal interbedded with shale and other impurities that

may mask the true wettability properties of the coal. On the laboratory scale, a coal sample will consist of a heterogeneous mixture of organic and inorganic (i.e., mineral matter) components. The organic components of coal are generally expected to be more hydrophobic than the mineral matter components (Nelson, 1989). Additionally, the distribution of minerals in a cleat is important in terms of the wettability of the cleat surfaces. If the flow paths through the cleat cross over the carbonate minerals, these sites in the cleat would be hydrophilic (i.e., water-wet). Coal cleats with some mineralization would probably have a composite wettability, implying that some sites on the cleat surface would be hydrophobic and others would be hydrophilic.

By definition, the wetting phase consists of a fluid making a contact angle of less than 90° with a solid and another fluid (Scheidegger, 1974). The organic components of coal include varying amounts of paraffinic, naphthenic, and aromatic hydrocarbons. The contact angle of water on paraffin in air is 112–114° (Adam, 1964), i.e., the paraffin is hydrophobic and the water is nonwetting. Measurements of the contact angle of water on coal in air have yielded values ranging from 30° (Arnold and Aplan, 1989) to 132° (Surinova and Polushkin, 1987), and the water ranges from wetting to nonwetting. Therefore, it is uncertain what inferences can be drawn about the wettability of coal surfaces from measurements of air–water–coal contact angles and whether these wettability data can be extrapolated to reservoir conditions where the coal would not have been altered by aerial oxidation and where the second fluid is methane rather than air. Aerial oxidation would increase the overall wettability of the coal surface (Nelson, 1989). Given the present state of knowledge, the wide range of contact angle values reported for water on coal in air are caused by variations in (1) oxygen functionality of the organic component of the coal surface, (2) the mineral matter content of the coal surface, (3) impurities, (4) porosity, and (5) surface roughness (Arnold and Aplan, 1989). Conclusions about the wettability of coal surfaces from air–water–coal contact angle measurements may be misleading, unless both the physical and chemical composition of the coal surface and the experimental conditions under which the measurements were made are known.

Critical elements for coal-bed sequestration will be the understanding of ubiquitous cleat systems in coal and the integrity of the confining beds bounding the coal seam. Cleats are naturally occurring fractures that provide the permeability necessary for fluid (i.e., gas and water) flow. As in other reservoirs (see the Geomechanics section), the geometry and distribution of void spaces in the cleat system will control the overall permeability of coal. Complications may arise from changes in reservoir permeability over time as injection of gas occurs and the coal begins to swell (Harpalani and Zhao, 1989). During methane production, losses of volatiles caused by desorption (Briggs and Sinha, 1933; Moffat and Weale, 1955) results in volumetric shrinkage of the coal matrix and a possible increase in

fracture apertures. Conversely, during gas or CO₂ injection, the net confining pressure within the reservoir system will decrease to alter the geometrical properties of the cleat network. Knowledge of the impact that the change in net stress has on cleat permeability is essential for accurate simulations of CO₂ injection potential of coal reservoirs. The role of fractures and the dependence of cleat permeability on stress have been treated more prominently in coal-bed analyses than in oil and gas reservoir simulations. Several of these aspects will be discussed later in detail from the viewpoint of geomechanics.

The importance of cleats suggests the need for research on remote characterization concerning cleats and cleat systems. Pyrak-Nolte *et al.* (1997) and Montemagno and Pyrak-Nolte (1999) used x-ray computerized tomographic (CT) imaging to obtain quantitative aperture data for three-dimensional interconnected fracture networks in coal. This work revealed that the aperture distribution of the networks was spatially anisotropic and dependent on the number and geometry of the individual fractures. Void area in the individual fractures ranged between 45 and 58%, while total volumetric porosity of the samples was on the order of 0.1%. A three-dimensional, autocorrelation analysis on the fracture network and a two-dimensional analysis on the individual fractures found that the apertures were correlated over distances of 10 to 20 mm in the direction of flow. Further research is needed to determine how the aperture distribution and connectivity of the fracture network (and thus, the relative permeability) in coal is affected by gas adsorption, which produces swelling in coal. In addition, research is needed to determine how laboratory results can be used on the field scale if apertures are only correlated over 10 to 20 mm.

3. GEOCHEMISTRY

3.1. Introduction

A useful way of identifying key issues in connection with CO₂ sequestration is to begin by considering the simple model problem of injecting CO₂ into a closed mineral/fluid system and to ask how well can we predict its subsequent evolution. Initial conditions need to be specified and a minimum characterization at $t = 0$ will involve pressure, temperature, fluid fraction and solute chemistry, and mineral fractions including their spatial distribution. The ability to calculate the state of the system at long times requires thermodynamic data, and for this there exist a number of software packages (e.g., EQ3/6 maintained by Lawrence Livermore National Laboratory) believed to be quite adequate for present purposes. Although the final state of the system can in many cases be calculated with reasonable confidence, predicting the path and rate by which the system evolves to this final state is extremely problematic. The main source of uncertainty derives from our inability

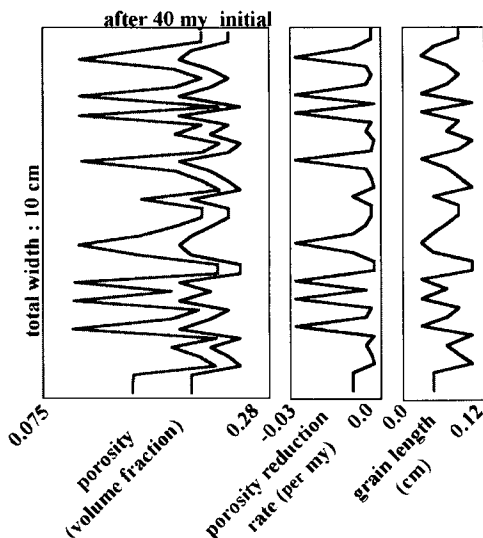
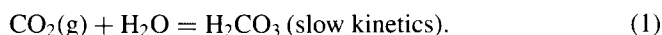


FIG. 11. Enhanced heterogeneity resulting from coupled pressure-solution and diffusive mass transfer. Initial heterogeneity is due to differing quartz volume mass transfer. Changes in heterogeneity are caused by varying rates of pressure-solution associated with grain sizes and porosity. In carbonate systems similar processes can occur three to five orders of magnitude faster due to greater kinetic reaction rates of carbonate minerals (modified from Park and Ortoleva, 1999).

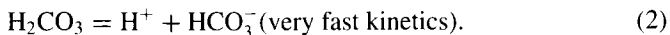
to realistically specify the kinetics of the various homogeneous and heterogeneous reactions that take place (Fig. 11).

Uncertainties in the rates of reactions expected to take place following CO₂ injection severely limit our present ability to predict the ultimate storage capacity and storage integrity of natural reservoirs associated with trapping injected CO₂ by the precipitation of carbonate phases. Several potentially important trapping mechanisms are discussed, and some indication is given as to whether the key reactions are expected to be fast or slow. However, quantitative statements regarding the effectiveness of any given trapping mechanism requires realistic kinetic information, but such information is not currently available for anything but the very simplest of situations.

Beginning with a simplified approach that focuses on geochemical reactions, we can examine elements of the sequestration problem by following the evolution of CO₂ upon injection into the subsurface and resulting physical displacement of the existing pore fluids. Figure 12 shows that CO₂ injection initiates a complex network of reactions that involve aqueous solutions and host rock minerals. First, CO₂ transfers across the gas–water interface to become an aqueous ion by the reaction



This is followed by rapid dissociation of carbonic acid



The formation of bicarbonate ion, HCO_3^- , and production of acidity by release of H^+ leads to a series of secondary reactions with complex feedbacks that buffer solution properties and mineral reactivity. These reactions greatly complicate estimates of CO_2 storage volumes as well as the geophysical characteristics of the host rock. However, it is these same reactions that suggest land disposal may have an enormous capacity for the safe, long-term sequestration of CO_2 by the same mechanisms that nature has employed for millennia on a global scale. The following discussion addresses the probable fate of this aqueous CO_2 from the point of view of geochemical thermodynamics and kinetics.

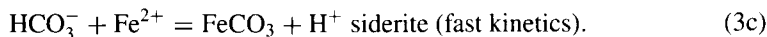
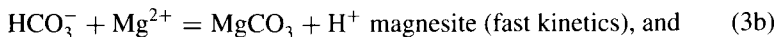
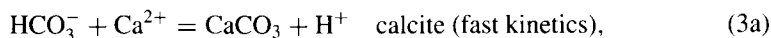
There are at least three ways in which CO_2 can be sequestered in subsurface processes involving chemical reactions, as shown in Fig. 12.

3.2. Aqueous Trapping

In the first mechanism, pore fluids can accumulate dissolved CO_2 by Rxn (1) and (2) through “aqueous trapping.” The pressure (P), temperature (T), and salinity (TDS as total dissolved solids) conditions of most subsurface disposal environments limit CO_2 accumulation by thermodynamic constraints that are well understood in comparison with other uncertainties. Although solubilities are maximized in formation waters with low salinities, generally speaking, pore fluids can hold only a small percentage of HCO_3^- regardless of TDS or the PCO_2 at injection (Bachu *et al.*, 1996). Thus, the capacity of subsurface fluids to capture CO_2 by aqueous trapping is relatively small.

3.3. Mineral Trapping

In a second type of trapping, dissolved CO_2 reacts with divalent cations to form carbonate mineral precipitates. This “mineral trapping” mechanism offers the greatest potential for increasing CO_2 sequestration capacities while also rendering CO_2 immobile for longer time scales (Perkins and Gunter, 1996). Overall reaction stoichiometries for the most common minerals show that carbonate precipitation consumes bicarbonate ion while producing acidity by the reactions



Rates of these reactions are known to be relatively fast but have a complex dependence on reactant concentrations, in situ pH, temperature, and salinity (e.g.,

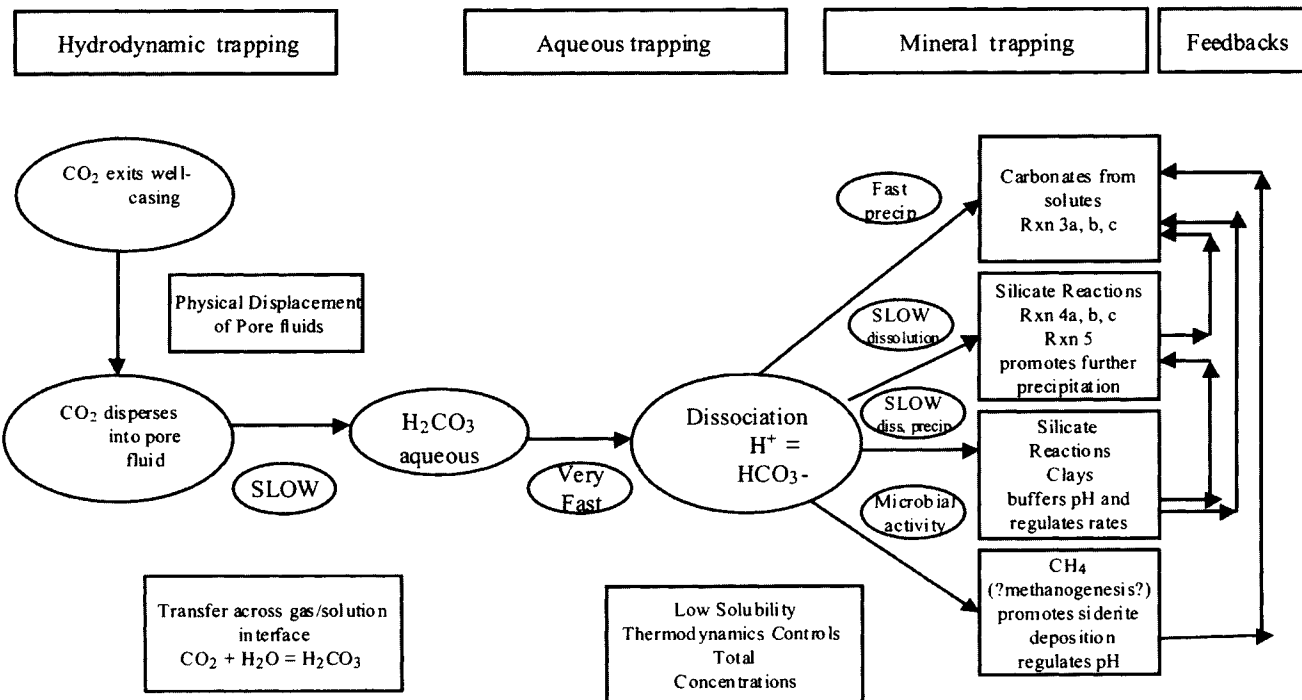


FIG. 12. CO₂ terrestrial sequestration-chemical processes and reservoirs (Dove, unpublished).

Morse, 1983; Zuddas and Mucci, 1998). Dreybrodt *et al.* (1996) and Liu and Dreybrodt (1997) have also shown that an important rate-limiting step for calcite precipitation and dissolution in this kind of system can be Rxn (1). If the host reservoir is initially poor in carbonate minerals, the HCO_3^- concentration is approximately constant and limited by CO_2 solubility; rates of precipitation are primarily constrained by the much larger supply of divalent cations (reactants) and consumption of protons (products). A closer look shows that three general scenarios affect these constraints to control the extent of mineral sequestration: (1) Formation of carbonates by reaction with pore-water solutes, (2) formation of carbonates by reaction with siliciclastic minerals, and (3) formation of carbonates by reaction with carbonate minerals.

3.3.1. Formation of Carbonates by Reaction with Pore-Water Solutes

The reactant cations arise from two sources. First, they can be indigenous to the pore fluids with ratios that are governed by the mineralogy of host formation(s) and concentrations that are approximately covariant with TDS. Zuddas and Mucci (1998) show that precipitation rates increase with solution ionic strengths. However, there is a competing effect where TDS also enhances calcite solubility, particularly at higher temperatures (e.g., Holland and Malinin, 1979). Second, cations can be released by the H^+ -promoted dissolution of silicate minerals. As shown in Fig. 11, reactions that release cations to solution can promote carbonate formation through a feedback mechanism. Quantifying mineral–solution interactions in this dynamic system to predict the conditions that maximize mineral precipitation requires a thorough understanding of carbonate–electrolyte chemistry and ion pairing models for aqueous complexation.

3.3.2. Formation of Carbonates by Reaction with Siliciclastic Minerals

In geologic environments enriched in silicate minerals, the same reactions that nature uses to recycle CO_2 may be employed by analogous reactions in the subsurface (Siefritz, 1990). Biogeochemists have long recognized that CO_2 is returned to the solid earth by silicate weathering and the subsequent deposition of carbonate minerals (e.g., Lasaga, 1981; Dunsmore, 1992). For example, the acidity produced in Eq. (2) is neutralized by promoting silicate dissolution as illustrated by the reaction



Figure 12 indicates that this release of cations further enhances bicarbonate consumption by promoting Rxn (3a) in a feedback mechanism. Similar mineral–water reactions favor additional formation of magnesium and iron carbonates by

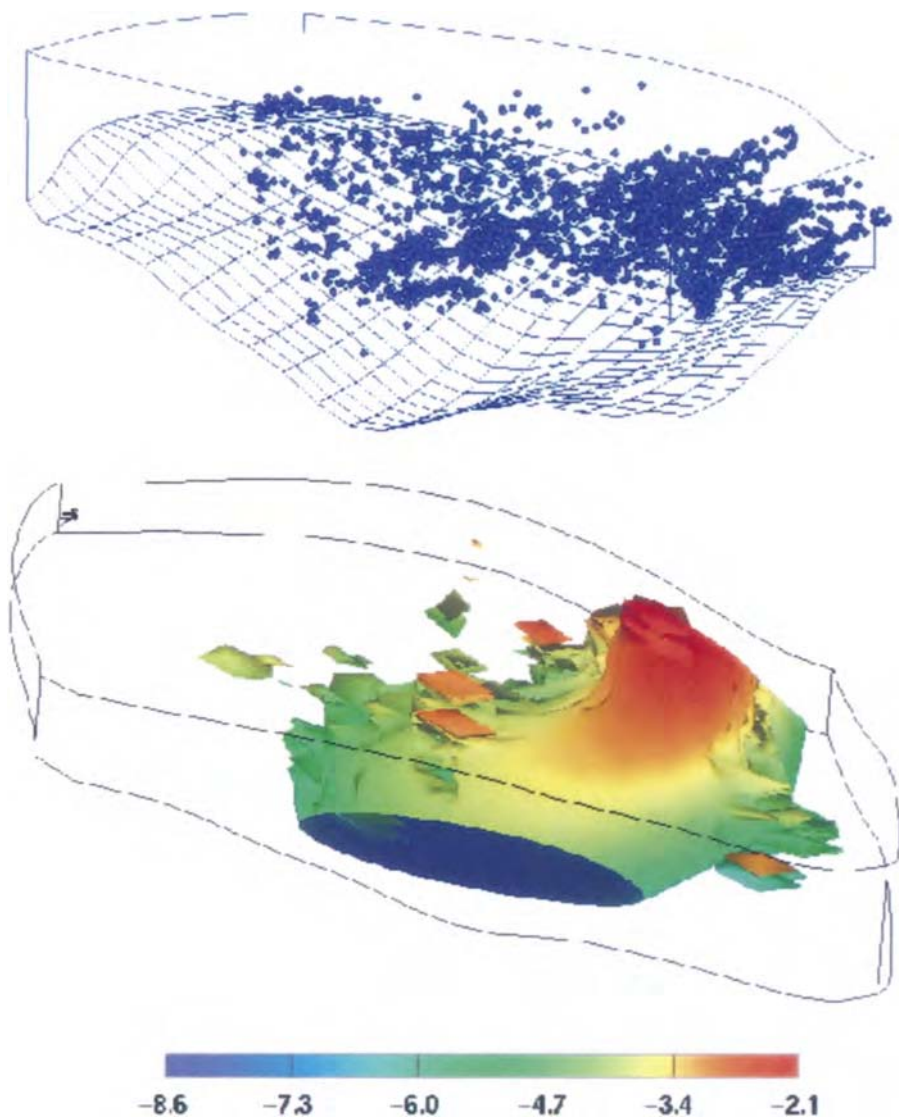


FIG. 2. (a) The three-dimensional view of the Anadarko Basin is seen from the south showing locations where high-quality pressure data are available. Note the high density of data in the deeper zones where compartmentation is generally believed to be most significant (from Ortoleva, 1998; data from Al-Shaieb *et al.*, 1994). (b) Isosurface of 100 kPa overpressure developed from data of frame (a) (from Ortoleva, 1998).

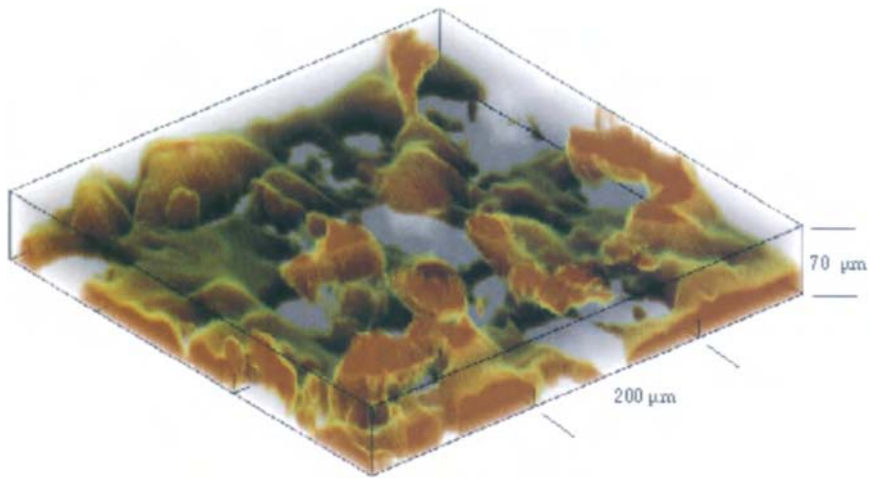


FIG. 5. High-resolution 3D image of pore space in Berea sandstone obtained with Laser Scanning Confocal Microscopy. The pore phase and solid grains are opaque and translucent, respectively. The data illustrate a complex fine-structure including conspicuously thin pore necks and throats connecting the larger (nodal) pore bodies (from Fredrich, 1999).

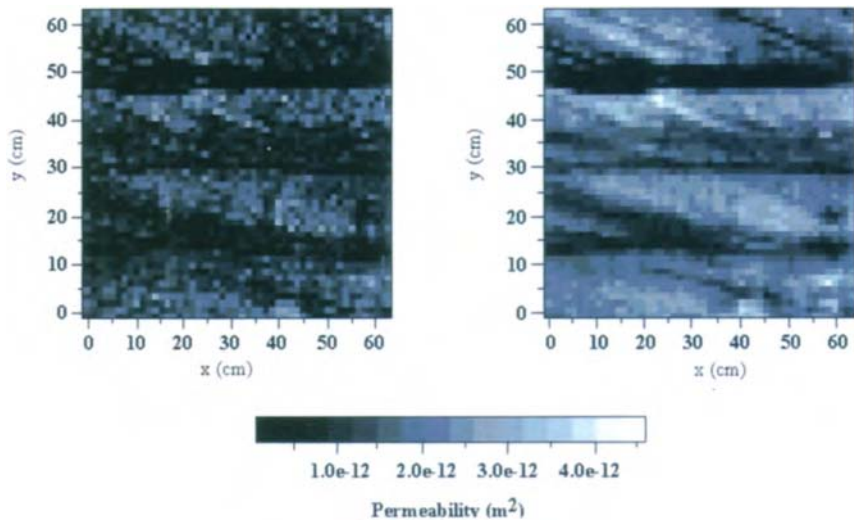


FIG. 6. Not only does permeability heterogeneity vary from rock to rock, it is also a function of the scale of measurement or simulation. Above are two permeability maps, each based on 2,500 individual measurements on one face of a meter-sized block of Massillon sandstone (from V. Tidwell and J. Wilson, personal communication, 1999). The sampling device used for the measurement on the right (b) integrates over a volume 64 times larger than the device used for measurements on the left (a). Note the distinct smoothing.

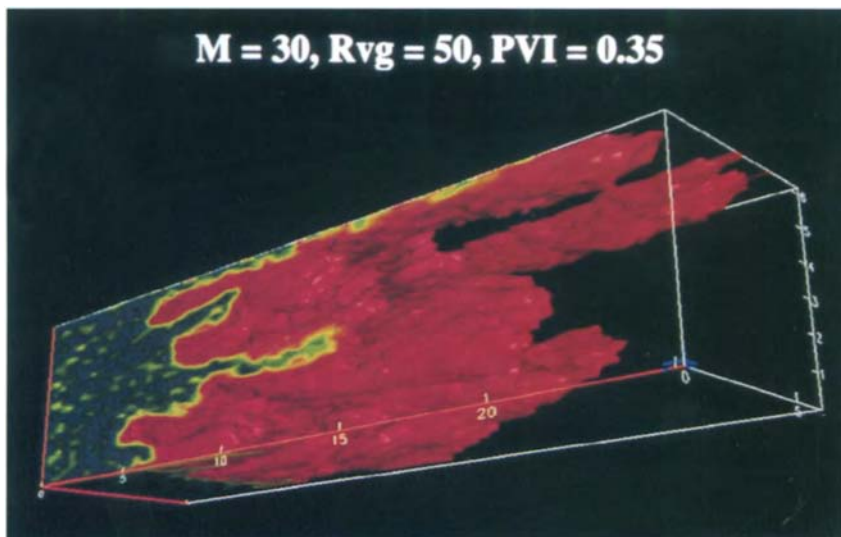


FIG. 7. A three-dimensional view of particle tracking simulations of viscous fingering and gravity segregation in a three-dimensional, homogeneous porous medium (from Tchelepi and Orr, 1994). A CO₂-like low viscosity fluid displaces another fluid 30 times more viscous from left to right. Viscous fingers move rapidly through the zone of low density, low viscosity fluid that forms at the top of the porous medium. Viscous fingers also form lower in the porous medium, but the gravity-dominated preferential flow that occurs at the top of the medium carries more of the low viscosity fluid.



FIG. 8. Calculated flow behavior for injection of CO₂ into a heterogeneous oil reservoir resulting in viscous fingering under the combined effects of gravity and heterogeneity. The lower panel (b) shows the spatial distribution of permeability in the two-dimensional cross-section. The upper panel (a) shows the portion of the reservoir invaded by CO₂. The low-viscosity CO₂ invades the higher permeability zones preferentially, and gravity forces cause the lower-density CO₂ to invade the upper zone as well. Similar behavior will occur in aquifers (K. K. Pande, personal communication).

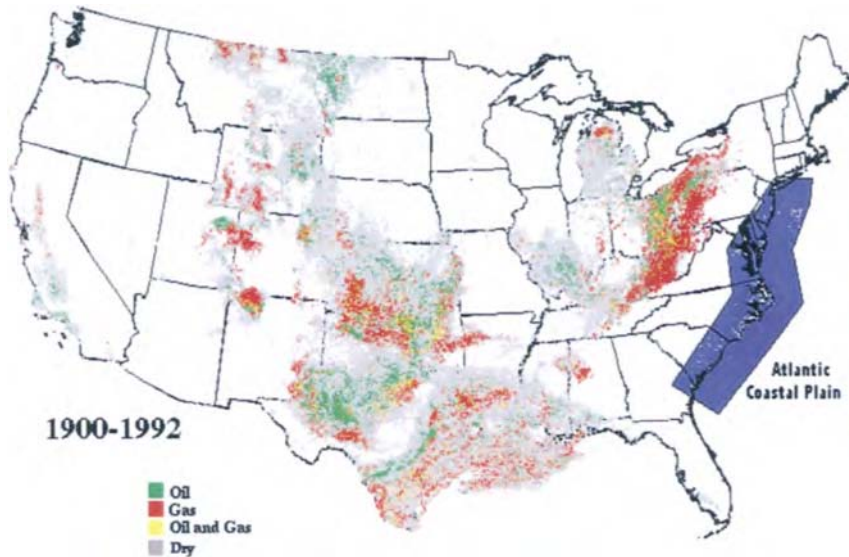


FIG. 9. Map of petroleum wells drilled in the U.S. (lower 48 states) from 1900 to 1992, illustrating the sedimentary basins located over vast portions of the U.S. that could be used for deep injection of supercritical CO_2 . Productive gas wells indicate a formation capable of storing natural gas, and thus also capable of storing CO_2 . Dry wells, especially dry wells close to productive gas wells, indicate that although the geologic interpretation suggests gas storage, natural gas either never developed or it escaped during the formation's history. It may not be possible to successfully sequester CO_2 in these areas. The blue region shown on the east coast indicates the clastic portion of Atlantic coastal plain aquifers that might be used for shallow injection of dissolved CO_2 (from Gautier *et al.*, 1996, modified by J. L. Wilson, 1999).

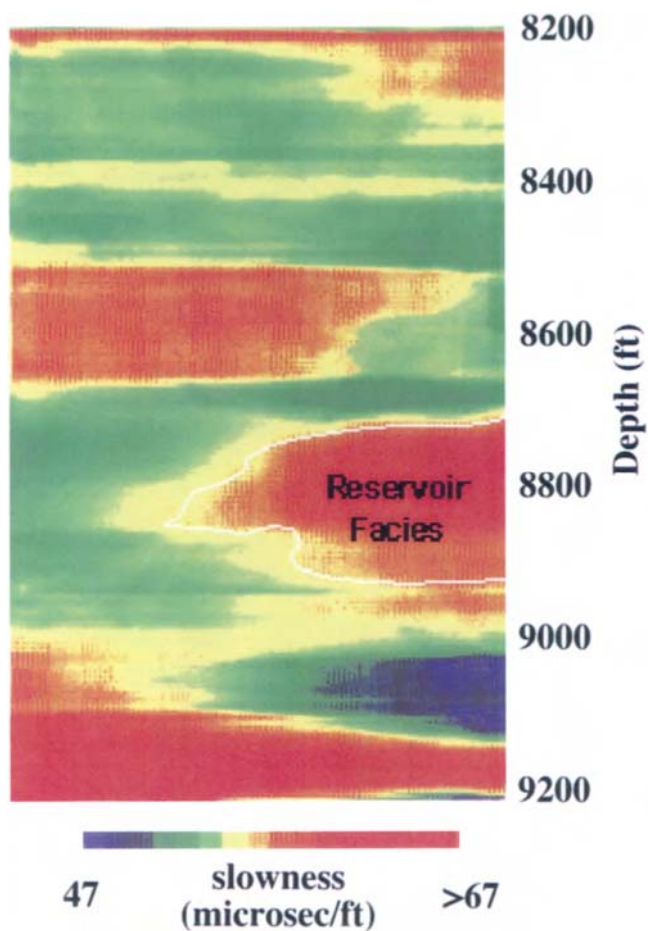


FIG. 39. High-resolution image produced with crosswell seismic tomography (from Langan *et al.*, 1997). The tomogram delineates an oval-shaped low-velocity zone representing a high porosity reservoir facies anomaly. The anomaly can be seen at a depth of approximately 2785–2660 m (8700–8950 ft) in the right hand side of the image. Crosswell methods are potentially capable of producing these high-resolution images in 2D. Research is needed to extend this capability to three dimensions.

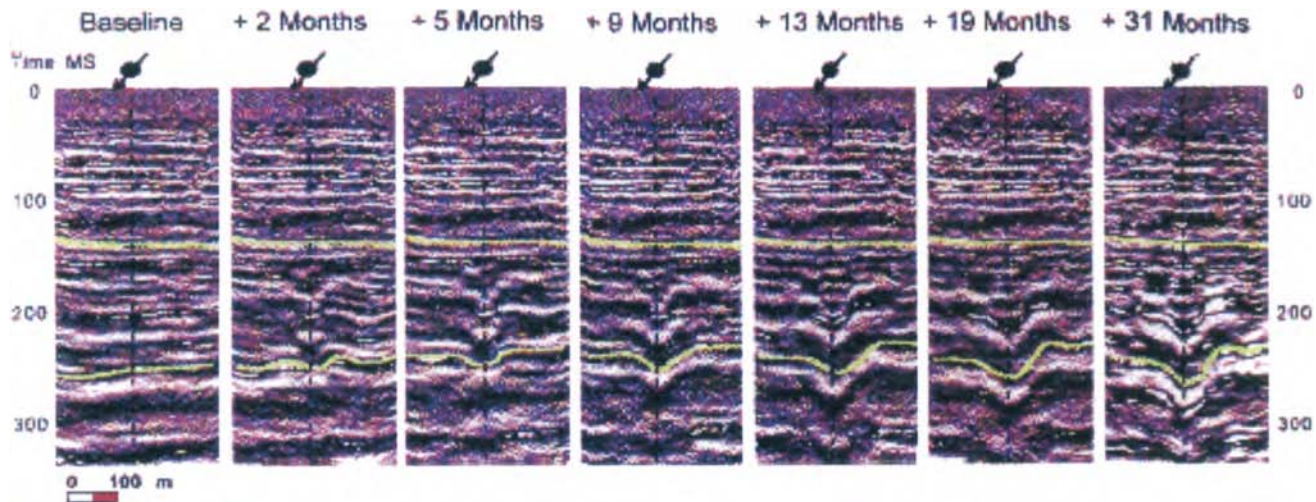


FIG. 40. Vertical sections from 3D surface seismic monitoring of steam injection. The yellow lines delineate the top and bottom of the steam injection interval. While the data do not change above the injection interval, the sag below is caused by the steam (from Jenkins *et al.*, 1997).

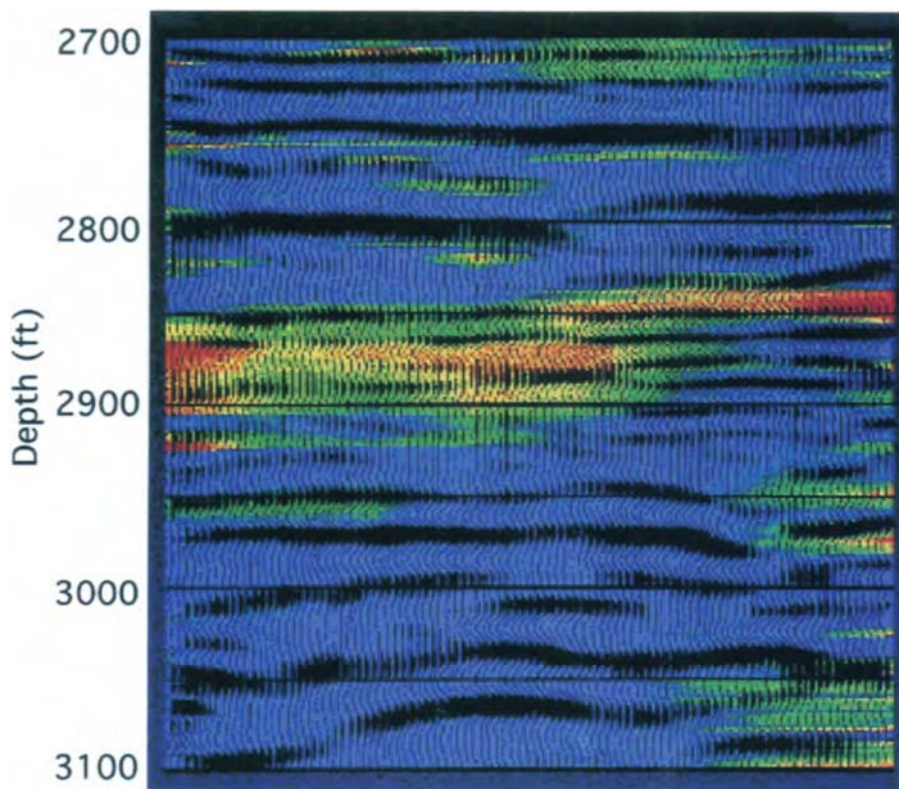


FIG. 41. Crosswell velocity difference tomogram overlaying a crosswell reflection image. The zone flooded with carbon dioxide is delineated by the yellow–red colors at 880–895 m (2850–2900 ft) that indicate a velocity decrease of about 5–10%; blue indicates no change in velocity (from Lazaratos and Marion, 1997).

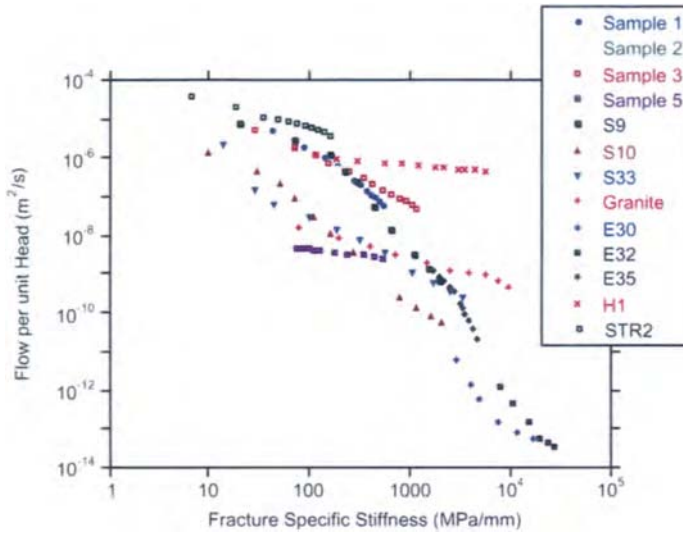
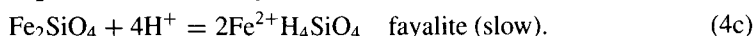
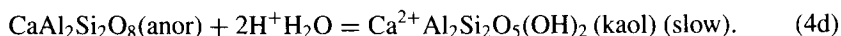


FIG. 42. Observed interrelationship between fluid flow and fracture-specific stiffness for 10 samples each containing a single fracture. The data for 13 samples have been obtained from Witherspoon *et al.* (1980), Raven and Gale (1985), Gale (1985), Gale (1987), and Pyrak-Nolte *et al.* (1987). (From Pyrak-Nolte and Morris, 2000.)

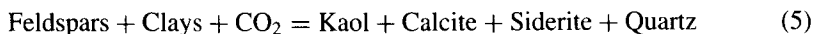
the respective reactions



Gunter *et al.* (1993) concluded that the calcium and magnesium (or other divalent) bearing silicate minerals have the greatest potential for enhancing CO₂ disposal capacities because they also act as enormous proton sinks during dissolution. Building on these simple examples, we can see that dissolution of the aluminosilicates also promotes precipitation of carbonate mineral as well as formation of clay minerals. For example, anorthite dissolution follows the stoichiometry



More generally, an overall reaction shows that feldspar dissolution can lead to CO₂ trapping as a variety of carbonate minerals



Siefritz (1990) and Fyfe *et al.* (1996a and b) have further noted that the exothermic properties of these mineral reactions also provide an energy bonus of 24 kCal per mole of feldspar dissolved that could potentially be recovered to offset costs.

3.3.3. Formation of Carbonates by Reaction with Carbonate Minerals

A third environment that modifies the extent of CO₂ by sequestration is the carbonate-rich environment. Mineral trapping in this system is not generally promoted because the decreased pH associated with H⁺ release by dissociation increases the solubility of carbonate minerals, whereupon they quickly dissolve. In some situations, this could be potentially hazardous to the reservoir host or seal integrity. Bergman and Winter (1995) have noted that reaction of acidic fluids with limestone or dolomitic formations can overpressure the formation through rapid CO₂ release. Note that carbonate minerals can, however, be precipitated when other minerals can act as rapid proton sinks to buffer H⁺ production (Hitchon, 1996). The literature suggests considerable uncertainty in our ability to predict the behavior of carbonate-hosted, subsurface systems.

3.4. Microbial Trapping

Several studies have suggested that microbial trapping may offer a third mechanism for sequestering CO₂ (e.g., Fyfe *et al.*, 1996a; Ferris *et al.*, 1994). Because most of these studies have focused on promoting biomineralization by mechanisms that depend upon photosynthesis by direct or indirect mechanisms, it is unlikely

they can promote CO₂ sequestration by terrestrial disposal. We could also consider that microbial conversion of CO₂ to methane via the simplified reaction



may enhance CO₂ capacities. This reaction has been documented in deep sediments (Kieft and Phelps, 1997) and deep aquifers of the Columbia River Basalts (Stevens and McKinley, 1995). However, the volume increase associated with methane production would decrease reservoir capacity, and work by Anderson *et al.* (1998) indicates CO₂ consumption by reaction with hydrogen is unlikely. Perhaps more likely is a secondary role of microbes in CO₂ sequestration by promoting feedback on the trapping mechanisms proposed earlier. Metabolic activities can promote silicate dissolution and therefore, secondary precipitation of carbonate minerals, particularly siderite (e.g., Brown *et al.*, 1994). The possibility of harnessing microbes to promote CO₂ sequestration is intriguing.

The foregoing summary suggests that the ideal chemical trapping mechanisms are characterized by their abilities to enlarge reservoir capacities and transfer CO₂ into an unreactive form through fast kinetics. While the long-term capacity of mineral traps is enormous, the kinetics of the reactions required to form these minerals is problematic. Hence, research should focus on the rates and mechanisms of chemical reactions that improve our ability to (1) make quantitative model predictions of how a system responds to CO₂ injection, (2) identify the "bottlenecks" that occur along the path from transferring supercritical CO₂ across the gas–water interface to the final sink as carbonate minerals, (3) investigate means of "widening" the bottlenecks, and (4) determine the long-term capacity of system for sequestering CO₂ by mineral trapping. Another possible limit on rates of silicate reactions is the precipitation of SiO₂ as a secondary product. The importance of understanding clay mineral formation should not be overlooked. These fine-grained constituents have enormous capacity for buffering mineral–water chemistry as well as affecting hydrodynamic properties by modifying formation permeability. Because CO₂ injected from a fossil fuel burning facility likely will contain trace gases, research may also be needed to determine the potential for gaseous contaminants to interact with mineral surfaces within the formation. Passivation by surface sorption and isolation of reactant sites from the fluid environment could greatly inhibit rates of mineral dissolution and precipitation. The feasibility of microbial trapping also should be investigated. Microbial processes are intertwined with the systems approach described above, but subsurface microbial studies are only beginning to document these unique ecosystems.

Up to this point, we have dealt only with the very oversimplified situation of a spatially uniform (on scales larger than mineral grains) closed system. But even in this idealized limit, we would argue that the present capability to specify the time evolution of the system is seriously compromised for lack of reaction kinetic information. It is important to keep in mind that the sort of kinetic information

needed is in the form of continuum-scale constitutive equations which, especially in cases of heterogeneous reactions, can involve complex averages over a variety of atomic scale processes. A full characterization and understanding of the reaction kinetics relevant to CO₂ sequestration in geological environments will require an extensive program of laboratory experimentation, along with carefully chosen field measurements to validate the upscaling of the laboratory behavior to the time and length scales of interest.

The next level of complexity that one might consider is that of spatially nonuniform open systems or potentially open systems. A potentially open system is one that is initially enclosed by a “seal” that effectively isolates it from the surroundings, but with time could become open because of mechanical or chemical breaching of the seal. In order to deal with open or potentially open systems, a number of additional constitutive equations need to be specified. Of special interest are the relationships of permeability to fluid content and mineral texture, and those relating rheology to fluid content, mineral fractions, and their texture.

3.5. Role of Coupled Processes and RTM Instability

As suggested in Fig. 13, there are many factors and processes operating naturally or during injection that are strongly coupled. Thus, simulation of the development of repositories over long time periods or their response to injection must be based on multiprocess models that account for all cross-coupling relations in the network of reaction, transport, and mechanical (RTM) processes. Furthermore,

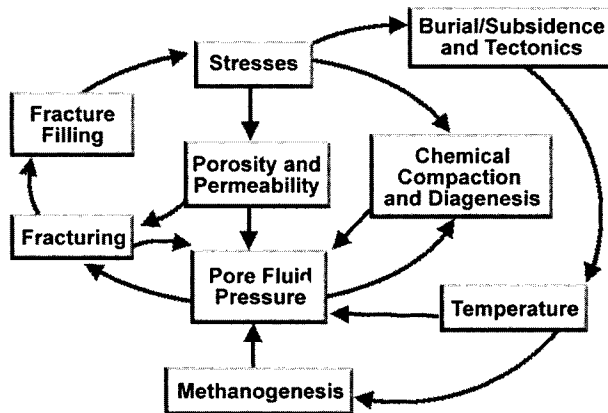


FIG. 13. Schematic of parameters and complex feedback between coupled reaction, transport, and mechanical *in situ* processes (Ortoleva, unpublished).

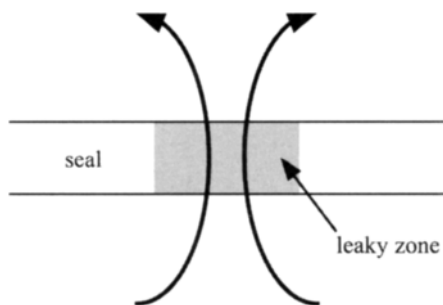


FIG. 14. Schematic view of flow self-focusing leading to a reaction-induced breaching of a seal (Ortoleva, unpublished).

these RTM simulators must be three-dimensional so that all geometric effects are accounted for (i.e., CO₂ waste fluids must be contained in all directions to ensure their sequestration from the accessible environment).

Flow self-focusing is an example of the strong effect of coupled processes that cannot be understood in terms of independent ones. (See Ortoleva, 1994b, for a review of this and other geochemical strong-coupling phenomena.) As shown schematically in Fig. 14, a slightly leaky region in a seal focuses fluid escape through it. If the fluids retained by the seal dissolve one or more minerals within the seal and thereby increase its permeability, then the escaping fluid will enhance the permeability in the leaky zone. Consequently, it will concentrate further flow there, and an efficient fluid escape pathway develops. This process illustrates the notion of geochemical seal stability: flow self-focusing can make a seal unstable with respect to fluid escape even if the minerals in the seal could not be appreciably affected when these fluids uniformly enter the seal (i.e., in an overall mass balance sense) in contrast to the destabilizing, strongly focused flow dynamic. Similarly, a front of injection-induced alteration can become unstable to fingering when that alteration increases permeability. In three spatial dimensions, these flow self-focusing phenomena are enhanced over those in two dimensions. These examples illustrate that reliable simulation of CO₂ repository behavior during injection or long afterwards requires the use of fully coupled, three-dimensional RTM models. Such modeling studies could help identify potential instability phenomena. They should also be used to tabulate chemically stable seal and reservoir lithologies as well as to analyze specific demonstration sites. Such three-dimensional, fully coupled RTM models should be developed for use as an integral part of a CO₂ repository.

Models for use in CO₂ repository analysis should be developed that account for effects of wormholing and cavitation. Such phenomena involve the interplay of free flow and Darcy flow zones, coupled to geochemical reactions. An attractive

approach seems to be the use of Brinkman's equation (Liu *et al.*, 1997). This model should be generalized for the multiphase regime.

3.6. Textural Models and RTM Dynamics

CO₂-induced clay dewatering could decrease rock strength, while CO₂-induced precipitation could increase it. Even small changes in grain geometry induced by CO₂ could alter the integrity of grain–grain contacts, and thereby affect rock strength, sound speed, and other properties.

The dynamics of the repository system depend on the distribution of rock mechanical and transport properties as well as mineralogy. In order to predict reservoir response, a complete set of texture geometric variables must be identified, and the laws for their evolution must be set forth (Fig. 15). The importance of these parameters and the interrelationship among texture parameters; porosity, permeability, capillarity, etc., are discussed in further detail in related sections.

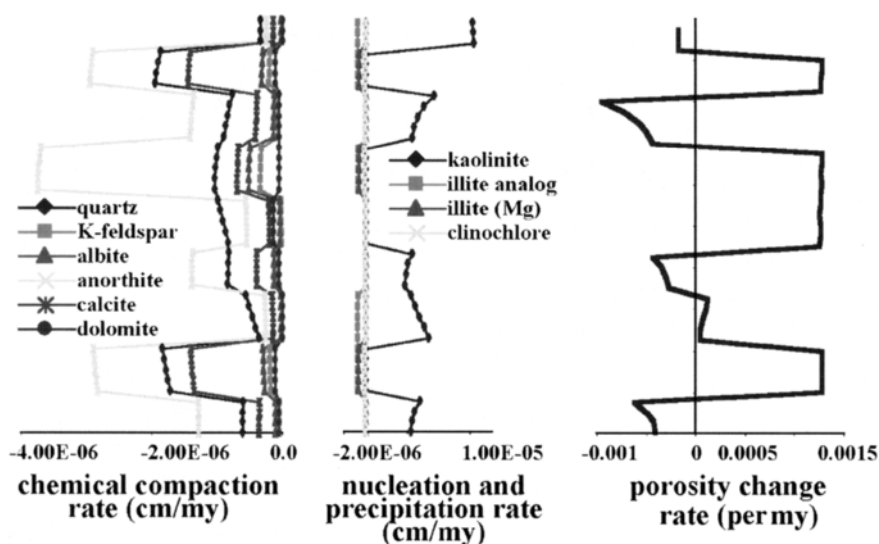


FIG. 15. Calculated reaction rates of minerals and porosity change rates for a system consisting of 10 minerals and 9 sedimentary layers. Water saturated with calcite and quartz are injected from below at a rate of 1 m/year. Coupled to water–rock chemical interaction mechanisms, advective and diffusive flow and complex mineralogy and texture result in complex mineralization patterns with potentially major effects on permeabilities and fluid pathways. In similar open systems, carbonate minerals, with higher rates than the silicates, are often the most mobile components (modified from Park and Ortoleva, 1999).

3.7. Nucleation and Ostwald Processes

A central theme in the subsurface CO₂ repository strategy is the formation of CO₂-bearing mineralization. Key geochemical processes that are poorly accounted for in most models are nucleation and Ostwald ripening and step-rule processes (Ortoleva, 1994b). Models should account for the resulting geometry of the new minerals, the mineral surfaces on which their nucleation is promoted, and the effect of Ostwald ripening. The practical challenge of embedding Ostwald ripening (and hence, the particle-size distribution) in three-dimensional RTM models should be addressed. The competition between various polymorphs (i.e., Ostwald step-rule phenomena) should also be considered (Ortoleva, 1994b; Fig. 16).

4. GEOMECHANICS

4.1. Introduction

The assessment of reservoir storage capacities and the efficient injection and sequestration of CO₂ are directly linked to modeling geologic systems. Credible geomechanical models require the formulation of realistic constitutive models, the site-specific identification and measurement of rock properties, and the determination of boundary conditions (Fig. 17). Boundary conditions include not only the *in situ* stress states, but also the location and properties of faults bounding reservoirs or compartments within reservoirs. Uncertainties and the need for research result from the heterogeneity of geologic systems emphasized previously, the presence of fracture networks, and changes in rock properties and stress state with pore pressure, fluid content, and time during and after oil or gas production, and CO₂ injection. Some of these attributes and the extent to which reservoir characteristics change with time ultimately require that geomechanics analyses are integrated into systems analyses in order to account for the interaction or “coupling” between diverse processes referred to as RTM (reaction, transport, and mechanical) processes.

4.2. Reservoir Characterization

4.2.1. Faults as Seals or Conduits to Fluid Flow

The effects of faults on fluid-flow ranges from prevention (barrier) through little or none to enhancement (conduit). The reasons for these differences are not presently apparent, although research on the structure of fault zones has suggested some relevant factors.

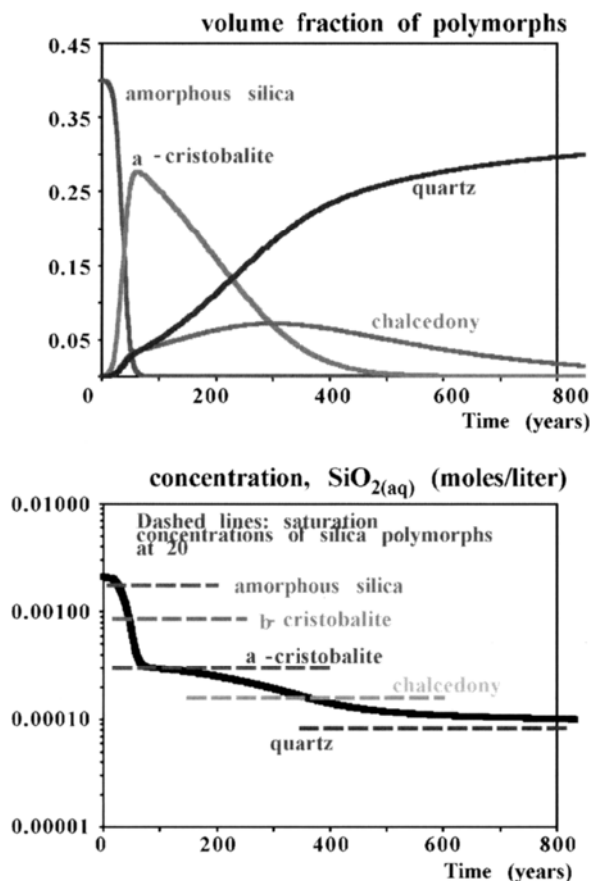


FIG. 16. Simulation showing nucleation and competitive growth (step-rule) among various silica polymorphs under room-temperature conditions. Changing physical and chemical conditions of sediments can invoke similar reaction mechanisms in carbonate systems, with the potential of large amounts of carbonates precipitating out from water (modified from Ozkan and Ortoleva, 1999).

The geometry of individual faults is complex in both strike and dip directions, but studies have established a general cross-sectional geometry that appears to characterize many faults. The nominal fault zone width—or that which is often mapped as the “fault”—is a damage zone where the fracture density is significantly higher than the surrounding country rock (Fig. 18). Within the damage zone is fault rock or gouge, a region of fine-grained material much narrower than the damage zone and often only 5–10% of that width (Fig. 19). The fault rock has been deformed by a variety of mechanisms depending upon the pressure and temperature regimes. These range from mechanical comminution and “smearing”

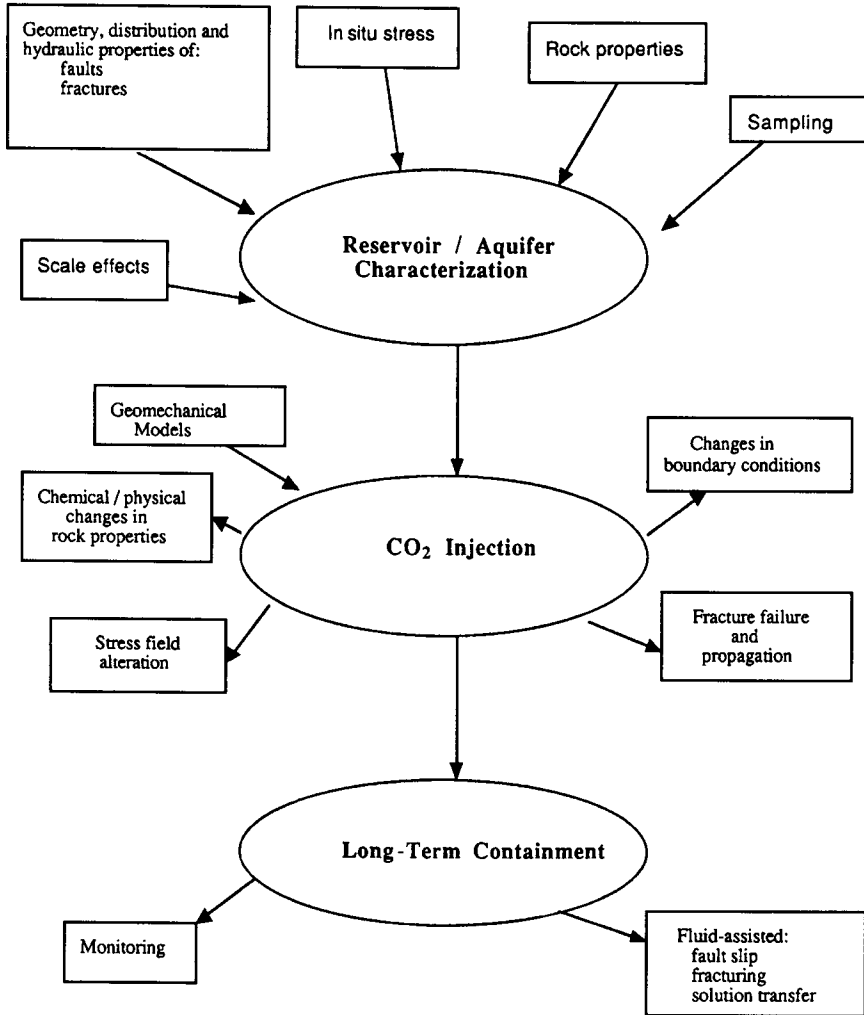


FIG. 17. Geomechanics considerations of CO₂ sequestration from reservoir characterization through long-term containment (Logan, unpublished).

of more ductile material such as some shales (Weber *et al.*, 1978) at lower temperatures and pressures, through dislocation glide, creep, and recrystallization, to solution transport at higher temperatures and pressures. Typically, deformation is not homogeneous, but is localized along fractures that evolve with increasing shear strain. The result is a grain-size reduction and heterogeneous porosity and permeability (Logan *et al.*, 1992).

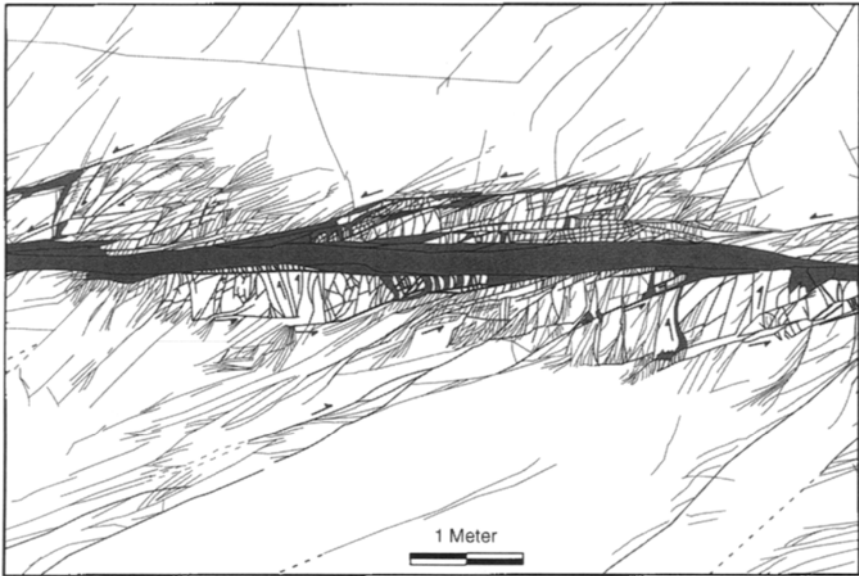


FIG. 18. Section of medium-scale fault in the Valley of Fire State Park, Nevada. Note well developed fracture network and through-going gouge zone. Most of the original joints and sheared joints are obliterated by fault slip; however, some sheared joints are preserved along the margins of the central damaged core (from Taylor *et al.*, 1997, and Myers and Aydin, 2000).

Because fracture porosity and resulting permeability are much higher in the damage zone than in the relatively unfractured country rock adjacent to it, fluid flow parallel to the fault is enhanced in this region. Flow parallel to the fault is also enhanced by the presence of fractures within the fault rock, which tend to align parallel or subparallel to the displacement vector of the fault. Transverse to the fault rock, flow is restricted by a decrease in grain size and a corresponding increase in the tortuosity of the migration path. Additionally, few major fractures cut across the fault rock. Consequently, any fault rock is potentially a barrier to fluid flow. This restricted flow may produce significantly higher values of pore pressure within the fault rocks than in the adjacent country rock. There is little evidence, however, that faults are absolute seals to fluid flow. Some leakage is expected (Surdam, 1997), but the rates are largely unknown.

Research is needed to better understand the origin of faults to predict their location, structure, extent, recurrence (or periodicity) of motion on them, and hydromechanical properties. Current hypotheses can be grouped into three categories: (1) fault formation along planes of critical shear stress, (2) faulting by cooperative deformation and growth of en echelon fractures and fracture clusters (Fig. 20),

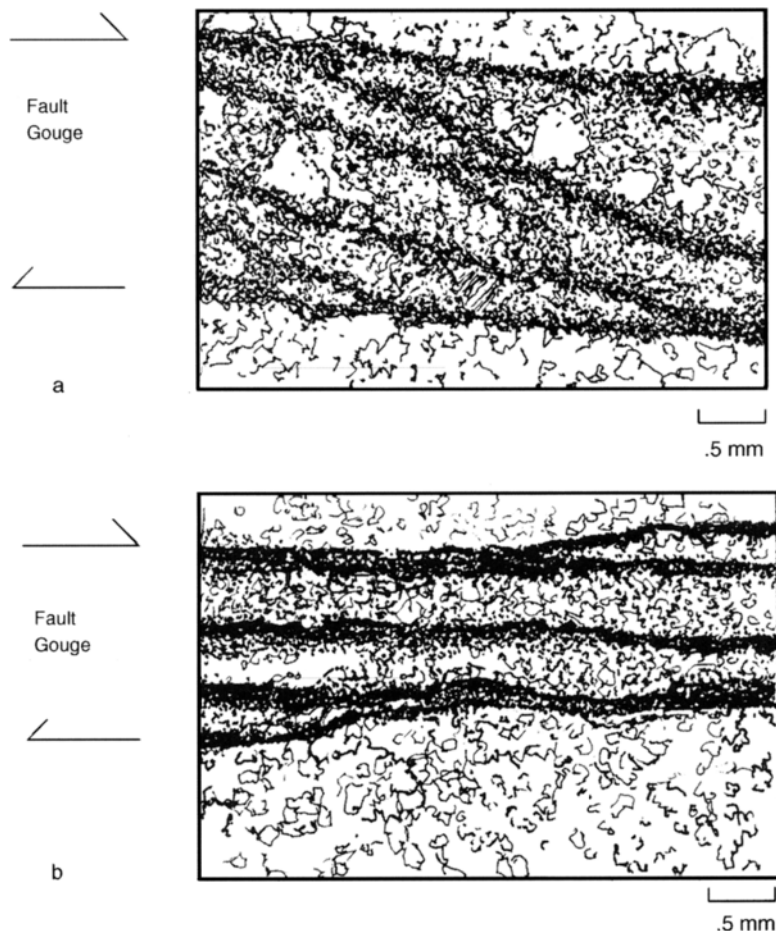


FIG. 19. Sketches of fault gouge produced in laboratory experiments in quartz sandstone showing fabric evolution. (a) Shear strain is relatively low, about 4. (b) Shear strain is about 14. The darker patterns are regions of finely comminuted grains, generally less than one micron in diameter produced by localized shear within overall gouge proper. These are boundaries of low permeability separating less deformed areas where the grains are coarser. The result is inhibited fluid flow normal to the shear direction. Sense of shear is indicated at the boundary of the gouge and country rock (Logan, unpublished).

and (3) faulting as localized shear resulting from material instabilities (Fig. 21). The second and third hypotheses offer mechanistic interpretations of rock failure and are supported by field observations and laboratory measurements (Thomas and Pollard, 1993; Taylor *et al.*, 1997; Myers and Aydin (in press); Moore and Lockner, 1995; Antonellini *et al.*, 1994; Ord *et al.*, 1991; Rudnicki and Rice, 1975; Olsson,

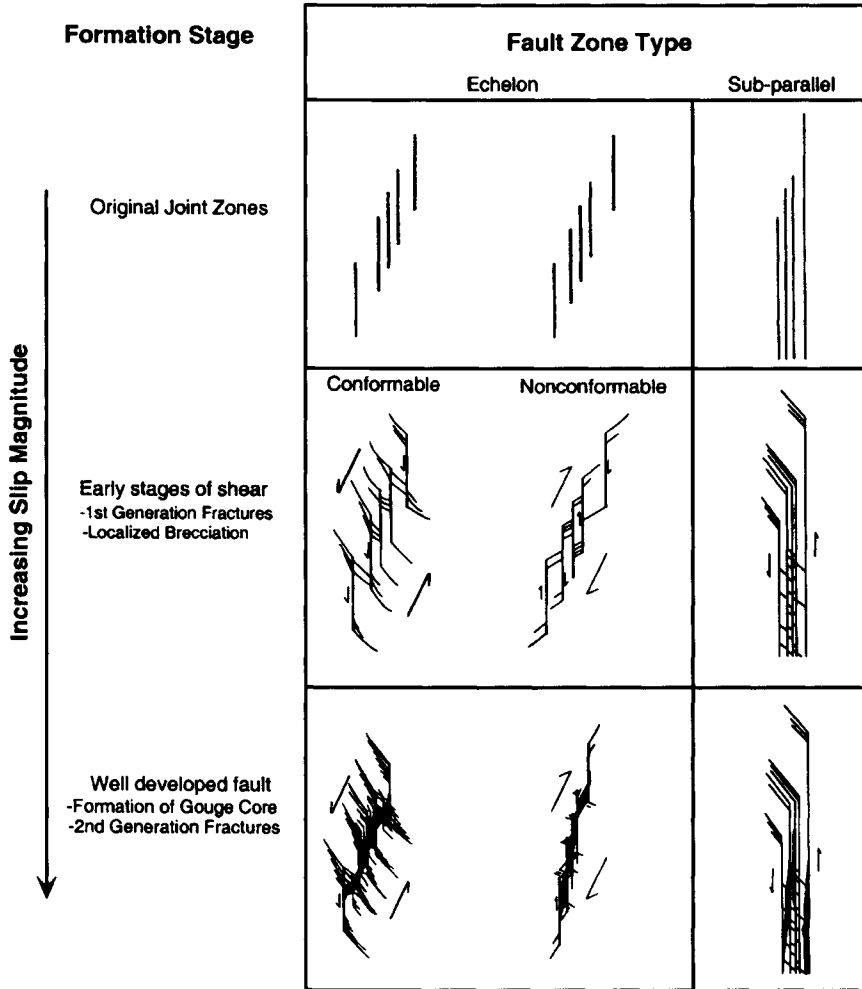


FIG. 20. Fault development by cooperative fracture growth: schematic illustration of three fault types and their major evolutionary stages (from Taylor *et al.*, 1997, and Myers and Aydin, 2000).

1998). Application and extension of these theories require an understanding of the development of fracture clusters (Taylor *et al.*, 1997) and of the evolution of the constitutive parameters of rocks (Holcomb, 1992; Olsson, 1998). Research on faulting is especially important in porous rocks (which are typical of reservoirs) and must encompass not only the initial formation of faults, but also criteria for extension and changes in structure and hydromechanical properties. Research into faulting and its relation to fluid flow has been hampered because of difficulties in

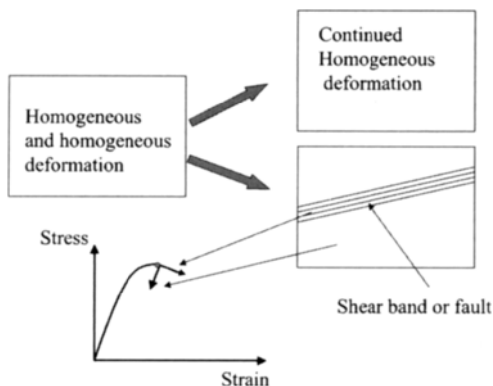


FIG. 21. Schematic illustration of fault formation (shear localization) as a bifurcation from homogeneous deformation (Rudnicki and Rice, 1975).

characterizing the three-dimensional structure of faults and a shortage of three-dimensional (as opposed to planar or axisymmetric) laboratory experiments to constrain realistic constitutive models.

4.2.2. *In Situ Stress State and Measurement of In Situ Stresses*

Rock behavior is determined by the effective *in situ* stress. Often, it is assumed that the total *in situ* stress state is the same as the lithostatic state of stress, and the pore pressure is distributed uniformly. Structural geologic evidence and field measurements indicate that reservoir stresses often are far more complicated (Teufel and Farrell, 1990; Warpinski and Teufel, 1992; Lorenz *et al.*, 1995). For example, Teufel and Farrell (1990) showed that a domal structure strongly affects the orientation of the maximum horizontal principal stress in the Ekofisk reservoir in the North Sea (Fig. 22). Similarly, Lorenz *et al.* (1995) have documented the dominant influence of basin-margin structures on the *in situ* stress distribution throughout in the Green River Basin, Wyoming. Knowledge of the tectonic history of such areas coupled with the pore fluid and compaction histories of the strata are essential for anticipating sources of stress-field perturbations and for interpreting and generalizing local *in situ* stress measurements by means of numerical modeling. Some knowledge of the *in situ* stress history over geologic times also is indispensable to characterizing fracture systems.

The importance of *in situ* stresses for reservoir characterization and monitoring mandates further research on methods of measuring *in situ* stresses and stress changes with time (Warpinski *et al.*, 1993; Amadei and Stephansson, 1997), especially at great depth as well as in anisotropic, fractured, and poorly consolidated strata. *In situ* stress states may be particularly complex in 'depleted' reservoirs

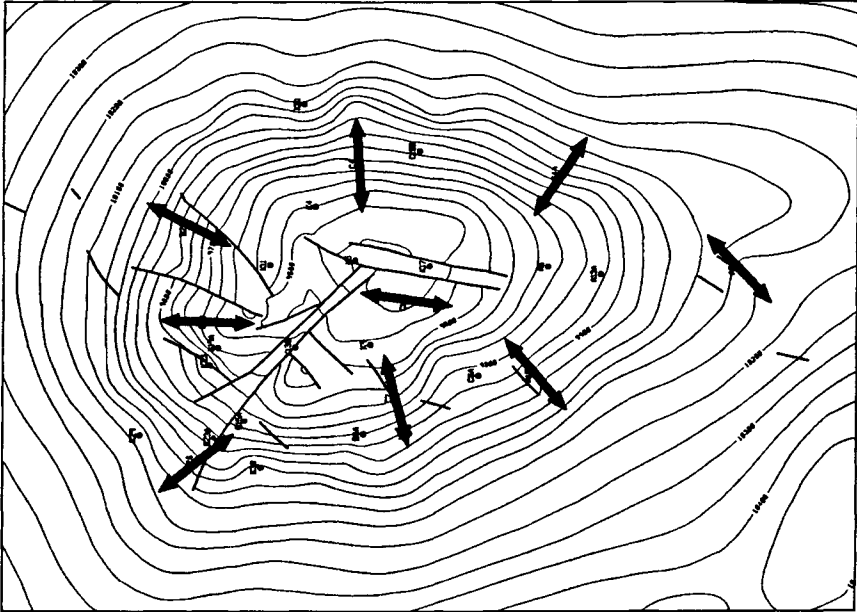


FIG. 22. Structure contour map for the top of the Ekofisk formation showing azimuth of the maximum horizontal stress. The crest of the domal structure is at a depth of approximately 2.9 km, and contour intervals are 15.2 m (from Teufel and Farrell, 1990).

being considered for CO₂ sequestration because of past anelastic deformations and heterogeneous pore pressure caused by patchy distribution of residual fluid.

4.2.3. Rock Properties

Earlier hydrologic discussions focused on the importance of rock porosity and permeability to fluid transport in reservoirs, but reservoir flow was assumed to be largely independent of many other physical rock properties and the influence of *in situ* stress state (Fig. 23). The hydrologic perspective in this chapter also stressed the use of continuum-type simulations, coupled with geostatistical approaches, to address reservoir heterogeneities. The discussion below encompasses some of the same issues, but with added attention to the effects of stress and the coupling of processes. This discussion also identifies difficulties in the complete constitutive characterization of rocks, which include the connection of grain-scale rock attributes and macroscopic response. Subsequent geophysical considerations will return to the topic of rock properties once more within the context of remote geophysical characterization of CO₂ sequestration sites and monitoring of injection processes, fluid distribution, and long-term site integrity.

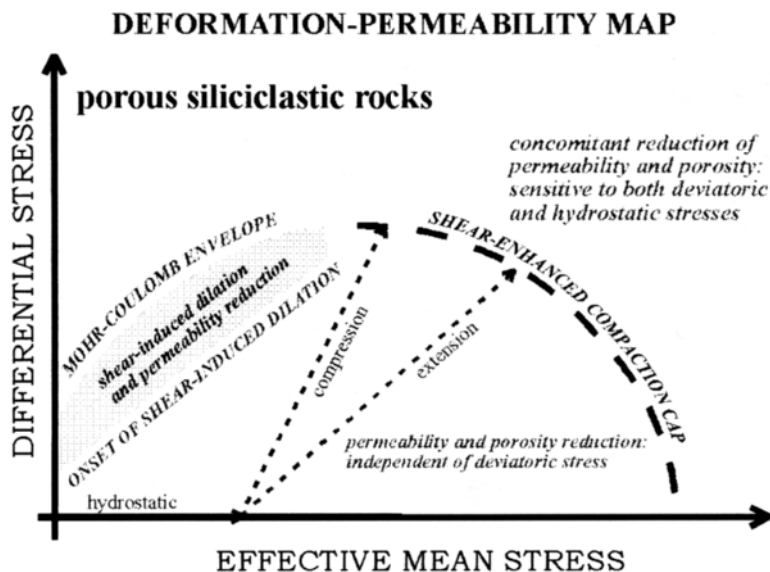


FIG. 23. Example of coupled phenomena—deformation-permeability map for porous siliciclastic rocks showing interrelationship between stress state, stress path, porosity reduction, and reduction in matrix rock permeability. The shaded area represents the brittle regime. The dashed lines with arrows represent load paths in conventional triaxial (axisymmetric) compression and extension (from Zhu and Wong, 1997, modified by Zhu, 1999).

Reliable reservoir characterizations require constitutive models, measurements of the associated material properties, and a description of the spatial heterogeneity of rock properties, including the properties of matrix rock, fractures, and faults on all scales. Often, predictions are based on an idealization of reservoir rocks as linearly elastic continua, with elastic and failure properties determined from laboratory tests. More realistic phenomenological models should incorporate inelastic deformation, dilatancy or compaction, stress-dependent and, in some cases, anisotropic porosity structure and permeability, etc. In addition to phenomenological models, models based on microscale mechanisms have been successful in qualitative and quantitative interpretations of geomechanical rock-mass behavior at high homologous temperatures. Insufficient field data and computational limitations, however, have left much uncertainty about the level of detail needed for adequate reservoir descriptions (such as the need to include inelastic behavior and the properties of natural fractures in analyses).

In the majority of reservoir studies, analyses are restricted to two-dimensional idealizations. Simulations of a diatomite reservoir (Fredrich *et al.*, 1998; Hilbert *et al.*, 1999) may provide the first large-scale example to assess important differences in rock and well bore response between two- and three-dimensional

calculations. Another example using a relatively complex elastic-plastic material model resulted in subsidence predictions above a diatomite oil field that under-predicted the magnitudes of vertical and horizontal surface displacement by some 25% (deRouffignac *et al.*, 1995). The discrepancy between measurements and calculations was tentatively attributed to the omission of time-dependent material behavior (creep).

The foregoing discussion implies that constitutive modeling, the determination of rock properties, and numerical or analytical solutions of boundary-value problems are inextricably linked. Consequently, a full understanding of rock behavior and the identification of dominant parameters require parallel research in all three of these areas. In particular, research is needed on (1) rock properties under fully three-dimensional stress states, (2) the influence of stress path on inelastic properties such as pore collapse as well as directional permeability, (3) the validity of the effective stress principle under large pore-pressure changes, (4) physical and hydromechanical properties of shales and the influence of clays, (5) microscopic and macroscopic processes governing rock behavior and the evolution of the constitutive properties, and (6) the connection between static and dynamic rock properties.

Existing experimental and computational evidence (Blair *et al.*, 1993; Winkler, 1983; Dvorkin *et al.*, 1991; Bruno, 1994; Zang and Wong, 1995) provides details about how macroscopic rock behavior and changes in rock response are directly related to grain-scale properties including elastic properties of grains and intergranular cements, grain anisotropy, grain size, and grain strength. They are also related to the fine-structure of the rock fabric (including pore and crack porosity, pore shape in terms of aspect ratio, and intergranular distribution of cementing materials (Fig. 24). It is logical to assume that the storage capacity, transport properties, and reactivity of reservoirs will be affected by the local distribution of matrix rock permeability. This, in turn, is a function of the shape, distribution, connectivity, and surface area of pore spaces and how these attributes change with stress and rock-fluid interactions. Grain shape, grain-size distribution, and surface roughness (surface area) will likely influence the local reactivity—both within individual pores and in the connection between pore spaces. Experiments and computations have demonstrated that aperture distribution in discrete, rough-walled fractures (Brown, 1987) can lead to flow channeling (Fig. 25). It is possible that heterogeneity in grain, cement, and porosity-fine structure could result in channel flow in matrix rock as well. At a minimum, anisotropy in the fine structure caused by stress or deposition is expected to alter both the local and the macroscopic permeability of reservoir rocks (Bruno, 1994).

Promising work concerning the grain-scale properties and fine structure of matrix rock should be expanded using a number of observational tools, some of which combine high resolution with the possibility of real-time measurements (e.g., Wood's metal impregnation, electron microscopy, laser-scanning confocal microscopy (Fig. 5), nuclear magnetic resonance, synchrotron radiation, and

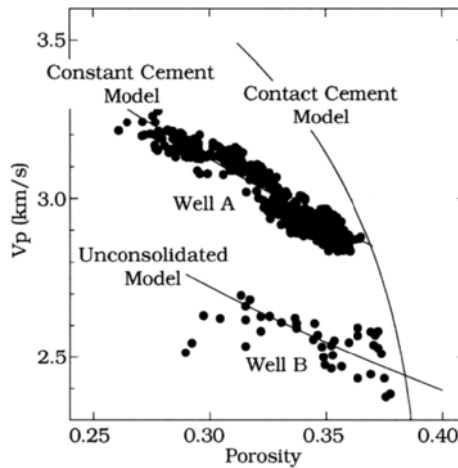


FIG. 24. Plots of P-wave velocities versus porosity demonstrate the significant effects of grain-scale properties on the bulk properties of rocks. The solid lines are theoretical curves. Their character depends on the mechanical properties of the grains and the cements and on the distribution of the intergranular cements at and away from grain contacts. Rock physics diagnostics make it possible to fine-tune velocity–porosity transforms to specific depositional environments (from The Stanford Rock Physics Laboratory, personal communication, and Avseth *et al.*, 1998).

acoustic and x-ray tomography) (Schlueter *et al.*, 1991, 1994; Fredrich *et al.*, 1995; and others). In principle, advanced algorithms for defining and representing pore geometries, and large computers, make it feasible to implement observational results in numerical simulations (O'Connor, 1996; O'Connor and Fredrich, 1999; Fredrich *et al.*, 1995; Fredrich, 1999; Lindquist *et al.*, 1996; Lindquist, 1998). Mathematical algorithm development, however, must be complemented by new experiments that measure local material properties (e.g., along grain contacts) or that derive local properties from the bulk behavior of small- or large-particle assemblages. Recent fluid-flow models at the pore scale take advantage of lattice Boltzman simulations. These and other approaches can extend and complement continuum damage models that relate bulk nonlinear rock behavior and pressure dependence to the growth and interaction of preexisting microcracks in elastic continua (Costin, 1983; Kemeny and Cook, 1991; Lockner and Madden, 1991; Rudnicki and Chau, 1996; Rudnicki *et al.*, 1996). New approaches based on grain-scale properties and matrix fine structure (texture) also promise to expand results obtained from contact analyses using highly idealized grain shapes and cement distributions (Digby, 1981; Dvorkin *et al.*, 1991, 1994; Bruno, 1994; Zang and Wong, 1995) to infer grain- and subgrain-scale micromechanical and transport processes, including preferentially aligned cement-grain bond failures, intragranular microfracturing, massive grain disaggregation, and pore collapse. Individual

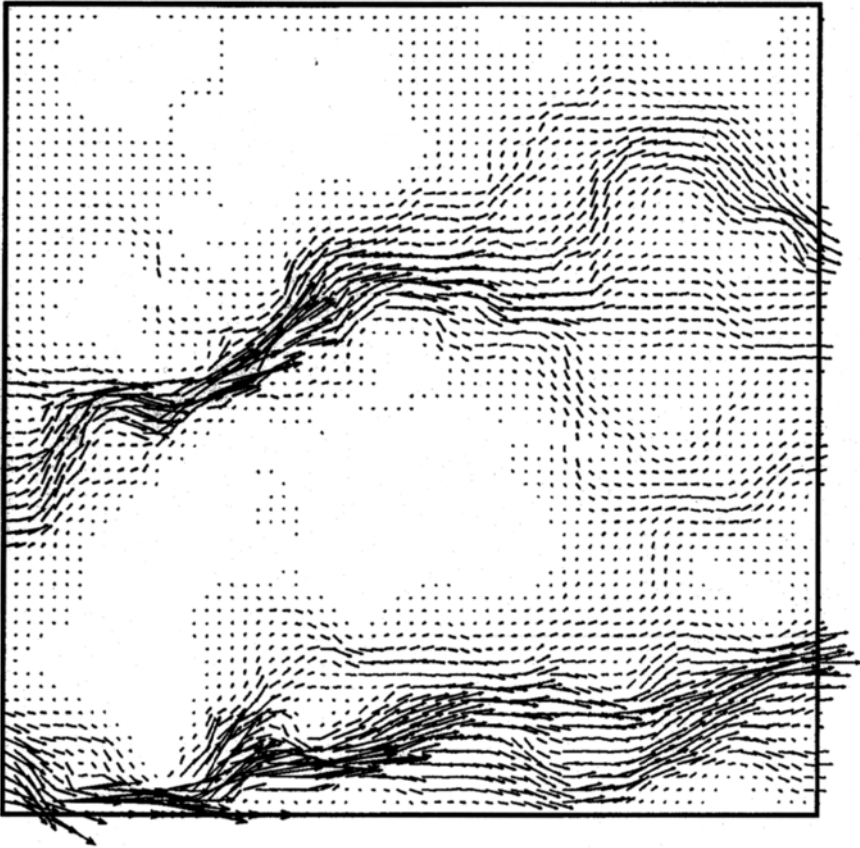


FIG. 25. Volume-flow-rate vectors demonstrating channeling in rough-walled natural fracture (from Brown, 1989).

research elements in these developments should address the influence of clays and the need to establish criteria for microfracture initiation and growth below the continuum scale (20 grain diameters?), which are influenced by local stress heterogeneity, crystal anisotropy, and local contrasts in thermomechanical material properties.

Although there are uncertainties in the properties of polymineralic rocks, such as clay- or calcite-cemented sandstones or even dolomitic limestones as reservoir materials, shales are a major area of ignorance. Except for some specialized facies, such as oil shales, little systematic research has been done on shale properties because of the sampling and preparation problems. Shales are particularly important because they frequently form reservoir boundaries or the boundaries of

high-pressure compartments within reservoirs. These shales are usually of Mesozoic age or younger and commonly contain about 45–65% quartz and feldspars and 40–45% phyllosilicates. The few extant laboratory studies show extremes in mechanical behavior depending upon the ratio of clay species to quartz and feldspar. With increasing amounts of quartz and feldspar, the materials become progressively more brittle and stronger. In a dry state, the shales behave in a manner similar to limestone and some sandstone. Studies on the frictional resistance to sliding have shown that a decrease in frictional strength begins only when the amount of clay approaches 25–30% of the rock volume. The frictional strength then decreases monotonically until the percentage of clay reaches 70–75%, after which little change occurs (Logan and Rauenzahn, 1987). Another uncertainty is the nature of the phyllosilicate species. Illite and kaolinite alter the strength of rocks much less than do species containing interlayer water such as smectites. This is a major factor in reservoirs deeper than the smectite-to-illite transition that occurs at about 125°C. In the Gulf of Mexico, this transition corresponds to a depth of about 3.2 km. The largest volume of shales in the world occurs, however, in the lower Paleozoic and is composed of 85–90% quartz, which dominates the mechanical properties. These rocks typically contain the fractured reservoirs mentioned earlier. The extremely brittle behavior and relatively high strengths of these quartz-rich shales sustain relatively large fracture apertures in contrast to the behavior of the younger shales.

4.2.4. Rock Sampling and Scale Effects

Rock sampling and scale effects are critical to linking the geomechanical and geophysical rock properties as well as interpreting geophysical measurements *in situ* (Fig. 26). Sampling and generalizing rock-property measurements to inaccessible areas is a major concern in reservoir characterization. This problem is dominated by the heterogeneity intrinsic to all reservoirs, but is exacerbated by an absence of proven scaling rules for property measurements made on core material. Further difficulties arise within the time frame of sequestration because almost all laboratory measurements on core material done today fail to consider time effects. The state of knowledge of the effects of potentially chemically active pore fluids such as CO₂ on all rock types is even more limited. The presence of CO₂ may not only result in mineral deposition in pores or along fractures, but it may also alter the mechanical properties of resident minerals.

Sampling strategies and data extrapolations suffer from poor understanding about the differences between static and dynamic data on elastic properties. Most data on reservoirs come from down-hole measurements or dynamic values derived from laboratory acoustic measurements. Because most modeling assumes static behavior, some static values of elastic properties are selectively made from core material. These static data are, however, sporadic and seldom sample overlying

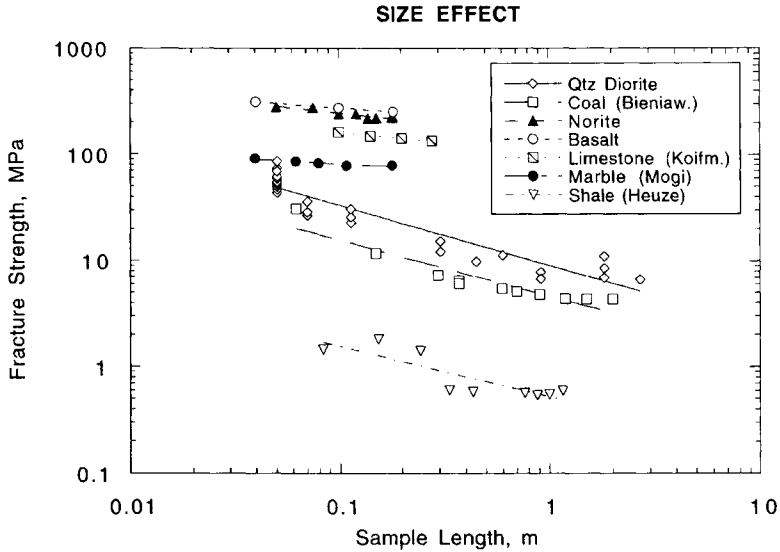


FIG. 26. Scale effects indicated by plots of the strengths of competent rock versus sample size (from Lockner, 1995).

sequences. In principle, it should be possible to determine static properties from dynamic measurements; but in practice, dynamic and static values usually differ, sometimes by large factors and often in an unpredictable fashion (e.g., Jaeger and Cook, 1979; and Yale *et al.*, 1995). Studies on a variety of rock types show static values of Young's modulus are often lower than dynamic determinations for sedimentary rocks, but they have been found to be higher for crystalline material. Quasi-static values of Poisson's ratio are frequently higher (Schatz *et al.*, 1993; and Yale *et al.*, 1995). Unfortunately, the differences are neither systematic nor consistent with the rock or investigator. This is an especially critical issue if old, abandoned reservoirs are to be considered for storage.

Down-hole logging offers an abundance of information on the reservoir and surrounding rocks, but is unable to identify inelastic properties. Given lithologic characteristics such as composition, mineral distribution, grain size, porosity distribution, and fracture frequency, it is desirable to make reliable predictions of strength and failure properties. An unrealized goal of petroleum companies has been to better constrain the inelastic properties needed for mechanical modeling of reservoirs.

Difficulties in translating down-hole logging data into laboratory data and vice versa exemplify the chronic problem of trying to characterize field properties, both elastic and inelastic, based upon laboratory measurements. This problem relates partly to the issue of laboratory sample size (i.e., scaling issues beyond

the considerations of differences between the subgrain and multigrain scales). Generally, laboratory samples range up to 5 cm in diameter and 15 cm long; most laboratories use half that size for work at elevated pressures and temperatures. In selecting samples, macroscopic fractures are generally avoided; consequently, the numbers and effects of fractures are not assessed. The usual assumption, which is qualitatively supported by a few studies, is that elastic properties and rock strength decrease with increasing rock volume because of the presence of fractures, reaching asymptotic, but unknown values. The magnitude of decrease depends, however, upon the specific circumstances. A number of theoretical models (e.g., Cuisiat and Haimson, 1992) try to deal with the difficulty, but these models are largely untested.

Field measurements of igneous rocks have shown Young's modulus decreases about 30% from laboratory values in one granite, but remains the same in another; Poisson's ratio was generally unchanged (Pratt *et al.*, 1972). In an investigation of sandstones and shale from the Mesaverde Formation in the United States, decreases in Young's modulus ranged from about 5 to 30%, but little change was found for Poisson's ratio (Lin and Heuze, 1987). Theoretical modeling combined with laboratory and field data suggests, however, decreases up to one order of magnitude in Young's modulus and possible increases in Poisson's ratio (Schatz, 1995).

4.3. Joints and Fracture Networks

Joints and fracture networks may fundamentally alter the behavior of reservoir rocks, including strength, deformability, permeability, and geophysical properties (Fig. 27). These sometimes consist of regular patterns of discontinuities but more frequently are complex sets of joints, fracture clusters, and deformation bands (Friedman and Logan, 1973; Pollard and Aydin, 1988; Lorenz and Laubach, 1994; NAS/NRC, 1996; Antonellini and Pollard, 1995; Mollema and Antonellini, 1996). Because rocks *in situ* are hardly ever free from natural fractures, greater attention should be paid to the documented effects of preexisting fracture networks on reservoir performance than may be indicated by history matching and reservoir simulations without regard to fractures.

Joints and the development of fractures in CO₂ sequestration are important in evaluating not only reservoir properties but also long-term site integrity and the possibility of breaching seals, traps, or cap rocks. Primary research issues fall into three broad groups: (1) the evolution of joint systems and fracture networks including joint lengths, spacing, and joint interactions with one another and with other rock mass heterogeneities such as lenses, bedding planes, and faults (Lorenz and Laubach, 1994; and NAS/NRC, 1996), (2) the need to understand joint connectivity in fracture networks, and (3) the interaction of the mechanical behavior of joints and joint systems, fluid flow, and geochemical activity including the development and distribution of fracture fillings over time.

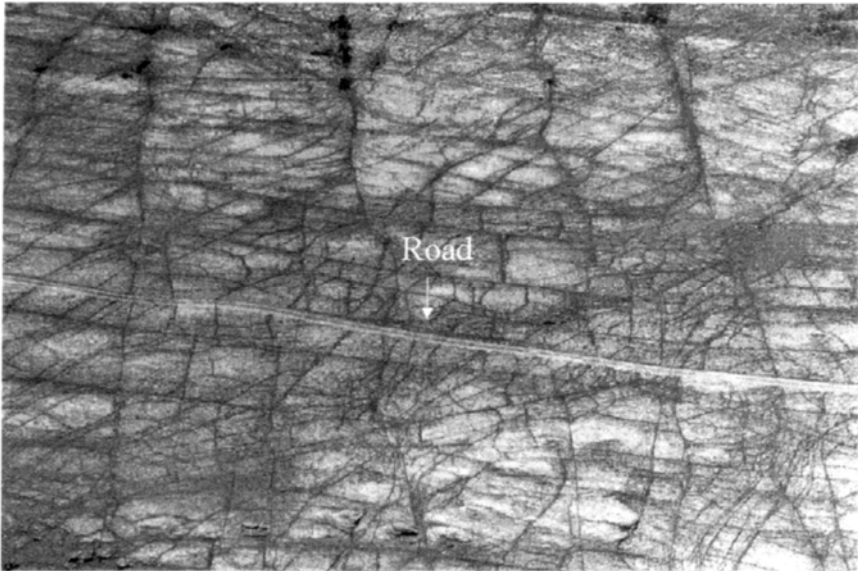


FIG. 27. Photograph of fracture network within a marine sandstone unit of the Frontier formation east of Kemmerer, Wyoming. Note road for scale (from Lorenz and Laubach, 1994, printed by permission of Gas Research Institute).

In situ principal stress directions and principal stress ratios probably are the most important parameters affecting joint orientation and the paths of growing fractures (Wu and Pollard, 1991). Great uncertainty exists concerning, for example, fracture spacing (Wu and Pollard, 1991). The influences of lithology and three-dimensional, fracture–fracture (Germanovich *et al.*, 1994) and fracture–interface interactions need clarification, especially in high-porosity, weakly consolidated rocks. Fracture interactions resulting in fracture clusters are of particular interest as major flow channels and potential precursors to faulting (Taylor *et al.*, 1997). Additional study concerning fracture development in high-porosity, weakly consolidated formations is important for hydraulic fracture design and response to fluid injection. Although joints are extensional features, generally it is unclear which and when one of several fracture growth hypotheses predominated: lithostatic stress changes, tectonic stresses, changes in pore pressure and effective stress, thermal stresses, or stresses arising from material heterogeneities dominated by differences in material properties across bedding planes.

The importance of fracture connectivity and the interdependence between fluid flow and geochemistry were subjects of earlier sections. The evaluation of fracture connectivity partly hinges on the ability to describe the geometries of fracture systems. For dense fracture systems and modest differences in fracture

conductivity, some success has been achieved in statistical descriptions of fracture patterns (Long and Hestir, 1990; NAS/NRC, 1996) without regard to fracture origin and fracture interactions. Fractal rules have proven useful in the spatial extrapolation of locally observed fracture patterns (Barton and LaPointe, 1995). This approach is bound to be less successful under conditions when fluid moves through only a few channels.

Although much work is needed to characterize both the geometry and the conductivity of fracture networks, important research needs to be continued concerning fluid-flow and fluid-rock interactions in discrete fractures. The hydrological literature appears to rely primarily on the so-called cubic flow law to describe the relationship between fluid flux and mean fracture aperture. Substantial deviations have been noted between this model and experimental measurements of aperture at high stresses normal to the fracture plane (Brown, 1989; Fig. 28). Systematic studies pertaining to fluid-flow behavior at fracture intersections do not appear to exist. Research should include the effect of shear deformation on joint normal deformation and fracture permeability.

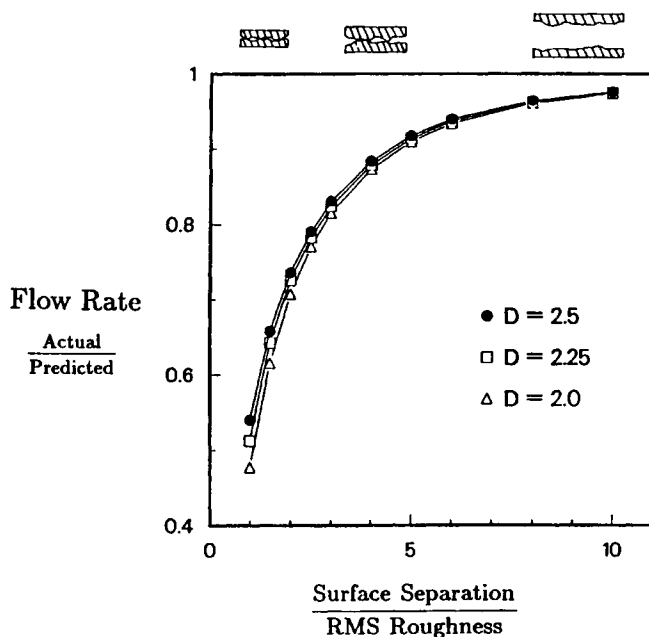


FIG. 28. Test of cubic flow law for fracture flow for fractures with different roughness characterized by fractal dimensions between 2.0 and 2.5. Significant deviation from cubic flow law occurs below abscissa values of approximately 4.1 when the fracture surfaces come into contact as shown schematically in the sketch above the plot (from Brown, 1987, modified by Brown, 1990).

4.4. Injection

Injection of any fluid (such as CO₂) into a reservoir under pressure will alter the effective stress state (Fig. 29). In addition, chemical reactions may result in spatial and temporal changes in the physical rock properties. To ensure the integrity and safety of the injection, it is necessary to evaluate whether alterations of stress will

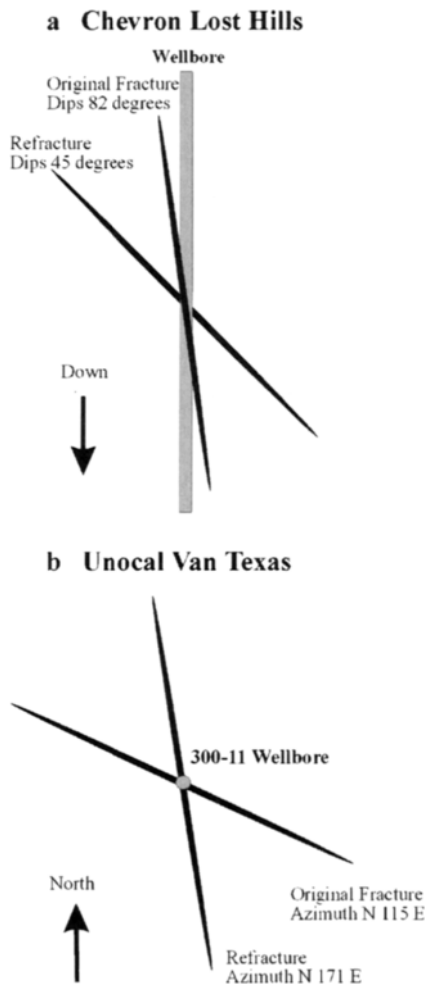


FIG. 29. Two examples of changes in *in situ* stresses due to fluid injection and production. The alteration in stress states resulted in changes in fracture orientations (azimuth and dip) between initial fracture and refracture treatments (from Wright *et al.*, 1995).

cause failure (seismic or otherwise) within the reservoir, along boundary faults, or in adjacent regions outside the reservoir. Furthermore, the alteration of stress may affect the storage capacity and hydrologic properties of the reservoir. For example, an increase in effective normal stress could substantially restrict flow along fractures that provide critical fluid pathways.

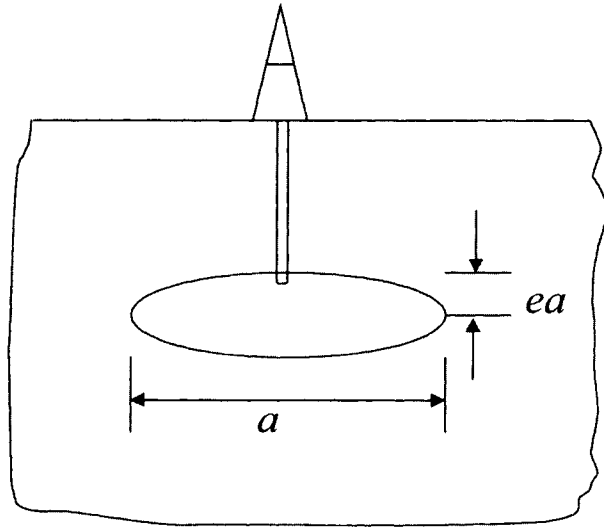
To predict the response of the reservoir to these alterations, it is necessary to adopt an appropriate theoretical framework, boundary conditions, and constitutive model to determine the relevant material properties and implement them in efficient and robust numerical algorithms.

4.4.1. Stress Changes and Boundary Conditions

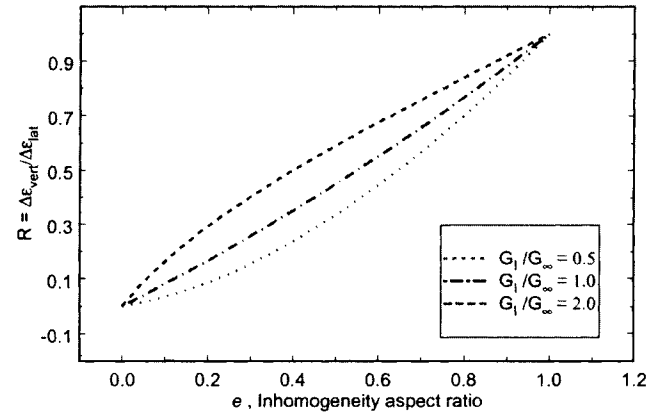
Adequate characterizations of reservoir stresses must combine local, often sparse, *in situ* stress measurements with numerical reservoir simulations. An analysis by Rudnicki (1999) demonstrates how fluid mass alterations in an idealized reservoir change the entire stress state, not simply the pore pressure as is sometimes assumed. The analysis indicates how stress changes depend on the geometry of the reservoir and the mismatch of elastic constants between the reservoir material and the surrounding formation. In the limit of a vanishingly thin planar reservoir, the strain state approaches uniaxial, but the rate of approach depends on the mismatch of elastic constants (Fig. 30). Rhett and Teufel (1992) demonstrate how the combination of measurements and analysis can explain and generalize puzzling observations about changes of the effective stresses with pore pressure drawdown in several oil reservoirs. Even highly idealized calculations prove the important connection among virgin *in situ* stress state, reservoir shape, and pore pressure distribution partly defined by well pattern and production rate. The influence of fluid withdrawal and withdrawal rate in oil and gas production is analogous to CO₂ injection and injection rate. In order to conduct complete site-specific analyses, careful consideration may have to be given to the added influence of adjacent geologic structures and how pore-pressure distribution is affected by the presence of natural fractures, fracture clusters, and fluid flow along major preferred channels.

4.4.2. Rock Properties and Geomechanical Models

Poroelasticity (or poro-thermo-elasticity, if temperature changes are important) provides a minimal framework for assessing the effects of injection. Even for this idealized model there is, however, uncertainty in the appropriate values of the poro- and thermo-elastic constitutive parameters. Determination from laboratory measurements is difficult because it involves small differences in measured quantities (Warpinski and Teufel, 1992). In addition, as discussed above, issues of scaling and the effects of larger fractures make the relation of laboratory measured values to



a



b

FIG. 30. (a) Sketch of the idealized geometry considered by Rudnicki (1999): Reservoir is idealized as an axisymmetric ellipsoidal inclusion with elastic properties different from the surrounding material and hydraulically isolated from the surrounding material. (b) Ratio of lateral strain increment to vertical strain increment in the inclusion due to a change of pressure as a function of the inclusion aspect ratio $e = a/c$. Results are shown for three ratios of the inclusion shear modulus to the shear modulus of the surroundings.

in situ conditions uncertain. More generally, accurate evaluation of stress changes in reservoirs is hampered by an inadequate understanding of the coupling of deformation with fluid flow and chemical reactions, i.e., RTM processes. Because of the complexity of the problem, current approaches have tended to focus on one aspect, e.g., idealizing the flow as occurring through a nondeforming matrix (neglecting deformation), or computing deformation, but neglecting coupling with flow and chemistry.

Although further progress can be made using poroelastic models, field and laboratory observations suggest that relatively small effective stress changes can alter flow properties and that inelastic volume changes, coupled with fluid flow and chemical alteration, and can play a role in reservoir response (Fig. 23). Shearing can cause dilation (inelastic volume increases), and compaction (inelastic volume decreases) can be caused by shearing and/or increases in mean effective compressive stress.

According to earlier discussions on geohydrology, many current simulations of fluid flow in fractured reservoirs appear to rely on the application of dual-porosity and dual-permeability models. These models contain two separate (possibly anisotropic) overlapping porous media, one for a permeable matrix and one for fractures in an impermeable medium, and incorporate fluid exchange between the two. These models admit spatial and temporal variations in the properties of the two components. They have, however, at least two fundamental shortcomings: (1) Fracture networks are idealized as orthogonal sets of infinitely long, perfectly smooth discontinuities whose fluid-flow properties meet the conditions of the cubic flow law, and (2) the fracture apertures and, therefore, fracture conductivities are assumed to be independent of (effective) stress state.

The importance of coupled simulations was demonstrated by a model of fluid flow through a fracture network in the Frontier formation, Wyoming (Brown and Bruhn, 1997). The elastic compliance and permeability properties of fractured rock are related to fracture geometry through tensors (e.g., Oda *et al.*, 1987) and the tensors for each physical property are derived by taking a volume average of the effect of each fracture population. The volume average contains functions of the fracture orientation, (finite) fracture length, and aperture in such a way that long or wide fractures contribute relatively more than small fractures. Elasticity is implicitly coupled to fluid flow through relationships between stress state, fracture-aperture distribution, and normal and shear deformation across fractures. One important result demonstrates that frictional sliding on favorably oriented fractures may cause extreme changes in the permeability tensor of the rock mass, including both magnitude changes and rotations of the principal stress axes (Brown and Bruhn, 1997). In one case, the maximum permeability direction was determined to lie at a 45° angle rather than parallel to the maximum principal stress direction.

4.4.3. Failure and Discrete Fracture Propagation

An issue of importance is whether injection will cause failure in any of a number of senses, including faulting as discussed previously. Experience at Rangely, Colorado (Raleigh, 1976) and elsewhere has demonstrated that fluid injection can cause seismic failure. Seismic events could damage pipelines, drill stems, and other structures associated with injection. Slip on faults, even if not seismic, could alter the properties of faults (whether barriers or conduits) and, consequently, the hydrological properties of the reservoir. Increases in pore pressure accompanying injection may cause (hydraulic) extension of fractures. In some instances, this may be desirable, but in others, fracture extension may breach seals or provide a rapid channel for fluid flow that prevents effective use of the reservoir volume for storage. Failure by shear localization, compaction, or disaggregation may have undesirable effects on the ability of the reservoir to store and contain CO₂.

The 1990s have seen great progress in the mechanics of earthquakes by using a constitutive relation for frictional slip in which the traction on the slip plane depends on the rate of slip and its history, as reflected in the current state of the sliding surface. The parameters of this relation, including a critical sliding distance, can be inferred from laboratory tests. Unfortunately, however, this critical length may be much larger *in situ* than as measured in the laboratory, and currently, there is no good means of determining values in the field (Scholz, 1990).

In practice, the possibility of seismic slip is most frequently assessed using the simple Mohr–Coulomb condition. As noted above, injection changes the entire stress state, not simply the pore pressure, and these changes must be considered in evaluating failure. The idealized analysis of Rudnicki (1999) can be used to determine whether injection causes the stress state to move toward or away from failure (Fig. 31). (Knowledge of the absolute *in situ* stress is needed to determine how far the stress state is from failure.) For example, if the reservoir strain state is uniaxial (a good approximation for a thin, tabular reservoir) and failure is assumed to be governed by a Mohr–Coulomb condition with friction angle ϕ , then injection at isothermal conditions will cause the stress state to move away from the failure condition if the following inequality is satisfied

$$\zeta > \frac{2(1 - \nu) \sin \phi}{(1 - 2\nu)(1 + \sin \phi)}$$

Here ν is the drained Poisson's ratio and ζ is a porous media constant, equal to $1 - K/K'_s$, where K is the drained bulk modulus of the porous material, and K'_s can, in certain idealized cases, be identified with the bulk modulus of the solid constituents. Application of even this simple condition is impeded by uncertainties about the appropriate value of the porous media constant ζ and friction angle. Furthermore, temperature changes of only a few degrees can alter the conditions for

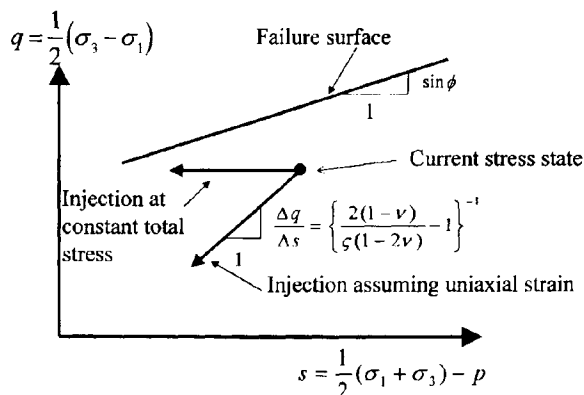


FIG. 31. Comparison of the different stress paths due to fluid injection if the total stress in the reservoir is assumed to be constant and if the reservoir is assumed to deform in uniaxial strain. The Poisson ratio of the reservoir is ν and ζ is the Biot porous media parameter (modified from Rudnicki, 9th Congr. Int. Soc. Rock Mech. Proc., 1999).

stability. Segall (1989) has used an analogous approach, based on poroelasticity, to determine stress changes outside the reservoir and the Mohr–Coulomb criterion to evaluate the potential for inducing failure (seismic slip) in regions adjacent to the reservoir. Neither approach takes into account the effect of stress alterations on boundary faults. At issue is not only whether stress alterations could cause either aseismic or seismic motions on these faults, but also whether stress alterations inducing slip could compromise the sealing ability of these faults. Despite the wide use of the Mohr–Coulomb condition, it has a number of shortcomings. It does not distinguish between rapid (seismic) and slow slip; it implicitly assumes homogeneous stress conditions, takes no account of the alteration of stress accompanying slip, and includes no means of predicting the size of an event.

The Mohr–Coulomb condition is also used to predict shear localization (fault formation), but has inadequacies in this application as well. Laboratory experiments demonstrate a clear dependence on deviatoric stress state (e.g., axisymmetric extension vs axisymmetric compression) that is absent from the criterion (Rudnicki and Olsson, 1998). Furthermore, the parameters of the relation (friction angle and cohesion) are purely phenomenological and bear little or no relation to constitutive parameters. For example, it is likely that fault formation differs in materials that compact vs those that dilate, but the Mohr–Coulomb prediction would be the same if the cohesion and friction angles were the same.

Understanding discrete fracture is a prerequisite for understanding the interaction and link-up of fractures and their behaviors at lithologic boundaries. Of particular importance for injection and containment of CO_2 are the growth and extension of fractures to form hydrological networks. Further work is needed on

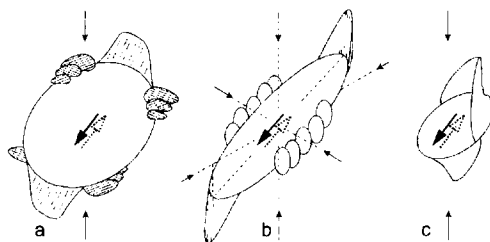


FIG. 32. Combined laboratory–field-based three-dimensional idealizations of shear fracture growth with associated development of secondary fractures [from Martel and Boger, 1998 with reference to (a) Adams and Sines, 1978, (b) Scholz, 1990), and (c) Germanovitch *et al.*, 1994].

three-dimensional effects and the effects of inelasticity and damage associated with fracture including, for example, an apparent influence of pressure and fluid diffusion in the crack-tip region.

The mechanics of discrete fracture propagation can be largely understood in terms of two-dimensional models, but three-dimensional effects are critical to fracture interactions and fluid flow (Germanovitch *et al.*, 1994; Martel and Boger, 1998; Fig. 32). In particular, for a fracture with a smoothly turning edge in a linear-elastic material, the asymptotic near-tip field decomposes exactly into separate plane and anti-plane, two-dimensional problems. But in a two-dimensional model, an asperity will completely block flow, whereas in three dimensions, flow can simply go around this obstacle.

The most prevalent models of fracture are those that treat the crack-tip as a singularity of stress in an otherwise linear elastic body or cohesive zone models in which the inelasticity is confined to a line ahead of the crack. Although these models are often adequate, the inelasticity and damage near the crack-tip may dramatically alter the out-of-plane growth and interaction of cracks.

4.5. Long-Term Containment and Monitoring

It was stated earlier that analyses of geologic systems must be built on an understanding of the interdependence of processes and coupled RTM simulations. This requirement is especially important for predicting the long-term containment of CO₂ and monitoring sequestration sites. CO₂-induced geochemical processes may weaken rock strength within a reservoir compartment leading to the potential for porosity collapse, buildup of fluid pressure, and seal failure. Associated changes in rock properties and fluid distributions are likely to affect the geophysical rock properties, such as *P*- and *S*-velocities, seismic attenuation, and electrical resistivity. While credible long-term predictions require an integrated approach, they also mandate targeted research in geomechanics.

4.5.1. Fluid-Assisted and Time-Dependent Fracturing

Surface-chemical effects of water on crack growth may be a significant factor in the long-term containment of CO₂. (See Kirby and Scholz, 1984, for a special issue of the *Journal of Geophysical Research* on the chemical effects of water and the deformation and strengths of rocks.) Many experiments (Atkinson and Meredith, 1987) have shown that the presence of water or other pore fluids can enhance crack growth in brittle rocks. In particular, the presence of pore fluid allows slow growth of cracks at stress intensity factors below the critical value corresponding to rapid (dynamic) crack growth. Das and Scholz (1981) have attributed a variety of time-dependent earthquake phenomena to this mechanism, and there is evidence (Dieterich and Conrad, 1984; Dove, 1995) that the micromechanical mechanism of rate and state-dependent friction is related to surface-chemical effects of pore fluid. Information from laboratory experiments on environmentally assisted crack growth has been incorporated into constitutive relations and these have achieved reasonable success at describing the time-dependent deformation of bulk specimens (Costin and Mecholsky, 1983; Costin, 1987). Segall (1984) has applied a model based on relations derived from laboratory experiments to rate-dependent extensional deformation in rocks.

Despite this progress, the coupling of chemical effects of pore fluid with strength and deformation remains poorly understood and may be a significant impediment to predictions about the long-time containment of CO₂. Few, if any, observations exist on crack growth in CO₂ contaminated environments. Laboratory experiments have, for the most part, considered the time-dependent growth of macrocracks under tensile loadings and assumed that crack-tip fields can be characterized in terms of the elastic singular field. Surface chemical effects, however, may be strongly related to inelastic processes near the crack-tip. Furthermore, the long-term, time-dependent behavior of rock may be due primarily to the growth of microcracks in stress fields that are locally tensile but overall compressive. For microcracks under overall compressive loads, branching and turning complicate growth. Additional complicating factors are different responses of various constituents to pore fluid and interface effects. Laboratory experiments of crack growth rates of less than 10⁻¹⁰ m/s are impractically long, yet this rate corresponds to about 3 mm/year, which is relatively rapid over the 50–100 year intended life-time of sequestration. Thus, sound extrapolations to time scales of interest require a thorough understanding of the underlying physical mechanisms.

Subcritical crack growth is important for the long-term constitutive description of sequestration sites for evaluating the potential of macroscopic fracture development and seal degradation and for incorporating changes in (geophysical) rock properties in interpreting geophysical measurements. Important changes may also result from inter- and intergranular creep. Creep may lead to significant, possibly anisotropic, changes in rock porosity, permeability, and local rock

strength—all of which could have profound consequences for pore-pressure distribution and fluid flow, as mentioned earlier. Although studies of creep mechanisms are most readily controlled in laboratory experiments, extrapolations of laboratory data to *in situ* conditions again may entail leaps in temperature, stress, and time (strain), with attendant but unrecognized changes in the rate-controlling physical or chemical processes.

5. GEOPHYSICS

5.1. Introduction

Successful CO₂ sequestration in active or depleted oil/gas reservoirs or aquifers requires an accurate map of the hydraulic and mechanical integrity of a site. Sub-surface reservoirs consist of solid, liquid, and gaseous phases that produce heterogeneity on multiple length scales and may vary temporally and spatially because of geochemical interactions and variations in stress, pressure, and temperature. The ability to detect these changes in reservoirs over time requires an understanding of the relationship among rock properties, spatial resolution, and time resolution. The rock properties most important for site selection, injection, and monitoring will dictate spatial and temporal resolution and thus the geophysical techniques used. The inversion of geophysical data maps to maps of reservoir properties will depend on the spatial and temporal resolutions achieved as well as an understanding of the relationship between geophysical information and rock properties.

With any geophysical method there is a tradeoff between the volume of rock sampled and the ability to image heterogeneity. For example, a three-dimensional seismic survey (50 Hz) can easily sample the entire volume of a reservoir 3000 m deep. However, the reservoir is sampled with a resolution of only a few tens of meters. Figure 33 indicates the tradeoff between the volume sampled and the resolution length scale for a variety of seismic methods. Laboratory measurements on cores can resolve submillimeter to millimeter features but can sample only a small fraction of the entire core volume. On the field scale, the type of seismic method used also will determine which portions of the reservoir are sampled. For example, sonic logs (10 kHz) sample the region immediately adjacent to the borehole with a submeter resolution, whereas crosswell seismic profiles (1000 Hz) sample the limited volume between wells with meter-scale resolution.

Geophysical methods have the potential to be a quantitative diagnostic tool for monitoring CO₂ sequestration, but progress is hindered by incomplete understanding of the effect of rock properties (especially porosity, permeability, saturation, geochemical alteration, and natural fractures), reservoir conditions (i.e., stress, pressure, and temperature), heterogeneities, and scaling on quantitative remote imaging. Active monitoring techniques need to be refined to quantify the changes.

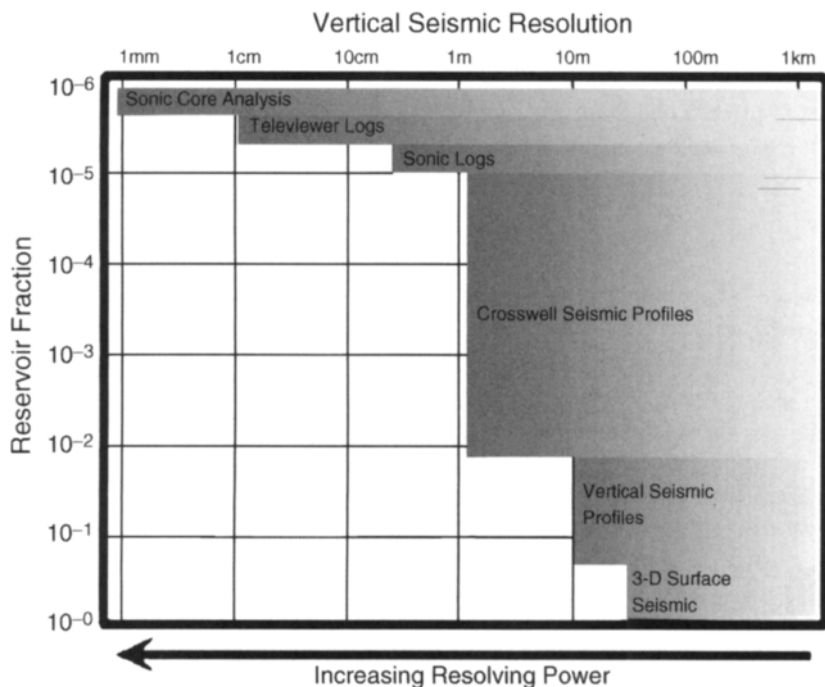


FIG. 33. Schematic of seismic resolution vs coverage as a function of seismic method (Harris, unpublished).

5.2. Rock Properties

Some of the key concerns for geophysical monitoring and interpretation involve gaps in the knowledge of the interrelationships among geophysical rock properties and geochemical, geomechanical, and flow-induced alterations. As discussed in the Geomechanics section, these gaps can be filled through an intensive program of theoretical, laboratory, field, and computational investigations at a variety of length and time scales using a combination of techniques. The geophysical characteristics of a reservoir or rock mass are strongly dependent upon the porosity and permeability characteristics of the formation. In addition, the micro-scale (pore and grain distributions, grain contacts, and cracks) and macro-scale (fractures, stratification, laminae, and other physical structures) heterogeneity in a reservoir modify the seismic, electromagnetic, and deformation responses.

Micro-scale sources of heterogeneity affect the macroscopic behavior of seismic waves propagated through rock by delaying and attenuating a wave as well as altering the frequency content of a signal. The micro-scale phenomena can be viewed in terms of discontinuity and interface phenomena, such as fractures,

grain-to-grain contacts, fluid–solid interaction, and liquid–gas interaction within the pores or fractures. Nihei (1992) identified the micromechanical behavior of the grain contacts in rock as the primary source of attenuation in dry and fluid-saturated rocks. From laboratory measurements (Suarez-Rivera, 1992), a five-micron-thick coating of clay in a fracture caused significant attenuation, although the scale of the heterogeneity (clay) was 0.001 of a wavelength. The effect of non-aqueous phase liquids (NAPLs) on compressional wave propagation through soils (Geller and Myer, 1995) showed that compressional wave velocities were sensitive to increased NAPL saturation in the soil cores. However, no research has been performed to determine if the fluid–fluid interface (or front) can be resolved from seismic measurements. The ability to resolve correlated pore/grain distributions or fluid-phase distribution from seismic data is not well established.

The development of velocity and attenuation relationships from seismic and electromagnetic data is required to interpret near-surface seismic data acquired through continuous on-line seismic monitoring and to detect and identify the alteration of a rock matrix from interaction with CO₂ and other pore fluids. Fluid flow through a porous or fractured medium depends on the size and spatial distribution of the pore space and the interconnectivity of the pore space. Fundamental physicochemical changes can occur in the transport of particles or fluid chemicals through a porous medium (Imdakh and Sahimi, 1991; Fryar and Schwartz, 1994; Bertrand *et al.*, 1994; Lappan *et al.*, 1997). The change in pore structure occurs either from chemical interaction between the fluid and rock matrix resulting in dissolution of the solid, or from various forces that result in physical adsorption of a particle onto the rock matrix surface (i.e., precipitation).

In general, CO₂ has properties very different from those of the water and oil that remain in the reservoir. Figure 34 shows the measured compressional wave velocity of CO₂ as a function of pressure at three different temperatures (Wang and Nur, 1989). For example, at high pressures, the density of CO₂ approaches that of water, yet its bulk modulus is much lower than that of water. The seismic detectability of sequestered CO₂ depends not only on this contrast in fluid properties, but also on its saturation and the properties of the host rock and the local environmental conditions, e.g., temperature and pressure. Other changes are demonstrated (Fig. 35) by the effects of CO₂ on the seismic velocity of Beaver sandstone originally saturated with *n*-hexadecane (Wang and Nur, 1989). The compressional wave velocity decreases markedly with the introduction of CO₂. The magnitude of the changes in velocity may not be this large in other rocks. Nevertheless, this example illustrates the underlying basis in rock properties for potentially monitoring a CO₂ sequestration process.

As stated in the previous sections, the presence of CO₂ may lead to significant changes in mineralogy through a complex series of reactions. Dissolution of the rock matrix may occur, increasing the size of the pores and the connectivity of the pore space. Dissolution can occur in regions with high surface energies, such

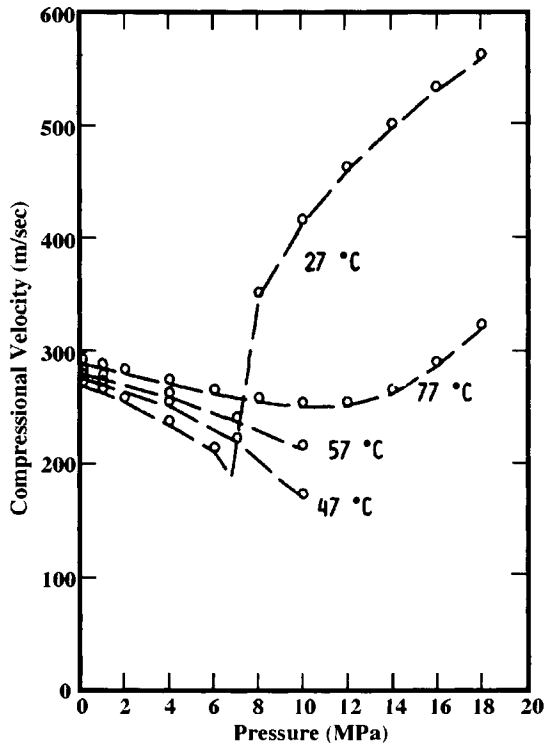


FIG. 34. Compressional wave velocity in carbon dioxide as a function of pressure at three different temperatures (from Wang and Nur, 1989).

as grain contacts under high stress. Dissolution at a grain contact reduces the mechanical stiffness of the contact by lowering the surface energy (Murphy *et al.*, 1984). A reduction in contact stiffness increases attenuation of transmitted acoustic waves (Nihei, 1992).

Precipitation or fines migration can block pore space and reduce the permeability of the rock (Gash *et al.*, 1992; Narayan *et al.*, 1997). It can also form cement at grain contacts and alter the grain-contact stiffness (Li, 1997; Li and Pyrak-Nolte, 1998). Dvorkin *et al.* (1994) found theoretically that the stiffness and amount of cement at the grain contacts controlled the elastic properties of the rock and, thus, the seismic properties.

The only laboratory investigation of the effect of sediment–pore water interaction on acoustic wave propagation was performed by Li (1997) and Li and Pyrak-Nolte (1998) on fully saturated synthetic sediments. The acoustic wave amplitude increased and decreased relative to the exchange of ions between the pore water and the sediment as indicated by electrical conductivity measurements (Fig. 36).

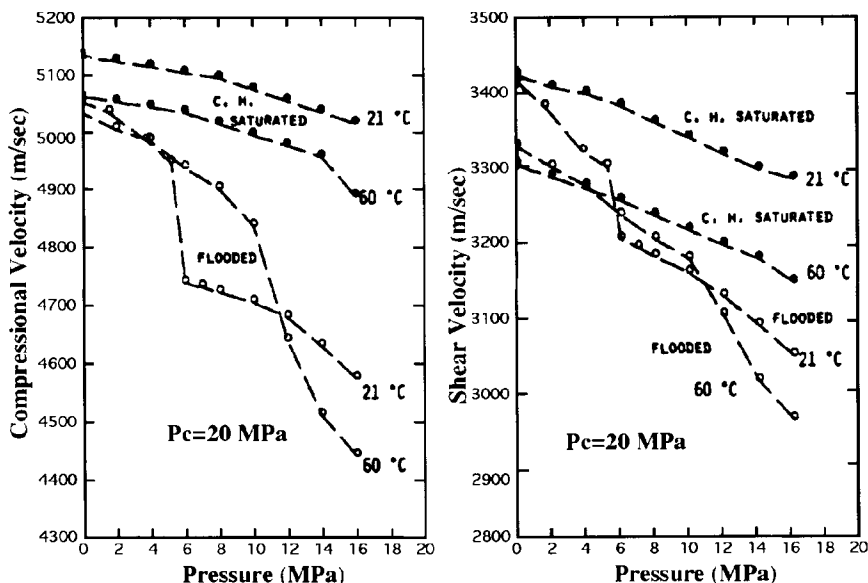


FIG. 35. Compressional wave and shear wave velocities in *n*-hexadecane-saturated and carbon dioxide-flooded Beaver Sandstone versus pore pressure (from Wang and Nur, 1989).

The lowest transmitted amplitude occurred when the ionic strength reached a minimum. Over a four-month period, the sediment sample underwent diagenesis and formed synthetic sandstone. The acoustic attenuation was observed to be sensitive to the ion exchange between the pore fluid and the sediment. However, the wave velocity was insensitive to the ion exchange, but was sensitive to compaction and cementation at the grain contacts. Microscopic investigation determined that precipitation had welded the grain contacts and reduced the porosity of the sample from 35% to 15–30%. Thus, if the geochemistry analyses demonstrate that the CO₂-related processes produce sufficient amounts of acids to significantly alter grain-to-grain contacts or fracture geometry, seismic methods have the potential to track chemically induced time-dependent changes.

To obtain the best geophysically derived maps of reservoir properties, it is important to understand how rock properties determined on the laboratory scale relate to field-scale measurements. The ability to resolve multi-scale heterogeneity depends on the type of heterogeneity present—fractures, pore/grain distributions, multiphase fluid distributions, etc. Mukerji *et al.* (1995) investigated scale-dependent velocity by comparing seismic velocities on the laboratory scale (wavelength ~ 0.01 cm) with the well log scale (wavelength ~ 0.1 – 1 m), and with the surface seismic scale (wavelength ~ 10 m). The observed scale dependence of the seismic velocity occurs because the length scale of the heterogeneity present

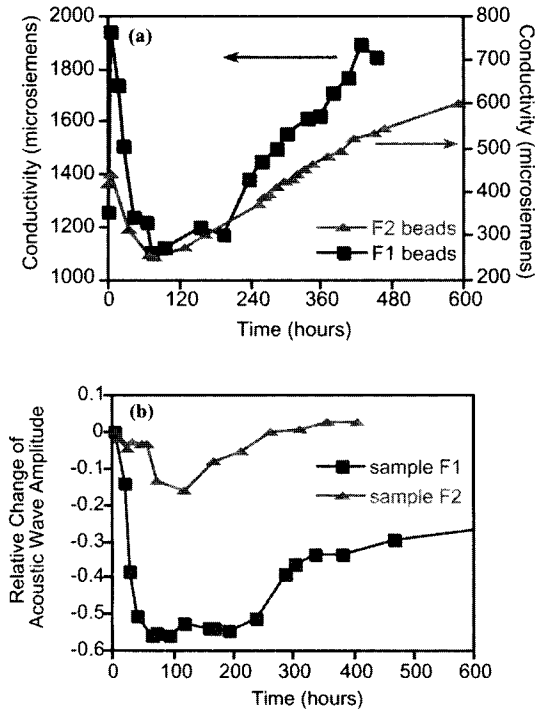


FIG. 36. (a) The electrical conductivity of the pore water and (b) the relative change in amplitude of a compressional wave as a function of time for two water-saturated synthetic sediments composed of soda-lime glassbeads. The minimum in electrical conductivity is concurrent with a minimum in compressional wave amplitude (from Li and Pyrak-Nolte, 1998).

may vary with the size of the volume of rock sampled. The seismic velocity was found to depend on spatial statistics of the petrophysical properties of the rock, the seismic wavelength, and the path length. Seismic waves would find “fast” paths of high-velocity material to propagate through the material.

Laboratory measurements of the seismic response of fractures may not be representative of the seismic response of all of the fractures observed in the field. Laboratory-scale fractures tend to have smaller apertures and possibly more contact area resulting in larger values of fracture-specific stiffness (the ratio between the stress and the magnitude of the displacement discontinuity produced by the stress). Therefore, fractures in the laboratory may exhibit less attenuation and produce fewer delays in a transmitted signal than in larger fractures in the field. However, the displacement discontinuity description (Pyrak-Nolte *et al.*, 1987, 1990a) of seismic wave propagation across a fracture contains a built-in scaling parameter in terms of a normalized frequency. Normalized frequency is the

product of the frequency of the incident signal, with the seismic impedance (product of density and phase velocity) of the rock divided by the fracture-specific stiffness. This ratio indicates which fractures can be located in the field for a given source frequency based on the specific stiffness of the fracture and whether amplitude data or velocity data will contain more information on the presence of a fracture based on the source frequency. This theory allows laboratory results to be scaled to field frequencies.

For fractures modeled as non-welded contacts, the limit of the ability to resolve fractures with field frequencies depends on the frequency of the source signal and the fracture-specific stiffness (Pyrak-Nolte, 1990a). Fracture-specific stiffness is a function of the size and distribution of contact between the two fracture surfaces. For the laboratory range of fracture-specific stiffness ($\kappa > 10^{11}$ Pa/m), the displacement discontinuity theory predicts that an incident wave with a frequency of 1.0 MHz will show a large increase in transmitted wave amplitude as the stiffness of the fracture increases, but will show very little change in seismic velocity. The theory also suggests that, on the laboratory scale, seismic amplitudes will yield more information on the presence of fractures and changes in fracture stiffness than seismic velocities. On the other hand, at field frequencies (e.g., at 10 Hz) a fracture with stiffness greater than 10^{11} Pa/m cannot be detected with either velocities or amplitudes. However, a fracture with a specific stiffness in the range of $10^5 < \kappa < 10^{11}$ Pa/m can be detected, and changes in contact stiffness could also be monitored. Other complications such as the effect of time-dependent geochemistry changes on the fractures (e.g., dissolution or rehealing) will need to be evaluated.

5.3. Characterization

Geophysical site characterization involves three tasks that range from qualitative reconnaissance through assessment to quantitative site description. The reconnaissance phase is needed to delineate the boundaries of the site, which include storage capacity, faults, etc. An assessment is also needed to determine the hydraulic integrity of the site that may be compromised by old wells, tunnels, seeps, etc. A quantitative description must set bounds on parameters such as saturation, porosity, and heterogeneity. These three characterization tasks are essential for establishing the baseline for subsequent monitoring and guidelines for site management. A variety of standard and state-of-the-art integrated geophysical techniques, including borehole and surface seismic, logs, core, potential fields, and electromagnetics, can be used with new technologies, yet to be identified, to perform these tasks.

The technologies for acquiring, processing, and interpreting seismic data are mature, but continue to evolve in their capability to image smaller and smaller

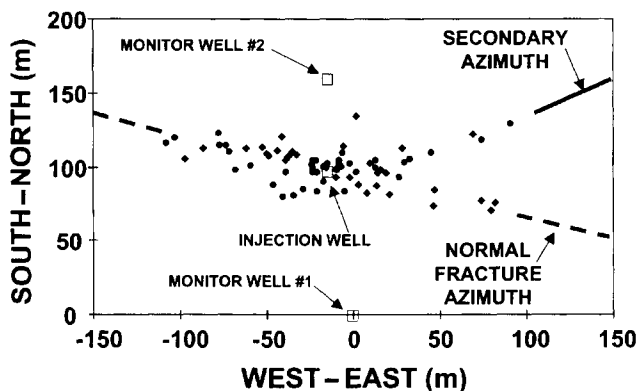


FIG. 37. Example of microseismic imaging from the GRI/DOE Multi-Site experiment (from Warpinski *et al.*, 1998).

features over larger and larger volumes. Notable improvements are occurring in the acquisition of higher frequencies and in pre-stack imaging. Stacking is the process of adding repetitive source shots to improve signal-to-noise ratios. These improved images are subsequently combined with rock physics and used as weak constraints in reservoir modeling schemes, such as geostatistics. Moreover, there is considerable research within the petroleum industry, government labs, and industry in translating these geophysical images (e.g., amplitude attributes) into more quantitative estimates of reservoir storage and flow properties, in addition to their well-established uses for structural imaging. The critical need is the development of capabilities (acquisition, processing, and interpretation) to resolve sufficient detail to ensure site integrity and efficient injection of CO_2 .

Figure 37 shows an example of imaging capabilities that can be obtained with downhole arrays of seismic receivers monitoring a hydraulic fracture injection. The plot provides a plan view of the locations of numerous microseisms that were produced in the early stages of a fracture stimulation (Warpinski *et al.*, 1998) and detected from arrays in two offset monitoring wells. Of particular interest is the formation of a secondary fracture, a result that was unanticipated and not evident in any of the other fracture data. Imaging technologies such as this should help delineate the flow paths that develop during injection processes.

Figure 38 relates to drill-cuttings injection (Griffin *et al.*, 1999) monitored with downhole tiltmeters in a well offset about 43 m. As shown on the left side, the fracture creates a deformed zone that is detected by sensitive downhole-tiltmeter arrays. By matching the tilt data with an appropriate model (in this case an elliptic fracture), an integrated image of the overall size of the fracture can be estimated. This particular injection appears to be nonvertical (about 15° inclination) and of very limited height.

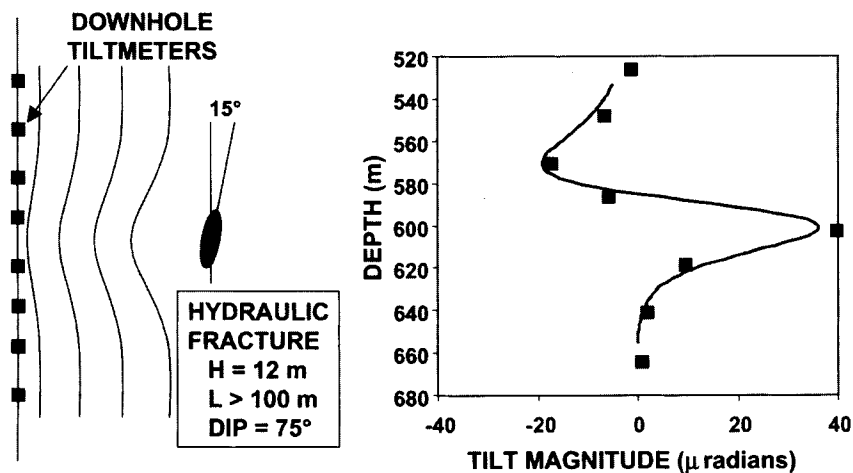


FIG. 38. Example of downhole tiltmeter imaging from the Mounds Drill Cuttings Injection Experiment (from Griffin *et al.*, 1999).

High-resolution images have been produced with crosswell seismic tomography (Langan *et al.*, 1997). The tomogram in Fig. 39 (color insert) defines an oval-shaped low-velocity zone representing an anomaly in the high-porosity reservoir facies. The anomaly is apparent at a depth of approximately 2785–2660 m (8700–89,500 ft) in the right hand side of the image. Crosswell methods are potentially capable of producing these high-resolution images in 2D. Research is needed to extend this capability to three dimensions.

To improve our ability to delineate and quantify porosity and permeability in potential CO₂ sequestration reservoirs, it is necessary to understand the effect on the mechanical-seismic response caused by (1) heterogeneity within a fracture, i.e., void space distribution, asperity heights, variation in stiffness, fluid saturation, etc.; (2) heterogeneity from multiple fractures and fracture networks, i.e., fracture orientation, number of fractures, geometrical properties of intersections, fluid saturation, etc.; and (3) other heterogeneities in porous media such as the grain contacts, fluid–grain contacts, fluid saturation, correlated grain/pore distributions, etc.

Will partial saturation of a reservoir with CO₂ be visible to geophysical techniques? If a CO₂ sequestration reservoir had a slow leak into a water or oil saturated fracture, displacement of liquid from the void space within a fracture by a gas reduces the stiffness of the fracture. The reduction in fracture stiffness delays and attenuates a wave transmitted across the fracture and enhances the reflected energy from the fracture. Seismic waves propagated along a fracture with reduced stiffness give rise to fracture-interface waves that depend on fracture-specific stiffness (Pyrak-Nolte and Cook, 1987; Pyrak-Nolte *et al.*, 1992). Thus, if during the injection process CO₂ displaces a liquid phase in a fracture, the seismic signal will

be dramatically altered. This has been observed on the field scale (Majer *et al.*, 1997; Myer, 1998) in high-frequency (1–10 kHz), crosswell seismic data taken during gas injection into a water-filled fracture in limestone. Specifically, interface waves were recorded as the gas displaced the water in the fracture. Further investigation is needed to determine the minimum gas saturation that can be detected seismically.

The integrity of the site and efficiency of the injection process require identification of heterogeneities (such as fractures and thin high-permeability layers) that may lead to the problems or failures discussed above. The ability to resolve such features using geophysical techniques is an issue. For example, fractures in rock extend over tens of meters, but the “thickness” or aperture of the fracture can be as small as microns to millimeters—much smaller than a wavelength. However, the small-scale micro-mechanics of the system strongly perturbs the wave front by partitioning energy into body waves, interface waves, and other guided modes. Majer *et al.* (1997) have shown using high-frequency (1–10 kHz) crosswell and single-well survey methods that air-filled fractures with a thickness of 1 mm could be resolved using wavelengths of 0.5 to 1 m (0.001 of a wavelength) for a well separation of 50–100 m over a 20-m depth. Another research issue is the detection of fracture orientation, fracture connectivity, and other rapid flow paths.

5.4. Monitoring

Monitoring during the injection process is important to identify the location and saturation of the gas, the potential for breach, and the overall reservoir dynamics, including changes in stress states referred to earlier. These tasks require a variety of geophysical techniques: tiltmeters, seismic, electromagnetic, and various geophysical logs. Necessary research involves determining the optimum techniques for repeatability at desirable resolutions. Methodologies for quantitative comparisons of time-lapse images must be developed. Monitoring will be useful for identifying changes rather than defining static properties of fluids or flow. For example, seismic velocity is usually sensitive to the type and saturation of fluids in the pore space and to the differential pressure (pore pressure minus confining pressure), but it also varies with lithology and cementation. Therefore, estimating relative changes in saturation from time-lapse changes in seismic velocity is a better posed problem than the direct inversion of velocity for absolute fluid saturation. Many good examples (Wang and Nur, 1989) of seismic monitoring come from thermal-recovery processes (e.g., steam floods) where the change in seismic velocity caused by steam can be as large as 30%. Despite the excellent time-lapse images showing the changes from thermal-recovery processes, interpreting the images to determine saturation levels is difficult because uncertainties persist in quantifying the combined effects of steam, hot water, and oil on the rock properties.

Seismic methods have been available for monitoring petroleum recovery processes for many years, though not used routinely. Recently, the effort has focused on developing low-cost techniques for repeated use in reservoir management. An example of monitoring steam injection for enhanced oil recovery is shown in Fig. 40 (color insert) (Jenkins *et al.*, 1997). These reflection seismic images show seven time-lapse snapshots taken as steam was injected over a period of 31 months. Expansion of the steam away from the injection well is readily seen by differencing snapshots (Jenkins *et al.*, 1997). Monitoring from the surface is successful in this case largely because the change in rock properties with steam injection is large and the reservoir target is shallow. The yellow lines delineate the top and bottom of the steam injection interval. While the data do not change above the injection interval, the sag below is caused by the steam. (Jenkins *et al.*, 1997).

The potentially large contrast in the seismic properties of rocks partially saturated with CO₂ versus those saturated with water and oil suggests that both the location and the saturation of CO₂ can be monitored in a manner similar to the steam example above. However, detection of CO₂ is potentially more difficult because it depends on volumetric factors such as the thickness and lateral extent of the zone undergoing changes in saturation and the depth of the reservoir. When possible, surface seismic methods are preferred because of their large coverage and ease in deployment of instrumentation. However, in some situations, borehole methods such as vertical seismic profiles and crosswell and well logs may be required because of their capability for high resolution and ability to detect small changes in small volumes.

Recently, crosswell tomography was used to identify simultaneous *in situ* changes of saturation and pressure caused by CO₂ injection in a carbonate reservoir (Harris *et al.*, 1996a,b). More work is needed to separate these two effects in the actual time-lapse images. Shear waves are not significantly affected by fluid changes; therefore, time-lapse, S-wave images should provide a pressure map, whereas time-lapse, P-wave images sense the combined changes of pressure and saturation. Laboratory results and rock physics modeling need to calibrate and support these field observations. Moreover, laboratory data show that the magnitude of the seismic changes (2 to 20% in seismic velocity) associated with the typical west Texas CO₂ injection process varies depending on the porosity and permeability of the formations. Through monitoring, it should become possible to identify high-permeability zones by quantitatively interpreting the magnitudes of the seismic changes. Based on these crosswell results, large-scale three-dimensional, time-lapse seismic experiments are recommended.

Figure 41 (color insert) is an example of crosswell tomographic monitoring of injected CO₂ in a west Texas carbonate reservoir (Lazaratos and Marion, 1997). In this field pilot study, compressional velocity was seen to decrease by more than 1000 ft/s (305 m/s) or about 6% in a 50-ft-thick (15.2 m) zone of the reservoir. The change is easily observed with high-frequency crosswell data, but due to its

depth, small volume, and small contrast, the change would be difficult to image with surface seismic. Also, the observed velocity changes in this example are due to the combined effects of an increase in pore pressure and the increase in CO₂ saturation, both associated with the injection process in oil recovery.

Geomechanics discussions alluded to the possibly significant alteration of stress state in reservoirs and the surrounding rocks by injection of high-pressure fluids or conversely, withdrawal of reservoir fluids (Warpinski and Branagan, 1989; Warpinski and Teufel, 1991; Wright *et al.*, 1995). Hydraulic fracturing and waterflooding generally result in both fracturing of the rocks and leakoff of high-pressure fluids into the reservoir. Large stress changes can occur, both locally around the injection/production well and throughout the reservoir. The magnitude of these stress changes is usually a significant fraction of the change in reservoir pressure, which typically is 10–50 MPa. These changes can be measured and modeled (although with some difficulty) by means of standard microacoustic stress testing equipment and other reservoir information. If CO₂ injection is similar to waterflooding, gas reinjection, and CO₂ flooding, the layout of the injection wells will result in a highly heterogeneous pressure surface within the reservoir, changing CO₂ solubility and fluid permeability throughout.

Monitoring the consequences of CO₂ injection would be similar to the problems of monitoring fracturing, waterflooding, subsidence, drill-cutting injections, or gas storage. Various technologies are applicable here, including microseismic monitoring of pressure-induced shear slippages in the disposal reservoir (e.g., Warpinski *et al.*, 1997), and surface and downhole tiltmeters (Wright, 1998) for detecting reservoir deformation. Tiltmeter measurements are important diagnostic tools because they yield reservoir strains (poro-thermo-elastically induced, in this case). Tiltmeters also aid in identifying fracturing, subsidence, and *in situ* stress changes. It is emphasized, however, that the foregoing diagnostic techniques have been used primarily during hydraulic fracturing and EOR operations, but have never been applied to long-term monitoring that may require new procedures and processing techniques.

5.5. Containment Integrity of CO₂

The most important consideration for ensuring the integrity of the site over extended periods of time is the frequency of the measurements. The frequency of monitoring measurements will depend on the required temporal and spatial resolution, the ability to use automatic sensing equipment, and the ability to maintain and interpret a large data set. Through time-lapse monitoring, geophysical imaging may be used to characterize the reservoir, to assess both vertical and horizontal changes, and to monitor the long-term integrity of containment. The permanent placement of geophysical sources and receivers can provide the means necessary

for cost-effective monitoring and differentiating injection-related changes from background changes. There are, nevertheless, several issues to be investigated:

- The magnitude of the seismic changes associated with CO₂ injection
- The dependence of the geophysical changes on lithology, pore structure, pressure, temperature, etc.
- The reservoir-specific issues, such as depth, heterogeneity, etc.
- The repeatability of the geophysical experiment
- The resolution required
- The experience to be gained from studying existing natural-gas storage sites

Research issues in containment related to the use of geophysical techniques include (1) quantitative definition of fast-flow paths and (2) identification of fracture formation caused by geochemical alteration or changes in local stress. Seismic methods have the potential for identifying fracture paths along which CO₂ may leak from the reservoir. Here again, the experimental, theoretical, and numerical investigations of seismic response of a fracture and fracture-specific stiffness are relevant (Pyrak-Nolte *et al.*, 1990a,b; Pyrak-Nolte and Cook, 1987; Gu *et al.*, 1996a,b). To identify fast paths in a network of fractures, the fracture stiffness for each fracture within the network could be mapped seismically. The hydraulic property of each fracture within the network would then be inferred from fracture-specific stiffnesses, if the interrelationship among fracture properties is fully understood.

Fractures in rock often are highly conductive, rapid flow paths that can connect rock formations that are otherwise hydraulically isolated. Laboratory data show that the fracture-specific stiffness and volumetric flow rate of a fracture are linked (Pyrak-Nolte, 1996) through the size and spatial distribution of the apertures and contact area of the fracture. This interrelationship (Fig. 42, see color insert) between fracture-specific stiffness and fracture flow has been observed over three orders of magnitude of specific stiffness and nine orders of magnitude in flow rates for laboratory samples of granite ranging in size from 0.052 to 0.29 m (Pyrak-Nolte, 1998). However, there were two classes of behavior for the interrelationship: low data fell on a universal curve, or the flow data were independent of stiffness. Several questions remain, such as:

- Will rocks from the same tectonic setting fall on the same fracture-specific stiffness-fluid flow curve,
- Or will there be different universality classes based on rock type or stress history?
- Will repeated stress cycling alter the relationship?
- Will the relationship be scalable to the field scale?

These questions cannot be addressed without more experimental results or without experimental validation of numerical codes to simulate fluid flow and fracture deformation.

Detection of crack formation can be performed using microseismic techniques or specialized active-monitoring techniques. When a fracture forms through the linkage of microcracks, this zone of material undergoes a reduction in mechanical strength and change in volume. The reduction in mechanical strength is confined to a region much smaller than a typical seismic wavelength. Therefore, it is suggested that the weakened zone can be represented as a non-welded contact with a defined stiffness. As the stiffness of the zone decreases with increased microcrack linkage, seismic waves propagated along this zone will form guided-wave modes that are a function of the stiffness of this zone and are dispersive. Pyrak-Nolte *et al.* (1996) found that shear waves are especially sensitive to crack formation when the wave-particle motion is perpendicular to the fracture plane because these shear waves couple into interface waves propagating along a fracture. Long before catastrophic failure, when a macroscopic fracture is formed, the energy in shear wave signals shows a dramatic frequency shift. This frequency shift is a signature of the partitioning of energy out of a bulk wave and into interface waves. Because this signature is observed prior to failure, it suggests that the presence of an incipient interface wave is supported by the network of oriented, but disconnected microcracks. The change in the amplitude, velocity, and frequency content of the signals with time can indicate that failure is imminent, and CO₂ leakage may occur.

If the formation of a macroscopic fracture produces a damaged zone immediately adjacent to the fracture, the thickness or extent of this zone will have altered the seismic properties relative to the undamaged portions of the rocks and possibly the fracture itself. This is an area that needs further research to determine if the damaged zone would support guided-shear modes similar to Love waves (Nihei *et al.*, 1994), as opposed to the fracture interface waves (Pyrak-Nolte and Cook, 1987; Gu *et al.*, 1996a). The distinction between these two types of guided modes would be the polarization of the shear-wave particle motion. The ability to resolve the damaged zone from the fracture may not be possible or will depend on the spatial resolution of the probe.

6. SUMMARY AND PRIMARY RESEARCH NEEDS

This paper explores the state of knowledge and uncertainties of terrestrial sequestration of CO₂ in active hydrocarbon reservoirs, depleted reservoirs, deep saline aquifers, and (to lesser extent) coal beds. Deliberations started from the premise that CO₂ disposal in geological formations is technically feasible based on (1) applicable industrial experience in hydraulic fracturing and the use of CO₂ for enhanced oil recovery, and (2) more recent experience in CO₂ disposal in saline aquifers in Norway and hydrocarbon producing regions in the Far East. It also became evident that studies of CO₂ sequestration could draw on current

geoscience research in several areas such as the influence and quantification of reservoir heterogeneities on a variety of scales; low-temperature geochemistry; micromechanical processes; the evolution of fracture systems and faults; coupled processes and their numerical treatments; and geophysical measurements of rock properties and reservoir conditions.

Fundamental differences, however, exist concerning the resolution needed in reservoir characterization for oil and gas production vs long-term CO₂ disposal, reservoir response to CO₂ injection with associated hydrological, geochemical, and mechanical interactions with the host rock and its natural fluids, and long-term containment potential of the reservoir and its seals. For example, it is not possible at this time to specify the kinetics of the various homogeneous and heterogeneous reactions following CO₂ injection. Differences also were identified between oil/gas reservoirs, aquifers, and coal. Oil and gas reservoirs will be better characterized than aquifers, with recorded production histories and more existing drillholes that can be used for additional characterization activities. CO₂ injection, distribution, and containment in coal beds will be controlled by methane desorption and adsorption processes not found in oil and gas production.

Further questions concerning terrestrial CO₂ sequestration arise in predicting total storage capacities. Storage and containment evaluations are dominated by porosity and permeability distributions but also depend on the presence and contributions of natural fractures, fluid saturation, and residual fluid distribution. Additional uncertainties exist concerning the pressure limits and requirements for defined seals in saline aquifers and the origins of fracture systems in hydrocarbon reservoir rocks and coal whose contributions to fast transport and reservoir boundaries may well become important to predicting the fate of CO₂ over hundreds of years.

Special issues germane to CO₂ disposal arise in the assessment of depleted reservoirs, whose properties are known to have changed during single or repeated pore-pressure drawdown and fluid redistribution. Data about the potential effects of these changes on the integrity of the surrounding reservoir seals appear to be sparse. Other questions specific to CO₂ sequestration relate to the influence of chemical processes on reservoir flow properties and rock strength, approaches to verifying the long-term containment potential of reservoirs, and the potential need for monitoring small changes in reservoir characteristics with time (e.g., caused by slow CO₂ leakage).

In order to identify uncertainties and research needs for the terrestrial sequestration of CO₂, this study was organized around reviews from four different general perspectives: geohydrology (and reservoir engineering), geochemistry, geomechanics, and geophysics. Accordingly, some specific fundamental research areas, unique to CO₂ sequestration or common with hydrocarbon reservoir characterization and development, include the following:

- Understanding fault formation and fault sealing properties as a function of lithology, stress state, temperature, and fluid chemistry.
- Further research concerning the evolution of joint systems and fracture networks, including joint lengths and spacing, fracture interactions with one another and with other rock mass heterogeneities.
- Characterization of matrix rock porosity and permeability and their effects on single- and multiphase fluid flow. This research includes the definition of spatial organization of porosity in terms of depositional environment and diagenetic processes.
- Research on the effect of porosity heterogeneity and fractures on viscous fingering and fluid channeling on all scales (grain scale to field).
- Understanding the connectivity of fracture networks and determining differences in conductivity between individual fractures and fracture sets causing permeability anisotropy and fluid flow along a few major channels. Research in this area must be cognizant of the effect of total stress and pores pressure on the opening and closure of fractures, hence aperture distribution.
- Research on CO₂ trapping mechanisms starting with the three simplest mechanisms for predicting CO₂ migration and reservoir-storage volume: aqueous, mineral, and microbial trapping.
- Research on the kinetics of the various homogeneous and heterogeneous geochemical reactions to predict the paths and rates of rock–fluid interactions in the presence of CO₂.
- Development of models of heterogeneous reactions involving complex averages over a variety of atomic-scale processes for use in chemical and fully coupled constitutive equations.
- Geochemical studies combined with studies of the history of fracture networks to understand the development of infillings on fluid flow and fracture healing. Fluid flow, aperture distribution, and channeling may be similarly affected by dissolution.
- A better understanding is needed of fluid flow and geochemical fluid–rock interactions along fracture intersections.
- Understanding CO₂ effects on clay minerals and shales.
- Research on the (mechanical) constitutive behaviors of porous media and discrete natural fractures, with emphasis on identifying fine structure and grain-scale processes as well as scaling from grain-scale processes to bulk behavior.
- Test and extension of the concept of effective stress to large changes in pore pressure and associated inelastic changes in porosity and damage development.
- Research into the evolution of matrix rock permeability as a function of stress state, stress path, and damage.
- Measurement and analyses of the influence of lithology and geologic structure on virgin *in situ* stress states and the evolution of *in situ* stresses with changes in pore pressure and rock-mass deformation.

- Additional study concerning fracture development in high-porosity, weakly consolidated formations with impact on reservoir response to injection and hydraulic fracture design.
- Relationships between rock textures, mechanical rock properties, geophysical properties, and stress states are needed for translation of seismic images into maps of reservoir properties. Desired outcomes are, for example, the delineation of pore pressure distribution and location of over- and underpressurized reservoir compartments.
- Research on permissible aquifer pressures associated with CO₂ injection.
- Research related to CO₂ sequestration in coal beds, including the fundamentals of coal wettability, methane desorption, and CO₂ adsorption processes and a thorough understanding of complex fracture (cleat) networks and attendant consequences for fluid flow.
- Coalbed sequestration will require research concerning the sealing properties of the bounding lithologies and associated structural features.
- Research on the capabilities of different geophysical techniques (e.g., seismic or electromagnetic) is needed to monitor time-dependent changes caused by dissolution or precipitation associated with changes of rock textures and fracture infillings.
- Determination of the seismic “visibility” of partial saturation of CO₂ for monitoring CO₂ migrations in different lithologies and at different pressures and temperatures.
- Seismic research on the relationship between the hydraulic, mechanical, and seismic properties of fractures and thin layers to assess and predict CO₂ leaks.
- Resolution of advanced-monitoring techniques, such as microseismic receiver arrays, surface/downhole tiltmeters, or appropriately applied surface or cross-well geophysical surveys to detect fast-leak paths and ensure site integrity.
- Development of new methods for differential seismic imaging using phase, amplitude, and frequency information for improved spatial resolution from the current range of 10–1000 m to a spatial resolution as high as 0.1 m.
- Geophysical research on fault and fracture detection by wave trapping and interface wave measurements and analyses, including such variables as the effects of scale, stiffness, void structure, fluid saturation, fracture spacing, and cyclic injection.
- Extensive laboratory experimentation along with carefully chosen field measurements to validate the upscaling of laboratory behaviors to the time and length scales of interest ranging from injection to long-term containment.
- Advances are needed in mathematical algorithms and their numerical implementations, for example, for representing complex grain shapes and pore structures. Such developments are essential for understanding, simulating, interpreting, and generalizing grain-scale observations as well as for taking measurements on reservoir systems.

- Constitutive models need to be integrated into coupled analyses, with emphasis on identifying system instabilities.
- Fundamental research needs to be coupled with studies and interpretations of natural analogues and case histories.

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