Introduction. Geological storage of carbon dioxide has been proven to be a viable, yet partial, solution to the excessive carbon present in the atmosphere due to human activities. Deep saline aquifers appear to be the geological setting with the highest storage capacities, since the injected supercritical CO$_2$ dissolves in the brine. The presence of the gas in the bulk fluid changes the elastic properties of the medium, therefore it is possible to monitor the propagation of the CO$_2$ in the formation by means of an active seismic experiment. In this work, we present a synthetic, yet realistic, 2D anticlinal formation suitable for CO$_2$ injection, monitored with a cross-hole seismic experiment. Modeling consists of 4 steps: i) Propagation of the CO$_2$ plume via a 2-phase flow simulator ii) Computation of the p- and s-wave velocities via White’s model iii) Computation of the synthetic seismograms iv) Tomographic inversion of the synthetic seismograms using cat3d software.

Geological setting and numerical discretization. We consider a 2D sandstone aquifer with shale intrusions, as in Carcione et al. (2012), with shale above and below such formation. The formation is located from 0.7 to 1.5 km depth and is 800 m long in the horizontal direction. The depth has been chosen so that carbon dioxide is in supercritical state and better dissolves in the
brine. Furthermore, the grains consist of a mixture of quartz and clay. Porosity and permeability vary continuously in the domain; the latter ranging from 10% in the shales bounding the aquifer to 35% in the porous sands in the anticlinal structure; the former from $10^{-17}$ m$^2$ to $10^{-12}$ m$^2$.

The geological model, together with the distribution of the porosity, permeability and clay content can be seen in Fig. 1.

The domain was computed on a regular grid of 315x315 nodes, which implies a node size of 2.5 m. This had to modified for the fluid flow simulation for numerical stability.

In the z direction, the domain was divided in 244 nodes, with a spacing of 2 m in the area of the complex aquifer and 8 m where the medium consists of homogenous shale. In order to minimize the effects of the boundary conditions and enhance the numerical stability of the fluid flow simulation, the domain has been extended approximately 25 km to the east and west. Then, the domain was divided in 4 different zones; the first is the area of the aquifer, from 0 to 500 m, in which nodes are 2 m wide. In the other areas, the boundaries of which are located at 0.5, 6 and 20 km from the well, node size is let increase logarithmically. Therefore, node space increases from 2 m close to the well to 20 km at the furthermost node. This allows to have the necessary high resolution close the well and far enough boundary conditions using only 247 nodes.

Results of the fluid flow simulation were then interpolated using a natural neighbor interpolation algorithm to match the original 315x315 grid, on which the forward seismic modeling was launched.

**Fluid-flow simulation.** The STOMP-CO2 (White and Freedman, 2007), developed at the Pacific Northwest National Laboratories, commercial software is used to model the fluid transport equation in isothermal mode. The code solves the mass balance equation for the non-wetting (CO$_2$) and wetting phase fluid (brine) and for the dissolved salt.

The fluxes are computed with the Darcy equation, considering two different relative permeabilities for each of the two fluids.

Since we are dealing with a two phase flow, the interfacial forces between the wetting and non-wetting phase fluids will give place to capillary pressure. We use a Van Genuchten (van Genuchten, 1980) relation for both capillary pressure and relative permeability curves. In this simulation STOMP considers capillary trapping mechanisms due to hysteresis of the relative permeability curve.

Temperature was considered constant at 37°C for the entire simulation time, the aquifer was considered to be fully saturated with brine before the onset of the injection. Initial pressure is considered to be hydrostatic with a brine density of 1030 kg/m$^3$ (~15 MPa at the bottom of the formation), while salinity is set to 3.2%. Zero flux boundary conditions are set at all boundaries, even though the same results can be obtained if Dirichlet boundary conditions are set, given their distance from the injection well.

Van Genuchten’s pore size distribution parameter m is set to 0.4 on the entire domain. We consider the Mualem approximation for which $n=1-1/m=1.67$. Entry capillary head $\alpha$ is set to 0.16 in the shales and 2.84 in the sandstone.

Grain density is set uniformly to 2600 kg/m$^3$, its compressibility to $4.5\times10^{-10}$ Pa$^{-1}$ and a Miltlington and Quirk tortuosity function is used.

We inject 0.31 kg/s of pure CO$_2$ for 2 years in a well located at point (501 m,-1030 m) of the formation. STOMP is asked to give outputs at 0.5, 1, 1.5 and 2 years after start of injection.

In Figs. 2a and 2b we show the distribution of CO$_2$ saturation and pressure and density after 1 year injection respectively.

It has to be stressed that we incurred in strong numerical instabilities, convergence failures and crashes while performing this simulation. For this reason, we compared the results with those obtained with TOUGH2-ECO2N software used at INGV Catania. This other simulator showed similar instabilities, but finally we found a grid and a set of parameters with which both simulator showed similar results.
Velocity model. We now need to compute the seismic velocities and attenuations of the partially saturated medium. To do this, we use White’s mesoscopic rock-physics theory (White, 1975), which is well described in appendix A of Carcione et al. (2012). White’s model approximates the partially saturated medium by considering patches of CO$_2$ in an otherwise brine-saturated medium; more precisely, he considers an outer sphere of radius $r_1 > r_0$ saturated with brine and an inner sphere of radius $r_0$ saturated with gas. Therefore, saturation can be defined as $S_g = r_0^3/r_1^3$. White’s mesoscopic model allows to compute the p-wave phase velocity as a function of frequency and attenuation factors in an isotropic medium. In fact, the model allows to compute the complex bulk modulus as a function of porosity, permeability, gas saturation, clay content and fluid viscosity, knowing the high frequency bulk modulus when there is no fluid flow between the patches. Then, a complex phase velocity can be computed, the real and imaginary parts are the phase p-wave velocity and attenuation factor respectively.

In fact, the complex bulk modulus can be computed, knowing the high frequency bulk modulus when there is no fluid flow between the patches and the permeability of the medium. Furthermore, the density is given by an average of the densities weighted over porosity and clay content for the solid part and over saturation for the fluid components. White does not provide a mesoscopic model for shear deformations. Therefore, we assume that the complex shear modulus is described by a Zener element having a peak frequency. Practically, we assume that the stiffer the medium, the higher the quality factor. Actually, this is not a bad approximation, since, as shown by Picotti et al. (2010), White’s model is consistent with Zener’s and the computed velocities differ by less than 5% in this simulation.

Finally, we consider the grains forming the rocks to be a mixture of quartz and clay. The presence of the latter changes the value of the effective bulk and shear moduli of the rock. We follow Hashing and Strickman’s (1963) variational approach and take the arithmetic average of the upper and lower bounds.

This model confirms the empirical evidence that p-wave velocity decreases with increasing gas partial saturation, until a threshold value (depending on the clay content) is reached. After that, fluid density effects prevail and we observe an increase in velocity. As for the S-waves, we record an increase in velocity with increasing gas saturations.

In Figs. 2c and 2d, we show respectively the relaxed (at $f_0$) p- and s- wave velocities as computed with White’s model, while in (e) and (f) one can see the quality factors for p- and s- waves respectively.

Seismic modeling. The synthetic seismograms are computed with a modeling code based on an isotropic and viscoelastic stress-strain relation. The equations can be found in Section 3.9 of Carcione (2015). The attenuation is described by the standard linear solid, also called the Zener model, that gives relaxation and creep functions in agreement with experimental results.

Simulations are run using a 315x315 staggered grid. 99 shots were computed, the shallowest of which is at -750 m with a source spacing of 5 m. An array of 315 receivers is placed in the other well, covering an entire column with a receiver spacing of 2.5 m. The dominant source frequency is set to 80 Hz, with a Ricker wavelet as source time history. The time step is set to 0.1 ms.

The algorithm is based on a fourth-order Runge Kutta method to calculate the synthetic seismograms recursively in time, while spatial derivatives are computed with a Fourier pseudo-spectral method.

The receivers were set to start recording when the source wavelet reaches the maximum, in order to have zero-phase. Therefore, to perform a tomographic inversion of the direct arrivals, we picked the maximum amplitudes of the first break in the seismogram.

In Fig. 3 a sample shot is shown, with the evident anomalies in the velocity of the first arrivals. The source time history is also displayed.

Tomographic inversion. The last step of this work consists of a tomographic inversion of the first arrivals (direct waves) of the synthetic seismograms using CAT3D software (see, for
example, Accaino et al., 2005). The domain to be inverted consists of the space between the two wells, therefore it extends 150 m in the horizontal direction and we only invert in the depth interval (0.8-1.3 km), considering therefore only 200 receivers A grid of 10x34 pixels is set, staggered in both directions twice; therefore 9 inversions are performed in total.

For the forward ray-tracing CAT3D uses a minimum time algorithm The scheme can be summarized as follows; the initial guess is a straight line joining the source and receiver points.
Then, this straight line is gradually modified by applying Snell’s law to subsequent triplets of points of intersection with the grid. The scheme continues until the last computed ray path differs from the previous one by less than a certain threshold. The inversion scheme used assumes an initial homogenous medium with a p-wave velocity of 3500 m/s. Then, the difference between the travel times computed from the ray paths and the picked ones is minimized with a Simultaneous Reconstruction Technique (SIRT) algorithm for 200 iterations.

Since we want to resolve velocity anomalies which are generally horizontal, we select only those rays which have an angle lower than 30° from the horizontal line. Despite this, ray coverage is sufficient, with a total of 6775 rays.

Results of the inversion are shown in Fig. 3c. As one can see, the main velocity anomalies of the domain are well resolved. As for the residuals, mean RMS is 1.1 %, with residuals well distributed around 0, as can be seen in Fig. 3d.

![Fig. 3](image)

**Conclusions.** We presented modeling of a synthetic, yet realistic, geological sequestration of CO\(_2\) experiment. We setup a 2D geological model consisting of a deep (>800 m) sandstone aquifer with some lens-shaped shale intrusions, surrounded by shales. We simulated the two-phase flow of the supercritical CO\(_2\) and the brine using STOMP commercial software. Output of this simulation are saturation, pressure, density profiles for both gas and liquid phases. From here, using White’s model, we computed the seismic velocities, which are the input of the viscoelastic code used for the seismic modeling. The direct arrivals were then picked in these synthetic seismograms, which were inverted using our in-house tomographic code CAT3D.

The results are encouraging, confirming the validity of the modeling and that a tomographic inversion of direct arrivals is able to detect the velocity anomalies caused by the presence of the CO\(_2\).
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