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## Systems analysis of field and laboratory experiments considering impacts of CO<sub>2</sub> leakage in terrestrial systems

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### Abstract

Geological CO<sub>2</sub> storage will be designed to prevent any CO<sub>2</sub> leakage. However, as recognized by the European Commission's (EC) CO<sub>2</sub> Storage Directive, a capability is needed to assess leakage impacts, even though leaks are unlikely. The RISCS project, which is funded by the EC and industry, is developing approaches to assess possible CO<sub>2</sub> leakage impacts on near surface ecosystems. During the project the impacts of CO<sub>2</sub> on terrestrial ecosystems were investigated using field experiments and systems models. A comparison between results from the experiments and models builds confidence that the main CO<sub>2</sub> impacts on these systems can be adequately modelled.

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### 1. Introduction

Facilities for the geological storage of CO<sub>2</sub> as part of carbon capture and storage (CCS) schemes will be designed to prevent any leakage to the surface. However, it is important to be able to assess the consequences of any leakage in the unlikely event that it should occur. The need for such assessments is recognised by regulations, such as the EC Directive on storage and the OSPAR Framework, and other guidance such as the USEPA Vulnerability Evaluation Framework and the CO<sub>2</sub>QUALSTORE Guideline.

For this reason, the on-going RISCS (Research into Impacts and Safety in CO<sub>2</sub> Storage) project, which is funded by the European Commission and industry under Framework Programme 7, is acquiring knowledge necessary for both storage site operators and regulators to assess the potential impacts on near surface ecosystems - both in terrestrial and marine environments. This paper concerns the potential impacts that might arise in a terrestrial environment should CO<sub>2</sub> leak there.

In order that potential impacts may be predicted a near-surface systems model of CO<sub>2</sub> migration and interaction with plants has been implemented using the general-purpose modelling tool QPAC (Quintessa [1]) having been significantly developed from earlier versions used to represent the Latera natural analogue (Maul et al [2]). To build confidence in the applicability of the modelling approach, experiments at two sites were simulated and experimental and simulation outputs were compared. The field experiments are: (1) the ASGAR experiments conducted by Nottingham University (with the British Geological Survey, Bundesanstalt für Geowissenschaften und Rohstoffe and Università di Roma “La Sapienza”) in central England (Smith et al [3]) ; and (2) experiments conducted by Bioforsk at Grimsrud Farm in southern Norway (Moni et al [4]).

## 2. The near-surface systems model

Systems models aim to represent all the important processes throughout the system that is being studied, but possibly in a more simplified way than in detailed models for particular processes or parts of the system. In this paper consideration is limited to terrestrial environments, with near-surface processes relevant to such environments being represented.

The current terrestrial systems model consists of two main components (see Figure 1):

- Multi-phase flow model (MPF - air, CO<sub>2</sub> and water) of a porous medium representing the sub-surface component of the system.
- Soil-plant model (SPM), representing the roots, stem and foliage of the plants together with the air and CO<sub>2</sub> in the canopy and the wider atmosphere and their interaction through metabolic processes.

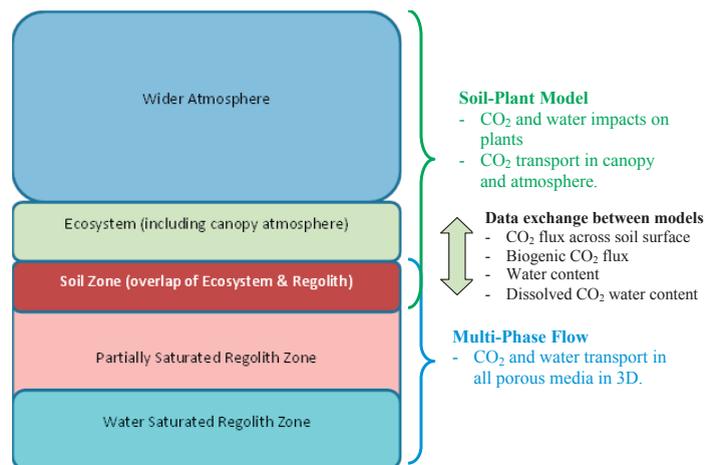


Figure 1 Schematic illustration of the systems model for terrestrial ecosystems (from Walke and Bond [6]).

The MPF model and SPM are fully coupled with the CO<sub>2</sub> in the sub-surface being metabolised by the plants as well as diffusing or advecting through the rock, soil, canopy and atmosphere. This allows all the CO<sub>2</sub> in the system to be ‘tracked’ and hence the consequence of the presence or absence of CO<sub>2</sub> in different parts of the system to be represented. The system can also be coupled with respect to water (e.g.

interception of rainfall by plants, uptake of water via plant roots), but this was not considered necessary or justifiable given the availability of data for the experiments to be considered.

The model can be spatially discretised in 1D, 2D or 3D using heterogeneous Cartesian or cylindrical type geometries, and all inputs can be time dependent or coupled to other system properties (e.g. CO<sub>2</sub> input from a source can be a function of time, space or any other feature) allowing the model to be used to represent spatially heterogeneous 1D, 2D or 3D physical geometries and complex couplings.

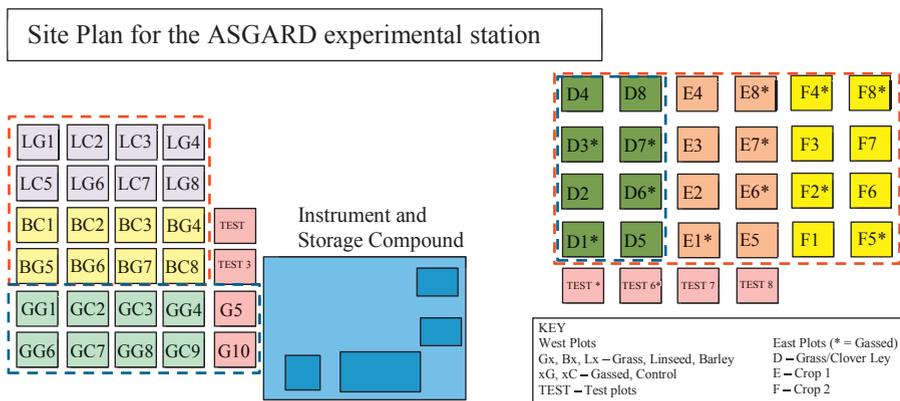
Key outputs from the model include: (1) saturations of air, CO<sub>2</sub> and water in the pore space; (2) fluid pressures; (3) fluxes of all fluids internally and across model boundaries; (4) dissolved quantities of CO<sub>2</sub> and air in the pore water; (5) biomass of the different plant species in the soil-plant model; (6) plant species height; and (7) canopy CO<sub>2</sub> concentrations.

### 3. Application of the systems model to the ASGARD experiments

The systems model was applied to represent the ASGARD experiments in which CO<sub>2</sub> has been injected below the ground surface and the subsequent transport and impacts of the CO<sub>2</sub> have been monitored. The aims were to: (i) demonstrate that the systems model is able to provide an appropriate representation of the ASGARD experiments; (ii) build understanding of CO<sub>2</sub> behaviour and impacts through interpreting the ASGARD results; and (iii) potentially improve the parameterisation/representation of processes within the systems model through iterative comparisons of model and experimental results.

#### 3.1. The ASGARD experiments

The area is characterised by up to 1.5 m of head deposit overlying mudstones. The head is very variable, but generally comprises a lower clay-dominated facies overlain in places by a sandy facies. A thin and highly variable mixed facies up to 60 cm thick (topsoil ‘A’ horizon and subsoil ‘B’ horizon) overlies these units across the entire site. Lithological variation also increases with depth. The site is divided into square plots, each 2.5 m by 2.5 m (Figure 2 and Figure 3). To mitigate the possible effects of lithological variation on gas migration, gas was injected at depths of 60 cm.



Note: Plots for Barely1-8, Linseed 1-8 and Grass 7-8 were used in 2010 (Year 1). Plots D, E and F were used in 2011 (Year 2) and 2012 (Year 3). The plots studied by University of Nottingham are within the red broken rectangles. The plots studied by BGS, BGR and University of Rome are within the blue broken rectangles.

Figure 2. Illustration of the ASGARD Plot Layout (modified from Smith et al. [3]).

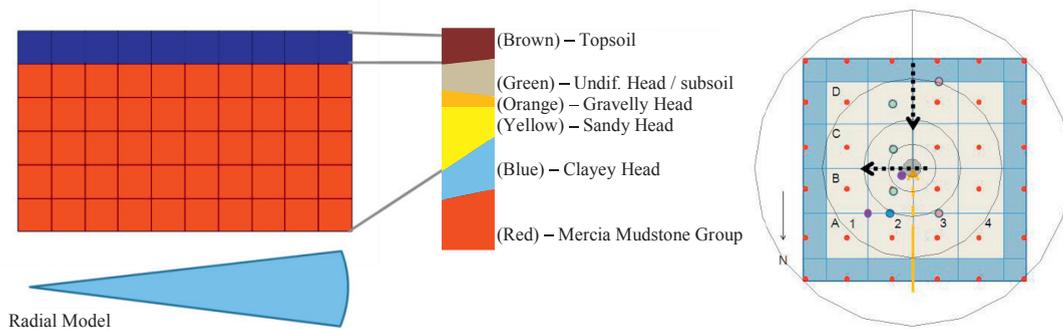


Figure 3 (left) Schematic illustration of the vertical extent of the ASgard plot models. Note that in the version of the model used here, the soil/rooting zone may be multiple compartments deep and the compartment sizes are radially uniform on a log-scale. (right) Plan view of radial grid (up to the edge of the rooting zone) overlaid on diagram of experimental sampling quadrants

### 3.2. Modelling the ASgard experiments

The modelling reported here focussed on plots B\*1-8, L\*1-8 and G7-G8, and data obtained from them during 2010 for oilseed rape, barley and grass, respectively. Both control plots (ungassed) and CO<sub>2</sub>-gassed plots were examined. The modelling aimed to represent the measured distribution of CO<sub>2</sub> from injection (fluxes and concentrations in the soil), and replicate the observed plant impacts for the four species being examined, primarily in terms of biomass and plant height. The experimental data shows the distribution of CO<sub>2</sub> from an injection source in the centre of a plot with only modest interaction between plots, and hence the consequent impacts to plants are also dominantly radial. The systems model was therefore configured to be 2D cylindrical in geometry, centred on the middle of a single plot. A radial extent of 100 m was selected with a logarithmic increase in discretisation size from the inner radius to the outer radius; the outer boundary condition is no-flow to water, air and CO<sub>2</sub>. The radial distance of 100 m was selected because initial scoping calculations showed little boundary interaction at this distance.

Vertically, the grid was divided into soil compartments and the remaining ‘bulked-up’ geology down to the saturated clay which forms the base of the model (Figure 3). A lack of hydrogeological information prevented a more complex definition of the hydraulic system, but such a simplification is consistent with the available data and the overall objectives of the modelling work. In the barley and oilseed rape models, the water table (normally greater than 0.6 m below the surface) lies within the rooting zone. The base of the model was set at 2 m below ground surface, approximately coincident with the depth of indurated clay at the site. The water pressure at the surface was defined using a hydrostatic pressure which would place atmospheric pressure (~0.1 MPa) at the elevation of the water table, assumed to be 0.6 m below ground surface. The reference grid used has 15 radial compartments by 8 compartments in the vertical direction. The radial compartments extend radially for 1.768 m so that they cover the entirety of the square 2.5 m by 2.5 m plot dimensions (Figure 4, right).

Models were run for ten years with the initial four full years allowing the system to reach dynamic equilibrium. Injection of CO<sub>2</sub> occurred in year 5 only, and the system was allowed to return to equilibrium in the following years. Runs were conducted on all three plot types to investigate parameter sensitivity and uncertainty (e.g. Figure 4).

When the MPF model and SPM were parameterized based on the experiment, reasonable agreement was obtained with experiments taking into consideration the degree of uncertainty in some model input

parameters, particularly those related to parameterisation of the soil properties, and of the degree of variability and uncertainty in the experimental data and environmental conditions.

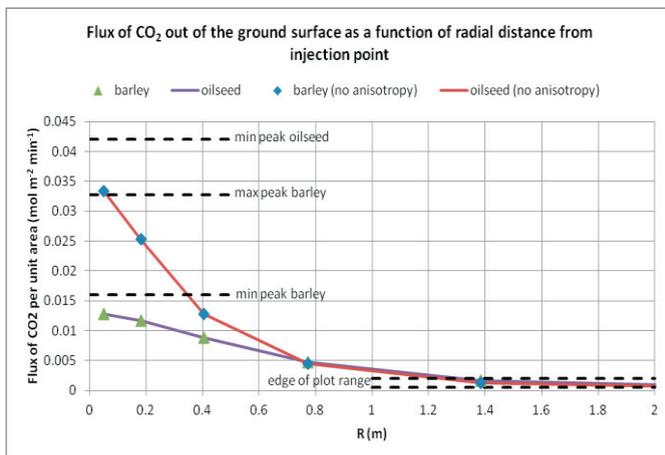


Figure 4 Flux of CO<sub>2</sub> per unit area from the ground surface after harvest as a function of radial distance from injection point. The dashed lines show peak experimental values measured at the plot’s centre. Dotted lines show experimental results where the precise measurement location is uncertain.

The concentrations and fluxes of CO<sub>2</sub> were of the right order of magnitude for both control and injection comparisons (e.g. Figure 5), and for any given crop the general temporal and radial trends were consistent with the experimental data (with peak CO<sub>2</sub> concentrations and plant die-back at the centre of the plot and a much weaker effect of CO<sub>2</sub> injection towards the edge – Figure 5). Given the lack of hydraulic data and the required simplifying assumptions, the agreement between the systems model and the experimental results are sufficiently good to provide confidence that the model is fit for its purpose of helping to understand the sensitivities of potential impacts to variable CO<sub>2</sub> fluxes.

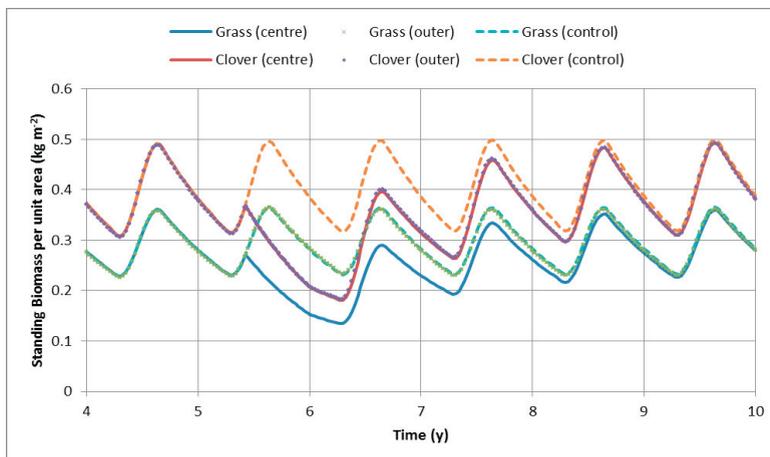


Figure 5 Calculated standing biomass per unit area against time showing values at the centre of the plot (directly above injection), at the edge of the plot, and for the control model, for grass and clover.

### 4. Application of the systems model to the Grimsrud experiments

#### 4.1. The Grimsrud experiments

The Grimsrud CO<sub>2</sub> experiment was designed to achieve a CO<sub>2</sub> gradient across the site (Figure 6), in contrast to the experiment at ASGARD which aims to represent approximately radial CO<sub>2</sub> leakage from the centre of the plot. In August 2010, four plots with horizontal dimensions of 6 x 3 m were excavated to a depth of 85 cm. “T” shaped injection pipes were installed in each plot and the excavation was refilled with 45 cm of sand and then 40 cm of local clayey topsoil on top. The plots were ploughed and sown with the rest of the field in May 2011, but due to water logging, the crops in plots 2 and 3 didn’t develop as in the undisturbed field. All plots were re-ploughed and re-sown in June 2011, but replanting did not improve crop cover.

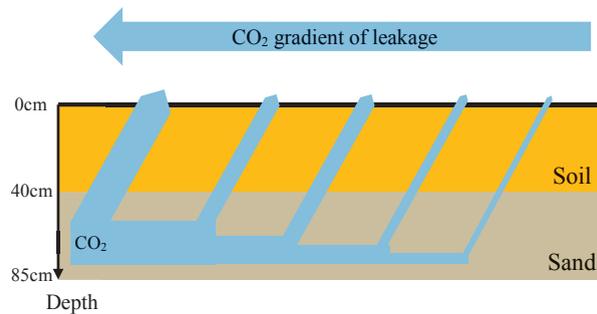


Figure 6. Depth cross section of the experimental setup at Grimsrud Farm.

Food-grade CO<sub>2</sub> was supplied continuously over the experimental period. The CO<sub>2</sub> had δ<sup>13</sup>C of -46 ‰, which distinguishes it from natural CO<sub>2</sub> found in the soil and plants. Soil gas was collected weekly using silicone tubes buried at 20 cm depth (Figure 7) and analysed for CO<sub>2</sub> concentration and δ<sup>13</sup>C ratio.

CO2 content (%)		Distance from gased side (cm)					Distance from gased side (cm)					Distance from gased side (cm)					Distance from gased side (cm)								
Date	DAI	50	150	250	350	450	550	50	150	250	350	450	550	50	150	250	350	450	550	50	150	250	350	450	550
05/07/11	12	2	2	2	2			3	1	1	3	1	1	85	22	4	2	4	3	1	1	1	1	1	1
11/07/11	18	3	1	2	1	3	3	0	1	1	1	1	2	100	100	28	2	4	5	3	1	0	1	1	0
20/07/11	27	4	3	3	3	3	3	2	3	1	3	2	4	48	40	17	4	5	5	4	2	2	2	3	1
25/07/11	32	4	2	1	2	3	3	6	5	6	6	3	5	100	36	7	4	4	4	7	5	6	5	6	6
29/07/11	36	7	6	6	3	5	4	2	2	3	5	2	3	100	25	13	4	6	5	3	5	4	2	2	
03/08/11	41	21	17	12	5	4	3	2	1	1	4	2	2	56	8	9	3	4	4	1	2	2	2	1	1
11/08/11	49	79	37	27	14	14	9	4	3	3	4	2	3	71	43	14	2	3	3	5	7	3	4	4	3
16/08/11	54	100	66	42	17	33	25	11	9	11	15	8	12	100	72	15	6	8	6	13	9	10	9	8	8
23/08/11	61	56	44	30	18	24	18	2	2	2	4	2	3	65	53	7	5	6	5	11	9	6	11	8	3
30/08/11	68	95	41	29	19	21	4	8	6	7	8	4	7	100	96	9	5	6	5	15	13	13	13	10	9
22/09/11	91	10	2	4	2	3	4	11	11	10	13	4	6	88	34	9	4	3	2	17	15	12	19	16	14
29/09/11	98	32	17	21	4	11	7	5	3	12	10	8	4	31	32	83	25		12	18	9	8	17	11	5

Delta 13C(permil)		Distance from gased side (cm)					Distance from gased side (cm)					Distance from gased side (cm)					Distance from gased side (cm)								
Date	DAI	50	150	250	350	450	550	50	150	250	350	450	550	50	150	250	350	450	550	50	150	250	350	450	550
05/07/11	12	-25	-25	-26	-25			-35	-35	-23	-24	-23	-24	-48	-41	-26	-24	-25	-24	-23	-23	-24	-23	-23	-23
11/07/11	18	-26	-26	-25	-26	-25	-25	-25	-32	-24	-24	-24	-26	-48	-42	-29	-26	-30	-28	-28	-25	-22	-23	-23	-22
20/07/11	27	-27	-27	-27	-26	-26	-26	-31	-38	-25	-26	-25	-27	-49	-44	-36	-27	-27	-27	-49	-44	-25	-26	-27	-24
25/07/11	32	-28	-27	-25	-25	-27	-26	-32	-31	-28	-28	-28	-27	-50	-46	-34	-27	-28	-26	-29	-28	-28	-27	-28	-27
29/07/11	36	-33	-29	-27	-26	-27	-26	-29	-26	-26	-25	-24	-25	-49	-42	-36	-26	-27	-25	-24	-27	-25	-24	-24	-24
03/08/11	41	-46	-45	-40	-33	-26	-24	-32	-28	-25	-25	-24	-24	-49	-47	-36	-25	-24	-25	-21	-22	-22	-22	-20	-21
11/08/11	49	-49	-48	-46	-41	-40	-34	-31	-30	-28	-27	-27	-28	-50	-47	-41	-28	-27	-27	-28	-28	-27	-29	-28	-27
16/08/11	54	-51	-49	-49	-42	-42	-37	-31	-29	-29	-27	-27	-28	-50	-49	-38	-28	-26	-26	-28	-27	-27	-26	-26	-27
23/08/11	61	-52	-50	-50	-44	-43	-40	-28	-27	-27	-26	-27	-26	-52	-51	-47	-28	-26	-25	-27	-27	-25	-26	-27	-24
30/08/11	68	-50	-50	-50	-46	-40	-50	-32	-31	-29	-28	-27	-28	-50	-50	-41	-29	-29	-27	-28	-25	-26	-26	-26	-26
22/09/11	91	-44	-41	-41	-34	-34	-33	-32	-31	-29	-28	-27	-27	-48	-51	-50	-29	-27	-26	-25	-27	-26	-26	-23	-24
29/09/11	98	-47	-47	-46	-41	-37	-33	-29	-29	-29	-26	-28	-28	-52	-51	-48	-36		-26	-27	-26	-25	-25	-21	-24

Figure 7. CO<sub>2</sub> concentration and δ<sup>13</sup>C values for the four plots, at 20 cm depth, where Plots 1 was gassed from DAI (day after injection) 32 onwards, Plot 2 was gassed prior to DAI 32 and Plot 3 was gassed for the whole trial (from Moni et al, [4]).

#### 4.2. Modelling the Grimsrud experiments

The model incorporates MPF model and a SPM, and an additional capability to track δ<sup>13</sup>C from the injection source, in-situ air and biomass (δ<sup>13</sup>C of -46 ‰, -25.8 ‰ and -25.8 ‰ assumed respectively). A single plot at the Grimsrud site was modelled. All the side boundaries are no flow boundaries reflecting the low permeability of the soil surrounding the excavated plots compared to the soil fill within the plots. The top boundary has a water infiltration term and is coupled to the soil-plant model to get the concentration of CO<sub>2</sub> in the atmosphere. The bottom boundary was at hydrostatic pressure just above a water table (at -1 m depth) and results were obtained for two cases, one in which there is diffusion of CO<sub>2</sub> out of the bottom of the model, and one in which no CO<sub>2</sub> crosses the bottom boundary.

A 40 cm thick clayey soil overlies a 45 cm thick sand layer, with hydraulic properties taken from Bosson et al. [7] (Table 6 5). No data is available yet for hydraulic properties at Grimsrud Farm so values are used from a Swedish site where soils have developed on glacial material. Parameters for a generic arable crop (Maul et al., [2]) have been used to represent the oat crop at Grimsrud. The plants were sown in June and harvested in September and therefore a 100 day growing period was specified.

The CO<sub>2</sub> δ<sup>13</sup>C values predicted by the model over the period of CO<sub>2</sub> injection are shown in Figure 8 for the case in which CO<sub>2</sub> is lost from the bottom of the model, and in Figure 9 for the case with no loss at the bottom boundary. In both cases, the observable anomaly in CO<sub>2</sub> concentration caused by the injected CO<sub>2</sub> is of more limited extent than the δ<sup>13</sup>C tracer anomaly. This observation from the modelling supports the finding in the field trials that δ<sup>13</sup>C is a much more sensitive tracer than CO<sub>2</sub> concentration for injected CO<sub>2</sub>.

The difference in results from the two models with different bottom boundaries is marked. When CO<sub>2</sub> is lost at the base of the model, the injected CO<sub>2</sub> does not reach the end of the 6 m long plot and travels further laterally in the top soil layer than in the sand. This is similar to the behaviour observed in Plot 3 in which the δ<sup>13</sup>C values are low (~-46 ‰ in the model, -52 to -47 ‰ in the data) within 3 m of the injection site and then increased rapidly to background levels as the distance to the injection site increases. When there is no loss of CO<sub>2</sub> at the bottom of the model, the injected CO<sub>2</sub> extends across the whole plot as observed in Plot 1.

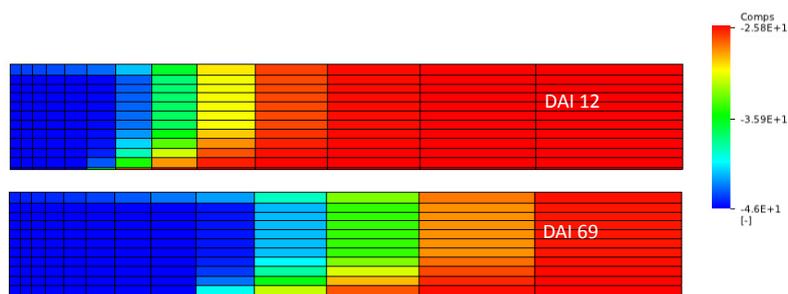


Figure 8. X-Z plane of δ<sup>13</sup>C of CO<sub>2</sub> in subsurface for case with CO<sub>2</sub> loss at the bottom boundary. Times are from the start of CO<sub>2</sub> injection and the model is 6 m long.

Since the extent to which CO<sub>2</sub> is leaking out of the bottom of the plot is unknown, it is unclear whether

the difference in the behaviour of Plots 1 and 3 is caused by different losses of CO<sub>2</sub> at the base, or even the side of the plot, but it is one plausible explanation.

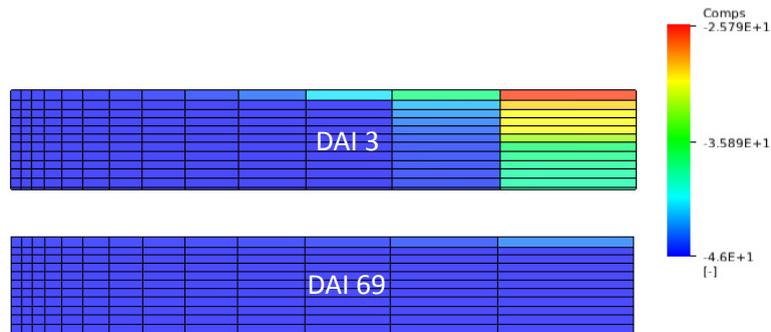


Figure 9. X-Z plane of  $\delta^{13}\text{C}$  of CO<sub>2</sub> in subsurface for case with no CO<sub>2</sub> diffusion at the bottom boundary. Times are from the start of CO<sub>2</sub> injection and the model is 6 m long.

## 5. Conclusions

A terrestrial systems model has been applied to two sets of field experimental data; ASGARD, near Nottingham UK and Grimsrud in southern Norway. While significant uncertainties remain, mainly pertaining to data and some aspects of the conceptual model, the systems modelling tool has been able to replicate the major features of both experiments, including  $\delta^{13}\text{C}$  tracer migration (Grimsrud only), CO<sub>2</sub> fluxes and concentrations in the sub-surface and plant canopies and biomass impacts. In general, the model has proven remarkably robust for a range of plant species and the different experimental configurations of the two sites.

## Acknowledgements

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