## CO2BLOCK user guide

CO2BLOCK provides the automatic estimate of the  $CO_2$  storage capacity of an aquifer. Please refer to De Simone and Krevor (2021) for details about the theoretical framework.

The tool is written in Matlab language and it is composed by six scripts. Users only need to open and modify the script **CO2BLOCK.m**. There is no need to open or modify the other scripts, which is instead not recommended.

## Input

It is necessary to provide an input file containing the aquifer parameters data, which must look as presented in the provided example file **example\_data.xlsx** (do not change the column order). There is a set of strictly required parameters, whereas others are calculated by means of default values, when not provided (Table 1). Although default values provide reasonable estimations, we recommend the use of precise data which would allow for a more accurate prediction of the storage capacity.

In the CO2BLOCK.m script, users have to define directory and name of the input data file. Users also need to set some parameters. They are:

- correction: set on or off to apply correction for superposition (off is the most conservative option)
- dist\_min: minimum inter-well distance [km] (considering operational requirements)
- dist\_max: maximum inter-well distance [km]. If auto is set, the tool automatically calculate the maximum distance according to the reservoir area
- nr\_dist: number of inter-well distances to explore (high numbers can cause slow calculation)
- nr\_well\_max: maximum number of wells. If auto is set, the tool automatically calculate the maximum number of wells according to the reservoir area and the minimum interwell distance
- rw: well radius [m]
- time\_yr: time of injection [years]

• maxQ: maximum sustainable injection rate per well because of technological limitations [Mton/years]

The code work-flow is the following:

- 1. Acquisition of the parameters by reading the input data
- 2. Set some parameters with default values if they are not provided in the input data. Details are provided in Table 1.
- 3. Evaluation of the maximum sustainable pressure
- 4. Evaluation of the pressure build-up due to a reference injection rate for all the scenarios
- 5. Estimate of the maximum sustainable injection rate for all the scenarios
- 6. Inclusion of constraints and rescaling of the maximum injection rates if necessary
- 7. Evaluation of the plausible scenarios

## Output

The tool calculates the storage capacity for each scenario of well number and distance. Output results are the maximum sustainable per-well injection rate and the maximum sustainable injected mass. They are provided both in graphical plots and in excel tables, as shown in Figure 1.

## References

- Altunin, V. and Sakhabetdinov, M. (1972). Viscosity of liquid and gaseous carbon dioxide at temperatures 220-1300 k and pressure up to 1200 bar. *Teploenergetika*, 8:85–89.
- Batzle, M. and Wang, Z. (1992). Seismic properties of pore fluids. *Geophysics*, 57(11):1396–1408.
- De Simone, S. and Krevor, S. (2021). A tool for first order estimates and optimisation of dynamic storage resource capacity in saline aquifers. *International Journal of Greenhouse Gas Control*, 106:103258.
- Redlich, O. and Kwong, J. N. (1949). On the thermodynamics of solutions. v. an equation of state. fugacities of gaseous solutions. *Chemical reviews*, 44(1):233–244.
- Spycher, N., Pruess, K., and Ennis-King, J. (2003). Co2-h2o mixtures in the geological sequestration of co2. i. assessment and calculation of mutual solubilities from 12 to 100 c and up to 600 bar. *Geochimica et cosmochimica acta*, 67(16):3015–3031.

 Table 1: Required and default parameters assumed when not provided.

Required parameters	Default parameters	Default values
Domain BC (open/closed)	Rock compressibility, $c_r$	$5 \times 10^{-4} \text{ MPa}^{-1}$
Shallowest depth, $\zeta$	Brine compressibility, $c_w$	$3 \times 10^{-4} \text{ MPa}^{-1}$
Mean depth, $\zeta_m$	Brine salinity, $\chi$	180000 ppm
Thickness, $H$	Shallowest pressure, $p_0$	10 MPa/km $\times \zeta$
Surface area, $A$	Mean pressure, $\overline{p_0}$	10 MPa/km $\times \zeta_m$
Permeability, $\kappa$	Mean Temperature, $\overline{T_0}$	$33^{\circ}/\mathrm{km} \times \zeta_m + 15^{\circ}$
Porosity, $\phi$	$\mathrm{CO}_2$ density, $\rho_c$	calculated with respect to $\overline{p_0}$ and $\overline{T_0}$ , according to Redlich and Kwong (1949) (with the parameters proposed by Spycher et al. (2003))
	$\mathrm{CO}_2\mathrm{viscosity},\mu_c$	calculated with respect to $\overline{p_0}$ and $\overline{T_0}$ , according to Altunin and Sakhabetdinov (1972)
	Brine viscosity, $\mu_w$	calculated with respect to $\overline{T_0}$ and $\chi$ , according to Batzle and Wang (1992)
	Vertical stress, $\sigma_v$	23 MPa/km $\times \zeta_m$
	Stress ratio, $k_0$	0.7
	Friction coefficient, $\varphi$	$30^{\circ}$
	Cohesion, $C$	0 MPa
	Tensile strength, $S_0$	0 MPa

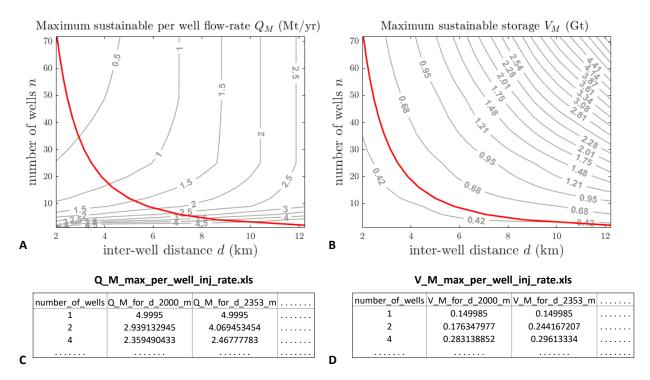


Figure 1: Examples of CO2BLOCK output plots and tables. Pressure-limited scenarios of sustainable mass injection rate (Mt/yr) (A and C) and of total mass for the injection period (Gt) (B and D) for different number of wells and inter-well distance. In A and B, plausible scenarios are on the left of the red line. In C and D, rows correspond to different scenarios of well number, while columns correspond to different scenarios of inter-well distance.