1	Assessment and Uncertainty Quantification of Onshore Geological CO2 Storage Capacity in
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#### Abstract

We provide a probabilistic assessment of  $CO_2$  storage capacity in major sedimentary basins in China. Our approach embeds constraints associated with the increase of reservoir pore pressure due to injection of  $CO_2$  in the presence of resident brine. Pressure build-up must be limited to avoid fault reactivation, caprock failure, and possible leakage, resulting in more conservative estimates of  $CO_2$  storage capacity as compared to volumetric estimates.

22 We rely on a numerical Monte Carlo framework considering uncertainty in the values of 23 reservoir size and major geological formation attributes (i.e., absolute permeability, porosity, and 24 reservoir compressibility). Our work shows that 10 major basins can potentially store, on average, 25 1350 Gt of CO<sub>2</sub> during the next 30 years (lower and upper quartiles being 1100 and 1700 Gt of CO<sub>2</sub>, 26 respectively). This far exceeds the likely amount (up to 175 Gt of CO<sub>2</sub>) required to be stored by 2050. Our analysis also suggests that 6 basins (located close to the largest emission areas) can store about 27 93 Gt (on average) of CO<sub>2</sub> during the next 30 years. Underground carbon storage in China, coupled 28 29 with other possible solutions, could meet the aims of the Announced Pledges Scenario (International 30 Energy Agency) to mitigate global warming by 2060.

We also perform a global sensitivity analysis to determine how our predictions of storage capacity may be affected by uncertainties in the simulation model input parameters. Moment-based global sensitivity metrics suggest that geological formation attributes are major sources of uncertainty, significantly affecting model outputs and the associated uncertainty.

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*Keywords*: geological carbon storage; storage capacity; climate change; uncertainty quantification;
 Global Sensitivity Analysis.

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# LIST OF MEAN SYMBOLS and NOMENCLATURE

Α	Reservoir area	[km <sup>2</sup> ]
B <sub>o</sub>	Oil formation volume factor	
$AMAE_{\theta_i}^Y$	Sensitivity index of parameter $\theta_i$ for the mean of <i>Y</i>	
$AMAV_{\theta_i}^Y$	Sensitivity index of parameter $\theta_i$ for the variance of <i>Y</i>	
$AMA\gamma^{Y}_{\theta_{i}}$	Sensitivity index of parameter $\theta_i$ for the skewness of <i>Y</i>	
С	Cohesion parameter	[MPa]
С	Reservoir compressibility	[Pa <sup>-1</sup> ]
d	Inter-well distance	[km]
g	Gravity vector	
Н	Reservoir thickness	[m]
k	Absolute permeability	[m <sup>2</sup> ]
ε	Ratio between minimum and maximum effective stress	
M <sub>CO2</sub>	Mass of CO <sub>2</sub>	[Gt]
$N_P$	Number of uncertain model parameters	
n	Number of wells	
$p_0$	Pressure at the top of the reservoir	[MPa]
$\Delta p$	Pressure buil-up	[MPa]
$\Delta p_r$	Pressure build-up for reference flowrate	[MPa]
$\Delta p_M$	Maximum pressure build-up	[MPa]
Q	Volumetric flowrate	[m <sup>3</sup> /s]
$Q_M$	Maximum flowrate	[Gt/y]
$Q_M^{tot}$	Total injection flowrate	[Gt/y]
$Q_r$	Reference flowrate	[Gt/y]

l	Number of MC realizations	
r	Distance from injection well	[m]
$r_0$	Well radius	[m]
R	Radius of influence of the well	
S	Fracture pressure indicator	[MPa]
t	Time	[y]
T <sub>0</sub>	Representative reservoir temperature	[°C]
$U^{ heta i}$ , $U^+_{ heta i}$	Support range of $\theta_i$	
Y	Vector of model output	
$V(B_i)$	$CO_2$ storage capacity of the basin $B_i$	[Gt]
ε	Binary operator	
Ψ	Radius of a fictious equivalent vertical interface	[m]
$\mu_c$	Viscosity of CO <sub>2</sub>	[Pa s]
$\mu_w$	Viscosity of brine	[Pa s]
θ	Vector of uncertain model parameters, with entries $\theta_i$	
$\widetilde{oldsymbol{ heta}}$	Sample of $\boldsymbol{\theta}$	
$ ho_{co2}$	Density of CO <sub>2</sub>	[kg/m <sup>3</sup> ]
$\sigma_1, \sigma_2, \sigma_3$	Principal stresses	[MPa]
$\sigma_n$	Normal stress	[MPa]
τ	Shear stress	[MPa]
$\phi$	Porosity	
CCS	Carbon Capture and Storage	
CEC	China Electricity Council	
APS	Announced Pledges Scenario	

IEA	International Energy Agency
GSA	Global Sensitivity Analysis
KLD	Kullback-Leibler Divergence
MC	Monte Carlo
pdf	Probability density function

### **1. Introduction**

China currently accounts for 27% of global CO<sub>2</sub> emissions (IEA, 2021). It has been the most 42 rapidly growing major economy since 1980, its gross domestic product (GDP) having increased more 43 than 30 times. While promoting an impressive growth in renewables and hydropower since 2000, 44 45 there is still a marked dependence on fossil fuels. These were documented to meet around 85% of its total primary energy needs in 2020 (coal accounting for almost 60% and oil for about a fifth; CEC, 46 2021). China's emissions from the energy sector (fuel combustion and industrial processes) made up 47 48 almost 90% of total internal greenhouse gas emissions, compared to 60% in the rest of the world. Hence CO<sub>2</sub> emissions in China reflect a carbon-intensive energy sector. About 70% of China energy-49 related emissions in 2020 are associated with coal, 12% with oil, 6% with natural gas, and about 11% 50 51 with process emissions (IEA, 2021; FAO, 2021; Saunois et al., 2020; Friendlingstein et al., 2020; UNFCCC, 2021; He et al., 2020). 52

53 Carbon Capture and Storage (CCS) is expected to potentially provide significant support in 54 the reduction of emissions (Celia, 2017; Leung et al., 2014), while considering that additional 55 emissive plants might be developed in the future years. Indeed, considering the dependence of China 56 on fossil fuels, this is an essential technology to achieve net zero CO<sub>2</sub> emissions by 2050 or 2060.

Fig. 1 provides a depiction of the main CO<sub>2</sub> emission points in China, together with pipelines 57 which are already present and potential geologic storage formations considered in our study. The 58 59 north-eastern part of the country is characterized by the presence of most of the storage formations that are located close to sources of CO<sub>2</sub> emissions. The five provinces of Jiangsu, Shanxi, Shandong, 60 Xinjiang, and Guangdong account for nearly 40% of China's coal burning plants (IEA, 2021). Most 61 of these are located in the northern and eastern parts of the country. This geographical proximity, 62 together with the existing pipeline infrastructure, could contribute to saving transportation costs, 63 64 provided that these formations can provide sufficient storage capacity. Note that offshore reservoirs

- are not considered in this work since storage in these formations is likely to be more expensive than
- 66 onshore.





Fig. 1 Map of (a) major CO<sub>2</sub> sources and (b) potential geological storage basins (denoted as B<sub>1</sub>-B<sub>10</sub>)
selected for the analysis of storage CO<sub>2</sub> capacity in China (IEA, 2021).

An Energy Sector Roadmap to Carbon Neutrality in China is illustrated in IEA (2021). It is then estimated that if the existing emission intensive infrastructure in China continues to operate in the same way it has in the recent years, it could result in 175 Gt of  $CO_2$  emissions between now and 2060 (IEA, 2021). This is equivalent to one-third of the maximum permitted global  $CO_2$  emissions budget (IPCC, 2018) to limit rise in global temperature to 1.5 °C by 2050 (see Mechler et al., 2020 for details).

According to the Announced Pledges Scenario (APS) of the World Energy Outlook (IEA, 77 2021), China's primary energy demand will grow much slower through 2030 than the overall 78 79 economy. This is mainly the result of efficiency gains and a shift away from heavy industry. A transforming energy sector leads to rapid improvements in air quality. Solar becomes the largest 80 81 primary energy source by 2045. Moreover, it is predicted that demand for coal will drop by more than 82 80% by 2060, oil by around 60%, and natural gas by more than 45%. CO<sub>2</sub> emissions from fossil fuel combustion alone are foreseen to reach around 450 Mt by 2060. They are entirely offset by negative 83 84 emissions produced by bioenergy in conjunction with carbon capture and storage (BECCS). The APS predicts a growing deployment of CCS in China, reaching 2.6 Gt of CO<sub>2</sub> emissions reduction in 2060. 85 86 Considering a temporal window of 30 years, this yields a need for almost 80 Gt of cumulative emission reduction to meet the targets. 87

In this broad context, our objective is to assess the storage capacity (with associated uncertainties) of China to answer the needs of developing CCS projects in the next three decades. To this end, a robust stochastic approach is used to estimate the geological CO<sub>2</sub> storage capacity of 10 major basins (see Fig. 1b) in China and assess if there is sufficient storage capacity to meet the APS targets of CCS for China.

The most suitable formations to establish  $CO_2$  storage projects are deep saline aquifers and depleted oil and gas reservoirs (IEA, 2020). There are various techniques to evaluate  $CO_2$  storage capacity. These are generally comprised within two main groups, depending on whether they are based on (*i*) the evaluation of the gross rock volume or (*ii*) of the pressure build-up across the system (see Section 3 for more details). Several studies use gross rock volume-based techniques (Bachu et al., 2007) to evaluate  $CO_2$  storage capacity in selected regions, basins, and formations in China (e.g., Jiao et al., 2011; Li et al., 2009; Poulsen et al., 2011; Qiao et al., 2012; Vincent et al., 2009; Zhou et

100 al., 2011) and show very high storage capacities. National scale source-sink matching studies show 101 that the storage capacity of onshore aquifers could address the needs of CCS associated with 102 emissions from large, stationary  $CO_2$  point sources in China for several decades (Dahowski et al., 103 2009).

104 The works mentioned above mainly focus on a specific region/basin/formation. In this 105 context, our study is set within a broader (national scale) assessment of CO<sub>2</sub> storage capacity in China and a rigorous quantification of associated estimation uncertainties is included. It is further noted that 106 107 a critical issue associated with most of the available studies is that they solely consider the gross rock 108 volume while neglecting constraints on the rate of injection. The latter can be limited by injection 109 facilities and by the requirement to prevent fracturing the rock, which can in turn lead to escape of 110 the CO<sub>2</sub> intended to be stored. Ignoring pressure constraints can result in overestimation of the 111 reservoir storage capacity. Our study then relies on an integrated assessment model that considers overpressure at each well as a key constraint parameter. 112

113 Our work focuses on the assessment of the available capacity of CO<sub>2</sub> storage across 10 selected onshore basins. These encompass oil and gas fields and saline aquifers and are considered 114 115 to be some of the most suitable sites in China (Wei et al., 2013). We collect information regarding 116 the geophysical characteristics of the selected fields. Since the main traits and attributes of subsurface 117 systems are always affected by uncertainty, a rigorous uncertainty quantification of the storage capacity is performed. As stated above, a stochastic approach is applied based on a pressure build-up 118 119 assessment for the evaluation of storage capacity across the basins studied. The analyses are framed in a numerical Monte Carlo context. This relies on modern Global Sensitivity Analysis (GSA) 120 121 techniques to (a) quantify the relative importance on storage capacity of each uncertain parameter associated with our simulation model and (b) identify the most critical variables affecting the results 122 of the study. 123

Our workflow is motivated by the observation that understanding the effects of the uncertainty associated with the values of input parameters on the variability of the output of an interpretive model helps to identify the most influential parameters with respect to the model responses (Muleta and 127 Nicklow, 2005; Pappenberger et al., 2008; Wagener et al., 2009; Ruano et al., 2012; Hill et al., 2016; Ranaee et al., 2021a) while other parameters can be set at prescribed values without distorting the 128 results (Degenring et al., 2004; van Griensven et al., 2006; Chu et al., 2015; Punzo et al., 2015; 129 Nossent et al., 2011). Most applications of GSA rely on variance-based indices (e.g., Sudret, 2008) 130 to quantify the sensitivity of the response(s) of the system to variations in the values of the controlling 131 132 variables. Recently, Dell'Oca et al. (2017) developed a technique where the influence of uncertain model parameters on various (statistical) moments of a target model output can be quantified through 133 a moment-based GSA approach. Sensitivity is defined by these authors as the average variation of 134 135 key statistical moments of the probability density function of an output due to model parameter variability. Model parameter uncertainty is then propagated to a target model output (i.e., CO<sub>2</sub> storage 136 capacity) through a Monte Carlo scheme. 137

The work is organized as follows. Section 2 provides a brief overview of current CCS activities in China. Section 3 introduces the mathematical model to evaluate the carbon storage capacity as well as the stochastic analysis underpinning our results. Implementation of the workflow and the ensuing results are discussed in Section 4. Concluding remarks are presented in Section 5.

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#### 2. CCS in China

Development of carbon capture and storage technologies in China is still in the early stages. 144 About 21 pilot, demonstration or commercial projects are currently in operation in China. These are 145 characterized by a combined capture capacity of more than 2 Mt/y of CO<sub>2</sub>, most of these being 146 associated with CO<sub>2</sub> - Enhanced Oil Recovery (EOR). The largest of these is possibly the commercial 147 148 600 kt/y China National Petroleum Corporation (CNPC) CO<sub>2</sub>-EOR project at Jilin, capturing CO<sub>2</sub> from natural gas processing. These CCS projects are located in northern and eastern China where 149 150 there is a high density of coal-based chemicals and power production as well as good opportunities of performing CO<sub>2</sub>-EOR. 151

Modern CO<sub>2</sub>-based enhanced oil recovery (CO2-EOR) processes can assist in mitigating CO<sub>2</sub>
 emissions. These yield a net reduction in carbon emissions from captured sources while improving

hydrocarbon production and (at least partially) revitalizing depleted oilfields. Oil production through
CO2-EOR is typically characterized by a less than average carbon intensity/footprint (Cooney et al.,
2015).

Bruce Hill et al. (2020) provide a comprehensive overview of key CO2-EOR projects across China. These authors note that China's CO2-EOR projects are typically confined to commercial projects of limited size, test or huff-n-puff injections associated with tens of thousands of tonnes per year, a strategy for recapture or recycle the produced  $CO_2$  not yet being implemented. They also note that China's 2019 roadmap for Carbon Capture, Utilization and Storage (CCUS) sets out goals with the aim of moving  $CO_2$  use from a research stage towards an industrial implementation scenario.

The potential for CO2-EOR in China has been preliminarily assessed by Advanced Resources International, with an estimate that implementation of CO2-EOR would lead to an incremental production of 1 billion barrels of oil following the use of 4 Gt of captured industrial CO<sub>2</sub> (Godec, 2011; Wei et al., 2015).

It is also noted that scarcity of water in China's arid oilfields have hampered waterfloodingbased EOR projects and has motivated research and development towards the use of  $CO_2$ , which is also favored considering the accessibility of substantially pure  $CO_2$  from industrial sources (Bruce Hill et al., 2020). The potential of enhanced water recovery methods in combination with  $CO_2$ injections is also being currently assessed. The latter is a saline geologic sequestration method and, when combined with reverse osmosis, might enhance availability of water resources in the areas of coal chemical industry and across petroleum basins in China (Li et al., 2019).

A critical element hampering the development and systematic implementation of enhanced oil recovery is related to the observation that the geological settings associated with China's depleted reservoirs typically require fracture stimulation to increase permeability and lead to an established commercial production. Thus, this can severely dampen potential benefits stemming from CO2-EOR projects in China. Zhang et al. (2015) provide some insights on the results of a monitoring campaign performed between 2008 and 2012 for the Jilin EOR project. The authors observed a breakthrough of  $CO_2$  in nearby production wells that approximately amounts to 20%. Ma et al. (2018) analyzed the 181 CO2-EOR project in Sinopec's Gaoqing 89 block and reported that almost all of the CO<sub>2</sub> injected
182 into the reservoir is vented from the produced oil.

183 CCS in China is expected to be critical to reach net zero and avert dangerous global warming. 184 To this aim, an all-around evaluation of conservative storage capacity coupled with an understanding 185 of the associated estimation uncertainties can effectively assist decision making for matching  $CO_2$ 186 emission sources with sites of potential storage. In Section 4 we address the way storage capacity of 187 the basins introduced in Fig. 1b can answer the needs of CCS in China.

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## 3. Materials and Methods

Our assessment of the overall storage capacity of a target formation rests on the methodology 190 191 developed by De Simone and Krevor (2021). The latter explicitly embeds constraints associated with 192 the increase of reservoir pore pressure due to injection of CO<sub>2</sub> in the presence of resident brine (see also e.g., Bachu, 2008; Rutqvist, 2012). It is noted that alternative, volumetric-based techniques for 193 the assessment of storage capacity currently consider at best crude approximations of pressure build-194 up. Accordingly, such techniques may be less conservative because they do not consider constraints 195 due to reservoir pressurization and possible plume migration through leakage pathways 196 197 (Szuluczewski et al., 2012).

Our estimates of the largest viable well injection rate and reservoir storage capacity used the open-source software CO2BLOCK (De Simone and Krevor, 2021). A variety of injection scenarios were considered expressed in terms of number of wells and inter-well spacing. This approach has been used recently to assess storage capacity in the North Sea (Karvounis and Blunt, 2021).

The workflow we consider for the assessment of  $CO_2$  storage capacity is depicted in Fig. 2. For simplicity, and consistent with the aim of our overall/global assessment, we assume (*i*) the reservoir to be conceptualized as a homogeneous system and (*ii*) *n* vertical injection wells to be placed across the domain. Wells are characterized by uniform spacing and operate at the same (constant) volumetric injection rate.



Fig. 2 Workflow of the analysis to assess the overall CO<sub>2</sub> storage capacity of a reservoir (De Simone
and Krevor, 2021).

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## 3.1.1 Pressure build-up due to single-well CO<sub>2</sub> injection

The study follows De Simone and Krevor (2021) and starts by considering the action of a single injection well and evaluate pressure build-up in the reservoir following injection of a reference CO<sub>2</sub> rate across a given time window. This result will then be used to evaluate the maximum possible injection rate.

From De Simone and Krevor (2021), pressure build-up following CO<sub>2</sub> injection from a single well into a homogeneous reservoir with open boundaries and under the assumption of no pre-existing fractures and negligible trapping can be evaluated as:

$$\Delta p(r,t) = \frac{Q\mu_w}{2\pi kH} \cdot \begin{cases} \frac{\mu_c}{\mu_w} \ln \frac{\psi}{r} + \ln \frac{R}{\psi}, & r \le \psi \\ & \ln \frac{R}{r}, & \psi < r < R \\ & 0, & r \ge R \end{cases}$$
(1)

here,  $\Delta p(r, t)$  is overpressure (or pressure build-up) at time *t* and radial distance *r* from the injection well operating at volumetric flow rate *Q*; *k*,  $\phi$ , and *H* are absolute permeability, porosity, and average thickness of the reservoir, respectively;  $\mu_w$  and  $\mu_c$  are brine and CO<sub>2</sub> dynamic viscosity, respectively;  $\psi(t)$  represents the radius of an equivalent vertical sharp interface between the injected plume and the resident fluid, which can be expressed as  $\psi = \exp(\omega)\xi$  (where  $\omega = \frac{\mu_c + \mu_w}{\mu_c - \mu_w} \ln \sqrt{\frac{\mu_c}{\mu_w}} - 1$ ;  $\xi = \sqrt{\frac{2\pi}{2}}$ 

224  $\sqrt{\frac{Qt}{\pi\phi H}}$ ; and *R* corresponds to the well radius of influence. The latter can be assessed according to 225 (Cooper and Jacob, 1946):

$$R = \sqrt{\frac{2.25kt}{\mu_w c}} \tag{2}$$

where *c* is reservoir compressibility. Equation (1) was introduced by De Simone and Krevor (2021; see their Equation (S1) in their Supplementary Material) and has then been recently employed by Karvounis and Blunt (2021) in their analyses. It stems from the formulation first introduced by Nordbotten et al. (2015; see their Equation (11)) after (*i*) integration across three regions around the injection well where all fluid is  $CO_2$ ,  $CO_2$  and water are mixed, and all fluid is pure water, respectively, and then (*ii*) introducing an appropriate formulation for the vertical interface between fluids (see also Villarasa et al., 2010).

# 233 The action of multiple wells can then be expressed through superposition, i.e.,:

$$\Delta p_{sup}(\boldsymbol{x}_i, t) = \sum_{j=1}^n \Delta p(d_{ij}, t)$$
(3)

where *n* is the number of wells,  $d_{ij}$  being the distance between wells at (vector) locations  $\mathbf{x}_i$  and  $\mathbf{x}_j$ ( $\mathbf{x}_i$  denoting the vector of spatial coordinates of well *i*). De Simone and Krevor (2021) assume no interference of CO<sub>2</sub> plumes related to each of the injection wells, (i.e.,  $d_{ij} > \psi$ ,  $\forall j$ ). They also suggest that the overpressure at a location  $\mathbf{x}_i$  of well *i* can be evaluated through superposition as:

$$\Delta p_{sup}(\boldsymbol{x}_i, t) = \frac{Q\mu_w}{2\pi kH} \left[ \frac{\mu_c}{\mu_w} \ln\left(\frac{\psi}{r_0}\right) + \ln\left(\frac{R}{\psi}\right) + \sum_{j=2}^n \ln\left(\frac{R}{d_{ij}}\right) \right]$$
(4)

where  $r_0$  is well radius (we recall that each well is characterized by the same injection rate *Q*). This approach allows various scenarios comprising a variety of well numbers and inter-well spacing to be evaluated for a total given injection rate into a reservoir.

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# 3.1.2 Limits to pressure build-up

Pressure build-up must be kept below a critical value, corresponding to the largest pressure,  $\Delta p_M$ , sustainable by the system. Jaeger et al. (2009) showed that formation failure may take place in either a tensile or a shear mode. The former state can take place along planes normal to the minimum principal stress, hereafter termed  $\sigma_3$  (i.e.,  $\sigma_1 \geq \sigma_2 \geq \sigma_3$ , subscripts being related to the principal directions of the local stress tensor) when pore pressure exceeds the sum of  $\sigma_3$  and the rock tensile strength,  $S_0$ . Thus, the limit value of pressure build-up ( $\Delta p_M^t$ ) for a tensile fracturing scenario is:

$$\Delta p_M^t = \sigma_3 - p_0 + S_0 \tag{5}$$

where  $p_0$  is the initial pressure at the top of the reservoir (which is typically considered to correspond to hydrostatic pressure).

250 Formation failure due to occurrence of high shear can be assessed on the basis of the Mohr-251 Coulomb failure criterion as:

$$\tau - [C + (\sigma_n - p)tan\varphi] \ge 0 \tag{6}$$

Here,  $\tau$  is shear;  $\sigma_n$  is the stress normal to the failure plane direction;  $\varphi$  is the angle of internal friction of the formation; and *C* is cohesion (i.e., intrinsic shear strength). Assuming that failure takes place along planes at angles of  $(45^\circ \pm \frac{\varphi}{2})$  with the direction of the largest principal stress,  $\sigma_1$ , the limit pressure build-up  $(\Delta p_M^s)$  for a shear mode scenario is evaluated as:

$$\Delta p_M^s = \frac{\epsilon - \theta}{1 - \theta} (\sigma_1 - p_0) + C \cdot \cot(\varphi)$$
(7)

where  $\epsilon \le 1$  is the ratio between the lowest and the largest effective stress values, i.e.,  $\epsilon = (\sigma_3 - p_0) / (\sigma_1 - p_0)$ , and  $\theta = (1 - \sin\varphi) / (1 + \sin\varphi)$ .

258 It is noted that a shear-related failure is typically expected in the presence of cohesionless rock systems (corresponding to C = 0). Otherwise, when considering reservoirs mainly characterized 259 by cohesive rocks, tensile failure is more common at shallow depths while shear-related failure can 260 take place at large depths. The largest sustainable overpressure  $(\Delta p_M)$  is then evaluated as the lowest 261 between tensile- and shear-related failure pressure values (i.e., Equations (5) and (7)). We emphasize 262 263 that quantification of these values is plagued by uncertainty due to a variety of sources. These include, for instance, the conceptual description of the system underlying the mathematical representation 264 (Equations (5) to (7)) as well as the associated parametrization which typically embeds uncertain 265 model parameters. Here, we focus on the effect of model parameter uncertainty while relying on the 266 modeling approach described above, which is consistent with the typical nature of a global assessment 267 268 CO<sub>2</sub> storage capacity project of the kind considered.

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## 3.1.3 Pressure build-up for multi-well injection

We adopt Equation (4) to evaluate the overpressure,  $\Delta p_r$ , due to a preliminary value set for the 270  $CO_2$  injection rate  $(Q_r)$  at a well. Such a value is taken as a reference and is maintained constant 271 across a given temporal window. We do so for a well located in the middle of the reservoir surface 272 area (where overpressure is typically highest). Here, a software default value of  $Q_r = \frac{M_0}{\alpha_r n}$  is 273 considered,  $M_0$  and n respectively being the value of total rate injected in the system and the number 274 of wells considered for such a reference scenario. Due to the lack of available data, values of 275 hydrostatic gradient (10 [MPa/km]), temperature gradient (33 [°C/km]), ratio between minimum and 276 maximum effective stress ( $\epsilon = 0.7$ ), and water salinity ( $1.8 \times 10^5$  ppm) are set to the default values 277 provided by the CO2BLOCK toolkit (De Simone and Krevor, 2021). 278

279 Several scenarios are built considering various numbers of wells and inter-well spacing for a 280 given total injection rate into the reservoir. De Simone and Krevor (2021) show that pressure build-281 up decreases with increasing (*i*) the number of wells, *n*, and (*ii*) the distance between wells,  $d_{ij}$ .

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3.1.4 Limits to the maximum flowrate

Once the maximum sustainable overpressure  $\Delta p_M$  is assessed and the overpressure,  $\Delta p_r$ , associated with the reference injection rate,  $Q_r$ , is evaluated, one can then evaluate the largest sustainable injection flowrate ( $Q_M$ ) into each well. In this context, De Simone and Krevor (2021) suggest the following formulation to evaluate  $Q_M$ , given the response (in terms of overpressure) for a reference scenario:

$$Q_M(t) = -\frac{Q_r \Delta \widetilde{p}_M}{W(-\Delta \widetilde{p}_M e^{-\Delta \widetilde{p}_r(t)})}$$
(8)

where *W* denotes the Lambert function (e.g., De Simone and Krevor, 2021; Corless et al., 1996) for  $-\Delta \widetilde{p}_M e^{-\Delta \widetilde{p}_r(t)} < 0$ ;  $\Delta \widetilde{p}_M$  and  $\Delta \widetilde{p}_r$  are evaluated as:

$$\Delta \widetilde{p}_M = \frac{\Delta p_M}{bQ_r} \tag{9}$$

$$\widetilde{\Delta p_r} = \frac{\Delta p_r}{bQ_r} \tag{10}$$

290 where  $b = \frac{\mu_w - \mu_c}{4\pi \kappa H \rho_c}$ , and  $\rho_c$  is the density of CO<sub>2</sub>.

Evaluation of the storage capacity for a given time t, i.e.,  $V_M = ntQ_M$ , is then straightforward. Finally,  $V_M$  for multiple scenarios is assessed encompassing various numbers of wells and inter-well distances to identify the maximum possible overall capacity of the reservoir.

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#### 3.1.5 Technical constraints

Given the scale and nature of the study, and consistent with Karvounis and Blunt (2021), each reservoir is assumed as homogeneous, with wells placed on a Cartesian grid and all operating with the same (constant) injection rate ( $Q_M$ ). Similar to Karvounis and Blunt (2021), for a given set of model input parameters (see also Section 3.2) we (*a*) generate a range of scenarios associated with various injection well numbers and inter-well distances and (*b*) identify the scenario which maximizes reservoir storage capacity,  $V_M$ .

In doing so, we follow De Simone and Krevor (2021) and consider a lower and an upper limit to the distance between well pairs i and j. The lower limit is set to minimize interference between CO<sub>2</sub> plumes as:

$$d_{i,j} > \sqrt{\frac{tQ_M(t)}{n\pi\phi H\rho_c}} \tag{11}$$

304 The upper limit is related to the reservoir surface area, A. The latter constraint is rendered as

$$d_{i,j} \le \sqrt{\frac{A}{n}} \tag{12}$$

305 Moreover, one could consider the presence of technical (engineering) limitations to the largest 306 injectable flow rate per well (hereafter termed  $Q_s$ ), so that:

$$n \ge \frac{Q_M^{tot}}{Q_s} \tag{13}$$

307 where  $Q_M^{tot}$  is the total injection rate, corresponding to the sum of the rates injected through the *n* 308 wells. Scenarios that do not satisfy technical constraints of (11)-(13) are not retained.

Note that, in line with De Simone and Krevor (2021), we set  $Q_s = 5$  Mt/y per well. This is also consistent with the study of Michael et al. (2011), who document that value of  $Q_s$  range between 4 and 20 Mt/y across the collection of industrial-scale CO<sub>2</sub> geological storage projects they reviewed.

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#### 3.2. Global Sensitivity Analysis and Uncertainty Assessment

Results of simulations of CO<sub>2</sub> storage practices may vary depending on uncertainties in the 314 values of the parameters embedded in Equations (1) to (13). Quantifying the way uncertainties 315 316 associated with model parameters propagate to model outputs (which are then ultimately employed 317 to estimate the maximum CO<sub>2</sub> storage capacity) can identify the most influential model parameters 318 with respect to the target model response. It can also address the viability of setting some parameter(s) (which are deemed as uninfluential) at prescribed value(s) without significantly affecting the model 319 320 results. In this sense, sensitivity analysis is a convenient framework to diagnose the behavior of a 321 given model in response to uncertainty associated with its parameters.

The parameters related to the reservoir size (*A* and *H*) and formation properties ( $\phi$ , *k* and *c*) included in the mathematical formulations presented in Section 3.1 are considered as uncertain. For the purpose of our application, uncertainties linked to CO<sub>2</sub>/brine properties (e.g., density and viscosity) are neglected. A vector  $\boldsymbol{\theta}$  whose entries  $\theta_i$  ( $i = 1, ..., N_P$ ) correspond to the values of these N<sub>P</sub> = 5 uncertain model parameters is introduced.

The study relies on modern Global Sensitivity Analysis approaches to diagnose the behavior of the model we consider in the presence of parametric uncertainty. We do so by focusing on the maximum CO<sub>2</sub> storage capacity of a target reservoir,  $Y = V(B_j)$ , and quantify the relative contribution of each uncertain model parameter to the uncertainty of *Y*.

We rely on random sampling the parameter space of variability  $\mathbf{\Gamma} = \Gamma_{\theta_1} \cdot ... \cdot \Gamma_{\theta_{N_P}}$ ,  $\Gamma_{\theta_i}$  being the support (range of variability) of parameter  $\theta_i$ , which is viewed as a random quantity (see, e.g., Saltelli et al., 2008; Muleta and Nicklow, 2005; Dell'Oca et al., 2017; Bianchi Janetti et al., 2019; Russian et al., 2019; Ranaee et al., 2021a; 2021b and references therein for additional details).

We focus on the recent moment-based global sensitivity metrics introduced by Dell'Oca et al. (2017). These are denoted as *AMA* indices and are defined as:

$$AMAE_{\theta_{i}}^{Y} = \begin{cases} \frac{1}{|E[Y]|} E[|E[Y] - E[Y|\theta_{i}]|] & if \quad E[Y] \neq 0\\ E[|E[Y|\theta_{i}]|] & if \quad E[Y] = 0 \end{cases}$$
(14)

$$AMAV_{\theta_i}^Y = \frac{E[|V[Y] - V[Y|\theta_i]|]}{V[Y]}$$
(15)

$$AMA\gamma_{\theta_i}^{Y} = \begin{cases} \frac{1}{|\gamma[Y]|} E[|\gamma[Y] - E[Y|\theta_i]|] & if \quad \gamma[Y] \neq 0\\ E[|\gamma[Y|\theta_i]|] & if \quad \gamma[Y] = 0 \end{cases}$$
(16)

where  $AMAE_{\theta_i}^{Y}$ ,  $AMAV_{\theta_i}^{Y}$ , and  $AMA\gamma_{\theta_i}^{Y}$  represent the sensitivity indices associated with the mean, variance, and skewness of  $Y(\theta)$ , respectively ( $E(\bullet)$  denotes expected value,  $V(\bullet)$  denotes variance and  $\gamma(\bullet)$  is skewness). Note that indices  $AMAE_{\theta_i}^{Y}$ ,  $AMAV_{\theta_i}^{Y}$  and  $AMA\gamma_{\theta_i}^{Y}$  quantify the expected change of mean, variance, and skewness of Y due to variations of  $\theta_i$ , respectively. The combined use of these indices enables one to perform a comprehensive GSA of the target model response,  $Y(\theta)$ , quantifying the impact of each entry of  $\theta$  on the variability of Y. When considered in the context of typically used variance-based methods (such as, e.g., methods based on Sobol indices; Sobol, 1993), this approach
provides enhanced understanding on the way uncertain parameters are acting through the model onto
key statistical moments characterizing the distribution of the selected model output.

Considering that probability densities of the values of a reservoir storage capacity can be 346 different from a classical normal distribution, relying on a traditionally used variance-based 347 348 sensitivity criterion (e.g., Sobol, 1993) may provide an incomplete picture of a system response to uncertainty in model parameters. Instead, moment-based sensitivity metrics of the kind we consider 349 350 enable one to analyze the system response in terms of its main statistical moments. As seen above, 351 these include the expected value of the simulation response, Y, the spread around the mean, and the degree of symmetry and tailedness of the probability density function (pdf) of Y. These indices allow 352 for a comprehensive description of how the structure of the pdf of Y is affected by variations of 353 354 uncertain model parameters.

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4. Results

# 4.1. Characteristics of the main sedimentary basins in China

The characteristics of the basins introduced in Fig. 1b are analyzed here for a (preliminary) assessment of suitability for CO<sub>2</sub> storage.

The study of Bruce Hill et al. (2020) is referred for a detailed description of the main 359 geological traits characterizing the lithology of typical continental reservoir rocks across China. Only 360 a brief summary is included here for completeness. Sedimentary reservoirs across China are typically 361 consolidated depositional basins filled with sedimentary sequences from fluvial and lacustrine 362 geologic settings (Petroleum Geology of China, 1992). Key elements associated with these have been 363 driven by burial, compaction, and related diagenetic processes (Bruce Hill et al., 2020). Basins in 364 north-eastern China are chiefly characterized by a marked overall thickness of sedimentary bodies 365 and several sets of reservoir-caprock layers, offering a setting of potential interest for geological 366 storage of captured CO<sub>2</sub> (Zeng et al., 2013). In this scenario, Diao et al. (2017) document that argillite 367 (mudstone and shale) and evaporites (gypsum and rock salt) constitute the most commonly found 368

369 caprocks for oil and gas fields in China; caprocks formed by carbonate rocks and frozen genesis caps
370 are also found in some fields.

371 Sandstone reservoir formations in Erlian sub-basins are buried at depths of 1-3 km and potential storage sites are formed by structural and fault traps. Wang et al. (2018) showed that key 372 373 lithological traits of the Dongving and Shahejie formations in the Bohai bay Basin encompass pebbly 374 sandstone, siltstone, sandstone intercalated with mudstone, and oil shale. Oilfields and surrounding aquifers across the Ordos basin could be considered as a potential target for storage of CO<sub>2</sub>, due to 375 the presence of sandstones characterized by a thickness of about 200 m at suitable depths and potential 376 377 structural and lithological traps. Mudstone interbedded with fine-grained sandstone of the Pliocene 378 Wulantuke formation and mudstone intercalated with fine-grained sandstone and marlite of the 379 Miocene Wuyuan formation form the caprock in the Hetao Basin, silt to medium-grained sandstone of the Oligocene Linhe formation (thickness of 260-340 m) providing a good potential for storage. 380 Saline aquifers in the Sichuan Basin are characterized by an overall very low porosity and 381 permeability. Otherwise, natural gas fields in the Sichuan Basin are characterized by suitable caprock 382 conditions for CO<sub>2</sub> storage (Diao et al., 2017). The reader is referred to the work of Sun et al. (2021) 383 for an exemplary stratigraphy of the Sichuan Basin. Su et at (2013) performed a (basin scale) 384 385 assessment of the potential CO<sub>2</sub> storage capacity in the deep saline aquifers of the Songliao Basin. 386 These authors suggest that spatial heterogeneities therein (in terms of e.g., pore volume, temperature, or pressure distribution) pose significant challenges for the quantification of storage potential. 387

Wei et al. (2013) implemented a GIS-based framework of analysis (first developed by Bachu, 2003) and reported that the basins illustrated in Fig. 1b are potentially suitable for CO<sub>2</sub> storage (due to their makeup, mainly associated with large sedimentary thickness, tectonic stability, and several sets of reservoir-caprock pairs). Their analysis considered four elements: (*i*) storage capacity and injectivity; (*ii*) risk minimization and storage security; (*iii*) environmental restrictions; and (*iv*) economic considerations. It was then shown that 90% of CO<sub>2</sub> sources are within 160 km of a CO<sub>2</sub> storage reservoir. This suggests that the technology is economically feasible (Dahowski et al., 2009).

For the purpose of our analysis, suitable layers within the same formation are conceptualized as different basins (e.g.,  $B_6$  and  $B_7$  in Fig. 1b). Basins which are suitable to  $CO_2$  storage and are at the same time close to emissions sources are included in our study (see Fig. 1).

398 The Erlian basin (see Fig. 1b) is a highly heterogeneous continental basin with generally low permeability and porosity. The Manite and Tengger subbasins belong to the Erlian basin and are 399 400 denoted as B<sub>1</sub> and B<sub>2</sub>, respectively, in Fig. 1b. These include sandstone rich formations with a thickness of the order of hundreds of meters buried at depths of 1-3 km. These elements potentially 401 provide a substantial CO<sub>2</sub> storage potential. Additionally, analysis of potential sources and sinks 402 403 reveals that marked CO<sub>2</sub> emission point sources (i.e., the Datang Group Hexigten Qi, a coal to gas 404 factory, estimated to emit about 8.56 Mt/y) are located less than 100 km away from these subbasins (Fig. 1a). The Bohai Bay basin (which includes subbasins  $B_3$  and  $B_{10}$  in Fig. 1b) contains porous 405 406 sandstone and conglomerate rich formations. These are sealed by mudstones and lithological and structural traps, thus being associated with potentially favorable conditions for CO<sub>2</sub> storage. The 407 408 Hebei Kaiyue Chemical Group (with about 4 Mt/y of CO<sub>2</sub> emissions) is located within 50 km from these subbasins. The Hetao basin (B<sub>4</sub> in Fig. 1b) comprises a well-defined succession of mudstone, 409 410 fine-grained sandstone, marlite, and silt to medium-grained sandstone (with a thickness of 260-340 411 m). It thus forms an ideal environment for storage of CO<sub>2</sub>. Source-sink matching identifies CO<sub>2</sub> 412 emissions from a coal to olefin factory in Baotao City (associated with about 2.4 Mt/y of CO<sub>2</sub> emissions). The Ordos Basin (B<sub>5</sub> in Fig. 1b) is characterized by sequences of sealed reservoir layers, 413 414 with seemingly good potential for CO<sub>2</sub> storage. Emission sources that can be found in its proximity include the Shenhua Ningxia Coal industry Group (about 3 Mt/y of CO<sub>2</sub> emissions). Furthermore, it 415 416 is noted that a pilot project with a storage potential of about 1 Mt of CO<sub>2</sub> is already in place (Zeng et al., 2013). Wei et al. (2013) suggest that Ordos (B<sub>5</sub> in Fig. 1b), Sichuan (B<sub>6</sub>-B<sub>7</sub> in Fig. 1b), and 417 Songliao (B<sub>8</sub>-B<sub>9</sub> in Fig. 1b) basins are the most promising sites for CO<sub>2</sub> aquifer storage projects in 418 419 China. The Sichuan basins (B<sub>6</sub> and B<sub>7</sub>) are approximately in the central part of China. These consist of different reservoir-cap combinations of lenticular sand body capped by brown-red mudstone and 420 sandy mudstone with siltstone layer. They are close to emission sources of about 100 Mt/y overall. 421

422	The Songliao basin (B <sub>8</sub> and B <sub>9</sub> ) is a large sedimentary basin in north-eastern China. It is an important
423	area due to the presence of mineral resources and well-established industrial bases, i.e., it accounts
424	for one-third of the total oil production in China (Su et al., 2013). Sandstone and siltstone with
425	caprocks of low permeable mudstone constitute the main lithology of the potential storage formations.
426	There are several CO <sub>2</sub> sources in the area, i.e., the Northern Songliao basin alone with several sources
427	emitting more than 10 Mt/y of CO <sub>2</sub> (National Bureau of Statistics of China, 2008). Wei et al. (2013)
428	evaluated the Tarim, Junggar, Turman-Hami, and Qaidam basins (all located in of the north-west of
429	China) as suitable sites for $CO_2$ storage. These are not included in our assessment because of ( <i>i</i> ) their
430	large distances from major emission sources and (ii) socio-political concerns that reduce the potential
431	of these basins to firmly establish CO <sub>2</sub> storage projects. Table 1 lists some key characteristics of the
432	selected basins (B <sub>1</sub> -B <sub>10</sub> ) collected from prior studies (e.g., Zeng et al., 2013; Diao et al., 2017; Fan et
433	al., 2014; Wang et al., 2014; Jin et al., 2017; Wang et al., 2018). Such information is required for the
434	assessment of carbon storage capacity, following Equations (1)-(13) in Section 3. For the purpose of
435	illustration, Fig. 3 provides a schematic depiction including the main parameters listed in Table 1.
436	The overall thickness of a basin is evaluated across the whole geological formation containing an
437	ensemble of permeable layers (suitable for CO <sub>2</sub> sequestration). Shallowest- and mean-depths of the
438	reservoir are referred to the mean sea level as depicted in Fig 3.



441 **Fig. 3.** schematic illustration of the main parameters listed in Table 1 onshore reservoir 442 characteristics suitable for  $CO_2$  sequestration. The thickness includes only the permeable layers 443 shaded.

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Unit name	Depth -	Depth -	Thickness*	Area	Permeability	Porosity
(subbasin)	shallowest [m]	mean [m]	[m]	[km <sup>2</sup> ]	[mD]	[-]
Manite subbasin (B <sub>1</sub> )	1000	2000	300	10000	1000	0.15
Tengger subbasin (B <sub>2</sub> )	1000	2000	300	12170	1000	0.15
Bohai Xialahoe (B <sub>3</sub> )	700	2240	200	428	1550	0.23
Hetao basin (B <sub>4</sub> )	1800	2650	300	2000	285	0.175
Ordos basin (B <sub>5</sub> )	870	1400	200	150	125	0.184
Sichuan Jurassic (B <sub>6</sub> )	3500	3650	300	37000	5	0.1244
Sichuan upper Triassic (B <sub>7</sub> )	4000	4500	500	37000	1	0.05
Songliao Yaojia (B <sub>8</sub> )	1287	1809	150	260000	200	0.2
Songliao Qingshankou (B9)	1469	2424	150	260000	210	0.188
Shahejie Formation (B <sub>10</sub> )	1600	2000	300	2500	10000	0.2

445 **Table 1.** Characteristics of the selected basins ( $B_1$ - $B_{10}$  in Fig. 1b).

\* It is noted that the overall thickness (termed thickness, for brevity) of the basin formation is assessed
across the whole geological formation and its evaluation encompasses solely the permeable layers
without including cap rock and impermeable layers (see also Fig. 3).

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## 4.2. Uncertainty Assessment

As mentioned in Section 3.2, we select a set of uncertain model parameters  $\theta_i$  (with i= {1, ...,5}). We consider the values of the uncertain parameter to be characterized by uniform probability densities. This modeling choice is consistent with scenarios where prior information (e.g., measurements) on model parameters is not available and enables one to give equal weight to each value across the space of variability of a given parameter. We refer to information reported in the

457 literature (Zeng et al., 2013; Diao et al., 2017; Fan et al., 2014; Wang et al., 2014; Jin et al., 2017; 458 Wang et al., 2018) and consider broad ranges of variability for the values of each uncertain model parameter  $\theta_i$  (see Table 2). Selection of the support ranges of each  $\theta_i$  values is set to represent broad 459 ranges of variability based on typical measurement uncertainties (see, e.g., Sifuentes et al., 2009; Li 460 and Liu, 2016; Ajayi et al., 2019; Barros et al., 2021). We set the support of  $\theta_1 = H$  and  $\theta_2 = A$ 461 considering a  $\pm$  50 % and  $\pm$  20% range of variability around the corresponding mean values reported 462 in the literature.  $\theta_3 = log_{10}(k)$  to vary across the range of  $\pm 1$ , to encompass a broad range of 463 variability. Porosity is correlated to permeability as  $\phi = \alpha \log_{10}(k)$ . We set the values of  $\theta_4 = \alpha$  to 464 range across the support  $\pm 0.03$  (accounting for possible inaccuracies of the empirical equation used 465 466 for porosity modeling). Accordingly, the distribution of  $\phi$  corresponds to the product of two uniformly distributed random variables. Sample values of  $\theta_5 = log_2(c)$  are described through a 467 468 uniform distribution within the support range of  $\pm 1$  around mean values reported in the literature (see Table 2). 469

471 **Table 2** List of the uncertain model parameters. Each uncertain parameter  $\theta_i$  (i = 1, ..., 5) is 472 characterized by a uniform distribution with support  $[U_{\theta_i}^-, U_{\theta_i}^+]$ .

Uncertain parameters	$\theta_1 = H$ [m]	$\theta_2 = A$ $[km^2] \times 10^3$	$\theta_3 = log_{10}(k)$ [ k in mD]	$\theta_4 = \alpha$ $[-] \times 10^{-3}$	$\theta_5 = log_2(c)$ [c in Pa <sup>-1</sup> ]
	$[U^{\ddot{\theta}_1}, U^+_{\ddot{\theta}_1}]$	$[U^{\ddot{ heta}_2}, U^+_{\ddot{ heta}_2}]$	$[U^{\ddot{ heta}_3}, U^+_{\ddot{ heta}_3}]$	$[U^{\ddot{ heta}_4}, U^+_{\ddot{ heta}_4}]$	$[U_{\ddot{\theta}_5}^-, U_{\ddot{\theta}_5}^+]$
Manite subbasin (B1)	[150, 450]	[8, 12]	[2, 4]	[48, 51]	[-31, -29]
Tengger subbasin (B <sub>2</sub> )	[150, 450]	[9.7, 14]	[2, 4]	[48, 51]	[-31, -29]
Bohai Xialahoe (B <sub>3</sub> )	[100, 300]	[0.34, 0.52]	[2.2, 4.2]	[70, 75]	[-31, -29]
Hetao basin (B <sub>4</sub> )	[150, 450]	[1.6, 2.4]	[1.5, 3.5]	[69, 73]	[-31, -29]
Ordos basin (B <sub>5</sub> )	[100, 300]	[0.12, 0.18]	[1.1, 3.1]	[85, 91]	[-31, -29]
Sichuan jurassic (B <sub>6</sub> )	[150, 450]	[29, 44]	[0, 2]	[21, 13]	[-31, -29]
Sichuan upper triassic (B7)	[250, 750]	[29, 44]	[0, 2]	[48, 51]	[-31, -29]
Songliao Yaojia (B <sub>8</sub> )	[75, 225]	[210, 310]	[1.3, 3.3]	[84, 90]	[-31, -29]

Songliao Qingshankou (B <sub>9</sub> )	[75, 225]	[210, 310]	[1.3, 3.3]	[78, 83]	[-31, -29]
Shahejie Formation (B <sub>10</sub> )	[150, 450]	[2, 3]	[3, 5]	[48, 51]	[-31, -29]

A collection of Monte Carlo (MC) realizations is generated by randomly sampling from the 474 distributions of the uncertain model parameters and the storage capacity of each reservoir j,  $V(B_i)$ , is 475 evaluated. The total storage capacity,  $V(B_{tot})$ , is evaluated considering all of the realizations 476 477 generated across the 10 basins studied. Fig. 4 depicts the way mean, variance, skewness, and coefficient of variation of the values of storage capacity depend on the number of realizations 478 479 considered. Results for each of the basins are depicted together with those associated with total storage capacity. These results suggest that stability of MC simulation results (in terms of moments 480 481 of CO<sub>2</sub> storage capacity) is attained after about 5000 MC realizations.



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483 **Fig. 4.** Mean (E[Y]), variance (V[Y]), skewness ( $\gamma$ [Y]), and coefficient of variation (CV[Y]) of the 484 values of storage capacity (i.e.,  $Y = V(B_j)$ ) versus the number of MC realizations considered. Results 485 for each of the basins (colored curves;  $V(B_1) - V(B_{10})$ ) are depicted together with those associated 486 with total storage capacity (black curves;  $V(B_{tot})$ ).

488 The degree of similarity/difference between two sample probability density functions (pdfs) of the storage capacity evaluated with different numbers of MC realizations is quantified (see Table 489 3) through the Kullback - Leibler divergence, KLD (Kullback and Leibler, 1951). Note that small 490 values of KLD correspond to small differences between the selected pdfs. 491

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Table 3. Values of the Kullback - Leibler divergence, KLD, for selected pairs of MC realizations (i.e., 493 1000 vs 2000, 3000 vs 4000, 5000 vs 6000, 7000 vs 8000, 9000 vs 10000). 494

Basin	KLD	KLD	KLD	KLD	KLD
	( <i>l</i> =1000 vs 2000)	( <i>l</i> =3000 vs 4000)	( <i>l</i> =5000 vs 6000)	( <i>l</i> =7000 vs 8000)	( <i>l</i> =9000 vs 10000)
$\mathbf{B}_1$	$2 \times 10^{-3}$	$4 \times 10^{-4}$	$1 \times 10^{-4}$	$8 \times 10^{-5}$	$8 \times 10^{-5}$
$B_2$	$3 \times 10^{-3}$	$8 \times 10^{-4}$	$2 \times 10^{-4}$	$2 \times 10^{-4}$	$1 \times 10^{-4}$
<b>B</b> <sub>3</sub>	$4 \times 10^{-3}$	$5 \times 10^{-4}$	$2 \times 10^{-4}$	$2 \times 10^{-4}$	$1 \times 10^{-4}$
$\mathbf{B}_4$	$4 \times 10^{-3}$	$5 \times 10^{-4}$	$1 \times 10^{-4}$	$1 \times 10^{-4}$	$8 \times 10^{-5}$
<b>B</b> 5	$4 \times 10^{-3}$	$1 \times 10^{-3}$	$4 \times 10^{-4}$	$2 \times 10^{-4}$	$1 \times 10^{-4}$
$B_6$	$4 \times 10^{-3}$	$8 \times 10^{-4}$	$2 \times 10^{-4}$	$2 \times 10^{-4}$	$4 \times 10^{-5}$
<b>B</b> <sub>7</sub>	$9 \times 10^{-3}$	$8 \times 10^{-4}$	$4 \times 10^{-4}$	$2 \times 10^{-4}$	$2 \times 10^{-4}$
$B_8$	$3 \times 10^{-3}$	$7 \times 10^{-4}$	$3 \times 10^{-4}$	$2 \times 10^{-4}$	$2 \times 10^{-4}$
<b>B</b> 9	$4 \times 10^{-3}$	9 × 10 <sup>-4</sup>	$5 \times 10^{-4}$	$2 \times 10^{-4}$	$2 \times 10^{-4}$
<b>B</b> <sub>10</sub>	$1 \times 10^{-2}$	$6 \times 10^{-3}$	$1 \times 10^{-4}$	$1 \times 10^{-4}$	$5 \times 10^{-5}$
B <sub>tot</sub>	$2 \times 10^{-3}$	$3 \times 10^{-4}$	$1 \times 10^{-4}$	$9 \times 10^{-5}$	$4 \times 10^{-5}$

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Overall, the set of analyses performed imbues us with confidence that a number of MC 496 realization approximately equal to 5000 guarantees stable results for the ensuing pdf of the storage 497 capacity for each of the target basins. As a result, 10<sup>4</sup> random Monte Carlo realizations are run for 498 499 each of the basins considered.

## 4.3. Sensitivity Analysis

We quantify the sensitivity of the simulated model outputs (i.e.,  $Y = V(B_i)$ ) with respect to variations in the values of uncertain parameters,  $\theta_i$ , referring to the approach introduced in Section 3.2. Figures 5-7 depict values of the *AMA* indices (Equations (14) - (17)) evaluated for each basin ( $B_i$ ; i = 1, ..., 10) and associated with mean, variance, and skewness of  $V(B_i)$  with respect to  $\theta_i$ .

When considering the mean value of storage capacity (as rendered through  $AMAE_{\theta_i}^{Y}$ ; Equation 506 13), one can see that all parameters are characterized by the same strength in B<sub>1</sub>, B<sub>2</sub> and B<sub>10</sub>. These 507 508 are intermediate size basins with reasonably high values of permeability. Reservoir compressibility 509 and the height of the reservoir are instead the most important quantities driving the potential storage capacity of B<sub>8</sub> and B<sub>9</sub> (very large basins with intermediate values of permeability). Otherwise, the 510 intrinsic properties of the geological system appear to be most significant for basins B<sub>3</sub>, B<sub>4</sub> and B<sub>5</sub> 511 (small basins with intermediate values of permeability), as well as  $B_6$  and  $B_7$  (large basins with low 512 513 permeability). These results confirm that formation properties are the key parameters effecting 514 storage capacity for the basins with low permeability values, even as the total volume of the reservoir 515 is large (e.g., B<sub>6</sub>, B<sub>7</sub>). Equation (4) shows how overpressure is linked to the rock attributes. In such 516 cases, low values of permeability constrain displacement of the resident brine by the injected CO<sub>2</sub>. 517 Accumulation of CO<sub>2</sub> can then locally lead to overpressure conditions (Karvounis and Blunt, 2021). It is noted that in the presence of high permeability values the main controlling factors to avoid 518 519 excessive overpressure are (a) the height of the system (which enables accumulation of CO<sub>2</sub>) and (b)520 reservoir compressibility (which allows for additional space for CO<sub>2</sub>).

With reference to the impact of uncertain model parameters on model output variance,  $AMAV_{\theta_i}^{Y}$  (Equation (15)) values show almost the same trend as the corresponding  $AMAE_{\theta_i}^{Y}$  for all reservoirs. An exception is given by B<sub>6</sub> and B<sub>7</sub> where, in addition to rock attributes,  $AMAV_{\theta_i}^{Y}$  shows also high sensitivities to *c* (i.e., reservoir compressibility). This can indirectly be linked to the low permeability values associated with these basins. Indeed, low permeability can result in local accumulation of CO<sub>2</sub> and local increases of pore pressures. Hence, high values of CO<sub>2</sub> compressibility 527 can alleviate some effects of low permeable formations on a local increase of pore pressures. 528 Accordingly, basins  $B_6$  and  $B_7$  show higher sensitivity to the values of the parameters directly 529 influencing flow of CO<sub>2</sub> across the system (i.e.,  $\phi, k, c$ ) due to their extremely low values of 530 permeability and porosity.

531 Values of  $AMA\gamma_{\theta_i}^{\gamma}$  reveal that skewness is mostly impacted by model uncertain parameters in 532 small basins (i.e., B<sub>1</sub>, B<sub>2</sub>, B<sub>3</sub>), where almost all uncertain parameters are important.

In summary, our results reveal that uncertainty in geological attributes and in reservoir size influence the CO<sub>2</sub> storage capacity of basins with reasonably high values of permeability (i.e., B<sub>1</sub>, B<sub>2</sub>, B<sub>10</sub>). Otherwise, system properties (i.e.,  $\phi$  and k) appear to be the most important parameters for evaluating storage capacity of the basins with small (to intermediate) values of permeability (B<sub>3</sub>, B<sub>4</sub>, B<sub>5</sub>, B<sub>6</sub>, B<sub>7</sub>). Reservoir compressibility and the height of the reservoir mainly influence model outputs in very large basins with high values of porosity/permeability (i.e., B<sub>8</sub>-B<sub>9</sub>).







541 *Fig. 5.* Evaluation of the moment-based  $AMAE_{\theta_i}^{Y}$  indices associated with the mean storage capacity

<sup>542</sup> of each basin studied  $B_j$   $(j = \{1, ..., 10\})$ .



**Fig. 6.** Evaluation of the moment-based  $AMAV_{\theta_i}^{Y}$  indices associated with the variance of the



*distribution of storage capacity of each basin studied*  $B_j$  ( $j = \{1, ..., 10\}$ ).

549 **Fig. 7.** Evaluation of the moment-based  $AMA\gamma_{\theta_i}^Y$  indices associated with the skewness in the 550 distribution of storage capacity of each basin studied  $B_j$   $(j = \{1, ..., 10\})$ .

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# 4.4. Uncertainty Quantification for CO<sub>2</sub> Storage Capacity

Our results illustrate that sample pdfs of the potential storage capacity show remarkable 553 variability across the basins analyzed (see Fig. 8). Sample pdfs of  $V(B_i)$  for intermediate size basins 554 with high permeability (i.e., B<sub>1</sub>, B<sub>10</sub>) are typically characterized by almost symmetrical distributions. 555 556 Distributions associated with small (and highly permeable) basins (i.e., B<sub>3</sub>, B<sub>4</sub>, B<sub>5</sub>) are skewed towards high values of  $V(B_i)$ . Large and low permeability basins (i.e., B<sub>6</sub>, B<sub>7</sub>) are characterized by 557 positively- (right-) skewed distributions, with frequent high values of storage capacity. Sample 558 559 distributions of very large (highly permeable) basins (i.e., B<sub>8</sub>, B<sub>9</sub>) are positively skewed, with long 560 tails to high values of storage capacity.

The emergence of left-skewed distributions (e.g.,  $B_2$ ) can be related to the constraint imposed 561 to the range of variability of inter-well distances (Equations (11) and (12)). This severely limits the 562 number of wells that can be placed in small reservoirs. Consequently, many realizations are 563 characterized by an estimated storage capacity limited by this constraint, with a tail of less likely 564 smaller capacities limited by other properties (see Fig. 8). Otherwise, the emergence of a right-skewed 565 distribution is mainly driven by the engineering constraints adopted (i.e.,  $Q_s = 5$  Mt/y per well). These 566 limit the storage capacity that can be obtained by a given number of wells. Basin B<sub>7</sub> is characterized 567 by a high frequency of low values of  $V(B_i)$ . It is noted that these values are mainly related to 568 569 realizations characterized by very low permeability values that are subject to the constraint on 570 permeability (i.e., k > 1 mD) associated with the simulation toolbox (De Simone and Krevor, 2021).



572

573 *Fig. 8.* Sample pdfs of  $CO_2$  storage capacity,  $V(B_j)$  ( $j=\{1,...,10\}$ ) for the basins studied. Results are 574 associated with  $10^4$  MC realizations.

One can then relate these probabilistic results to  $CO_2$  emissions documented across nearby regions (Cui et al., 2021). An average (mean) of 55.3 Gt of  $CO_2$  is seen (Fig. 9a) to be potentially stored in 30 years in B<sub>1</sub> and B<sub>2</sub> (associated with the Erlian basin). This value is compatible with accommodating about 16 Gt of  $CO_2$  (in 30 years) of emissions from power and industrial sectors located in the provinces of Beijing and Inner Mongolia. An average value of 13.8 Gt of  $CO_2$  potential 581 storage capacity is associated with the Hetao basin (i.e., B<sub>4</sub>). This can satisfy the storage needs in the Gansu and Ningsia provinces, corresponding to about 10 Gt of CO<sub>2</sub> in 30 years (Cui et al., 2021). 582 Fig.9b shows that the Bohai Bay basin (encompassing  $B_3$  and  $B_{10}$ ) can serve (in an average sense) 583 23.4 Gt of CO<sub>2</sub> storage capacity in 30 years. This basin is close to the Tianjin, Shandong, Jiangsu, 584 Shanxi, Henan, and Hebei provinces. These provinces are estimated to be characterized by a 585 586 cumulative emission of about 82 Gt of CO<sub>2</sub> by 2050 (Cui et al., 2021). Accordingly, underground storage could only partially satisfy the projected requirements in this region. Thus, one would need 587 to either design a proper management scheme for (a) transporting some parts of the captured  $CO_2$  to 588 589 other basins or (b) combining applications of CCS with fossil free and renewable power generation. It is estimated that the Shaanxi, Hubei and Qinghai provinces will produce almost 20 Gt of CO<sub>2</sub> in 590 the next 30 years. Our results show that the nearby Ordos basin (i.e., B<sub>5</sub>) cannot satisfy the totality of 591 the needs of carbon storage in this region. 592





595 Fig. 9. Sample pdf of CO<sub>2</sub> storage capacity in the Erlin basin (with  $B_1$  and  $B_2$  subbasins) and Bohai 596 Bay basin (with  $B_3$  and  $B_{10}$  subbasins). Results correspond to  $10^4$  MC realizations for each 597 basin/subbasin.

599 Fig. 10 summarizes our results depicting the sample pdf of  $V(B_{tot})$ , corresponding to the overall storage capacity. For ease of interpretation, the associated boxplot representation is 600 juxtaposed. This shows a median value of approximately 1350 Gt of CO<sub>2</sub> (red line) and an 601 602 interquartile (25% to 75%) range spanning between 1100 and 1700 Gt of CO<sub>2</sub>. As stated in Section 2.2, CO<sub>2</sub> emissions to be abated across China for the next 30 years are expected to range from 80 Gt 603 of CO<sub>2</sub> (according to APS; IEA, 2021) to 175 Gt (without further intervention). These values are 604 much lower than those associated with the probability distribution of  $V(B_{tot})$  evaluated from our 605 606 modeling approach (see Fig. 10). Accordingly, our probabilistic analysis supports the idea that the storage capacity of China can meet the needs of most of the CO<sub>2</sub> emissions and offers multiple 607 possibilities to pair emission sources to storage sites. 608

609



610

611 Fig. 10. Sample pdf of total  $CO_2$  storage capacity,  $V(B_{tot})$ , in the 10 studied basins across China.

612 *Results are based on*  $10^4$  *MC realizations for each basin.* 

For example, if only the basins within the immediate proximity of the regions in China associated with the most severe carbon emissions are considered (i.e., the group denoted as B<sub>s</sub> in Fig. 1b and comprising basins  $B_1 - B_5$  and  $B_{10}$ ), one can evaluate the total storage capacity available and assess the possibility that these basins fulfill the APS projected requirements of 80 Gt of CO<sub>2</sub>. Fig. 11 depicts the sample pdf of storage capacity for group  $B_s$ . These results reveal an average storage capacity of about 93 Gt of CO<sub>2</sub> over the next 30 years, with lower and upper quartiles of 70 and 117 Gt of CO<sub>2</sub>, respectively. Thus, our results suggest that group  $B_s$  is associated with about 68% probability of providing a storage capacity of at least 80 Gt of CO<sub>2</sub>. Thus, this group of sites is potentially capable of satisfying the needs for CO<sub>2</sub> storage foreseen by APS within the year 2060. 



*Fig.* 11. Sample pdf of total  $CO_2$  storage capacity,  $V(B_s)$ , for 6 strategically selected basins of China.

*Results are based on*  $10^4$  *MC realizations for each storage basin.* 

# **5.** Conclusions

Carbon capture and storage is a key technology needed to reach net-zero. This study provides an estimate of the total storage capacity in major sedimentary basins in China close to emissions sources. A total of 10 basins are analyzed to estimate onshore  $CO_2$  storage capacity in China. Capacity is constrained using a semi-analytical model of pressure build-up.

Uncertainties in the estimation of each basin storage capacity are evaluated in a numerical
 Monte Carlo simulation framework based on a collection of basin model realizations generated with
 different plausible input geological properties.

This study suggests that an average of 1350 Gt of  $CO_2$  (with lower and upper quartiles of 1100 and 1700 Gt of  $CO_2$ , respectively) can be stored in onshore geological formations in eastern China within the next 30 years. In this context, considering the current emission scenario yields the expectation that up to 175 Gt of  $CO_2$  will be emitted across China over the next 30 years. Meanwhile, according to the Announced Pledges Scenario suggested by IEA (IEA, 2021) China will require about 80 Gt carbon capture and storage over the next 30 years. Hence, our analysis supports the conclusion that that CCS technology can fully sustain the currently foreseen needs of  $CO_2$  storage in China.

The results of the study suggest that a group of six basins can provide a viable answer to the needs for geological  $CO_2$  storage in China by 2060. This subgroup is close to major emissions sources and may have sufficient capacity alone to store likely emissions for the next 30 years.

Application of a rigorous Global Sensitivity Analysis framework provides insights into (i) the most important (uncertain) model parameters affecting CO<sub>2</sub> storage capacity, and (ii) how these quantities affect the ensuing probability distribution of storage capacity. The GSA results show that for the basins with very low permeability rocks it is misleading to evaluate storage capacity referring to the size of reservoir. Instead, formation properties are the key parameters effecting pressure buildup and storage capacity of such reservoirs.

The results provided in this work can be used as a first step for further decision making, detailed investigations, and development of CCS projects. The uncertainty analysis performed offers critical insights on the most important parameters in storage assessment, providing suggestions for

655	further data acquisition. Important sources of uncertainties that deserve future research include an
656	assessment of the impact of reservoir heterogeneity and better characterization of formation
657	properties. Coping with the combined effects of such sources of uncertainty would require significant
658	theoretical and operational work to incorporate model and parameter uncertainties in the analysis and
659	is still an open research challenge. Further source-sink matching analysis can also contribute to assist
660	an economical and feasible implementation of CCS technology in China.
661	
662	<b>Conflicts of interest/Competing interests</b>
663	The authors declare they have no known of conflicts of interest or competing interest that could have
664	appeared to influence the work reported in this paper.
665	
666	Availability of data and material
667	Data are available upon request
668	
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670	Ranaee, E. Software, design and implementation of the research, methodology, analysis of the
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673	design and supervision of the research, conceptualization, methodology, analysis of the results,
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