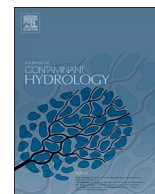




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## A predictive estimation method for carbon dioxide transport by data-driven modeling with a physically-based data model

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### ABSTRACT

In this study, a data-driven method for predicting CO<sub>2</sub> leaks and associated concentrations from geological CO<sub>2</sub> sequestration is developed. Several candidate models are compared based on their reproducibility and predictive capability for CO<sub>2</sub> concentration measurements from the Environment Impact Evaluation Test (EIT) site in Korea. Based on the data mining results, a one-dimensional solution of the advective–dispersive equation for steady flow (i.e., Ogata-Banks solution) is found to be most representative for the test data, and this model is adopted as the data model for the developed method. In the validation step, the method is applied to estimate future CO<sub>2</sub> concentrations with the reference estimation by the Ogata-Banks solution, where a part of earlier data is used as the training dataset. From the analysis, it is found that the ensemble mean of multiple estimations based on the developed method shows high prediction accuracy relative to the reference estimation. In addition, the majority of the data to be predicted are included in the proposed quantile interval, which suggests adequate representation of the uncertainty by the developed method. Therefore, the incorporation of a reasonable physically-based data model enhances the prediction capability of the data-driven model. The proposed method is not confined to estimations of CO<sub>2</sub> concentration and may be applied to various real-time monitoring data from subsurface sites to develop automated control, management or decision-making systems.

### 1. Introduction

Risk assessment provides important information regarding the potential hazards imposed by CO<sub>2</sub> leakage. During the operational phase of CO<sub>2</sub> storage, timely information from risk assessment enables decision-makers to prepare plans preemptively to mitigate or avoid such risks, and heavily relies on monitoring.

Because of the importance of monitoring techniques, the Intergovernmental Panel on Climate Change (IPCC) evaluated existing monitoring, measurement, and verification (MMV) techniques and suggested that site-specific MMV plans should be applied for individual geological storage sites (Metz et al., 2005). Therefore, several small-

scale controlled CO<sub>2</sub> release tests have been performed to evaluate site-specific MMV technologies alongside commercial-scale CO<sub>2</sub> injection (Jones et al., 2015). Well-designed controlled release testing is important to improve monitoring and site-characterization techniques, which aid in the development of continuous monitoring and estimation tools for the operation period. In a controlled CO<sub>2</sub> release test conducted by the Zero Emissions Research and Technology (ZERT) project in Montana, USA, CO<sub>2</sub> was released from a line source buried at depths of 1.3–2.5 m in an agricultural field (Strazisar et al., 2009; Zheng et al., 2012). Soil CO<sub>2</sub> flux measurements, in conjunction with numerical simulations, indicated that CO<sub>2</sub> leakage patterns at the surface are primarily governed by both subsurface heterogeneity and the dynamic

*Abbreviations:* AIC, Akaike information criterion; ASGARD, Artificial Soil Gassing and Response Detection; CPS, cyber-physical system; DHM, data-driven hydrogeological model; EIT, Environment Impact evaluation Test; EWS, early warning system; GPR, Gaussian process regression; IPCC, Intergovernmental Panel on Climate Change; K-COSEM, Korea CO<sub>2</sub> Storage Environmental Management; MMV, monitoring, measurement and verification; PHM, process-based hydrogeological model; RSS, residual sum of squares; ZERT, Zero Emissions Research and Technology

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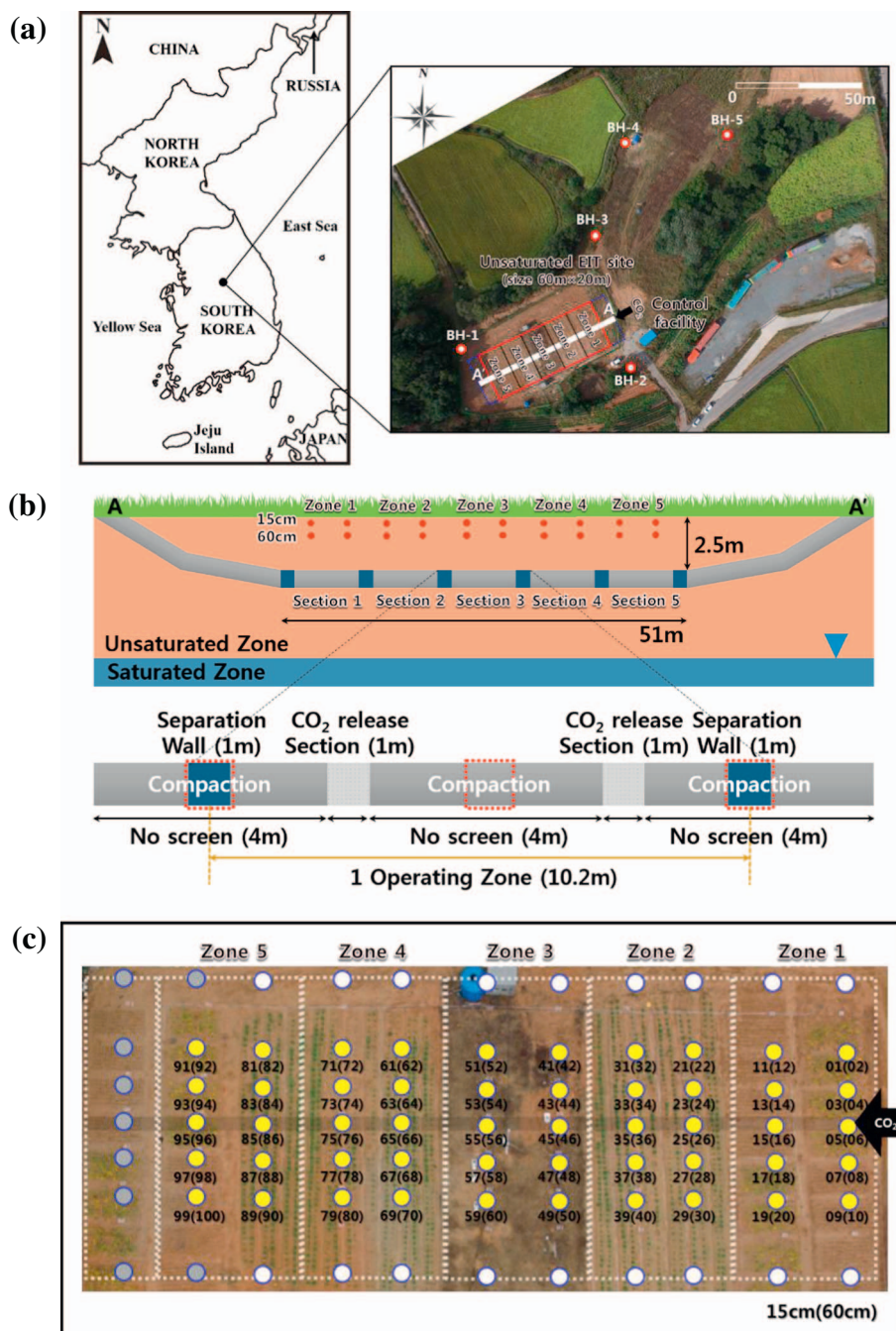


Fig. 1. (a) Location and an aerial photograph of the study area and the controlled CO<sub>2</sub> release test facility, (b) a schematic cross-sectional view of the installed horizontal well for CO<sub>2</sub> injection and the detailed design of the wellbore, and (c) the location of the monitoring points and their identification numbers.

fluctuation of the groundwater table (Lewicki et al., 2007). In an example from the Artificial Soil Gassing and Response Detection (ASGARD) project in Nottingham, UK, continuous monitoring of CO<sub>2</sub> concentration and flux revealed distinct damage to both soil microbiology and vegetation growth caused by CO<sub>2</sub> release (Smith et al., 2013). Similarly, a controlled CO<sub>2</sub> release experiment was performed in the Ginninderra site (NSW, Australia) by Geoscience Australia and the CO2CRC during 2012–2013 (Feitz et al., 2014). Based on > 10 different near-surface monitoring techniques, it was found that climatic conditions, groundwater fluctuation, and soil moisture substantially affected subsurface CO<sub>2</sub> migration. In these previous studies, a range of suitable monitoring technologies was identified. Nevertheless, uncertainties regarding measurements must be addressed when these technologies are applied for risk assessment and forecasting of CO<sub>2</sub> leakage.

Operational risk assessment, which is based on a framework of a real-time monitoring, includes, as the principal components, one or more predictive estimation methods. Estimation methods can be categorized into (1) process-based and (2) data-driven models. Process-based hydrogeological models (PHMs) generally adopt the mathematical form of a partial differential equation (PDE), which is solved using either analytical or numerical techniques. Strictly following physical laws, the PHMs directly solve conservation equations for fluid flow (e.g., Darcy's law) or solute transport (e.g., Fick's law) with several constitutive equations (e.g., equations of states, relative permeability, and capillary pressure) for cases with interdependent parameters. In terms of risk assessment of CO<sub>2</sub> leakage, PHMs are employed in the interpretation of CO<sub>2</sub> leakage potential associated with geological or anthropogenic conduits, such as faults and abandoned wells (Nordbotten et al., 2005; Stauffer et al., 2009; Oldenburg et al., 2010;

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