Seismic modeling to monitor CO2 geological storage: The Atzbach-Schwanenstadt gas field

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[1] We develop a petro-elastical numerical methodology to compute realistic synthetic seismograms and analyze the sensitivity of the seismic response when injecting carbon dioxide (CO2) in a depleted gas reservoir. The petro-elastical model describes the seismic properties of the reservoir rock saturated with CO2, methane and brine, and allows us to estimate the distribution and saturation of CO2 during the injection process. The gas properties, as a function of the in-situ pressure and temperature conditions, are computed with the Peng-Robinson equation of state, taking into account the absorption of gas by brine. Wave attenuation and velocity dispersion are based on the mesoscopic loss mechanism, which is simulated by an upscaling procedure to obtain an equivalent viscoelastic medium corresponding to partial saturation at the mesoscopic scale. Having the equivalent complex and frequency-dependent bulk (dilatational) modulus, we include shear attenuation and perform numerical simulations of wave propagation at the macroscale by solving the viscoelastic differential equations using the memory-variable approach. The pseudo-spectral modeling method allows general material variability and provides a complete and accurate characterization of the reservoir. The methodology is used to assess the sensitivity of the seismic method for monitoring the CO2 geological storage at the Atzbach-Schwanenstadt depleted gas-field in Austria. The objective of monitoring is the detection of the CO2 plume in the reservoir and possible leakages of CO2. The leakages are located at different depths, where the CO2 is present as gaseous, liquid and supercritical phases. Even though the differences can be very subtle, this work shows that seismic monitoring of CO2 from the surface is possible. While the identification of shallow leakages is feasible, the detection of the plume and deep leakages, located in the caprock just above the injection formation, is more difficult, but possible by using repeatability metrics, such as the normalized RMS (NRMS) images. Considering real-data conditions, affected by random noise, a reference detection threshold for deep leakages and the CO2 plume in the reservoir corresponds to a signal-to-noise ratio of about 10 dB.


1. Introduction

[2] The emission of CO2 to the atmosphere from the combustion of fossil fuels is one of the possible causes of the greenhouse effect. In order to avoid these emissions, one of the options is the geological storage of carbon dioxide in depleted hydrocarbon reservoirs or deep saline aquifers. An example of the latter is the Sleipner field in the North Sea [Arts et al. 2004; Chadwick et al., 2010], where CO2 is stored in the Utsira formation, a highly permeable porous sandstone 800 m below the sea bottom [Faerseth, 1996; Carcione et al., 2006].

[3] There are more saline aquifers than hydrocarbon reservoirs but they require more exploration because they have not been surveyed. The storage can be hydrodynamic as dissolved CO2 in the formation waters. However, the storage should be made at supercritical pressures to avoid the presence of the gas phase. The best conditions start at a minimum depth of nearly 1 km (the critical pressure and temperature of CO2 are 7.4 MPa and 31 °C, respectively). When CO2 is stored into depleted oil and gas fields or unmineable coal seams, enhanced oil/gas recovery (EOR/EGR) and coal-bed methane production make CO2 geological storage cost-effective [e.g., Baines and Worden, 2004].
Like EOR the effectiveness of EGR is due to the pushing effect of the CO₂ cushion. However, while EOR is a well established technology, EGR is not yet common practice [e.g., Oldenburg and Benson, 2001; Oldenburg, 2003].

[6] Injection is already active in the K12-B gas-field [Vandeweijer et al., 2006], offshore Netherlands, and in the Weyburn-Midale oil field [Wilson and Monea, 2004], located in southeast Saskatchewan, Canada. For all these options, a critical issue for geological storage is ensuring that the captured and stored CO₂ does not escape from the host formation during and after the injection. A key point, particularly when the site is onshore, is to provide confidence in predictions of the long-term location of CO₂ in the subsurface and to identify and measure any potentially hazardous leaks to the surface, requiring an efficient monitoring program.

[5] The choice among the wide range of available monitoring tools depends on the site characteristics, the objectives and the costs [e.g., Benson et al., 2004; Arts and Winthagen, 2005]. Among the geophysical methods, the multichannel seismic methods (i.e., 3D/2D surface reflection seismics, vertical seismic profiling and cross-well seismics) provide, with the highest resolution, information about possible changes of the petro-elastical characteristics occurred in the storage zone. The effects of pore pressure on the frame of the host rock and the contrast between the acoustic properties of oil and brine and those of CO₂ are important factors. Wang et al. [1998] measured a pore pressure increase from 8 to 16 MPa due to CO₂ flooding at the McElroy field in West Texas. Xue and Ohsumi [2004] performed laboratory experiments and measured a P wave velocity change of 6% caused by gaseous CO₂ injection and 10% due to supercritical CO₂ injection. As noted by Oldenburg [2003], the density change of CO₂ is large in the transition from gaseous to supercritical conditions, and can approach that of liquid water. Instead, pure CH₄ (methane, hydrocarbon gas) exhibits no such drastic change. Also, the viscosity of CO₂ is low but always higher than the CH₄ viscosity. These variations may indicate that seismic methods can be used to monitor the presence and movement of the CO₂ plume into depleted oil and gas fields.

[6] In general, the sensitivity of the time-lapse (4D) seismic method depends on the survey plan (type of sources, number and location of receivers on the surface and/or well, etc.) and on the specific characteristics of the storage site [e.g., Arts et al., 2004; Chadwick et al., 2010]. It can be evaluated a priori through numerical modeling that takes into account the reservoir characteristics and storage process. These simulations allow to optimize the seismic surveys, which should be repeated over time to monitor the evolution of the injected CO₂. Seismic modeling is a suitable tool to image specific geological settings and to simulate different CO₂ geological storage scenarios, but its success depends on a correct description of the physical properties of the CO₂-bearing rocks.

[7] One of the main phenomena occurring in rocks, in particular partially saturated with gas, is the mesoscopic-loss effect. It has been shown that it is the major cause of P wave attenuation at seismic frequencies [e.g., Pride et al., 2004]. It is caused by heterogeneities greater than the pore size but much smaller than the predominant wavelengths. A fast P wave traveling in a heterogeneous fluid-saturated porous material induces fluid-pressure gradients in the different regions of the medium. This in turn generates slow P waves that diffuse away from the interfaces separating the heterogeneities, causing energy loss and velocity dispersion. Carcione and Picotti [2006] and Carcione [2007] present a detailed physical description of this mechanism that it is present where there is any kind of mesoscopic heterogeneity. Because the mesoscopic-scale heterogeneities in the solid frame and fluid properties, typically on the order of centimeters, are much smaller than the wavelength, any finite element or finite difference numerical procedure based on Biot’s equations is impractical. To overcome this difficulty, we present an alternative approach, based on an equivalent viscoelastic medium.

[8] This work investigates the sensitivity of the seismic properties to variations in CO₂ and CH₄ within a reservoir, as a feasibility study for future seismic time-lapse surveys. First, we define the fluid properties as a function of pressure and temperature, with the gas acoustic properties obtained from the real-gas Peng-Robinson equation of state (PR-EoS). We take into account the possibility that CH₄ and CO₂ can go into solution in the brine. This process affects the saturation of the gaseous phases and the density and bulk moduli of the liquid phases. Secondly, we obtain the dry-rock bulk and shear moduli as a function of porosity and clay content using the Hashin-Shtrikman theory and the Krief model [Carcione et al., 2006]. Then, an equivalent complex dilatational modulus is determined by solving at the mesoscale local boundary value problems representing oscillatory compressibility tests on a representative volume of bulk material containing stochastic heterogeneities characterized by their statistical properties. Only heterogeneities in fluid properties are considered in this paper. The oscillations of these mesoscopic scale heterogeneous rock samples are assumed to obey Biot’s equations of motion. The computed displacements allow us to determine the equivalent bulk modulus at the macroscale as functions of frequency. Moreover, by averaging over many realizations of the stochastic heterogeneities we obtain an average bulk modulus. The final viscoelastic model is obtained by fitting the computed modulus with a suitable viscoelastic causal model, i.e. the Zener model [e.g., Carcione, 2007], which is used to perform numerical simulations to obtain synthetic seismograms. Picotti et al. [2010] showed that mesoscopic models can effectively be approximated by using a Zener viscoelastic element. The anelasticity of shear waves is also described by the Zener model. Numerical simulations of wave propagation at the macroscale are performed in the time domain, using a single-phase viscoelastic algorithm, including wave attenuation [Carcione, 2007]. The advantages of this approach are that the use of very small grid spacings due to the presence of the Biot slow wave can be avoided, with a substantial computer memory saving. Moreover, the viscoelastic modeling algorithm uses fewer material properties and field variables than the corresponding poroelastic modeling, with further memory and computer time reduction. The numerical algorithm, based on the viscoelastic velocity-stress elastodynamic equations, uses a pseudospectral method. This approach allows the calculation of the spatial derivatives with high accuracy [Carcione, 2007].

[9] The numerical experiments illustrate the implementation of the methodology to compute synthetic seismograms with the purpose of studying the sensitivity of the seismic response under varying CO₂ saturations in the reservoir and
for the detection of potentially hazardous leakages in the caprock and overburden. Note that for simplicity the term “leakage” is not used to indicate migration of CO₂ out of the storage complex, as formally specified in the European Directive, but rather to describe migration of CO₂ out of the reservoir. The methodology is applied to the Atzbach-Schwanenstadt gas field [Polak et al., 2006], a potential site for underground CO₂ sequestration. This almost depleted gas-field, located in Upper Austria and operated by Rohoel-Aufsuchungs AG, is one of the four potential sites considered within the EU-funded CASTOR (CO₂ from CApture to STORage) project (2004–2008) [Rossi et al., 2008]. Due to the presence of residual methane, the conditions for the seismic technique to map the CO₂ plume in the reservoir are less favorable than for a depleted oil reservoir or saline aquifer. Detection of leakages at early stages just above the injection formation is also very difficult, because the CO₂ can be present in the supercritical state. However, use of repeatability metrics such as the normalized RMS (NRMS [Kragh and Christie, 2002]) to assess the differences of repeated data sets increases the sensitivity of the seismic method, in particular if the monitoring is performed from the surface. Various scenarios have been considered, in order to model the seismic response of leakages containing CO₂ in different states (gaseous, liquid and supercritical states) and mixed with CH₄. The simulations confirm the suitability of the seismic method to monitor the evolution of the CO₂ plume in the reservoir and possible CO₂ leakages in the overburden and caprock.

1.1. Fluid Properties

[10] To correctly model the seismic response, it is necessary to calculate the physical properties of the fluids involved in the sequestration process. In this work, we consider brine and a mixture of methane and carbon dioxide. The fluid properties depend on temperature T and pressure p, which in turn depend on depth z. A simple – reference – situation is to consider a constant geothermal gradient, G, such that the temperature variation with depth is [Carcione et al., 2006]

\[ T = T_0 + Gz, \]

where \( T_0 \) is the average surface temperature and \( G \) is the average geothermal gradient (5 °C and 25 °C/km in our example, respectively). The pore pressure \( p \) at depth \( z \) depends on many factors, most of them of geological nature, such as low-permeability regions, sealing faults and hydrocarbons caps, which prevent pressure equilibration (communication) from the reservoir to the surface. The simplest case is when there are no permeability barriers and the fluids (say, water) are free to flow from depth \( z \) to the surface. In this case, the pore pressure is hydrostatic and is given by

\[ p = \rho_w g z, \]

where \( \rho_w \) is the water (brine) density and \( g \) is the acceleration of gravity. With \( \rho_w = 1 \text{ gr/cm}^3 \), the pore pressure ranges from 0 MPa at the surface to 30 MPa at 3 km depth. As shown in the CO₂ phase diagram of Figure 1 [Mahan and Myers, 1987], the injected CO₂ in the reservoir (R) is in the supercritical state.

[11] In-situ reservoir gas behaves as a real gas. In order to compute the density \( \rho_g \) of gases we consider the PR-EoS [Peng and Robinson, 1976], a cubic equation derived from the van der Waals equation (see Appendix A). Because of its simplicity and high performance, it is the most widely used EoS in chemical engineering thermodynamics. The bulk modulus of the gas \( K_g \) is given by [Morse and Ingard, 1986]

\[ K_g = \gamma \frac{\partial p}{\partial \rho_g}, \]
where $\gamma$ is the specific heat ratio. For air it is $\gamma = 3/4$. Batzle and Wang [1992] provide an empirical equation for the methane specific heat ratio:

$$\gamma = 0.85 + \frac{5.6}{p_r + 2} + \frac{27.1}{(p_r + 3.5)^2} - 8.7 \exp[-0.65(p_r + 1)].$$

where $p_r = p/p_c$ is the reduced pressure and $p_c$ is the critical pressure. For CH$_4$, $p_c = 4.64$ MPa and for CO$_2$, $p_c = 7.38$ MPa. From a regression of the experimental data of Wang and Nur [1989], we obtain a similar empirical equation for the CO$_2$ specific heat ratio:

$$\gamma = 1.37 + \frac{11.29}{p_r + 6} + \frac{15.55}{(p_r + 1.3)^2} - 38.89 \exp[-1.25(p_r + 1)].$$

Figure 2 shows also the corresponding theoretical plots for CH$_4$, which are in good agreement with those obtained using the empirical relations of Batzle and Wang [1992].

The parameters of the CO$_2$-CH$_4$ mixtures are computed with the same relations used for pure components. However, in this case the parameters of the PR-EoS require a modification using the so-called mixing rules, which allow us to compute mixture parameters equivalent to those of pure substances (see Appendix A). The specific heat ratio of fluid mixtures is assumed to obey the same mixing rules used for the parameters of the PR-EoS [Danesh, 2001]:

$$\gamma = \gamma_1 x_1^2 + \gamma_2 x_2^2 + x_1 x_2 (\gamma_1 + \gamma_2),$$

where $x_1$, $x_2$ and $\gamma_1$, $\gamma_2$ are the molar fractions and the specific heat ratios of the two pure components, respectively. The viscosity of the pure components, as well as those of the fluid mixtures (as a function of pressure and temperature), is determined using the Lohrenz-Bray-Clark (LBC) theory [Lohrenz et al., 1964].

The brine acoustic properties depend on temperature, pressure and salinity. Batzle and Wang [1992] provide a series of useful empirical relations for density, velocity and viscosity. Using these relationships, we can also obtain the brine bulk modulus. Part of the hydrocarbon gas and CO$_2$ can dissolve in brine and the rest remain as free gas. There is a maximum quantity of gas that brine can absorb. Carcione et al. [2006] provide the equations to model the absorption of gas by brine. The mixture of free CO$_2$ and CH$_4$ with brine behaves as a composite fluid with properties depending on the stiffness moduli of the constituents and their respective saturations. The brine-fluid mixture density $\rho_f$ is given by

$$\rho_f = S_g \rho_g + (1 - S_g) \rho_b,$$

where $S_g$ is the free gas saturation and $\rho_b$ is the brine density.

2. Formation Properties

Because of the presence of clay and quartz, the grains are formed by a mixture of two solids and the effective grain moduli of the composite rock are different than the moduli of the single components. The density is simply

$$\rho_g = (1 - C) \rho_q + C \rho_c,$$

where $\rho_q$ and $\rho_c$ are the sand-grain (quartz) and clay densities, and $C$ is the clay content. We assume that the grain bulk modulus $K_g$ and shear modulus $\mu_g$ are equal to the arithmetic average of the upper and lower Hashin-Shtrikman bounds [Hashin and Shtrikman, 1963], as described in detail in Carcione et al. [2006]. When available, we use the P wave interval velocity $c_p$ to compute the matrix bulk modulus $K_m$ using the inverse Gassmann’s equation [Carcione et al., 2006]:

$$K_m = \frac{(\phi K_g/K_b + 1 - \phi) K_G - K_s}{\phi K_s/K_b + K_G/K_s - 1 - \phi}.$$

Figure 2 shows a comparison between the experimental data of Wang and Nur [1989] and the densities and sound velocities computed using the PR-EoS and the above equations. We observe an excellent agreement between the theoretical and experimental results in the temperature and pressure range considered in this work. Figure 2 shows also the corresponding theoretical plots for CH$_4$, which are in good agreement with those obtained using the empirical relations of Batzle and Wang [1992].
where $\phi$ is the porosity, $K_p$ is the brine bulk modulus, $K_G = \rho C_p^2$ is the wet-rock (Gassmann) modulus, assuming the dry-rock shear modulus:

$$\mu_m = \frac{K_s}{K_i} K_m.$$  \hspace{1cm} (10)

[16] If the P wave interval velocity is not available, we use Krief model:

$$K_m = K_s (1 - \phi)^{4/[(1 - \phi)]},$$  \hspace{1cm} (11)

where $A$ is a dimensionless parameter. Carcione et al. [2005] verified that the value of $A = 3$ is appropriate for sediments composed by a mixture of quartz and clay. Clay content affects the permeability, which is not available for all the formations. Carcione et al. [2000] derived a model of permeability as a function of clay content. They assumed that a shaly sandstone is composed of a sandy matrix and a shaly matrix with partial permeabilities:

$$\kappa_q = \frac{R_q^2 \phi^3}{45 (1 - \phi)^2 (1 - C)}, \hspace{0.5cm} \kappa_c = \frac{R_c^2 \phi^3}{45 (1 - \phi)^2 C},$$  \hspace{1cm} (12)

where $R_q$ and $R_c$ denote the average radii of sand and clay particles, respectively. Assuming that permeability is analogous to the inverse of the electrical resistance, the average permeability of the shaly sandstone is given by

$$\frac{1}{\kappa} = \frac{1}{\kappa_q} + \frac{C}{\kappa_c} = \frac{(1 - \phi)^2}{A \phi^4} \left[ (1 - C)^2 + C^2 B^2 \right],$$  \hspace{1cm} (13)

where $A = R_q^2/45$ and $B = R_q/R_c$, or can be assumed as empirical parameters.

3. Modeling of Realistic Attenuation: Mesoscopic Loss

[17] The simulation of synthetic seismograms requires solving Biot’s differential equations with very small grid spacings, since the loss mechanism involves the conversion of fast P wave energy to diffusion energy in the form of the Biot static mode. Because the wavelength of this mode can be very small, the poroelastic solution requires a very large amount of memory and computer time [Picotti et al., 2007; Rubino et al., 2007]. An efficient approach to overcome this problem is to compute the complex moduli of the equivalent viscoelastic medium and then solve the single-phase viscoelastic differential equations [Carcione, 1998; Santos et al., 2008; Picotti et al., 2010]. We consider a fluid-saturated porous material composed of several subdomains, and assume that the whole aggregate is isotropic. We also assume that some of the subdomains contain multiscale mesoscopic heterogeneities in the fluid properties, which are statistically homogeneous and can be described by their statistical properties. A representative volume element is denoted by $\Omega$, and for simplicity let us assume that $\Omega$ is a square of side length $L$, i.e., $\Omega = (0, L)^2$. In the absence of external body sources, the oscillatory motion of $\Omega$ at the angular frequency $\omega$ is assumed to obey Biot’s equations of motion, stated in the form [Biot, 1962; Santos et al., 2009]

$$-\omega^2 \rho d (\ddot{x}, \omega) - \omega^2 \rho_f u_f (\ddot{x}, \omega) - \nabla \cdot \tau(u', u') = 0, \hspace{0.5cm} \ddot{x} \in \Omega,$$  \hspace{1cm} (14)

$$-\omega^2 \rho_f u_f (\ddot{x}, \omega) - \omega^2 \frac{S \phi}{1 - \phi} \ddot{u}_f (\ddot{x}, \omega) + i\omega \eta \kappa \ddot{u}_f (\ddot{x}, \omega)$$

$$+ \nabla p_f (u', u') = 0, \hspace{0.5cm} \ddot{x} \in \Omega,$$  \hspace{1cm} (15)

where $i = \sqrt{-1}, \ddot{x}$ denotes the local coordinate system at the mesoscale in $\Omega$, $u'$ and $u''$ are the solid and fluid relative to the solid displacement vectors, respectively, $\tau(u', u'')$ is the total stress tensor and $p_f (u', u'')$ is the fluid pressure. Also, $\rho$, $\rho_f$ and $\eta$ are the mass densities of the solid grains and of the saturating fluid and

$$\rho = (1 - \phi) \rho_s + \phi \rho_f$$  \hspace{1cm} (16)

is the bulk density of the material. Moreover, $\eta$ is the fluid viscosity, $\kappa$ the absolute permeability and $S$ the structure or tortuosity factor. The stress-strain relations are [Santos et al., 2009]

$$\tau_{jk} (u', u'') = 2 \mu \varepsilon_{jk} (u') + \delta_{jk} (\lambda \nabla \cdot u' + \alpha M \nabla \cdot u''),$$  \hspace{1cm} (17a)

$$p_f (u', u'') = -\alpha M \nabla \cdot u' - M \nabla \cdot u'',$$  \hspace{1cm} (17b)

where $\varepsilon_{jk} (u')$ denotes the strain tensor and $\delta_{jk}$ is the Kronecker delta. The shear modulus of the bulk material $\mu$ is considered to be equal to the shear modulus of the dry matrix $\mu_m$ and $\lambda = K_G - \frac{2}{3} \mu$, with $K_G$ being the Gassmann bulk modulus, i.e. the bulk modulus of the saturated material. The coefficients in (17a) and (17b) can be obtained from the relations

$$\alpha = 1 - \frac{K_m}{K_i}, \hspace{0.5cm} M = \left( \frac{\alpha - \phi}{K_s} + \frac{\phi}{K_f} \right)^{-1}, \hspace{0.5cm} K_G = K_m + \alpha^2 M,$$  \hspace{1cm} (18)

where $K_s$, $K_m$ and $K_f$ denote the bulk moduli of the solid grains, dry matrix and saturating fluid, respectively. The viscoelastic model to be used at the macroscale to perform the numerical simulations is defined in terms of the (undrained) average equivalent dilatational modulus $K_G(\omega)$. It is a complex and frequency-dependent modulus to be computed with Monte Carlo experiments, as described in detail in Santos et al. [2009]. Here, we briefly summarize the procedure. White’s theory considers a simplified model for the gas distribution in the pore space, consisting of plane layers alternatively saturated by liquid and gas [White et al., 1975], or spherical patches of gas in a background liquid [White, 1975]. Our methodology considers a more realistic medium consisting of fractal patches. Although the exact spatial distribution of these heterogeneities is in general unknown, they can be assumed to be stochastic functions characterized by their statistical properties. With this assumption, the idea is to average the properties over many patchy realizations of statistical parameters. To generate the quasi-fractal patchy saturated regions, we use a stochastic fractal field based on the so-called von Karman self-similar
correlation functions. Following Santos et al. [2005], we consider a particular case for which the spectral density of the stochastic field is given by

$$S_d(k_x, k_y) = S_0(1 + k^2a^2)^{(n+1)/2},$$

(19)

where $k = \sqrt{k_x^2 + k_y^2}$ is the radial wave number, $a$ the correlation length, $s$ a self-similarity coefficient ($0 < s < 1$), $n$ is the Euclidean dimension and $S_0$ is a normalization constant. Equation (19) corresponds to a fractal process of dimension $d = n + s - 1$ at scales smaller than $a$. Biot’s equations (14) and (15) are solved over a set of realizations of representative samples $\Omega$ containing stochastic heterogeneities characterized by their statistical properties, with boundary conditions representing compressibility oscillatory tests at a finite number of frequencies. The size of the rock sample $\Omega$ is not arbitrary: it has to be large enough to constitute a representative volume of the medium but, at the same time, it has to be much smaller than the wavelengths associated with each excitation frequency. To obtain the equivalent complex P wave modulus $E(\omega)$ associated with each realization of the reference sample, $\Omega$ is subjected to a time-harmonic compression of the form $\Delta P \exp(i\omega t)$ on its top boundary, and no tangential forces are applied on the boundaries of the sample. Also, the solid is neither allowed to move on the bottom boundary nor to have horizontal displacements on the lateral boundaries, and the fluid is not allowed to flow in or out of the sample. Thus, we solved equations (14) and (15) with the following boundary conditions:

$$\tau(u^f, u^f) \nu = (0, -\Delta P), \quad \text{on} \quad \Gamma^T,$$

$$\tau(u^f, u^f) \nu \cdot \chi = 0, \quad \text{on} \quad \Gamma^L \cup \Gamma^R,$$

$$u^f \cdot \nu = 0, \quad \text{on} \quad \Gamma^L \cup \Gamma^R,$$

$$u^f = 0, \quad \text{on} \quad \Gamma^B,$$

$$u^f \cdot \nu = 0, \quad \text{on} \quad \Gamma^L \cup \Gamma^R \cup \Gamma^B \cup \Gamma^T,$$

(20)

where $\Gamma^L$, $\Gamma^R$, $\Gamma^B$ and $\Gamma^T$ are the left, right, bottom and top boundaries of $\Omega$, respectively. In the expressions (20), $\nu$ is the unit outer normal and $\chi$ is a unit tangential oriented counterclockwise on the boundaries of $\Omega$, such that $\{\nu, \chi\}$ is an orthonormal system on $\Gamma$. For a given realization of the stochastic parameters, the computed displacements on the top boundary $\Gamma^T$ allow to measure the volume change of the sample, from where $K_G(\omega)$ is determined as $E(\omega) - (4/3) \mu_m$ [Santos et al., 2009]. Figure 3 shows a schematic representation of an alternative undrained oscillatory compressibility test allowing a more direct computation of $K_G(\omega)$.

To solve equations (14) and (15) with (20) as boundary conditions we used a finite element procedure employing bilinear functions to approximate the solid displacement vector, while for the fluid displacement a closed subspace of the vector part of the Raviart-Thomas-Nedelec space of zero order is employed [Raviart and Thomas, 1975; Nedelec, 1980]. The mesh size used in this local problem, has to be small enough, that the diffusivity process associated with fluid pressure equilibration is accurately resolved. For practical purposes, in this work we take the mesh size so that the minimum diffusion length is discretized with at least three mesh points at the highest frequency, which is sufficient to represent a (smooth) diffusion-type process. See Santos et al. [2009] for details on the finite element spaces and mesh sizes used to solve each oscillatory local problem.

The average and variance of the phase velocities and quality factors associated with these moduli are obtained by averaging over realizations of the stochastic parameters, and the Monte Carlo realizations are stopped when the variance of the computed quantities stabilize at an almost constant value. Once determined the average equivalent complex dilatational modulus $K_G(\omega)$, the complex P wave velocity is given by

$$v(\omega) = \sqrt{\frac{K_G(\omega)}{\rho} + (4/3)\mu_m},$$

(21)

since the dry- and wet-rock shear moduli are the same, according to Gassmann’s theory. The complex velocity has the following associated phase velocity and quality factor:

$$c = \left| \frac{\text{Re}(\frac{1}{\Gamma})}{} \right|^{-1},$$

(22)

$$Q = \frac{\text{Re}(\frac{\Gamma}{\text{Im}(\frac{\Gamma}{\Gamma})})}{\text{Im}(\frac{\Gamma}{\Gamma})},$$

(23)

respectively [e.g., Carcione, 2007]. In the next section, we approximate this medium by a viscoelastic equivalent medium and introduce shear wave attenuation.

4. Viscoelastic Representation of the Mesoscopic-Loss Mechanism

The computed complex and frequency-dependent modulus $K_G(\omega)$ must be approximated by a suitable causal viscoelastic model to compute synthetic seismograms in the time domain. Let us denote the fit of $K_G(\omega)$ by $K(\omega)$. Picotti et al. [2010] showed that the mesoscopic model can be effectively approximated by using a Zener viscoelastic element. At sufficiently low frequencies, the fluid pressure

![Figure 3. Schematic representation of the oscillatory compressibility test.](image-url)
is uniform (iso-stress state) and the effective modulus of
the pore fluid is given by Wood’s equation [Wood, 1955].
We fit the real and imaginary parts of \( K_G \) with the
corresponding viscoelastic ones by imposing the low-
frequency limit \( K(0) = K_G(0) = K_G \), where \( K_G \) is given by
equation (18), and

\[
K_G = \left( 1 - S_p + S_k \right) \frac{1}{K_b} K_G^{-1}
\]  
(24)

is the Wood average. Actually, imposing this condition, the
only fitting parameter is the minimum dilatational quality factor \( Q^{(1)}_0 \) (see [21]).

[21] The complex moduli associated with bulk and shear
deformations of a Zener element can be expressed as [Carcione, 2007]

\[
M_i = \frac{1 + i \omega \tau_i^{(0)}}{1 + i \omega \tau_i^{(0)}} = \varepsilon, 2
\]  
(25)

where \( \tau_i^{(0)} \) and \( \tau_i^{(0)} \) are relaxation times. They are given by

\[
\tau_i^{(0)} = \frac{\tau_0}{Q_0^{(1)}} \left( \sqrt{Q_0^{(1)} - 1 + 1 \right), \quad \tau_i^{(0)} = \frac{2 \tau_0}{Q_0^{(1)}}
\]  
(26)

where \( \tau_0 \) is a relaxation time such that \( 1/\tau_0 \) is the center
frequency of the relaxation peak and \( Q_0^{(1)} \) are the
dilatational quality factors. In order to introduce shear dissipation,
we assume that the complex modulus \( \mu \) is described by a Zener
element having a minimum quality factor given by

\[
Q_0^{(2)} = \frac{\mu_m}{K_m} Q_0^{(1)},
\]  
(27)

where \( Q_0^{(1)} \) is the dilatational quality factor associated with
\( K \). The complex P and S wave moduli are then given by

\[
E = K + \frac{4}{3} \mu,
\]
\[
\mu = \mu_m M_i,
\]  
(28)

respectively, where

\[
K = K_0 M_1
\]  
(29)

is the dilatational modulus. The complex P and S wave
viscoelastic velocities are given by

\[
v_p = \sqrt{\frac{E}{\rho}}, \quad v_s = \sqrt{\frac{\mu}{\rho}},
\]  
(30)

and the respective phase velocities and quality factors are
given by equations (22) and (23) but replacing \( v \) by \( v_p \) or \( v_s \).
The dilatational quality factor is

\[
Q_i = \frac{\text{Re}(K)}{\text{Im}(K)} = \frac{\text{Re}(M_1)}{\text{Im}(M_1)},
\]  
(31)

whose minimum value as a function of frequency is \( Q_0^{(1)} \) [e.g.,
Carcione, 2007].

5. Viscoelastic Differential Equations

[22] The time domain equations for propagation in a het-
erogeneous viscoelastic medium can be found in Carcione
[2007]. The two-dimensional velocity-stress equations for
anelastic propagation, considering the \((x, z)\)-plane, are
as follows:

\[
\dot{v}_x = \frac{1}{\rho} \left( \sigma_{xx} + \sigma_{xz} \right) + f_x,
\]  
(32)

\[
\dot{v}_z = \frac{1}{\rho} \left( \sigma_{xz} + \sigma_{zz} \right) + f_z,
\]  
(33)

where \( v_x \) and \( v_z \) are the particle velocities, \( \sigma_{xx} \), \( \sigma_{xz} \) and \( \sigma_{zz} \)
are the stress components, \( \rho \) is the bulk density (16) and \( f_x \)
and \( f_z \) are the body forces. A dot above a variable denotes
time differentiation.

[24] 2. Constitutive equations:

\[
\dot{\sigma}_{xx} = K_0 (v_{xx} + v_{xz} + e_1) + \mu_0 (v_{xx} - v_{xz} + e_2),
\]  
(34)

\[
\dot{\sigma}_{xz} = K_0 (v_{xx} + v_{xz} + e_1) - \mu_0 (v_{xx} - v_{xz} + e_2),
\]  
(35)

\[
\dot{\sigma}_{zz} = \mu_0 (v_{xz} + v_{zz} + e_3),
\]  
(36)

where \( e_1, e_2 \) and \( e_3 \) are memory variable and \( K_0 \) and \( \mu_0 \)
are the unrelaxed (high-frequency) bulk and shear moduli,
respectively, given by

\[
K_0 = K_0 M_1(x) = K_0 \frac{\tau_i^{(1)}}{\tau_i^{(2)}},
\]
\[
\mu_0 = \mu_0 M_2(x) = \mu_0 \frac{\tau_i^{(2)}}{\tau_i^{(2)}},
\]  
(37)

[25] 3. Memory variable equations:

\[
\dot{e}_1 = \left( \frac{1}{\tau_i^{(1)}} \right) (v_{xx} + v_{xz}) - \frac{e_1}{\tau_i^{(1)}},
\]  
(38)

\[
\dot{e}_2 = \left( \frac{1}{\tau_i^{(2)}} \right) (v_{xx} - v_{xz}) - \frac{e_2}{\tau_i^{(2)}},
\]  
(39)

\[
\dot{e}_3 = \left( \frac{1}{\tau_i^{(2)}} \right) (v_{xz} + v_{zz}) - \frac{e_3}{\tau_i^{(2)}},
\]  
(40)

[26] The differential equations are solved with a 4th-
order Runge-Kutta time stepping scheme and the staggered
Fourier method for computing the spatial derivatives, which
is noise-free in the dynamic range where regular grids
generate artifacts that may have amplitudes similar to those
of physical arrivals [Carcione, 2007].

6. Application to the Atzbach-Schwanenstadt
Injection Site

[27] The Atzbach-Schwanenstadt gas field is one of the
four test sites chosen by the EU co-funded CASTOR project
to test and validate the technology [Polak et al., 2006; Rossi
et al., 2008]. Rohoel-Aufsuchungs AG, which operates this
field, tested its transformation into a CO2 storage site as well
as the suitability of CO2 injection for EGR. Potential CO2
sources would have been a paper mill (emitting about 0.2 Mt
of CO2 per year) and a fertilizer plant (emitting about 0.1 Mt
6.1. Geological Model

The Atzbach-Schwanenstein gas field, and (b) 2D section of the geological model. The main geological formations are indicated. It is assumed that CO2 is injected in the reservoir, located in the A4 formation, at an average depth of about 1800 m, while the A3 formation is the caprock. L1, L2 and L3 indicate three possible leakages.

Figure 4. (a) Location of the Atzbach-Schwanenstein gas field, and (b) 2D section of the geological model. The main geological formations are indicated. It is assumed that CO2 is injected in the reservoir, located in the A4 formation, at an average depth of about 1800 m, while the A3 formation is the caprock. L1, L2 and L3 indicate three possible leakages.

of CO2 per year), while the transport of CO2 would be ensured by trucks. The possible CO2 injection rate could have been of about 0.2 Mt CO2/year. CASTOR project studied the site assessment, encompassing the construction of a digital geological model and an upscaled reservoir model. Reservoir simulations carried out in these models allowed to evaluate the feasibility of an injection at 0.3 Mt CO2/year for thirty years, starting from 2010, with and without EGR, and considering also new wells. The other project target was to investigate the effect of CO2 injection on the mechanical stability of the site, and the risk for CO2 migration to the groundwater or the atmosphere and the possibility of detecting CO2 in such cases [Polak et al., 2006]. This was guaranteed by soil gas measurements to provide background data for comparison to future soil gas monitoring, a feasibility study to assess the possibilities for seismic monitoring though the years, geochemical experiments and simulations to evaluate the effect of CO2-rich brine on the reservoir seal, and finally, geomechanical experiments and simulations to assess the mechanical stability of the site [Polak et al., 2006; Le Thiez et al., 2009].

6.1. Geological Model

The Atzbach-Schwanenstein gas field is located in central northern Austria (Figure 4a), in the Molasse Basin in the foreland of the Alpine mountain chain, outside the area affected by compressional deformation. Molasse basin filling started from the latest Eocene to the early Oligocene. The reservoir sandstone intervals, approximately 1600 m below the surface, were formed in the Puchkirchen Basin, a deep water trough parallel to the Alpine front. The geological model (Figure 4b) has been built on the basis of seismic interpretation, geological knowledge, and well log data [Polak et al., 2006], including the topographic surface and one low velocity layer to simulate the overburden.

[29] The model was then populated with the physical properties provided in part by the partners and in part from the existing literature [Polak et al., 2006; Rossi et al., 2008]. We revised all the parameters of Rossi et al. [2008]. Missing or unreliable parameters were computed using rock-physics theories (see section 2). The sedimentary sequence shows the presence of shaly sandstones with variable clay content from 30% to 50% (see Table 3). It is assumed that CO2 is injected in the reservoir, located in the A4 formation at an average depth of about 1800 m (see Figure 4), while the overlying formation with high clay content constitutes the caprock.

[30] We consider three scenarios for the reservoir, described as follows. The first scenario represents the baseline, before the CO2 injection, where the CH4 saturation in the reservoir is 56% [Polak et al., 2006]. The second scenario represents the reservoir half occupied by the CO2 plume, and we assume that the CO2 injection occurs at the bottom of the A4 formation (see Figure 4b). According to Oldenburg and Benson [2001], the CO2 and CH4 mixing would be limited because of the high density and viscosity of CO2 relative to CH4. Moreover, the relatively larger viscosity of CO2 will make for a favorable mobility ratio displacement of CH4 with diminished tendency to interfinger and mix with the displaced CH4. Thus, a strong vertical density stratification is expected in the reservoir during and after CO2 injection. Hence, we assume that the injected CO2 replaces and displaces the in-situ CH4 which, being less dense and viscous, migrates upward and is subjected to compression. Because of compression and a consequent further CH4 production by EGR, we expect a decrease of CH4 saturation. We assume a decrease of CH4 saturation from 56% to 40%, after some years of CO2 injection.

[31] Numerical simulations [Oldenburg and Benson, 2001] show that the mixed zone (where CO2 and CH4 are mixed together in equal proportions) after eight years is approximately 15 m thick, where mixing is due to molecular diffusion. Since CO2 can be present in gaseous, liquid or supercritical states, and mixed with small amounts of CH4, hereafter we will refer to these mixtures with the term fluid. Therefore, because of the density and viscosity difference between CO2 and CH4, we assume the presence of 90% CO2 and 10% CH4 at the bottom of the reservoir, pure CH4 at the top, and a 15 m thick fluid mixture zone of CO2 and CH4 in equal proportions (50%) in the middle. The saturation of the fluid mixture at the bottom, having replaced the previously in-situ CH4, should be 56%. The third scenario represents the reservoir fully saturated by a fluid mixture of 90% CO2 and 10% CH4.

[32] As shown in the geological model of Figure 4b, we simulate three possible leakage scenarios in a 2D model, caused by the degradation of the casing of an abandoned well. A realistic leakage scenario along a well with CO2
accumulating in a shallow structure is probably not described by a 2D feature. However, the 2D approach is sufficient to demonstrate the basic principles of the specific problems considered in this study. In this work we simplified the geometry of the leakages, which is flat lying, to concentrate our efforts on modeling the seismic response of leakages containing CO2 in different states (i.e., gaseous, liquid and supercritical). In fact, the state of CO2 changes during its migration toward the surface, according to the changes in the pressure and temperature conditions defined by the CO2 phase diagram (Figure 1). In any case, the flat lying geometry should not be considered a simplification in this kind of geological formations. In fact, they can be caused, for example, by the presence of thin layers with high clay content, which are common in sedimentary basins [Chadwick et al., 2005, 2010]. These thin layers force the CO2 to migrate horizontally. The leakages are composed by 90% CO2 and 10% CH4, which is the same fluid mixture present in the third reservoir scenario, with a saturation of 10%. The leakage size (in 2D) is approximately 500 m x 50 m. The reasoning behind the assumed saturation of only 10% is that the most important objective of monitoring is to detect small amounts of gas, i.e. CO2 migrations at early stages. Considering the CO2 phase diagram of Figure 1, the three leakages have the following characteristics: leakage 1 (L1) is located at 480 m depth, with the CO2 in the gaseous state; leakage 2 (L2) is located at 950 m depth, with the CO2 in the liquid state; leakage 3 (L3) is located at 1480 m depth, with the CO2 in the supercritical state. Figure 5 shows the density (Figure 5a), bulk modulus (Figure 5b) and viscosity (Figure 5c) as a function of depth of the considered fluid mixture (90% of CO2 and 10% of CH4).

[33] Tables 1, 2 and 3 give the properties of the fluids, solids and formations constituting the model (see Figure 4b), respectively. Assuming for the leakages an elliptical geometry in the plain view, with a secondary axis of about 50 m, the three leakages contain about 15,300 m3 (L1 and L2) and 10,000 m3 (L3) of CO2, which correspond to a total mass of about 2 kt (L1), 11.25 kt (L2) and 7 kt (L3) of CO2.

In Table 1, the brine has absorbed gas and $f_0$ indicates the peak frequency of the relaxation mechanism. The P wave velocities indicated in Table 3 are the experimental interval velocities used to obtain the dry-rock modulus (9), while $c_s$ is obtained from Krief model (10) and the density (7). [34] As explained in a previous section, we determine the equivalent complex bulk modulus solving at the mesoscale

### Table 1. Properties of the Leakages and Reservoir Fluids and Viscoelastic Parameters

<table>
<thead>
<tr>
<th>Medium</th>
<th>$z$ (m)</th>
<th>$S_g$ (%)</th>
<th>CO2 (%)</th>
<th>CH4 (%)</th>
<th>$K_s$ (GPa)</th>
<th>$\rho_e$ (kg/m³)</th>
<th>$\eta_e$ (cP)</th>
<th>$K_b$ (GPa)</th>
<th>$\rho_b$ (kg/m³)</th>
<th>$\eta_b$ (cP)</th>
<th>$f_0$ (Hz)</th>
<th>$Q_0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Leakage</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>L1</td>
<td>480</td>
<td>10</td>
<td>90</td>
<td>10</td>
<td>6.53</td>
<td>128</td>
<td>0.017</td>
<td>2.43</td>
<td>1036</td>
<td>1.17</td>
<td>15</td>
<td>10.2</td>
</tr>
<tr>
<td>L2</td>
<td>950</td>
<td>10</td>
<td>90</td>
<td>10</td>
<td>18.8</td>
<td>509</td>
<td>0.04</td>
<td>2.6</td>
<td>1036</td>
<td>0.94</td>
<td>15</td>
<td>12.4</td>
</tr>
<tr>
<td>L3</td>
<td>1480</td>
<td>10</td>
<td>90</td>
<td>10</td>
<td>61.7</td>
<td>587</td>
<td>0.047</td>
<td>2.65</td>
<td>1035</td>
<td>0.77</td>
<td>15</td>
<td>45</td>
</tr>
<tr>
<td>R1</td>
<td>1800</td>
<td>56</td>
<td>0</td>
<td>100</td>
<td>36.3</td>
<td>128</td>
<td>0.018</td>
<td>2.7</td>
<td>1032</td>
<td>0.68</td>
<td>50</td>
<td>95</td>
</tr>
<tr>
<td>R2</td>
<td>1800</td>
<td>40</td>
<td>0</td>
<td>100</td>
<td>36.3</td>
<td>128</td>
<td>0.018</td>
<td>2.7</td>
<td>1032</td>
<td>0.68</td>
<td>30</td>
<td>62</td>
</tr>
<tr>
<td>R3</td>
<td>1800</td>
<td>56</td>
<td>50</td>
<td>50</td>
<td>47.1</td>
<td>295</td>
<td>0.028</td>
<td>2.7</td>
<td>1033</td>
<td>0.68</td>
<td>60</td>
<td>120</td>
</tr>
<tr>
<td>R4</td>
<td>1800</td>
<td>56</td>
<td>90</td>
<td>10</td>
<td>86.2</td>
<td>609</td>
<td>0.05</td>
<td>2.7</td>
<td>1034</td>
<td>0.68</td>
<td>80</td>
<td>150</td>
</tr>
</tbody>
</table>

- $z$: average depth
- $S_g$: gas saturation
- $K_s$: fluid mixture bulk modulus
- $\rho_e$: density
- $\eta_e$: viscosity
- $K_b$: brine bulk modulus
- $\rho_b$: density
- $\eta_b$: viscosity
- $f_0$: peak frequency
- $Q_0$: quality factor

[33] Tables 1, 2 and 3 give the properties of the fluids, solids and formations constituting the model (see Figure 4b), respectively. Assuming for the leakages an elliptical geometry in the plain view, with a secondary axis of about 50 m, the three leakages contain about 15,300 m³ (L1 and L2) and 10,000 m³ (L3) of CO2, which correspond to a total mass of about 2 kt (L1), 11.25 kt (L2) and 7 kt (L3) of CO2. In Table 1, the brine has absorbed gas and $f_0$ indicates the peak frequency of the relaxation mechanism. The P wave velocities indicated in Table 3 are the experimental interval velocities used to obtain the dry-rock modulus (9), while $c_s$ is obtained from Krief model (10) and the density (7).

[34] As explained in a previous section, we determine the equivalent complex bulk modulus solving at the mesoscale
(and for a finite number of frequencies) boundary value problems representing oscillatory compressibility tests on a representative volume of bulk material containing multiscale heterogeneities. Since the exact spatial distribution of these heterogeneities is in general unknown, they are assumed to be stochastic fractal fields based on the von Karman self-similar correlation functions (19). Figure 6 shows two different fluid patchy realizations, corresponding to the leakages (a), where the fluid saturation is 10%, and the reservoir (b), where the fluid saturation is 56%. In this case we used a side length of 50 cm, \( d = 2.5 \) and \( a = 5 \) cm as fractal dimension and correlation length, respectively. [35] Santos et al. [2009] show that the variance of the equivalent compressional phase velocity averaged over the whole range of frequencies is stable after about 30 realizations. In our case, for the leakages, the variance is very small near the origin and around 0.01 and 10 m/s at 30 Hz, respectively for P wave attenuation and phase velocity. In the reservoir, at higher fluid mixture saturations, the variance reduces by an order of magnitude. Figures 7a–7d show the results obtained for the three leakages and reservoir. It is useful to compare these results with those obtained using White’s layered model [Carcione and Picotti, 2006]. The period width used for the White model is 17 cm. The strong differences in the attenuation curves of Figure 7b justifies the use of the oscillatory tests, because White’s model overestimates the attenuation. The results obtained for the reservoir show that the attenuation and velocity dispersion are lower than those obtained for the leakages. In particular, we observe that while the saturation of CH\(_4\) decreases, the attenuation increases and the relaxation peak moves to lower frequencies. On the other hand, attenuation and velocity dispersion for the injected supercritical CO\(_2\), which we assumed mixed with a small amount of CH\(_4\) (10%), is very weak. The fact that leakages with 10% fluid mixture saturation have higher attenuation/dispersion than the reservoir scenarios is a result of oscillatory compressibility tests. However, this is also confirmed by White’s model of patchy saturation. Using this model, Carcione and Picotti [2006] found that the most significant loss mechanisms are a result of porosity variations and partial saturation, where one of the fluids is very stiff and the other is very compliant. In particular, small amounts of free gas produce high attenuation and velocity dispersion effects, decreasing as free gas saturations increases. This phenomena can be intuitively understood by considering the energy transfer that occurs between the incident P wave and the

Table 3. Formation Properties

<table>
<thead>
<tr>
<th>Formation</th>
<th>C (%)</th>
<th>( \phi ) (%)</th>
<th>( k ) (mD)</th>
<th>( \eta_b ) (cP)</th>
<th>( \rho ) (kg/m(^3))</th>
<th>( c_p ) (m/s)</th>
<th>( c_s ) (m/s)</th>
<th>( Q_0 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Overburden</td>
<td>50</td>
<td>38</td>
<td>40</td>
<td>1.51</td>
<td>1827</td>
<td>800</td>
<td>400</td>
<td>50</td>
</tr>
<tr>
<td>HSCHT</td>
<td>30</td>
<td>26</td>
<td>42.6</td>
<td>1.11</td>
<td>2219</td>
<td>2600</td>
<td>1456</td>
<td>180</td>
</tr>
<tr>
<td>Hall</td>
<td>71</td>
<td>20</td>
<td>29.6</td>
<td>0.88</td>
<td>2298</td>
<td>3276</td>
<td>1890</td>
<td>260</td>
</tr>
<tr>
<td>A2</td>
<td>80</td>
<td>15</td>
<td>11</td>
<td>0.82</td>
<td>2373</td>
<td>3043</td>
<td>1710</td>
<td>210</td>
</tr>
<tr>
<td>A3</td>
<td>50</td>
<td>17</td>
<td>17</td>
<td>0.73</td>
<td>2353</td>
<td>3409</td>
<td>1984</td>
<td>240</td>
</tr>
<tr>
<td>A4</td>
<td>30</td>
<td>17</td>
<td>24.5</td>
<td>0.68</td>
<td>2362</td>
<td>3687</td>
<td>2365</td>
<td>165</td>
</tr>
<tr>
<td>Channel</td>
<td>40</td>
<td>15</td>
<td>15</td>
<td>0.65</td>
<td>2390</td>
<td>3752</td>
<td>2266</td>
<td>230</td>
</tr>
<tr>
<td>SST</td>
<td>50</td>
<td>15</td>
<td>15</td>
<td>0.63</td>
<td>2386</td>
<td>3200</td>
<td>1796</td>
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<tr>
<td>Eocene</td>
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<td>15</td>
<td>0.57</td>
<td>2700</td>
<td>5200</td>
<td>2855</td>
<td>270</td>
</tr>
</tbody>
</table>

\( C \) percentage clay content, \( \phi \) porosity, \( k \) permeability, \( \eta_b \) brine viscosity, \( \rho \) bulk density, \( c_p \) P wave velocity, and \( c_s \) S wave velocity. The baseline dilatational quality factors \( Q_0 \) correspond to the dominant frequency of 15 Hz.

Figure 6. Two examples of fractal patchy realizations, corresponding to (a) the leakages (the fluid saturation is 10%), and (b) the reservoir (the fluid saturation is 56%). In these examples, white regions correspond to a fluid mixture composed by CO\(_2\) (90%) and CH\(_4\) (10%), and black regions to brine with absorbed gas.
diffused slow-wave. Higher saturation of the stiffest fluid means more bulk flow of fluid inside the pore space, which requires more energy to be supplied by the propagating wave, resulting in increased attenuation value. Obviously, at the limit of full saturation of the stiffest fluid, there is no attenuation because there is no compliant pore space where the fluid can move.

[36] Then, we define an equivalent viscoelastic model to be used for the computation of synthetic seismograms in the time domain. Figure 7 shows the Zener best fit of the P wave velocities and quality factors. Despite that the fits are not mathematically perfect, these results show that the Zener model provides a good approximation for practical purposes. We also use the Zener model for all the other formations by fitting the properties of the White plane-layered model and assuming a very small gas saturation of 0.1%. In the overburden, we assume brine and air in the pore space.

6.2. Synthetic Seismograms

[37] We simulated a 2D seismic acquisition corresponding to the model shown in Figure 4b. We used a grid composed of 800 × 720 points. The mesh has squared cells with a grid spacing of 5 m. This grid size is sufficient to sample the shortest wavelengths, according to the Nyquist theorem. We locate a receiver at every grid point at the surface and 102 sources 35 m spaced, to simulate a realistic seismic survey. The source is an explosion with a Ricker-wavelet time-history. The dominant frequency is 15 Hz, which corresponds to the attenuation peak frequency of the leakages (see Figure 7b). The wavefield is computed by using a time step of 0.5 ms till a maximum time of 2.2 s. We obtained imaging sections by applying the Kirchhoff pre-stack depth and time migration [Yilmaz, 1987] to the simulated seismograms. A gain function is applied during migration only to compensate for geometrical spreading. Common Imaging
Gathers (CIG) are produced by the migration algorithm in order to find the best CIG stacking offset range and maximize the quality of the final imaging sections. Figure 8 shows a pre-stack time migration of the simulated seismograms corresponding to the baseline (first scenario), which can be compared to the real data published in Rossi et al. [2008]. Then, we migrated in depth the simulated seismograms after CO₂ injection, assuming that the velocity model has been refined, for example with a tomographic algorithm, to take into account the effect of the injected CO₂. Thus, any observed difference is attributed to changes in amplitude due to changes in attenuation and in the reflection coefficients.

A useful procedure, when assessing the similarity of two time-lapse data sets, is to use repeatability metrics. Time-lapse repeatability is a key parameter controlling what can be detected seismically. One very common used metric is the normalized RMS (NRMS), where [Kragh and Christie, 2002]

\[
\text{NRMS} = 200 \cdot \frac{\text{RMS}(\text{repeat} - \text{base})}{\text{RMS}(\text{repeat}) + \text{RMS}(\text{base})}
\]

The NRMS, which is expressed as a percentage, varies radically in space and travel-time, and it is extremely sensitive to the smallest changes in the data. For example, a 1° phase shift, which is equivalent to 1.1 ms at 25 Hz, gives rise to a 17.4% NRMS residual. Figures 9a and 9b show the depth-migrated simulated seismograms before and after CO₂ injection, corresponding to the first and second scenarios. Figure 9c, representing the NRMS section obtained by using the migrated sections of Figures 9a and 9b, shows that the detection of the carbon dioxide in the reservoir is possible.

We can clearly see that there is a difference between the pre-injection and post-injection phases, mainly concentrated in the bottom of the reservoir, because the second scenario represents the reservoir half saturated with CO₂, where the fluid mixture (90% CO₂ and 10% CH₄) accumulates at the bottom of the A4 formation. It indicates also the

![Figure 8](image)

**Figure 8.** Magnification of the pre-stack time migration of the simulated baseline.

![Figure 9](image)

**Figure 9.** (a) Pre-stack depth migration of the simulated baseline, and (b) of the simulation assuming that half reservoir (A4 formation) is saturated with a mixture of CO₂ (90%) and CH₄ (10%). The CH₄ saturation is 56% in the first, and 40% in the second, while the mixture saturation is 56%. (c) The NRMS section obtained by using the simulations before and after the CO₂ injection clearly shows the effects of the presence of the CO₂ in the reservoir.
The area is about 45%, which is comparable to the value of 35% because all the reservoir is saturated with CO2. The higher distributed on the whole reservoir area. This is plausible, case, the NRMS section shows lower NRMS residuals, but corresponding NRMS section. With respect to the previous the first and third scenarios, while Figure 11c shows the attenuation NRMS residual in the reservoir (mainly CO2). The average NRMS residual in the reservoir bottom of the second scenario are due to the presence of the new weak reflection caused by the interface between gas layer R2 (methane) and R4 (mainly CO2) in the middle of the reservoir.

In order to show a clear picture of the attenuation effect, we carried out an elastic simulation of the second scenario. The corresponding depth-migrated section is shown in Figure 10. A comparison between this section and the corresponding viscoelastic section represented in Figure 9b, shows the impact of attenuation on the modeling. There is a noticeable difference in amplitude between these two sections and, due to the absence of velocity dispersion, in the elastic case the reflection events can easily be discriminated.

Figures 11a and 11b show the NRMS footprint of leakage L3, where the average NRMS residual is about 50%. However, the differences are very subtle, and poor data quality can further reduce the detection sensitivity (presence of noise and/or non-repeatable acquisition patterns). In fact, repeatability depends mostly on time-lapse changes in ambient noise and in acquisition parameters. The former leads to random difference noise but the latter produces difference noise which depends systematically on baseline reflectivity. Repeatability also varies with depth. It is poorer at greater depths as signal penetration decreases, and also at shallow depths as fold decreases. These issues all affect what the time-lapse seismic can show at different levels. Here we study how the presence of random noise changes the NRMS signature of the deeper leakage L3, which is the most difficult to detect, assuming that the presence of this noise is the only factor controlling the repeatability. A complete treatment of repeatability requires also a rigorous modeling of acquisition patterns, which is beyond the aims of this paper. We contaminated the data with different amounts of random noise, in order to compute a detection threshold for this kind of leakage. A detection threshold can be expressed in terms of the signal-to-noise ratio, which is measured in

![Figure 10. Pre-stack depth-migrated section related to the elastic simulation assuming that half reservoir is saturated with a mixture of CO2 (90%) and CH4 (10%), where in this case we do not consider the effect of attenuation (the quality factor is infinite in all the formations). This section has to be compared with the migrated section of Figure 9b, which represents the result of the corresponding viscoelastic simulation.](image)
decibel [Sheriff and Geldart, 1996]. In this case, the detection threshold of leakage L3 corresponds to a signal-to-noise ratio of about 10 dB (see Figure 13). In other words, a signal-to-noise ratio lower than 10 dB can prevent its detection. This conclusion is also valid for the third reservoir scenario, because it shows an average NRMS residual very similar to that of the leakage L3. Note that as the signal-to-noise ratio decreases, the average NRMS residual tends to the value of

![Figure 11.](image)

(a) Pre-stack depth migration of the simulated baseline, and (b) of the simulation assuming that the reservoir is fully saturated with a mixture of CO$_2$ (90%) and CH$_4$ (10%). The mixture saturation is 56%. (c) The NRMS section obtained by using the simulations before and after the CO$_2$ injection clearly shows the effects of the presence of the CO$_2$ in the reservoir.

![Figure 12.](image)

Pre-stack depth migration of the simulation after the CO$_2$ injection with leakage (a) L3, (b) L2, and (c) leakage L1. The leakages are composed of a mixture of CO$_2$ (90%) and CH$_4$ (10%), with a saturation of 10%. Leakages L1 and L2, with the CO$_2$ in the gaseous and liquid state respectively, are evident, while leakage L3, with the CO$_2$ in the supercritical state, is hardly resolved.
141% (see Figures 13d–13f), which corresponds to the theoretical NRMS value of traces containing only noise [Kragh and Christie, 2002].

Finally, it should be noted that leakages can produce a velocity pushdown effect and an amplitude shadow effect on the reflected events below them. These effects are clearly evident in the pre-stack time migrated sections of Figure 14, where the details of the reflector below leakages L1 and L2 are shown. The velocity pushdown effect is also observable in the pre-stack depth-migrated sections (Figures 12b and 12c), because at the location of the leakages the seismic data are migrated using a velocity higher than it should be (we ignore the presence of leakages in the velocity field). These effects can easily be evaluated comparing the sections before and after the leakage. In the case of leakage L1 we have a maximum pushdown effect of about 5 ms and a lateral amplitude reduction of about 30% on the underlying reflector. Since leakages are generally small secondary accumulations with limited lateral extension, they produce seismic signals corresponding also to diffracted waves. Therefore, the amplitude shadow effect should be due to attenuation from scattering and mesoscopic loss, depending on the size of the leakage and the dominant frequency.

7. Discussion

[45] From Table 2, Table 3 and Figure 7 it follows that for shallow leakages, where the CO₂ is in the gaseous and liquid states, both P wave velocity and dilatational quality factors are very sensitive, while the sensitivity decreases significantly for deep leakages and the reservoir, where the CO₂ is in the supercritical state. S waves are less sensitive to the presence of CO₂ in the pore space. This is a consequence of the mesoscopic-loss effect, provided that the most
significant loss mechanisms are a result of porosity variations and partial saturation, where one of the fluids is very stiff and the other is very compliant. In particular, small amounts of free gas produce high attenuation and velocity dispersion effects, decreasing as free gas saturations increases. The implications on a seismic monitoring plan oriented to the quantification of CO2 accumulations are the following:

1. The acquisition pattern has to be accurately designed, so to guarantee a continuous and adequate coverage and a sufficient offset in order to obtain an accurate estimation of the interval velocity.

2. A seismic source with a wide frequency range is recommended to allow an accurate estimation of the quality factor.

3. 3C sensors are also recommended for multicomponent analyses, that represent an additional tool in order to better characterize the fluid content in the rocks.

4. If there is another gas in the reservoir (i.e. methane in the case of a depleted gas reservoir) and the saturation is high, the seismic response is small and it may be masked by noise. In this case, a cross-well seismic survey may help to better evaluate the changes within the reservoir, related to varying CO2 saturations. It may also help to distinguish between CO2 and CH4 saturated zones.

The methodology described in this work has global relevance. In fact, it can be applied elsewhere, in order to study the sensitivity of the seismic method to specific cases. From sensitivity studies it is possible to evaluate which seismic properties (P or S wave velocity or attenuation) show stronger variations in response to small CO2 saturation variations, and tune the monitoring plan accordingly. The monitoring methods are site dependent since the results depend on the depth and in-situ conditions of the reservoir. Borehole monitoring, cross-well surveys, and a real-amplitude processing, are the key to obtain valuable results also in difficult situations. Leakage quantification requires a sufficient resolution, in order to correctly evaluate the leakage size, and knowledge of the petrophysical parameters of the formations. The pushdown effect, as described by Chadwick et al. [2005], allows an approximated estimation of the CO2 saturation. Application of advanced tools such as travel-time and attenuation tomography based on the frequency-shift approach [Böhm et al., 1999; Rossi et al., 2007; Picotti and Carcione, 2006] will improve significantly the determination of the seismic velocity and quality factor. Together with rock-physics theories, these techniques can provide a more reliable quantification of the CO2 accumulations.

8. Conclusions

Time-lapse surface seismic technology represents a useful CO2 monitoring technique during and after CO2 injection, providing the temporal evolution of the CO2 plume in the reservoir, and allowing the detection of possible dangerous leakages. In this work, we present a numerical methodology to obtain realistic synthetic seismograms in heterogeneous media, with the aim of assessing the sensitivity of the surface seismic method in the case of a depleted gas field, where CO2 is stored. This methodology consists of rock-physics theories to calculate the properties of rocks and pore fluids, and in an upscaling procedure to obtain equivalent viscoelastic solids for heterogeneous fluid-saturated porous media. Oscillatory compressibility tests, based on a finite element solution of the classical Biot’s equations in the space-frequency domain, enable us to obtain the equivalent complex and frequency-dependent bulk modulus of reservoir rocks. Since at mesoscopic scales the rock parameter distributions are generally uncertain and of stochastic nature, we apply the oscillatory tests based on Monte Carlo experiments. Then,

![Figure 14. Pre-stack time migrations illustrating (a) the baseline, (b) the push down effect below the leakage L2 and (c) leakage L1.](image-url)
we approximate the Biot medium by an average equivalent viscoelastic solid based on the Zener model. This approach is computationally much less expensive than any numerical procedure based on the discretization of the full Biot’s equations for the same order of accuracy.

[52] To illustrate the methodology, we built a petro-elastical model of the Atzbach-Schwanestadt almost depleted gas-field, located in Upper Austria, and computed synthetic seismograms. Different 2D rock models were considered, with the purpose of analyzing the sensitivity of the seismic response with varying saturations of CO2 in the reservoir and for the detection of potentially hazardous leakages in the caprock and overburden, where the CO2 can be present in three different states: gaseous, liquid and supercritical. The simulations show that these three type of leakages have different thresholds and are more evident when the CO2 is present in the gaseous state, until about 600 m depth. However, they are also clearly visible when the CO2 is present in the liquid state, until about 1100 m depth. On the contrary, detection of leakages at early stages (just above the reservoir, in the caprock) where the CO2 is still present in the supercritical state, is more difficult. However, the use of repeatability metrics, such as the normalized RMS, when assessing the similarity of two repeated data sets, makes the time-lapse surface seismic technique suitable and more sensitive. A repeatability analysis of the simulated seismograms contaminated by random noise allowed us the computation of a reference detection threshold for this kind of leakages, which corresponds to a signal-to-noise ratio of about 10 dB. This is also valid for the reservoir, where the presence of another gas at high saturation makes the seismic response small and easy to be masked by background noise.

Appendix A: Density of the CO2 - CH4 Mixtures

[53] In-situ reservoir gas behaves as a real gas. The most common method used to compute the density \( \rho_g \) of real gases is to solve the equations of state. We consider the PR-EoS \[ \text{Peng and Robinson, 1976}. \] This equation expresses the fluid properties in terms of the critical temperature \( T_c \), the critical pressure \( P_c \) and the acentric factor \( \omega \):

\[
p = \frac{RT}{V_m - b} - \frac{a\omega^2}{V_m^2 + 2bV_m - b^2} \quad (A1)
\]

where \( p \) is the gas pressure, \( V_m \) is the gas molar volume and \( R = 8.31 \text{ J/(mol K)} \) is the gas constant. If \( m \) is the mass of one mole of gas, then the gas density is \( \rho = m/V_m \). For pure CH4, \( m = 16 \text{ g/mole} \) and \( \omega = 0.0115 \), while for pure CO2 it is \( m = 44 \text{ g/mole} \) and \( \omega = 0.225 \). For air it is \( m = 29 \text{ g/mole} \) and \( \omega = 0.078 \). Moreover,

\[
a = (0.45724R^2T_c^2)/p_c,
\]

\[
b = (0.07780RT_c)/p_c,
\]

\[
\beta = [1 + (0.37464 + 1.54226\omega - 0.26992\omega^2)(1 - \sqrt{T_c})^2],
\]

(A2)

where \( T_r = T/T_c \) is the reduced temperature and \( T_a = T(\text{C}) + 273.15 \) is the absolute temperature. For CH4, \( T_r = -82.6 \text{C} \), while for CO2, \( T_r = 31.1 \text{C} \). The critical pressures for CH4 and CO2 are \( p_c = 4.64 \text{ MPa} \) and \( p_c = 7.38 \text{ MPa} \), respectively. The gas density at the critical conditions, or critical density, is \( \rho_c = 162.7 \text{ kg/m}^3 \) for CH4 and \( \rho_c = 468.2 \text{ kg/m}^3 \) for CO2. For air it is \( T_r = -140.8 \text{C} \), \( p_c = 3.7 \text{ MPa} \) and \( \rho_c = 340 \text{ kg/m}^3 \).

[54] Earlier studies \[ \text{McQuarrie and Simon, 1999} \] have shown that the PR-EoS exhibits performance similar to other EoS, like the Redlich-Kwong EoS and the Soave-Redlich-Kwong EoS \[ \text{Soave, 1972} \], although it is generally better in predicting the densities of many species near the critical point, especially the non-polar ones. It also yields results comparable (and sometimes superior) to equations of higher complexity as the Valderrama-Patel-Teja EoS \[ \text{Valderrama, 1990} \].

[55] The equations of state were developed for pure fluids first and then extended to mixtures. The mixture extension requires mixing rules, which allow us to obtain mixture parameters equivalent to those of pure substances. More precisely, the EoS parameters \( a \) and \( b \) in (A2) are expressed as functions of the parameters \( a_i \) and \( b_i \), of the concentration \( x \), of the pure components in the mixture

\[
a = \sum_{i=1}^{N} \sum_{j=1}^{W} x_i x_j (1 - k_{ij}) \sqrt{a_i a_j},
\]

\[
b = \sum_{i=1}^{N} \sum_{j=1}^{W} x_i x_j b_i b_j \frac{k_{ij}}{2},
\]

(A3)

where the binary interaction parameter \( k_{ij} \), particularly useful in hydrocarbon mixtures with high concentration of CO2, takes into account the attractive term between pairs of non-similar molecules \[ \text{Danesh, 2001} \]. The above mixing rules, known as the van der Waals quadratic mixing rules, are used extensively in mixture calculations involving equations of state, and are well known to be suitable for hydrocarbon mixtures.

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