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Energy Procedia 1 (2009) 1871–1878
Energy Procedia
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GHGT-9

Large-scale numerical simulation of CO_2 geologic storage and its impact on regional groundwater flow: A hypothetical case study at Tokyo Bay, Japan

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Abstract

With the help of massively parallelized computing techniques, a comprehensive, large-scale numerical simulation of CO_2 geologic storage that predicts not only CO_2 migration but also its impact on regional groundwater flow was performed. As a case study, a hypothetical industrial-scale injection of CO_2 at the Tokyo Bay, surrounded by the most industrialized area in Japan, was considered. In the simulation, CO_2 is injected into a storage aquifer at about 1km depths under the Tokyo Bay from 10 wells with a total rate of 10 million tons/year for 100 years. A regional hydrogeological model with an area of about 60km × 70km around the Tokyo Bay was discretized into approximately 10 million gridblocks. To solve the high-resolution model efficiently, we used a parallelized multiphase flow simulator TOUGH2-MP/ECO2N on a highest performance supercomputer in Japan, the Earth Simulator (5120 CPUs). The results suggest that even if containment of CO_2 plume is ensured, pressure buildup in the order of tens of meters can occur in shallow confined layers of extensive regions including urban inlands.

Keywords: CO_2 storage; parallel computation, large-scale simulation; groundwater pressure; Tokyo Bay; Kanto Plain; Earth Simulator

1. Introduction

When a volume of CO_2 is injected into a virgin aquifer, it may eventually pushes the equivalent volume of water out of the aquifer. In industrial-scale projects of CO_2geologic storage, it is expected that the amount of CO_2 fluid injected into an aquifer can be several million tons per year for each storage site. Continuous long-term injections for more than several decades will buildup groundwater pressures in extensive regions. Recently, it has been suggested that large-scale CO_2 injections may have a hydrological and geochemical impact on even shallow

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doi:10.1016/j.egypro.2009.01.244

groundwater resources [1][2][3]. Birkholzer et al [2] conducted a sensitivity study on pressure response in radially symmetrical stratified systems. Nicot [3] investigated the impact of a hypothetical large-scale injection on regional groundwater at the Texas Gulf Coast Basin using a conventional groundwater flow modeling.

In this study, with the help of massively parallelized computing techniques, a comprehensive, large-scale numerical simulation of CO_2 geologic storage that predicts not only CO_2 migration but also its impact on regional groundwater system was performed. As a case study, a hypothetical, industrial-scale CO_2 injection at the Tokyo Bay, the most industrialized area in Japan, was considered. A regional hydrogeological model of about 60km x 70km area around the bay in the Kanto Plain was constructed, using the data from a few dozen deep boreholes and several seismic reflection surveys. The model includes the entire hydrogeological system in the area (i.e, the surface topography, a freshwater aquifer for drinking water, a sealing layer, and the CO_2 storage aquifer). The model domain was discretized into about 10 million gridblocks. To solve the high-resolution model efficiently, we used the parallelized multiphase flow simulator TOUGH2-MP [4][5] with ECO2N [6] fluid properties module of sub/supercritical CO_2 on a highest performance supercomputer in Japan, the Earth Simulator (5120 CPUs).

2. Massively Parallel Computation

TOUGH2-MP/ECO2N [4] is an efficient parallel simulator for large-scale, long-term CO_2 geologic storage in saline aquifers. The simulator is a three-dimensional, fully implicit model that solves large, sparse linear systems arising from discretization of the partial differential equations for mass and energy balance in porous and fractured media. The simulator is based on the ECO2N [6] module of the TOUGH2 code and inherits all the process capabilities of the single-CPU TOUGH2 code, including a comprehensive description of the thermodynamics and thermophysical properties of H_2O-NaCl-CO_2 mixtures. It is capable of modeling single and/or two-phase isothermal or non-isothermal flow processes, two-phase mixtures, fluid phases appearing or disappearing, as well as salt precipitation or dissolution. TOUGH2-MP uses MPI for parallel implementation, the METIS software package for simulation domain partitioning, and the iterative parallel linear solver package Aztec for solving linear equations by multiple processors.

The Earth Simulator (ES) is a high-speed supercomputer that was originally developed for, and greatly contributed to global climate change simulations. The ES had been the fastest supercomputer in the world from 2002 to 2004. It consists of 640 nodes with eight vector processors and 16 GB of computer memory at each node, for a total of 5120 processors and 10 TB of main memory. The total peak performance is currently 40Tflop/s and is scheduled to increase to 131 Tflop/s by March 2009. In this study, TOUGH2-MP was implemented and successfully run on the Earth Simulator. The code was specially tuned up to increase its vector operation ratio (VOR) for an efficient use of the vector processors of the ES. The CPU time for the two-phase flow simulations with about 10 million gridblocks in this study was generally 1 to 2 days.

3. Model Setup

3.1. Tokyo Bay and Kanto Plain

The Kanto Plain (Figure1a) is the largest coastal plain in Japan, surrounded by the Tokyo Bay, the Kanto Mountains, the Miura Peninsula, and the Boso Peninsula. The Tokyo Bay area is the most populated and industrialized area in Japan, where large stationary CO_2 emission sources, including coal-fired power, steel and cement plants, are located. Annual emission of CO_2 from those large emission sources around the Tokyo Bay is about 100 $MtCO_2$/year [7]. Since the 1950's, extensive explorative investigations and production of natural gas (mostly methane gas, dissolved in deep groundwater) have been carried out in the Boso Peninsula. The geologic structure in this area is well understood through a few dozens of deep borehole investigations and geophysical surveys for land subsidence and earthquakes [8][9]. In recent years, a number of hot spring wells for spa resorts have been drilled to the depths over 1km. A review work on deep groundwater and water quality in the area is found in Marui [10]. Due to these activities, a relatively abundant geologic information has been obtained in this area.

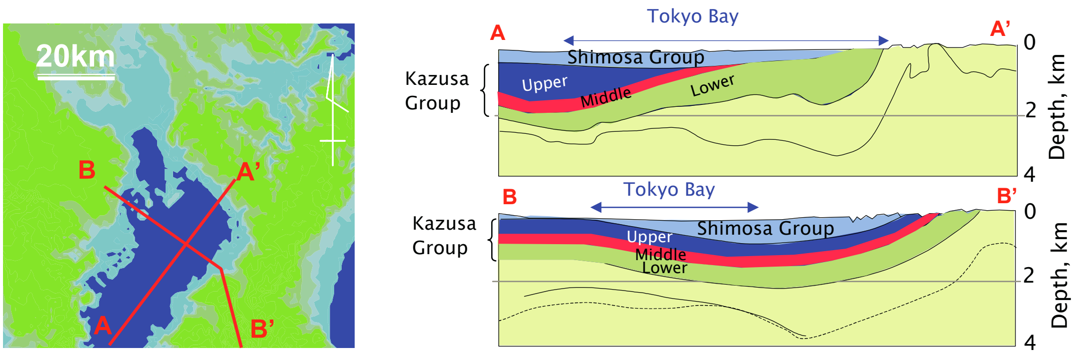
The plain is underlain by the Plio-Pleistocene Kanto sedimentary basin, composed of unconsolidated formations of silt, sand and gravel extending to a depth of more than 3,000 m. Figure 1b shows the conceptual geologic cross section across to a depth of around 4,000 m below the sea level. Primary geological formations at the site consist of the pre-Tertiary basement, the Tertiary Miura Group, the Plio-Pleistocene Kazusa Group, and the Pleistocene Shimosa Group. RITE [7] discussed the possibility of CO_2 geologic storage in the middle or lower part of the Kazusa Group at depths greater than 800m, supposing sealing capabilities of the overlying upper Kazusa Group and Shimosa Group. In Figure 1b, if we consider the CO_2 injections in the middle/lower Kazusa Group at the bottom of the basin under the Tokyo Bay, it could result in deep saline groundwater in the Kazusa Group being pushed up-dip into shallow aquifers, the buildup of groundwater pressures, and the change of water salinity of fresh water wells.

It should be emphasized that there is no plan of CO_2 geologic storage at the Tokyo Bay at present. We selected the Tokyo Bay area for a case study, because (1) the geologic data is relatively abundant for Japan excluding gas/oil fields, and (2) the basin structure under the Kanto plain is suited for demonstrating the impact of down-dip CO_2 injection on near-surface (up-dip) aquifer.

3.2. Conceptual model

We constructed a three-dimensional geological structure model for the 60km×70km area centered on the Tokyo Bay shown in Figure 1a. The surface topography are represented by 50m-grid DEM (digital elevation model) data published by the Geographical Survey of Japan, and the formation boundaries are defined by 200m-grid DEM data by Sasaki et al. [7]. For example, Figure 3 shows the contour map of the bottom elevation of the Kazusa Group, obtained by interpolating formation boundaries identified by borehole loggings and seismic reflection surveys. The locations of boreholes and seismic survey lines used for the interpolation are also shown in the figure.

The geological structure model is discretized into IFDM (integral finite difference method) gridblocks for



(a) Topographic map (b) Geologic cross section

Figure 1 Topographic map and geologic cross section around the Tokyo Bay (RITE [7])

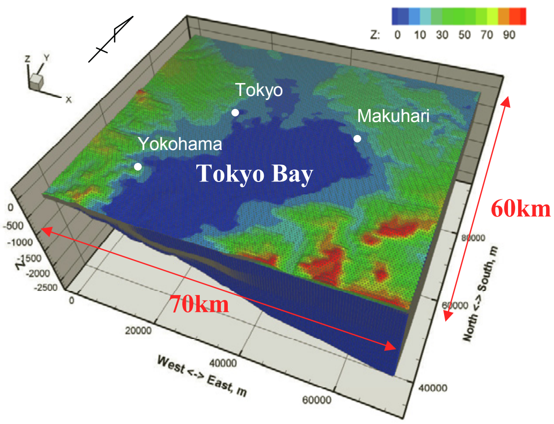


Figure 2 Modeled region

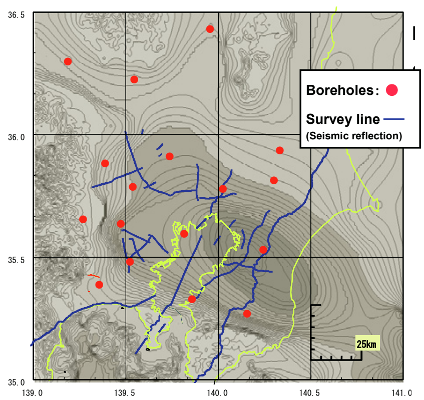


Figure 3 Bottom elevations of the Kazusa Group [9]

TOUGH2 simulations (Figures 2 and 8), using grid generation software VORLAY3D developed by Taisei Corporation. The 3D shapes of formation boundaries are represented explicitly as the interfaces between gridblocks. The horizontal surface is discretized by Voronoi polygons of about 250m resolution. The Voronoi discretization allows changing spatial resolution at desired regions, such as in the vicinity of injection boreholes as shown in Figure 8. The discretization results in approximately 121,100 gridblocks in each horizontal layer and 84 layers in the vertical direction with a total of about 10 million gridblocks and 40 million connections between these gridblocks.

A stratigraphic diagram of the Kazusa Group is shown in Table 1. The Kazusa Group is generally characterized by submarine sediment with thin-bedded sand-mud sequences. Thus, in the table, for example, 'muddy' represents a mud-dominated lithofacies, and is neither massive sand nor mud. In addition, the lithofacies in the Kazusa Group changes rapidly in lateral directions. At present, the regional distribution of lithofacies has not been modeled. We assume simplified lithofacies of sand and mud for the Kazusa Group, as shown in Table 1. In addition, perfect lateral continuities of all the layers are assumed as illustrated in Figure 4.

In the RITE report [7], the storage formation into which CO_2 is injected was selected in the middle part of the Kazusa Group located at depths of about 800m to 1000m below the ground surface. The selected storage formation, the Umegase (sandy) and Higashi-Higasa Formation (gravelly), is bounded at the top by a sealing layer, the Kokumoto Formation, followed by overlying sandy layers of the upper and middle part of the Kazusa Group, and the Shimosa Group. An additional sealing layer was assumed at the bottom of the Shimosa Group, based on some observations of pressure and salinity distributions that suggest the hydraulic communication between the Kazusa and Shimosa groups is weak (e.g., Nirei [11]).

Carbon dioxide is injected through 10 boreholes in the bay, with an annual rate of 1 $MtCO_2$/year/well over 100 years, resulting in a total annual rate of 10 $MtCO_2$/year. The simulation runs cover a time period of 1000 years including the post-injection period of 900 years. Prior to injection of CO_2, regional groundwater flow simulation is carried out until steady state has reached. In spite of the isothermal simulation, temperature is needed to calculate the fluid properties such as density and viscosity. Temperature varies linearly with depth, assuming a geothermal gradient of 2°C per 100m depth and the temperature of 15°C at the surface. The salinity is assumed to be very low and no density-driven flow occurs. Geomechanical effects such as land-surface uplift are not explicitly considered.

The surface and side boundaries are hydraulically open, while the bottom is closed. The large lateral extent of the 60km × 70km model was chosen to ensure that the boundary condition have minimal effects on the simulation results. At the lateral boundary, the initial hydrostatic pressure is specified and the boundary is open for fluids to escape from the model domain. The surface boundary is also open, so that the pressure is fixed at the atmospheric pressure. The bottom of the model is closed (no-flow) representing very low permeability of the Tertiary and pre-Tertiary basement rocks.

Table 1 Lithofacies of the Kazusa Group

(a) Lithofacies (modified from Sasaki et al.[9])

Age			Ma	Group/Formation				Lithofacies West/East	
Quarternay	Horocene			fluvial/river terrace sediments				–	
Quarternay	Pleistocene	Late		Shimosa Group				–	
Quarternay	Pleistocene	Middle		Kazusa Group	Upper	Kongochi		sandy	
Quarternay	Pleistocene	Middle		Kazusa Group	Upper	Upper Kasamori		muddy	sandy
Quarternay	Pleistocene	Middle	0.6	Kazusa Group	Upper	Lower Kasamori		gravelly	
Quarternay	Pleistocene	Middle		Kazusa Group	Upper	Chonan		sandy	
Quarternay	Pleistocene	Middle		Kazusa Group	Upper	Ichijyuku		gravelly	sandy
Quarternay	Pleistocene	Early	0.8	Kazusa Group	Upper	Kokumoto		muddy	
Quarternay	Pleistocene	Early		Kazusa Group	Upper	Umegase		sandy	
Quarternay	Pleistocene	Early	1.0	Kazusa Group	Upper	Higashi Higasa		gravelly	
Quarternay	Pleistocene	Early	1.2	Kazusa Group	Lower	Otadai		muddy	
Quarternay	Pleistocene	Early	1.7	Kazusa Group	Lower	Kiwada		muddy	
Neocene	Pleiocene			Kazusa Group	Lower	Tomiya	Tomiya	muddy	
Neocene	Pleiocene			Kazusa Group	Lower	Tomiya	Ohara	muddy	
Neocene	Pleiocene			Kazusa Group	Lower	Tomiya	Namihana	muddy	
Neocene	Pleiocene			Kazusa Group	Lower	Tomiya	Katsuura	muddy	
Neocene	Pleiocene			Kazusa Group	Lower	Kurotaki		gravelly	
Neocene	Miocene			Awa Group				–	–

(b) Simplified model

fluvial/river terrace	Sandy
Shimosa	Sandy
Shimosa	Muddy
Upper Kazusa	Sandy
Middle Kazusa	Sandy
Middle Kazusa	Muddy
Middle Kazusa	Sandy
Lower Kazusa	Muddy
Lower Kazusa	Sandy
Lower Kazusa	–

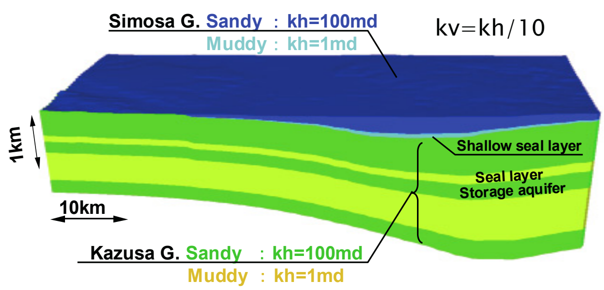


Figure 4 Hydrogeological model (base case)

Table 2 Base and sensitivity cases (changes from the base-case are highlighted)

Case name \ Parameters		Case	Pore Compressibility (Pa^{-1})	Permeability (md)				Porosity (%)	Side Boundary (Open/Close)
				Shimosa Group		Kazusa Group			
				Sandy	Muddy	Sandy	Muddy		
Base case		1	1×10^{-9}	100	1	100	1	40	Open
Pore compressibility		2a	1×10^{-8}	100	1	100	1	40	Open
		2b	1×10^{-10}	100	1	100	1	40	Open
Seal permeability	Shimosa	3a	1×10^{-9}	100	10	100	1	40	Open
		3b	1×10^{-9}	100	0.1	100	1	40	Open
	Kazusa	4a	1×10^{-9}	100	1	100	10	40	Open
		4b	1×10^{-9}	100	1	100	0.1	40	Open
Porosity		5	1×10^{-9}	100	1	100	1	20	Open
Boundary condition (BC)		6	1×10^{-9}	100	1	100	1	40	Close

3.3. Model parameters and sensitivity cases

The hydrogeologic parameters chosen for this case study are given in Table 2. For simplification, in most simulation cases, all sandy and muddy layers have been assigned the same set of sand and mud properties without variation in depth. Vertical/horizontal ratio of permeability is assumed to be 1/10 in all the layers. Horizontal permeability is 100md for sandy, and 1md for muddy in the base case. Porosity is set to 40%, based on well logs and laboratory core test data. The rock compressibility is set to 1×10^{-9} Pa^{-1} based on elastic moduli generally obtained from in-situ mechanical tests in this area. Van Genuchten model is used to calculate the capillary pressure and relative permeability of the two-phase flow of CO_2 and water. The model parameters are basically employed from Pruess [6], except for the residual water saturation for mud, which was increased from 20% to 40%. Sensitivity cases are also summarized in Table 2. The first sensitivity case (case 2) increases/reduces pore compressibility of the base-case by one order of magnitude. In the two following sensitivity cases (case 3 and 4), we change the permeabilities of the muddy seal layer in the Shimosa and Kazusa Group, respectively. In addition, the sensitivities to the porosity and the boundary condition are also explored in case 5 and 6.

4. Result and Discussion

4.1. Behavior of CO_2 plumes

Figure 5 shows the simulated distribution of CO_2 plumes from 10 injection points under the bay at 100 years after the start of the injection for the base-case. The evolution of CO_2 gas saturation for a plume on a cross-section is shown in Figure 6. After the stop of the injection at 100 years, the plume slightly enters into the seal layer and moves to shallower part by buoyancy, but basically continues to be contained under the sealing layer. As shown in Figure 7, the initially injected CO_2 is mostly stored as supercritical fluid, however, after the termination of the injection, the contribution of dissolution in groundwater gradually increases and eventually becomes dominant.

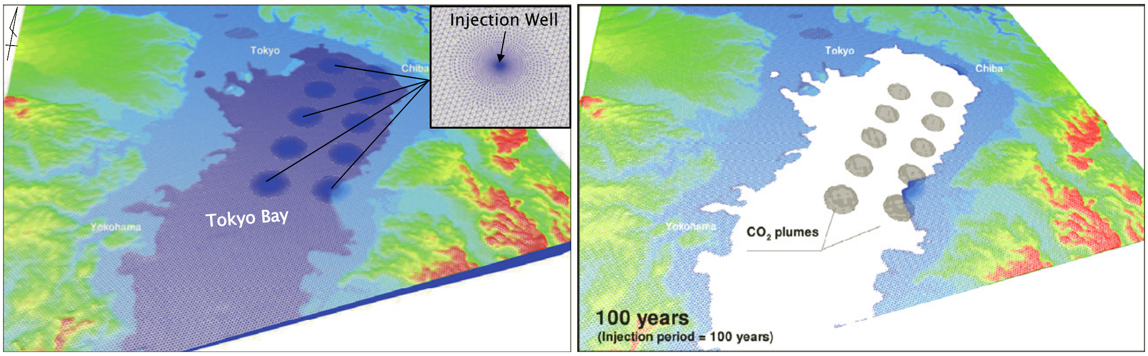
4.2. Impact on regional groundwater flow

4.2.1. Pressure buildup

Pressure buildup at the injection points was about 20 bars. Figure 8 shows spatial distribution of calculated hydraulic heads for the base case (a) at the initial time and (b) at 100years on a cross-section, showing that the pressure buildup can occur over a wide area of the region. Time evolutions of pressure buildup at some points around the Tokyo Bay are shown in Figure 9a. Note that these points are urban inlands that are few tens of km away from the injection points. Pressure recovery takes almost the same length of time as the buildup. Significant buildup of more than 1 bar is seen at 300m depths of the point C and G, while it is negligibly small at the point A. Figure 9b shows vertical-pressure profiles for the point A and G at the time of 100years. From this figure, it is clear that buildup at the point G is due to the shallow seal layer, assumed at the bottom of Shimosa Group. This result suggests that significant pressure buildup can occur in a confined aquifer even at a shallow depth. For the sensitivity cases, the comparison of pressure build-up at 300m depths of point G is shown in Figure 10. As easily expected, the larger the pore compressibility is, the slower the pressure buildup, and the longer the recovery time (Figure 10a). In the current model, the seal permeability is the most important factor for the pressure buildup as seen in Figure 10b. By lowering the permeability of the shallow seal layer in the Shimosa Group by one order of magnitude (case 3b), a pressure buildup of almost twice the base case was obtained, suggesting the importance of investigations on hydrogeological structure and flow parameters even in shallower depths. As shown in Figure 10c, porosity and boundary condition have minor effects on pressure perturbation in the current settings and the region size of the model.

4.2.2. Discharge/recharge area

Due to the large-scale injection, the equivalent volume of groundwater is pushed out and discharged on the land



(a) Grid refinement around the injection wells (b) Simulated CO_2 plumes (100 years since injection)
Figure 5 Numerical meshes (about 10 million gridblocks) and simulated CO_2 plumes (base-case)

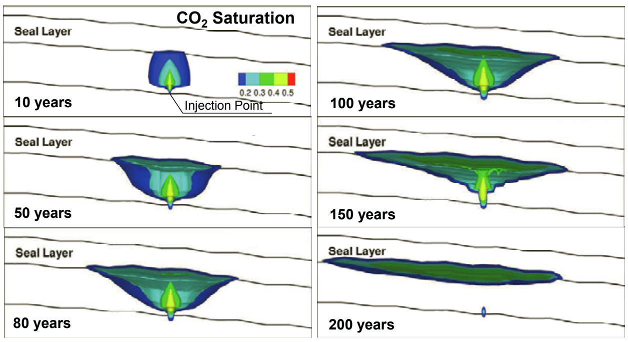


Figure 6 CO_2 plume during and post injection (base-case)

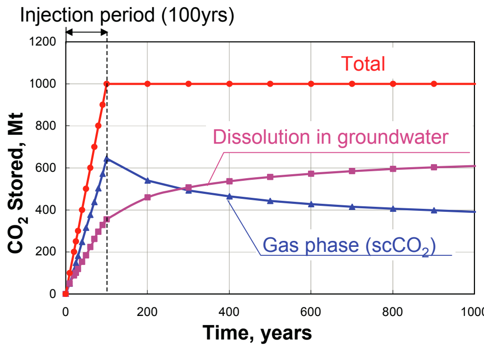
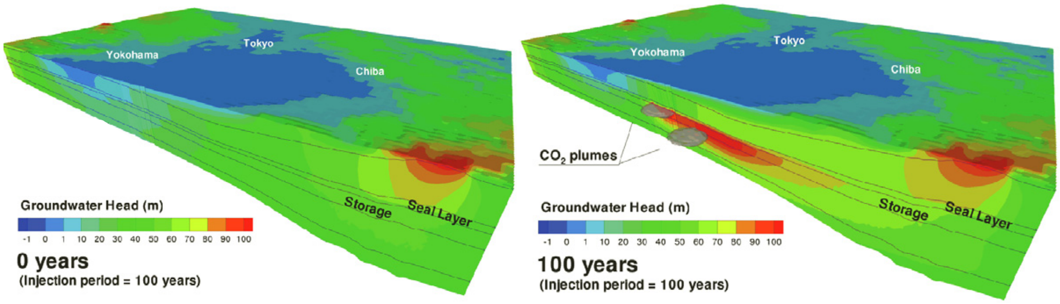
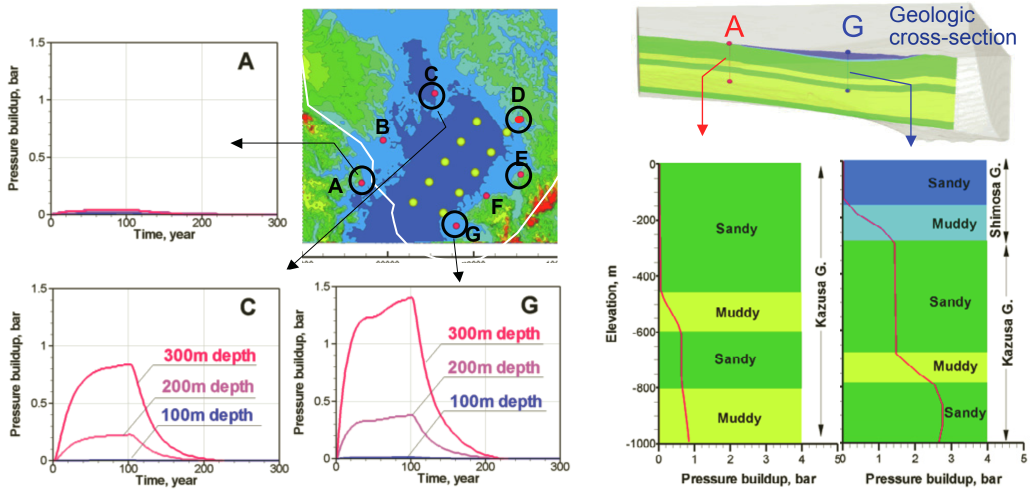


Figure 7 Stored CO_2 condition (base-case)

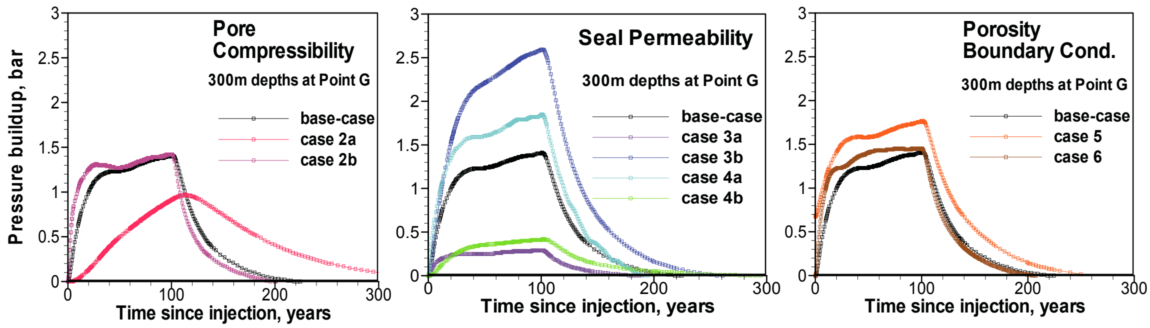


(a) Initial condition (b) After 100years injection
Figure 8 Regional groundwater head changes due to CO_2 injection (base-case)



(a) Change in time (b) Change in depth (after 100 years injection)

Figure 9 Changes of groundwater heads /pressures around the Tokyo Bay (base-case)



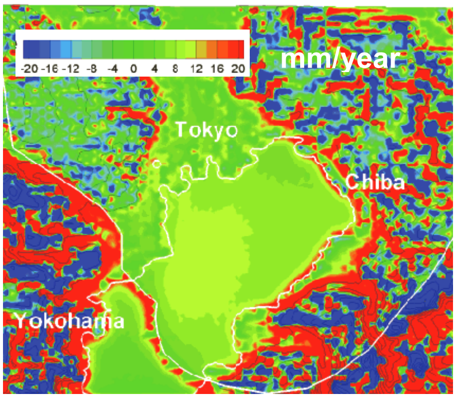
(a) Pore compressibility (b) Seal Permeability (c) Porosity and closed boundary

Figure 10 Comparison of pressure build-ups in the sensitivity cases (at 300m depths of point G)

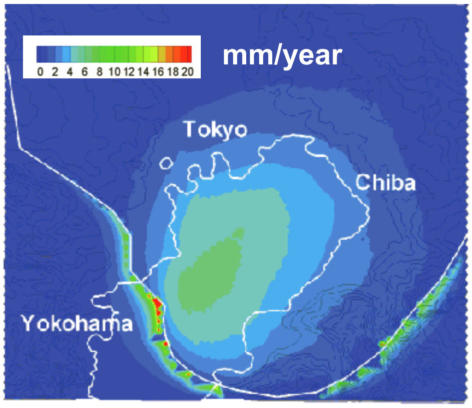
surface. Figure 11 shows the distribution of discharge and recharge rate on the surface. The change in discharge/recharge rate from the initial condition is shown in Figure 11b. The discharge is increased mainly in seabed, so that the impact on the land surface area should be small. Significant increase is also found along the boundary of the Shimosa and Kazusa Group, indicated in the figure by the white line. The increase of the discharge is in the order of few tens of mm/year as a local maximum, which is about 1% of annual precipitation of the Kanto area (about 1400mm/year) and is smaller than the annual variation levels. Dividing the discharge rate by porosity gives a rough estimate of transport velocity of groundwater in vertical direction near the surface. For example, with the discharge rate of 20 mm/year and 40% porosity, we obtain 0.05m/year, which is slower than that estimated in the natural groundwater at Alberta Basin (i.e., 0.1 to 1m /year; Bachu et al. [12]).

5. Concluding Remarks

The massively parallel computing technique makes it possible to perform comprehensive simulations that predict not only CO_2 migration but also its impact on regional groundwater system. It was successfully demonstrated that the Earth Simulator efficiently solves the two-phase flow model of about ten million gridblocks. The simulation runs for 1000 years period were finished within 1-2 days/run. The high-resolution model is useful to depict three-dimensional region of influence during/after injection of CO_2 and the possible implications for shallow groundwater resources. In terms of the impact of CO_2 geologic storage on groundwater flow that was hypothetically simulated at the Tokyo Bay, the following conclusions were obtained. (1) Build-up of groundwater pressure in shallow confined



(a) Discharge / recharge rate



(b) Increase in discharge rate to the surface

Figure 11 Increase in surface discharge of groundwater (100 years since injection, base-case)

layers can occur in extensive regions including urban inlands. (2) Groundwater discharge to the land surface and seabed can increase in the order of few tens of mm/year. In addition to the improvement of the hydrogeological model, the effect of faults and abandoned and existing wells will be addressed in the future.

Acknowledgement

We greatly appreciate Satoshi Imamura, Tomoyuki Aoki, Toyokazu Ogawa at Taisei Corporation, and Karsten Pruess at Lawrence Berkeley National Laboratory for encouragement and helpful discussions. Our sincere thanks also to Shinichi Nanai at Taisei Corporation, Satoru Shingu and Yuichi Hirokawa at Japan Agency for Marine-Earth Science and Technology (JAMSTEC), and Takaaki Noguchi at NEC system technologies Ltd. for their extensive helps and support for the use of the Earth Simulator. The authors wish to thank to Katsuji Sasaki and Akira Hyuuga at Suncoh Consultant Inc for providing us the digital data of geological structure model of the southern Kanto Plain. The use of the Earth Simulator was supported by "Open Advanced Facilities Initiative for Innovation (Strategic Use by Industry)" funded by Ministry of Education, Culture, Sports, Science and Technology (MEXT) of Japan.

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