British Geological Survey
NATURAL ENVIRONMENT RESEARCH COUNCIL

The status of the QPAC Player for the ASGARD site; implications for the RISCS project

Carbon capture and storage Programme

Open Report OR/10/004

BRITISH GEOLOGICAL SURVEY

CARBON CAPTURE AND STORAGE PROGRAMME

OPEN REPORT OR/10/004

The status of the QPAC Player for the ASGARD site; implications for the RISCS project

T Vounaki[a], P Maul[b], P Robinson[b]

[a] British Geological Survey [b] Quintessa Ltd

Keywords

Report; RISCS; QPAC; carbon leakage; CCS; modelling; monitoring; plant stress.

National Grid Reference

SW corner 450657,326445
Centre point 450655,326455
NE corner 450643,326445

Front cover

Bibliographical reference

THALIA VOUNAKI, PHILIP MAUL, PETER ROBINSON. 2011. The status of the QPAC Player for the ASGARD site; implications for the RISCS project. *British Geological Survey Open Report*, OR/10/004. 40pp.

Keyworth, Nottingham British Geological Survey 2011

BRITISH GEOLOGICAL SURVEY

The full range of our publications is available from BGS shops at Nottingham, Edinburgh, London and Cardiff (Welsh publications only) see contact details below or shop online at www.geologyshop.com

The London Information Office also maintains a reference collection of BGS publications, including maps, for consultation.

We publish an annual catalogue of our maps and other publications; this catalogue is available online or from any of the BGS shops.

The British Geological Survey carries out the geological survey of Great Britain and Northern Ireland (the latter as an agency service for the government of Northern Ireland), and of the surrounding continental shelf, as well as basic research projects. It also undertakes programmes of technical aid in geology in developing countries.

The British Geological Survey is a component body of the Natural Environment Research Council.

British Geological Survey offices

BGS Central Enquiries Desk
Tel 0115 936 3143 Fax 0115 936 3276
email enquiries@bgs.ac.uk

Kingsley Dunham Centre, Keyworth, Nottingham NG12 5GG
Tel 0115 936 3241 Fax 0115 936 3488
email sales@bgs.ac.uk

Murchison House, West Mains Road, Edinburgh EH9 3LA
Tel 0131 667 1000 Fax 0131 668 2683
email scotsales@bgs.ac.uk

Natural History Museum, Cromwell Road, London SW7 5BD
Tel 020 7589 4090 Fax 020 7584 8270
Tel 020 7942 5344/45 email bgslondon@bgs.ac.uk

Columbus House, Greenmeadow Springs, Tongwynlais, Cardiff CF15 7NE
Tel 029 2052 1962 Fax 029 2052 1963

Maclean Building, Crowmarsh Gifford, Wallingford OX10 8BB
Tel 01491 838800 Fax 01491 692345

Geological Survey of Northern Ireland, Colby House, Stranmillis Court, Belfast BT9 5BF
Tel 028 9038 8462 Fax 028 9038 8461

www.bgs.ac.uk/gsni/

Parent Body

Natural Environment Research Council, Polaris House, North Star Avenue, Swindon SN2 1EU
Tel 01793 411500 Fax 01793 411501
www.nerc.ac.uk

Website www.bgs.ac.uk
Shop online at www.geologyshop.com

Foreword

This report is the published product of a study by the British Geological Survey (BGS) and Quintessa reviewing the QPAC Player for the ASGARD site in preparation for the RISCS project.

Acknowledgements

The authors would like to acknowledge:

1. Quintessa who developed the QPAC Player and the soil-plant model that forms the base of the Player. Specific thanks go to Laura Limer, Mike Thorne and Alex Bond.
2. Julie West for providing guidance and support, and for reviewing the report.
3. Dave Jones and Jonathan Pearce for reviewing the report.
4. Majdi Mansour and Sarah Hannis for helping with the structure and content of the report.

Contents

FIGURES

PLATES

TABLES

Summary

The RISCS project is a 4-year EU funded project starting in January 2010 that will assess the impacts of CO_2 storage on ecosystems/near-surface environments. One of the experimental test facilities will be the ASGARD site at the Nottingham's University campus. Previous research at ASGARD has investigated the impacts of shallow injection of CO_2 on plants as part of the CO2GeoNet programme. BGS collected botanic data, and Quintessa developed an initial version of a soil-plant model for the site using Quintessa's general purpose modelling code QPAC. In preparation for RISCS, Quintessa developed prototype software for BGS to familiarise itself with the model and understand the model data needs in order to provide information relevant to discussions on the experimental design at ASGARD during the RISCS project kick off meeting.

The current version of the model has the following capabilities and limitations:

- It can represent the fertilisation and toxicity effects of CO_2 on plants in terms of plant biomass and height change
- Experimental data can be used to optimise model fertilisation and toxicity parameters
- It was initially developed to model a single plant species, but has been used to model two species, with one species assumed to be dominant. This could be further developed to allow species competition to be modelled in the presence of elevated levels of CO_2 effects.
- Currently CO_2 transport in the rooting zone is assumed to be primarily by diffusion. In the RISCS project it may be necessary to extend the model to consider advective transport. Depending on the purpose of the experiment, the model could include the movement of CO_2 from the injection point to the rooting zone by using the QPAC-CO2 code developed by Quintessa.

Conclusions relevant to the experimental design at ASGARD for RISCS include the following:

- Measurements of key parameters, such as CO_2 concentration and flux, will be needed. Depending on the measurement frequency, this might require automated instrumentation.
- The variability in the plant species in the grassed plots and the limited area of high CO_2 at the surface makes it hard to quantify the relationship between CO_2 concentration and effect on plant species. It is therefore suggested that the plots are planted with one or two species, such as grass and clover.
- Measurements of plant biomass and CO_2 concentration in the rooting zone, the surface and the canopy are needed for the model calibration.
- The application of herbicides on the plots should depend on what is aimed to be represented; grazed or uncultivated land might be expected to be herbicide free.
- Vertical barriers might be envisaged to prevent CO_2 from migrating to controlled sites, to have better control of where the CO_2 goes and thus facilitate comparisons between measurements and model calculations. They could help with increasing the surface area exposed to high CO_2 levels, which currently is very small.
- To better understand the effect of CO_2 on plants, it is necessary to expose the plants to a range of CO_2 concentration levels. This requires careful consideration of the injection type and depth and of the size of the plots.
- Different injection types might be envisaged depending on the plant composition; mixed pasture which contains several plant species would benefit from a uniform CO_2 concentration within the plot.

1 Introduction

The geological storage of CO_2 has the potential to be an effective and safe way to reduce anthropogenic CO_2 emissions (IPPC, 2005). However, many stakeholders require the scientific community to demonstrate that all possible scenarios have been evaluated including the potential impacts of leakages into the biosphere. As part of the CO2GeoNet project "Ecosystem Responses to CO_2 Leakage – Model approach", a number of natural and experimental test facilities were used to investigate the risk from leakage to the near surface, and initial examples of a system model to assess the impacts at a storage site were developed (West, 2007). Quintessa developed and applied a systems model for the Latera site in Italy where there are high natural fluxes of CO_2 to the surface, using Quintessa's general purpose modelling code QPAC (Maul et al., 2009). Quintessa then adapted the systems model to create a prototype model for the experimental field test facility at the University of Nottingham's ASGARD (Artificial Soil Gassing And Response Detection) site.

BGS and other organisations will now conduct experiments at the ASGARD site as part of RISCS, a 4-year EU funded project that will assess the impacts of CO_2 storage on ecosystems/near-surface environments. In preparation for RISCS, Quintessa produced a "wrapped" version of the ASGARD model, referred to as the Player for brevity, which allows the user to run the model with different values of the parameters and visualise the results. The aim of the Player was for BGS to familiarise itself with the model and understand the model data needs in order to provide information relevant to discussions on the experimental design at ASGARD during the RISCS project kick off meeting (28^{th} and 29^{th} January).

This report discusses the capabilities and the limitations of the preliminary ASGARD model and raises issues that should be addressed with regards to the experimental design of ASGARD in light the RISCS project. This report includes consideration of the output from the discussions at the kick off meeting.

The objectives of this report are the following:

- Introduce system modelling
- Summarise the application of systems modelling to the Latera site
- Develop a conceptual model of the ASGARD site
- Present the ASGARD model and the prototype version of the Player
- Identify model and experimental limitations
- Present the potential of the model through example outputs
- Conduct sensitivity analysis of some parameters
- Summarise information relevant to the experimental design of ASGARD within the RISCS project

2 Background to systems modelling

Real problems involve many processes that are better represented in separate models with well defined interfaces which are then integrated into a systems representation. Systems model s represent the whole system under consideration with the aim of including 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. The application of systems modelling may be undertaken using general-purpose modelling codes.

Quintessa has developed a general-purpose modelling code, called QPAC, to represent a wide range of physical problems, including geological storage of CO_2. As part of CO2Geonet, Quintessa applied QPAC to develop a systems model for key processes at the Latera site where there are high natural fluxes of CO_2 to the surface. Subsequently the model was adapted for the ASGARD site. This section provides a summary of the Latera site and of the systems model.

2.1 SUMMARY OF RESULTS FROM THE LATERA SITE

One of the natural test facilities used for the CO_2GeoNet project was the Latera site in Italy, where a detailed geochemical and biological study was conducted during two different seasons on a naturally occurring gas vent. The results showed that the significant impact was only observed in the 6 m wide centre core of the vent where CO_2 flux rates exceed 2000-3000 g m^2 d^{-1}. In this ''vent core'' there is no vegetation, pH is low (minimum 3.5), small changes are recorded in mineralogy and bulk chemistry, the microbial activity is controlled by near-anoxic conditions and extremely high soil gas CO_2 (>95%). A transition zone over a 20 m wide halo surrounding the core exists, over which there is a gradual decrease in CO_2 concentrations, a rapid decrease in CO_2 fluxes, and the absence of reactive gas species. In this transition zone grasses dominate near the vent core, but these are progressively replaced by clover and a greater plant diversity moving away from the vent centre (Figure 1). The results indicated that even at this high-flux site, the effects of the gas vent are spatially limited and that the ecosystem appears to have adapted to the different conditions through species substitution or adaptation (Beaubien et al., 2008).

Figure 1 Plant transition around a gas vent at the Latera Site (photo from West, 2007)

2.2 SYSTEMS MODELLING OF THE LATERA SITE

A systems model was applied to this site by Quintessa using the general purpose modelling code QPAC. The systems model had three subsystems: a deep geosphere model, a near-surface model and a soil-plant model (Figure 2). The deep model represented the transport of CO_2 through faults to the surface using multiphase flow modelling. Once the CO_2 reached the shallow aquifer, it entered the near surface model. In the near surface model the fluids were either assumed to be poorly mixed and the fluids formed distinct layers, or well mixed, for which multiphase flow was used. Some CO_2 also dissolves into groundwater. Once the CO_2 reached the rooting zone, it entered the soil-plant model, where the effect of CO_2 on plant biomass was simulated (Maul et al., 2008). Good comparisons were obtained between model calculations and observed data of surface venting patterns, soil gas concentrations and plant responses, give confidence that the key features of the system are well understood (Maul et al., 2009).

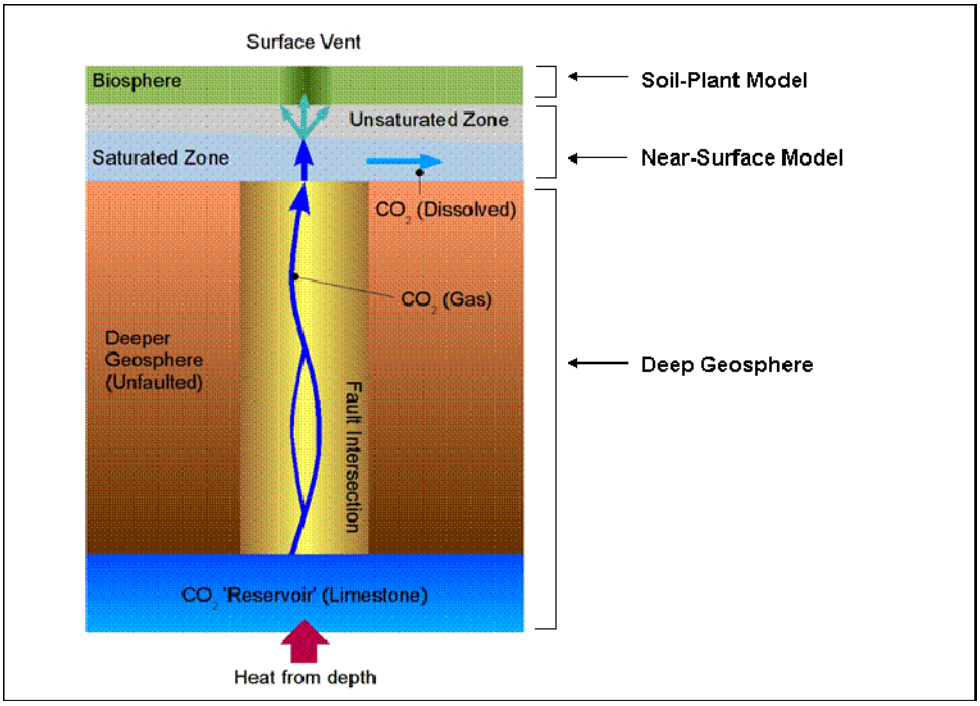

Figure 2 Conceptual model for the CO_2 transport at Latera (Maul et al., 2008).

2.3 CONCLUSIONS FROM THE SYSTEMS MODELLING OF THE LATERA SITE

The conclusions from the systems model of the Latera site were (Maul et al., 2008):

- A single integrated systems-level model was possible using the QPAC software
- The inclusion of near-surface processes which affect CO_2 transport and are observed at the Latera site could be useful in assessments for the geological storage of CO_2.
- The pattern of CO_2 venting calculated by the model was broadly consistent with field observations at the site.
- Model calculations of soil gas concentrations and plant response were overall in good agreement with observed data. This provided support to the idea that observable changes in ecosystems could provide early warning of leakage to the surface.
- Future experiments should consider biomass or height measurements for better comparison between observed and model results
- Future model developments should consider plant transition (and allow for more than two plant species).

3 The ASGARD site

3.1 BACKGROUND AND AIM OF TO THE ASGARD WORK

The principal objective of the ASGARD site was to develop a facility that could assess crop plant responses to elevated CO_2 concentrations, within the soil environment, as a simulation of a leak from a CO_2 storage facility. By creating a purpose-built facility, the volumes of CO_2 introduced could be precisely controlled and the exposures could be carefully constrained. Experimental test facilities such as ASGARD have the advantage that plants are not adapted like in naturally leaking CO_2 sites. Thus the observations at ASGARD are considered to be representative of what would be expected if CO_2 leaked from a storage site (West, 2007).

3.2 THE ASGARD SITE

The ASGARD site is located on the University of Nottingham's Sutton Bonington Campus, approximately 18 km south of central Nottingham. The site had been previously used for sheep pasture. Geologically, the study area is characterised by up to 1.5 m of head deposits overlying mudstones. The head deposit is quite variable in terms of lithology, especially below 60 cm depth. At the BGS plots the head deposits consist of a lower clay-dominated facies overlain by a thin and highly variable mixed facies up to 60 cm thick which is characterised by a gravel-rich base, typically 15 cm thick.

The ASGARD site consists of 30 plots measuring 2.5 m x 2.5 m which are arrayed in a rectangular grid pattern (5 x 6 plots) with pathways (~50 cm) between each plot The southern group of eight plots were kept as pasture and these were selected as the focus for all of BGS activities (Figure 3 and Figure 4). CO_2 was injected at atmospheric pressure and temperature at a 45 degrees angle into the centre of plots G1, G2, G6 and G8 through permanently installed pipework at a constant rate of 3 litres per minute between 50 and 60 cm below ground level over a period of 19 weeks (May to September 2006). The CO_2 entered the soil through the final 10 cm of the pipe, where it was screened. The rate was set such as to obtain a high concentration at the surface in order to observe stress on plants. After that period, injection continued in the non-BGS plots at a lower rate of 1 l/min.

Figure 3 The BGS grassed plots at the ASGARD site in June 2006 (fig from West, 2007)

BGS conducted botanic surveys and took CO_2 flux and concentration measurements for plots G1-G4 and G6-G9 prior and at the end of the injection. The botanic survey was conducted in March and in September and identified the percentage cover and type of flora in each plot species composition. Flux measurements were taken at the centre of the plot in May and August, and detailed flux was measured at G1 and G8 in September. Gas concentrations were measured around the perimeter of the plots in May and within each plot in September at the following depths: 20, 50 and 70cm. Detailed soil gas concentration measurements were taken in G7 and G8. A baseline characterisation of the microbiology, mineralogy and geochemistry of all plots was done prior and towards the end of injection. A full description of the geology, experimental methodology and site is given in West (2007).

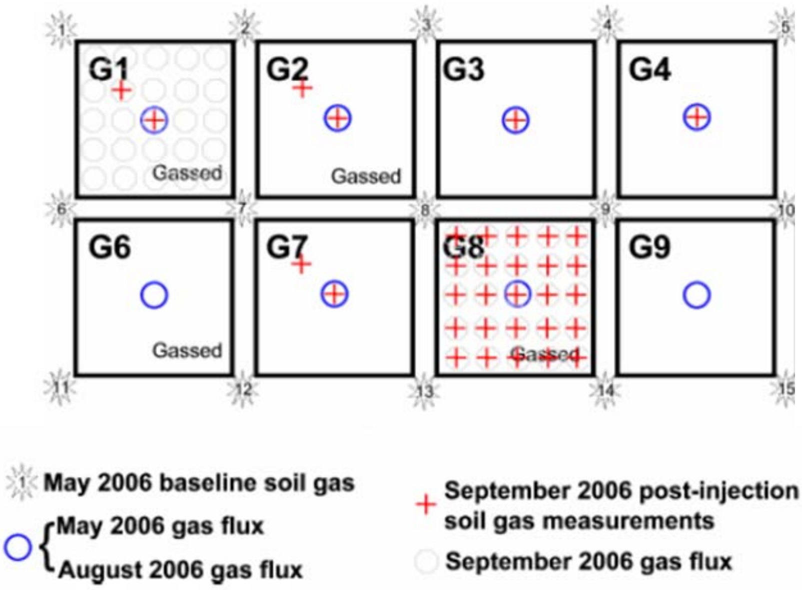

Figure 4 Soil gas concentration and flux sampling plan carried out in May (pre-injection), August (during injection) and September (end of injection) 2006. (fig adapted from West, 2007)

3.3 SUMMARY OF RESULTS

The plant species composition of controlled and gassed plots looked very similar in March prior to injection. All plots contained a range of monocotyledonous (e.g. grasses) and dicotyledonous (e.g. dandelions, thistle, plantain, chickweed, mallow, clover) plant species. In September however, controlled plots had higher proportions of minor plant groups than the gassed plots at the end of the injection period (Figure 5-G7). In very high CO_2 concentrations (more than 75% at 20 cm depth), plants turned yellow or brown and bare earth appeared (Figure 5-G8). At lower concentrations (up to 45% CO_2 at 20 cm depth), grass was the dominant plant group in the gassed plots (Figure 5-G8). Towards the end of the injection period, the area of significantly altered soil was 50 – 100 cm in diameter. Changes in the soil microbiology and geochemistry were also observed.

Soil flux measurements taken towards the end of the injection period indicated that about one third of the CO_2 injected into the soil was accounted for in the flux measurements at this time. This would suggest that soil flux measurements cannot be directly related to injection (or leakage) rates even over a depth of 60 cm. This mass imbalance is supported by CO_2 flux and gas measurements that indicate lateral movement was greater than vertical movement, particularly at depth (Figure 6) (West et al., 2009).

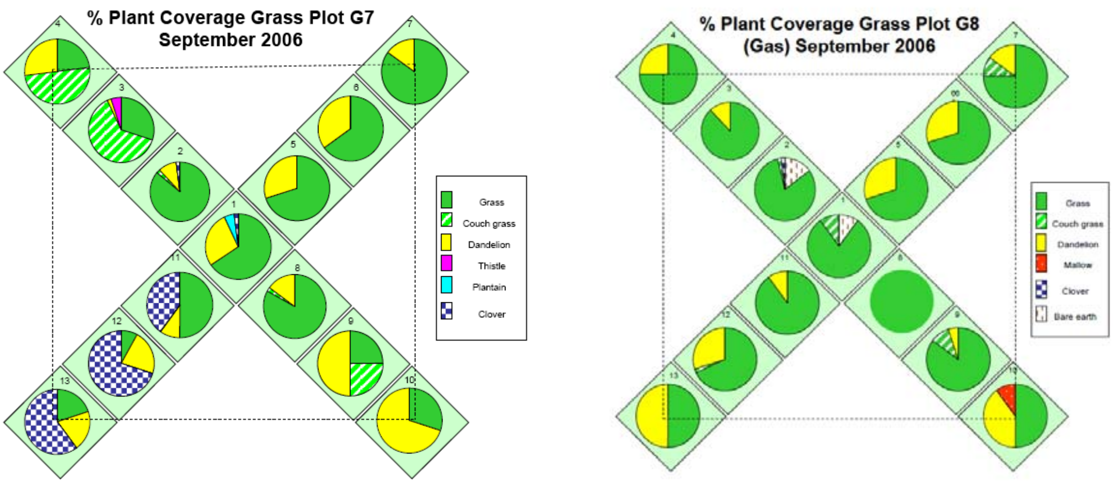

Figure 5 Botanic survey of plot G7 (control) and plot G8 (gassed) in September 2006 (fig from West et al., 2009)

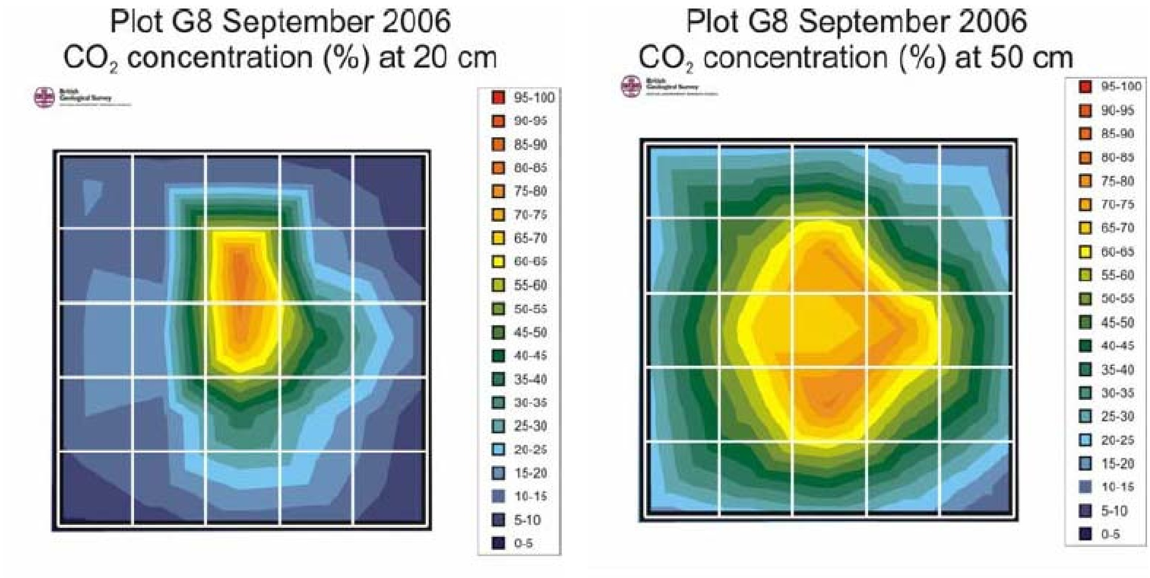

Figure 6 Distribution of CO_2 concentration at 20 and 50cm depth in G8 in September 2006(fig from West et al., 2009)

3.4 CONCEPTUAL MODEL OF THE ASGARD SITE

3.4.1 Processes in the soil zone

A schematic representation of the ASGARD site that summarises the key elements necessary for systems modelling in the soil zone is provided in Figure 7. Once the CO_2 enters the system, its transport is dictated by a combination of diffusion, advection and density-driven flow. Diffusion results in CO_2 moving in all directions as the gas moves to areas with lower concentrations. An advective component is also expected as the injected rate is significantly higher than the background flux. The direction of the advective movement depends on the pipe direction and the exit characteristics. Based on the injection rate and the initial plan that CO_2 would be contained within the plots, the pore space of a plot would be renewed 1.5 times a day with CO_2, assuming a porosity of 0.3 and a depth of 1.5 m. This implies a very rapid turnover rate of CO_2 in the soil, which indicates there must be an advective component to the flow. CO_2 is also expected to sink because it is denser than air. The elevated CO_2 concentration and the lateral spread at 70 cm depth suggest that both advection and density-driven flows take place.

The physical boundaries of the system are the Mercia mudstone at 1.2 m to 1.5 m depth which acts as a no flow boundary and the atmosphere starting from the top of the vegetation, where the CO_2 is at atmospheric concentration. Lateral boundaries that would separate the plots do not exist as the geology is continuous. The fluids in the soil zone include air and water. A water table has not been identified, so the system bounded by the Mercia mudstone is assumed to be unsaturated with respect to water. From a modelling point of view, a multiphase flow approach would be needed to represent the relevant processes.

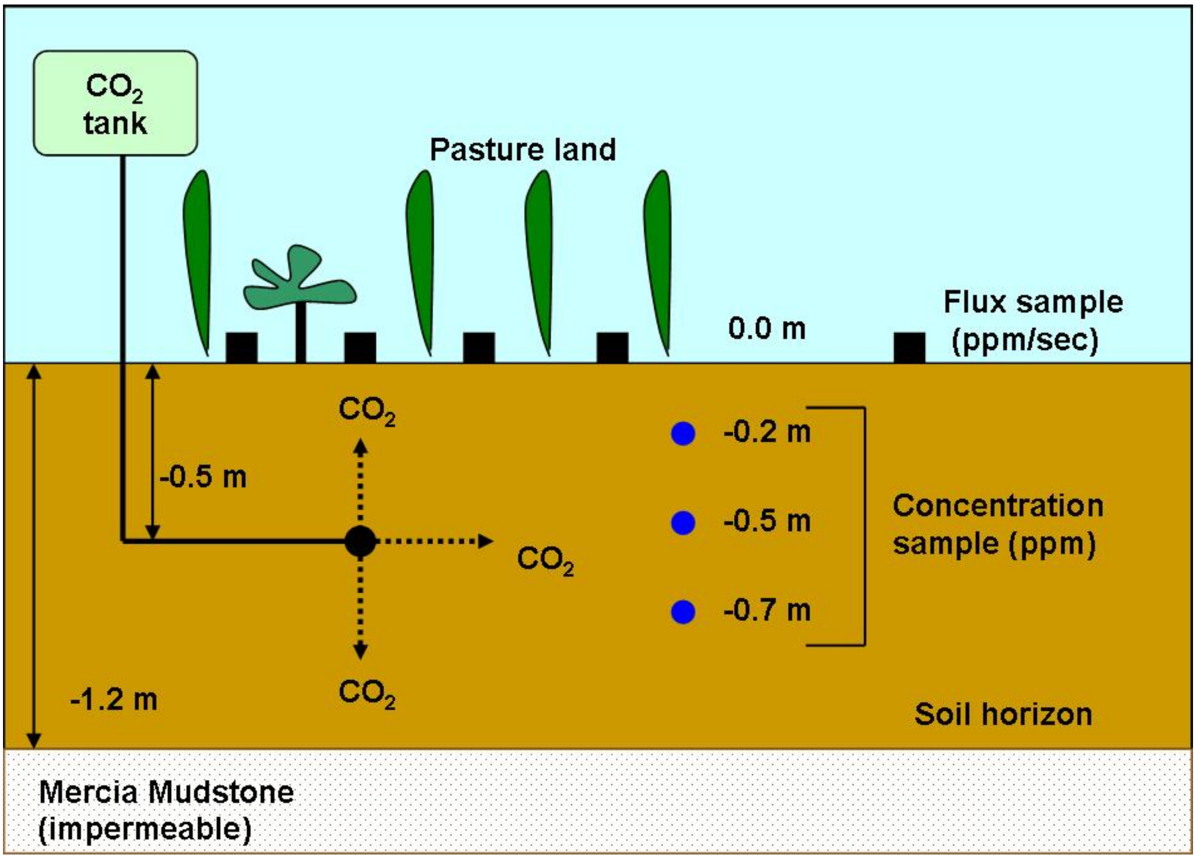

Figure 7 Schematic representation of the ASGARD experiment layout

3.4.2 Processes above the surface

Studies at analogue sites such as Latera, Italy, and Lacher See, Germany, have shown that monocotyledonous (e.g. grasses) plant species are more tolerant to high levels of CO_2 than dicotyledonous (e.g. clover) plants species (West, 2007). The results at the ASGARD site, although not as conclusive as those at the analogue sites, indicate a similar pattern. When comparing the plant species composition of plots G7 to G8 at the end of the experiment, the control plot (G7) contained a higher species variation, while only grass was regarded in the centre of G8 where plant die-off and the highest CO_2 concentration and flux were observed.

4 Status of the QPAC ASGARD Player

Quintessa has adapted the soil-plant model used at the Latera site for the ASGARD site to create a prototype ASGARD model. In preparation for RISCS, Quintessa produced a “wrapped” version of the model, referred to as the Player, which allows the user to run the model with different values of the parameters and visualise the results. The aim of the Player was for BGS to familiarise itself with the model and understand the model data needs in order to provide information relevant to discussions on the experimental design at ASGARD during the RISCS project kick off meeting (28th and 29th January).

The Player described in this report is a prototype that will be developed during the RISCS project. The aim is to be able to reproduce field observations of the impact of elevated levels of CO_2 on plants. Some model parameters will need to be adjusted in order to provide good modelled representation of experimental data. The calibrated model can then be used to make predictions for different possible scenarios.

The near surface model used at Latera was not represented in the prototype Player, but this may be necessary to fully understand the processes occurring at ASGARD. In the soil-plant model CO_2 movement in the rooting zone is controlled by vertical diffusion, although it may be necessary to develop the model to include vertical advection (Figure 8).

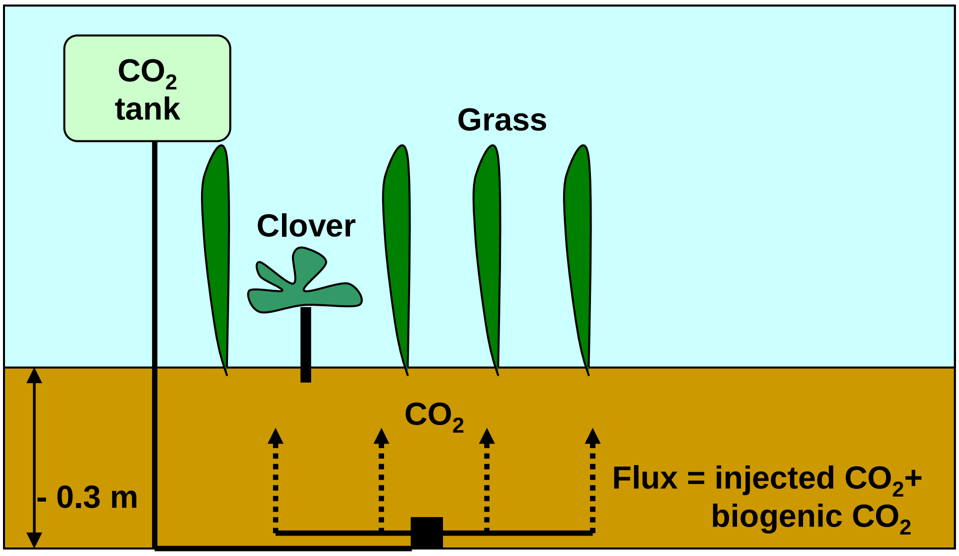

Figure 8 Schematic representation of the simulation of CO_2 movement in the Player

4.1 THE SOIL-PLANT MODEL

4.1.1 Conceptual understanding

The soil-plant model can simulate the impact of CO_2 on plants by calculating the evolution in plant biomass and height. This gives an indication of whether or not a species can survive at a given CO_2 concentrations and how quickly the plant recovers. The current version of the model allows one or two plant species to be represented; grass and clover were considered for the Latera model, where grass was shown to be more tolerant of CO_2 than clover (West, 2007). The soil-plant model can be used for to arable crops as well as pasture.

The biomass of a plant species is calculated based on the time history of soil moisture, temperature and fertilisation and toxicity effects from CO_2 (Limer et al., 2008). The height of the plant is derived from the biomass and the maximum specified height for that plant species. The CO_2 concentration (C_{CO2}) that the different parts of the plant see depends on the height (z) of that part, the flux and the soil (D_{soil}) and air (D_{air}) diffusion coefficients. The flux is the combination of the injected CO_2 and the CO_2 produced by the plants, called biogenic flux. The concentration decreases with height and reaches a minimum value (C_{min}) above the canopy, where it is at background atmospheric levels (Figure 9).

The CO_2 impact on a plant species depends on its sensitivity to CO_2 and its relation to the other plant species. The model assumes that the tallest species sets the upper boundary and thus the height at which the background atmospheric CO_2 concentration prevails. This determines the CO_2 vertical concentration profile. As a consequence of this assumption, the shorter of the two plants species is exposed to a higher canopy atmosphere CO_2 concentration (X2) than if the two plants were the same height (X1) (Figure 10).

In the calculations undertaken using the Player it was assumed that the plots were not mowed. In reality this was not the case, but mowing can be simulated in the soil-plant model.

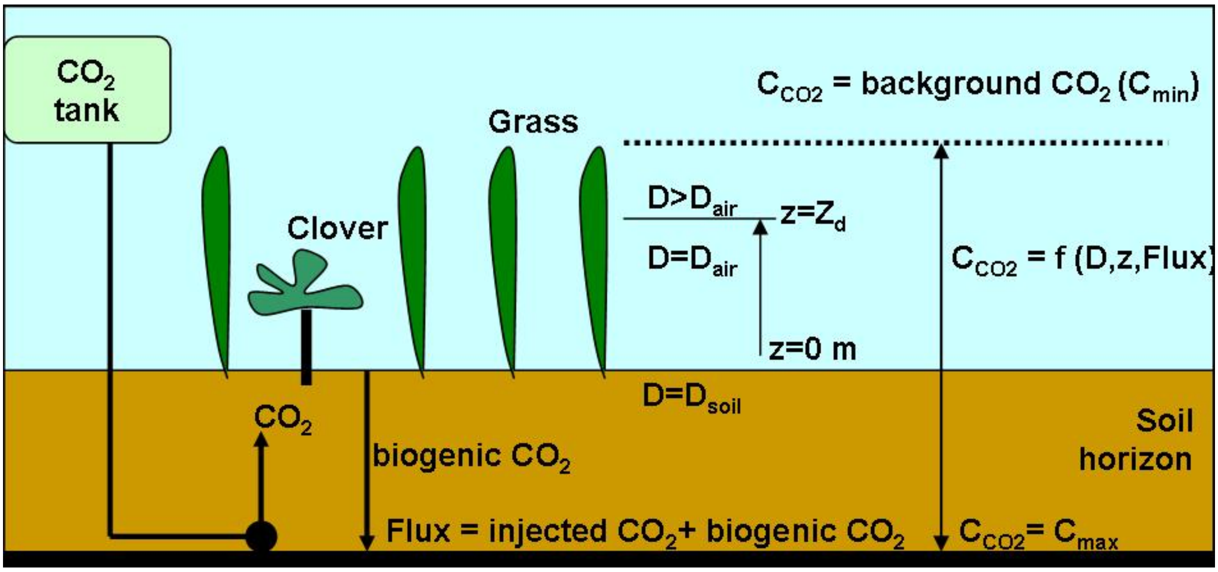

Figure 9 Sketch of parameters controlling the CO_2 concentration in the soil-plant model

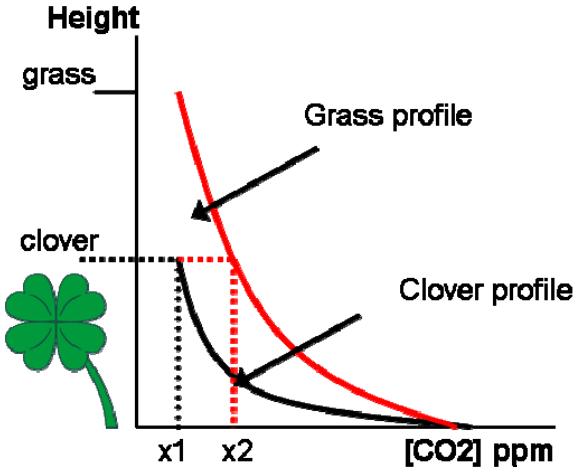

Figure 10 Sketch illustrating the effect of the dominant (tallest) species on the other

4.2 PARAMETERS

4.2.1 Parameters in the soil-plant model

A list of most parameters is given in Limer et a. (2008). These fall in general into the following categories:

a) **Plant specific parameters** that dictate growth under normal conditions and that assign the dominant species (maximum biomass for each plant part, maximum height). These have little influence on the effect of CO_2 on the plant

b**) Plant related** but not plant specific constants that are well documented in the literature, e.g. temperature related growth and soil decomposition rates

c) **Non plant related** constants that are well documented in the literature, e.g. density of air, friction velocity and critical soil water contents

d) **Site specific** parameters e.g. area and volume of the model

4.2.2 Parameters accessible in the Player

The Player can allow the user to modify whichever parameters are considered to be important. In this prototype version the user can modify parameters which control the effect of CO_2 on the plants. These include plant specific and non plant specific parameters (Table 1). The values taken for the parameters for application to the Latera site are given in Maul et al. (2008).

Soil moisture is set to 20% which is assumed to correspond to no effect on plant growth. This is an acceptable value if the soil moisture is between 10 and 20%. This assumption was made for illustrative purposes as no experimental data were available. If the soil is extremely dry, this would result in plant stressing. It is important therefore to have control plots in an experimental setup, in order to identify whether plant die-off in the gassed plots is due to CO_2 or to natural conditions.

The assumption in the default values is that grass has a higher resistance to toxic effects in the soil (k2) and benefits more from fertilisation effects (beta) than clover. The higher the k2 value, the more adverse is the effect on the plant. Beta relates to the fertilisation of the plant; a higher beta value results in a higher biomass growth for CO_2 concentrations that lead to an increase in photosynthesis. The default values for the toxicity effects in the air (k1) and the constant relating biomass and plant height (nu) are the same for both species. More detailed information on the derivation of the default values are provided in Maul et al. (2008).

A dispersion coefficient factor above the canopy was introduced for the ASGARD model due to the small sizes of the plots.

The grass/clover ratio is assumed to be 4:1. This ratio is constant throughout the simulation as species competition is currently not represented in the soil-plant model.

Table 1 Model Parameters that the user can adjust in the Player

Parameter	Parameter Name in Player	Description	Are values same for both species?	Relevant figure
C_{CA}^{**}	Air toxicity threshold	CO_2 concentration in the canopy atmosphere when toxic effects start to occur in the plant	YES	Figure 1
C_{SA}^{**}	Soil solution toxicity factor	CO_2 concentration in the rooting zone when toxic effects start to occur in the plant	YES	Figure 2
Δ	Delta	Fraction of the thickness of the plant canopy corresponding to the location of z_d	YES	Figure 3
K_1	Kappa_1	Constant that determines how rapidly toxicity effects are observed when atmospheric conditions deviate from optimality	YES	Figure 4
K_2	Kappa_2	Constant that determines how rapidly toxicity effects are observed when soil conditions deviate from optimality	NO	Figure 5
Canopy Dispersion Factor	Canopy Dispersion Factor	Coefficient that controls the horizontal dispersion above the canopy of the tallest plant species Parameter introduced in ASGARD only because of the small size of the plots	NA	Figure 6
k_m	Soil moisture	Growth rate modification factor due to soil moisture status. Referred to as k_1 in previous reports	NA	Figure 7
β	Beta	Parameter which determines the range over which enhanced CO_2 concentrations in air can result in increased productivity	NO	Figure 8
N	Nu	Power law index relating vertical growth to standing biomass	YES	Figure 9

4.3 GRID AND BOUNDARY CONDITIONS

The Player represents the plots G7 (control) and G8 (gassed). Each plot is divided in five columns and rows to obtain 25 subplots, shown as nodes in the QPAC Viewer (Figure 11). This structure is the same as the experimental layout. The model is delineated by a top and bottom boundary which applies to all model nodes. The top boundary is set just above the canopy, and the bottom one is the base of the model, here set to 30 cm below the ground. The lateral boundaries are the edges of the plot. The calculated flux of CO_2 in the model has only a vertical component, from the ground surface to the top of the canopy. The processes that occur in the soil profile are modelled at a point. As such the depth of the injection does not affect the calculations.

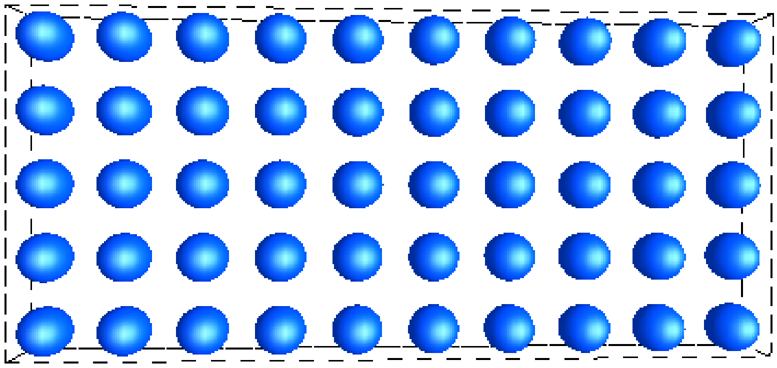

Figure 11 Model grid nodes representing plots G7 and G8. G7: column 1-5, G8: column 6-10

4.4 THE USER INTERFACE OF THE QPAC PLAYER

The user specifies the parameters in the Player under different window tabs that fall in four categories.

Timing

This tab allows the user to specify the duration of the injection and of the run (Figure 12). This is useful as it enables the simulation of what happens before, during and post injection. A run without injection could be useful for calibrating the model under normal conditions, which involve fewer parameters. Once the model is calibrated for the standard parameters, complexity can be added by simulating injection and more parameters can be calibrated by modifying the new parameters until the observed data match the modelled ones. Once injection stops, the run can continue and the recovery rate of plants can be estimated by the model.

Input A to E

These tabs were set in this version as a quick way to set the location and rate of the injection in the model. Each tab represents one of the columns of the gassed plot G8, each subdivided into five rows, producing a 5 by 5 grid (Figure 13). To inject in the middle of the plot, the user would have to set a value in Tab C, row 3. A more convenient method will be provided in the future.

Generic

The generic tab includes parameters that are land use but not plant specific (Figure 14). These include soil moisture content, CO_2 concentration thresholds in the air and in the soil above which plants die, and dispersion factors in and above the canopy. The type of land use is also specified here. The default values are considered to be reasonable starting points.

Grass/Clover/Arable/Pasture

Depending on the land use type selected in the Generic tab, the user adjusts the plant-specific parameters in the tabs grass and clover for pasture land, or arable for arable land (Figure 15).

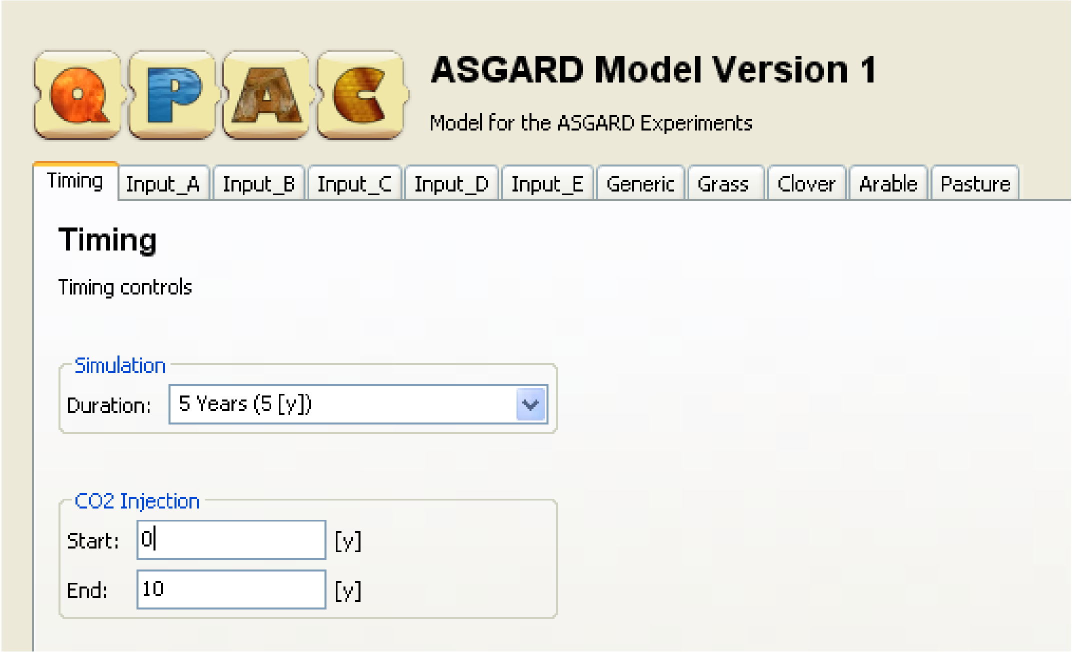

Figure 12 User specified parameters with regards to time

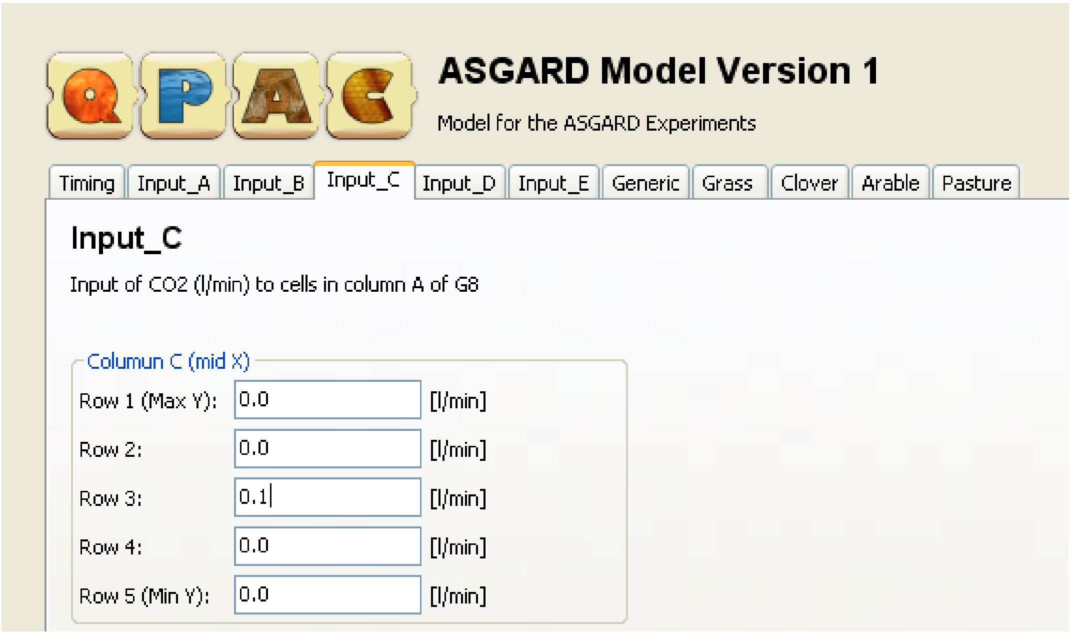

Figure 13 Example tab for specifying location and rate of injection within one of the five columns of G8.

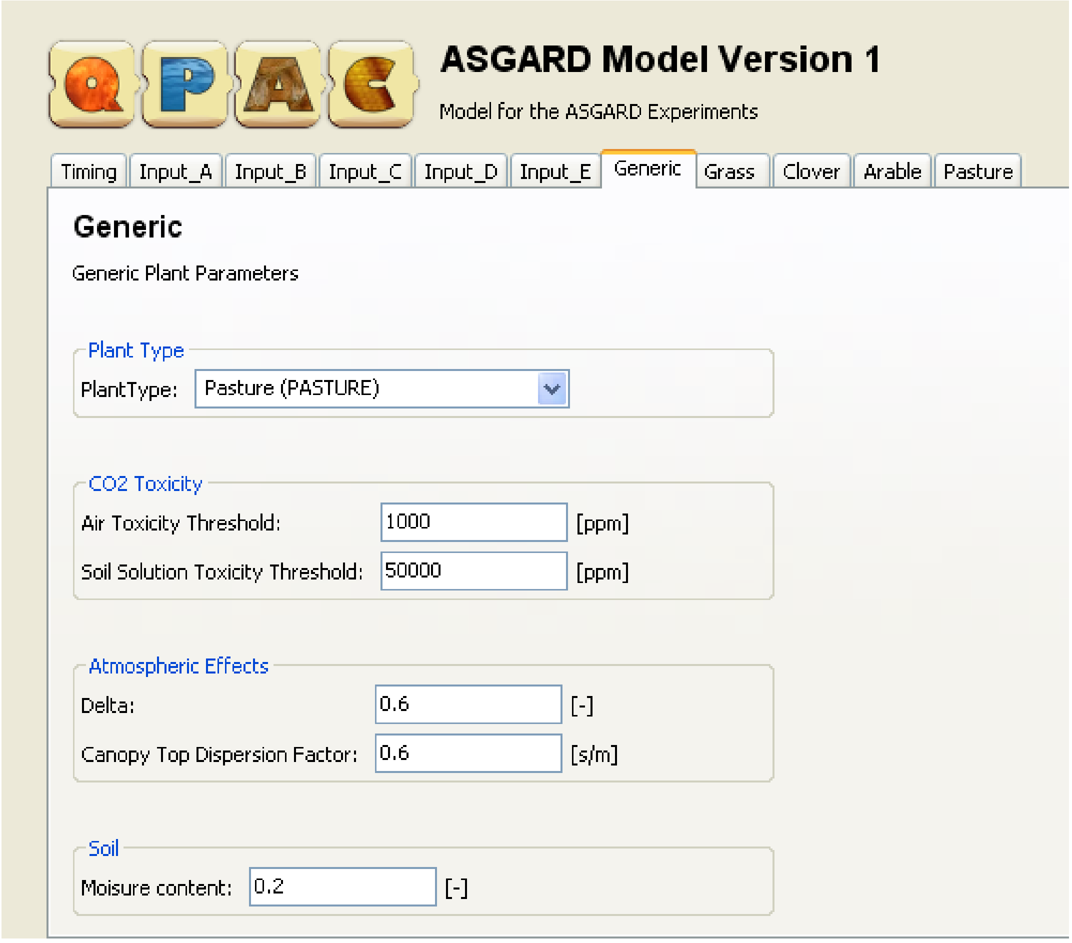

Figure 14 User Specified parameters that are not plant specific

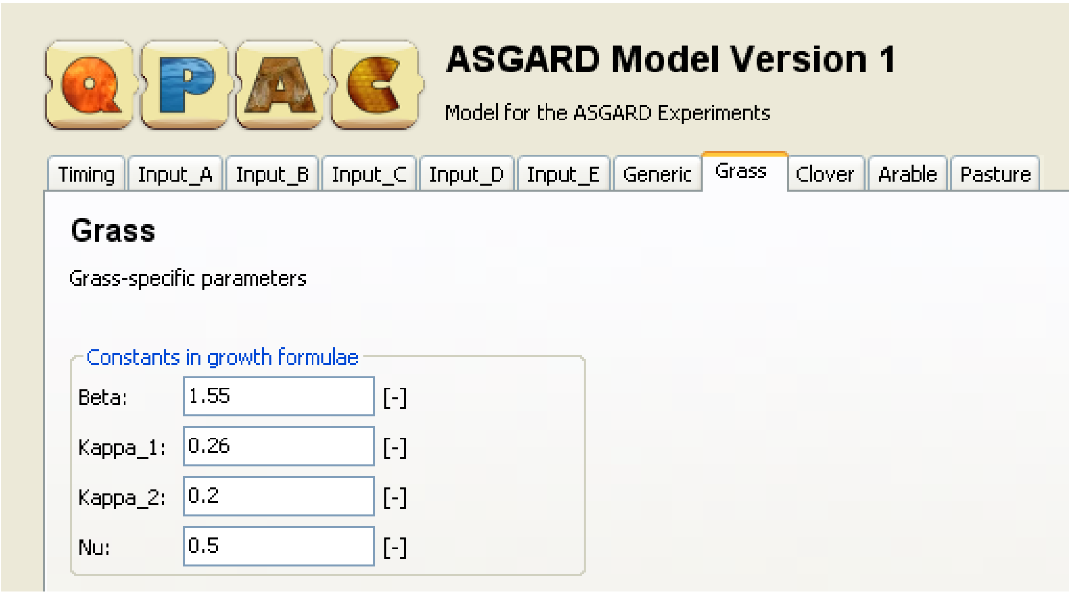

Figure 15 User specified parameters that are plant specific

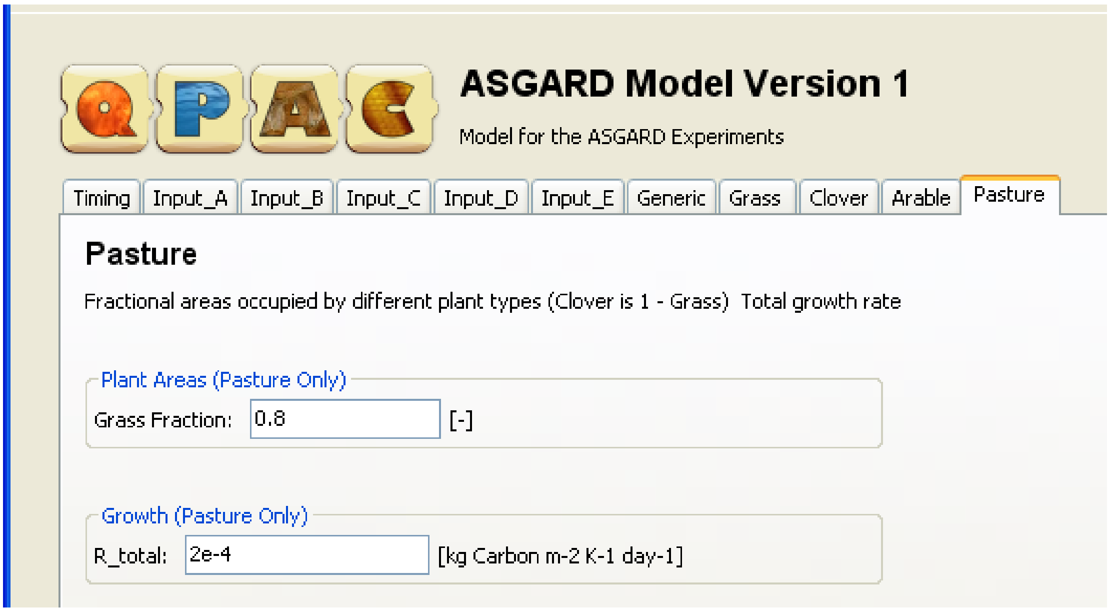

Figure 16 User specified parameters for plant composition

4.5 MODEL OUTPUT OPTIONS

Once the model has run, the user can view the results of the run in the QPAC viewer that is part of the QPAC Player. The results can be displayed spatially for the whole model for a given time or as time series of selected nodes. As with the model input, the Player can be configured to provide whatever outputs are considered to be useful. The outputs of the prototype Player are:

- Height of stem and foliage (m)
- Concentration of CO_2 in the canopy and top of the canopy (kg CO_2 m^{-3})
- Labile and recalcitrant organic Mass (kg C)
- Root, stem, fruit and foliage Mass (kg C)
- Biogenic flux (kg C m^{-2} day^{-1}) [flux from plant decomposition]
- Geosource (kg C m^{-2} y^{-1}) [geosource = injection rate, as no near-surface model]
- Total Flux (kg C m^{-2} y^{-1}) [Biogenic + Geosource]
- Concentration of C in the root zone, canopy and above canopy (ppm)
- Standing and Total Biomass (kg C m^{-2})

4.6 LIMITATIONS

Calculations from the prototype Player cannot be compared directly with currently available experimental data from ASGARD. This is because of a combination of a lack of information on some experimental data and of limitations of the current version of the software.

4.6.1 Player/Model limitations

The limitations of the Player fall into two categories; a) type of models included in the Player b) limitations of the processes represented in the soil-plant model.

Player limitations

The Player can represent what occurs at the ASGARD site from the root zone upwards but not what happens below, such as the movement of CO_2 from the injection point. This is acceptable if the aim is to investigate the effect of CO_2 on plants only. In this case the actual injection rate and location do not matter; instead the fluxes measured at the surface can be used in the model as the input value at the root zone. This approximation is reasonable because the CO_2 injected into a cell moves primarily upward in the rooting zone. The model includes consideration of the biogenic flux, but this is very small compared to the injected flux at ASGARD.

If the detection of CO_2 is one of the aims of the experiment, then its transport has to be modelled explicitly. This will require adding the near surface model developed for Latera.

Soil-plant model limitations

The soil-plant model currently simulates the effect of CO_2 on plant species through biomass change and can represent the effect of a taller species on a shorter one with regards to the CO_2 concentration profile. However, the fixed plant coverage ratio means that species competition is not represented. The incorporation of species competition in the model is difficult as it depends on a number of factors, including seasonal variations, but could be simplified to represent in only the effects from elevated levels of CO_2. Another limitation of the model is that it does not allow for advective flow in the rooting zone.

4.6.2 Experimental limitations

Data type

The key limitation in comparing observed to modelled data arises from the difference in the data type used to assess the effect of CO_2 on plants. The model outputs plant biomass and height while the experimental data collected by BGS were on plant type and coverage. As a result the model results cannot be compared directly to the collected data.

Different collection methods

The second limitation results from the difference in collection methods for the botanic survey, the CO_2 flux and the CO_2 concentration measurements. The botanic survey was done in a St Andrews cross while the CO_2 fluxes were taken on a regularly gridded pattern (Figure 17). As a consequence the measurements of the botanic survey could not easily be matched to the flux or gas concentration measurements.

Frequency of measurements

Botanic surveys were taken twice; before and at the end of injection (Figure 18). This established the maximum time within which an effect on plant was observed. It is possible that the same effect occurred earlier. It is recommended to take measurements at regular intervals in order to establish the minimum time after which plant die off occurs. The shape of the transition within time could also be obtained through regular measurements.

Plant species variation

Plant species variation between the quadrants within a plot becomes a limitation when the CO_2 flux differs between these quadrants too. Unless a similar plot with the same plant variation exists it is hard to correlate the one with the other as the tolerance to CO_2 differs among species.

Plot proximity

The third limitation arises from the fact that part of the injected CO_2 moved into control plots. As a result these could not act anymore as control plots. This could be attributed to the proximity between plots.

Plot size

The control and gassed plots differed in overall plant composition prior to injection. This meant it was hard to compare the effect of CO_2 on the species using species composition as an indicator of CO_2 impact on plants. The size of the plots might not have been big enough for plots to have statistically similar plant composition.

Mowing

During the experiment the grass plots were mowed to simulate grazing. This has direct impacts on the CO_2 concentration profile that plant species will see and on the interaction between species. In the Player it was assumed that the plots were not mowed as the focus was on the interaction between the species.

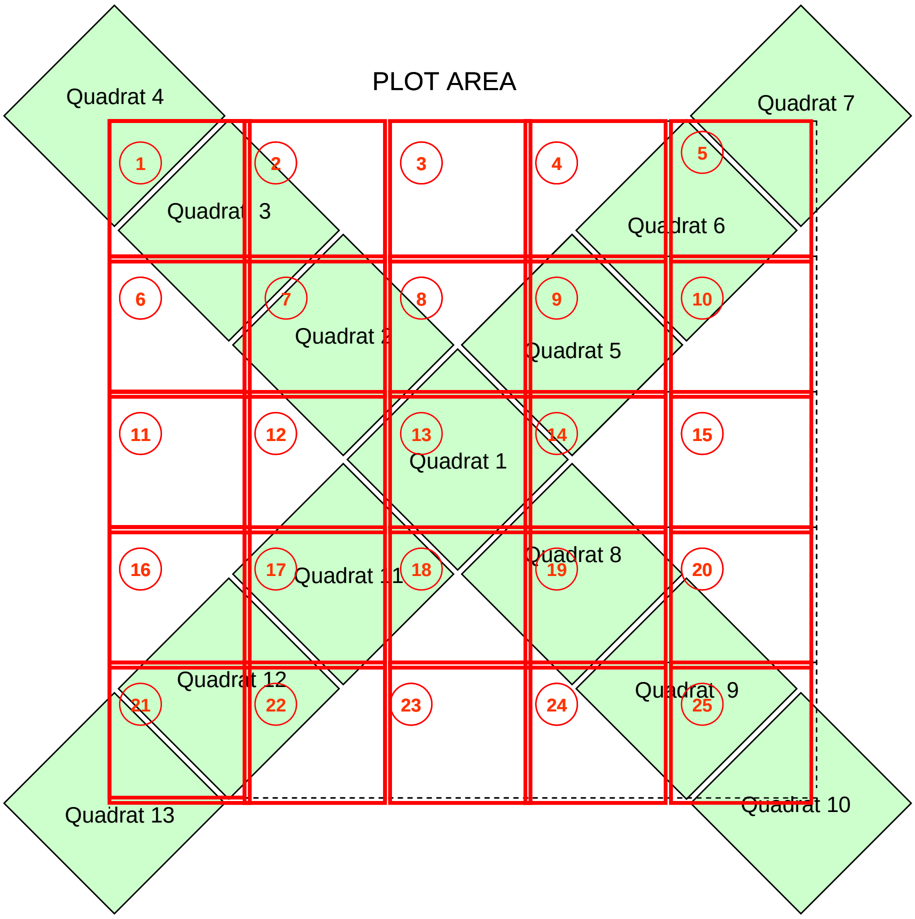

Figure 17 Sampling location for the botanical survey (green quadrats, 0.5 m^2 each) and for the flux survey (red rectangles, 0.25 m^2 each) (fig adapted from West, 2007)

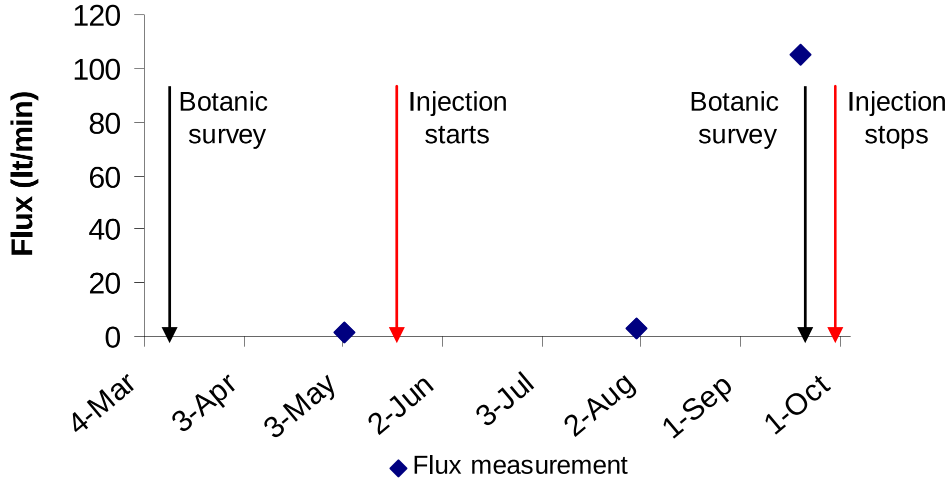

Figure 18 Timeline of injection period, flux measurements and botanic surveys.

5 Example of ASGARD Model calculations

A series of runs was conducted to show what the current version of the Player can do. These fall in three categories:

1. Base case without injection and default parameters
2. Base case with variable injection and default parameters
3. Sensitivity runs with modified parameters

As the field observations (plant species composition) can not be compared directly to the model output (plant biomass and height), the runs do not attempt to calibrate the model but rather to show the potential of the Player. Realistic values were assigned where possible in order for the output to be meaningful.

5.1 BASE CASE WITHOUT INJECTION

The default parameters are based on Maul et al. (2008), where explanations and references justifying the values are given. Their values are listed in Table 2. The normal seasonal biomass fluctuation for the two plant species is ± 20% (Figure 19). The overall slight biomass decrease of grass and increase of clover occurs because the model does not start from equilibrium. The peak CO_2 concentration is 0.4% in the soil, 0.1% in the canopy of clover and 0.05% in the canopy of grass (Figure 20). In comparison, the median measured background concentration at 20 cm depth was 1.7% in May 2006 and 3.8% in September (West, 2007). This suggests the model using the default values is underestimating the CO_2 seen by the plants at the root zone.

The concentration just above the canopy is below 0.04%. This is almost identical to the value of the atmospheric background concentration set in the model, because the canopy dispersion factor results in lateral spreading of CO_2 in the free atmosphere. The highest concentration is calculated in the rooting zone due to the biogenic production of CO_2 is. The calculated CO_2 concentration is higher in the canopy of clover than in the canopy of grass as the former is shorter.

Table 2 Default values of the parameters accessible to the user

Parameter	Units	Grass	Clover	Arable Crops
Parameters that are plant –specific				
β	-	1.55	1	1.55
κ_1	-	0.26	0.26	0.26
κ_2	-	0.2	0.5	0.2
N	-	0.5	1.0	0.5
Species cover %	-	0.8	0.2	0.0
c_{CA}^{**}		1E-3	1E-3	1E-3
c_{SA}^{**}		5E-2	5E-2	5E-2
Parameters that are not plant –specific				
Δ	-	0.6	0.6	0.6
Canopy dispersion factor	s/m	0.6	0.6	0.6
moisture content	-	0.2	0.2	0.2

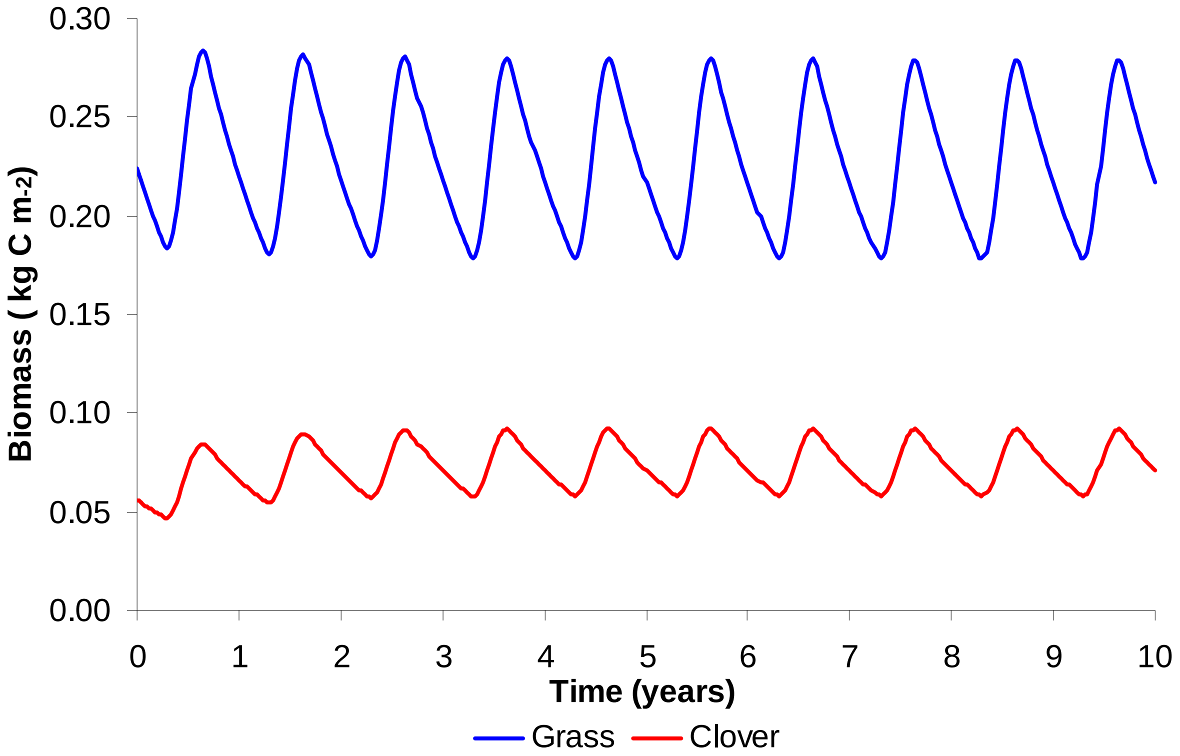

Figure 19 Standing biomass of grass and clover (composition: grass 80%).

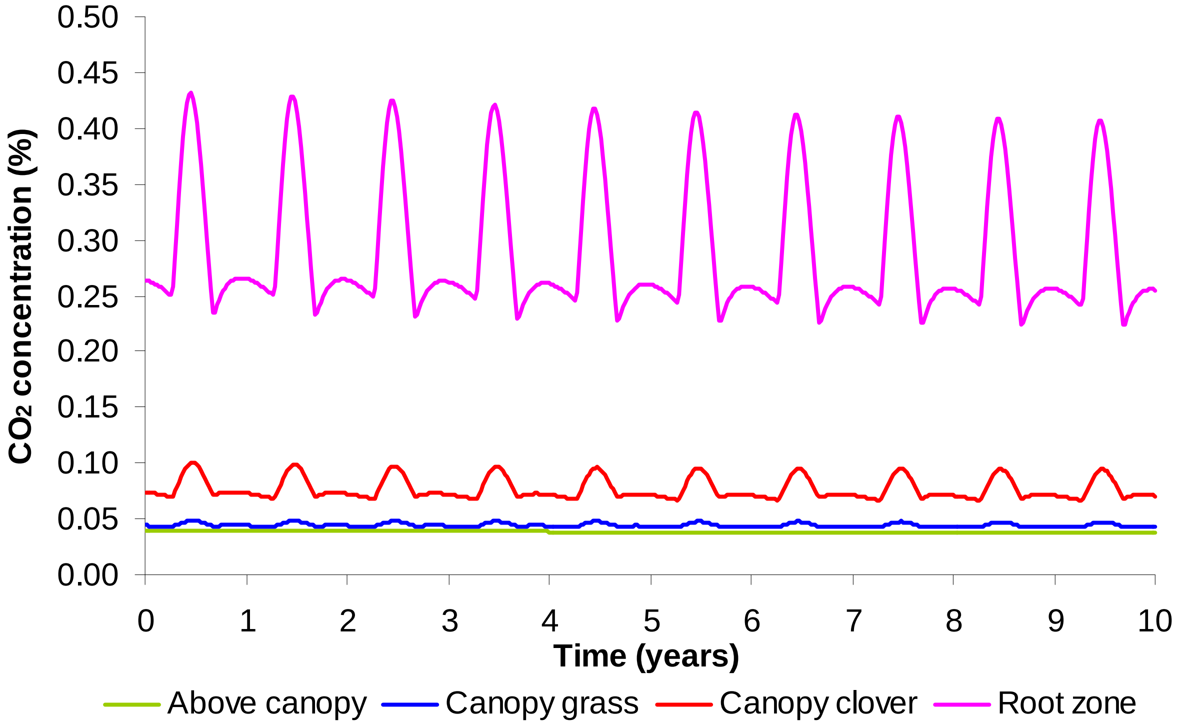

Figure 20 CO_2 concentration in the soil and in the canopy of grass and clover

5.2 BASE CASE WITH INJECTION

The focus of the first run is to simulate the plant die-off in the centre of the plot G8 where bare earth was recorded. The injection rate was set to 0.1 l/min as measured at the surface of subplot 13 (Table 3), which corresponds to the area of plant die-off (quadrat 1). This was preferred to the actual injection rate of 3 l/min as the injected CO_2 in the Player goes straight to the rooting zone, and remains the same at the surface. This record was chosen over the higher flux observed in subplot 8 for the following reasons a) the botanic and flux sampling quadrats match more closely (Figure 17) b) the flux in subplot 8 is not reliable as it went off the scale of the measuring device and c) a value closest to the minimum flux that leads to plant die-ff was sought.

Table 3 Observed CO_2 fluxes (l/min) in plot G8 in September. The blue and red cells correspond to the quadrats 1 and 2 respectively where there was plant die-off**.**

Col/Row	1	2	3	4	5
1	0.01	0.0075	0.0005	0.01	0.0075
2	0.01	**0.05**	**0.415**	0.0075	0.025
3	0.0125	**0.0225**	**0.1075**	0.0275	0.05
4	0.03	0.03	0.0625	0.0225	0.05
5	0.0075	0.015	0.015	0.01	0.01

The output from the Player is compared to the observed data for the time needed for plant biomass to reach zero or a very low value. The botanic survey showed that plant die-off occurred within 4 months and possibly in less than two as the flux two months prior the end of injection was still low (0.0075 l/min) in the centre of G8 compared to the flux measured in September. It is important to note that the flux was measured over a 0.005 m^2 area in the centre of each subplot and does not necessarily correspond to the location where die-off is observed in the 0.5 m^2 quadrat. Since the remaining part of the subplot was vegetated, the flux that corresponds to the plant die-off should be equal or bigger than the one measured. Thus if the model does not simulate plant die-off, this is not necessarily wrong.

The default values of the parameters were used. The run lasted ten years, with injection taking place during the first four years. Grass is assumed to cover 80% and clover 20% of the area.

The biomass of both plant species decreases steeply in the first year and more gradually in the following two years until it reaches a minimum after three years (Figure 21). Once injection ceases, biomass recovers fully within four years. The effect of CO_2 on plant height is similar to that on biomass (Figure 21).

The Player is able to represent the decline in biomass and height but not within the time observed in the field, nor does it predict full die-off. This suggests that the toxicity parameters need to be adjusted. It is also possible that the flux at the location of plant die-off was higher than the recorded flux.

The concentration of CO_2 in the canopy starts very high at 14% in clover and 2% in grass (Figure 23). It then decreases as the atmospheric concentration comes closer to the surface with decreasing plant height. Once the injection stops, the concentration drops to background levels.

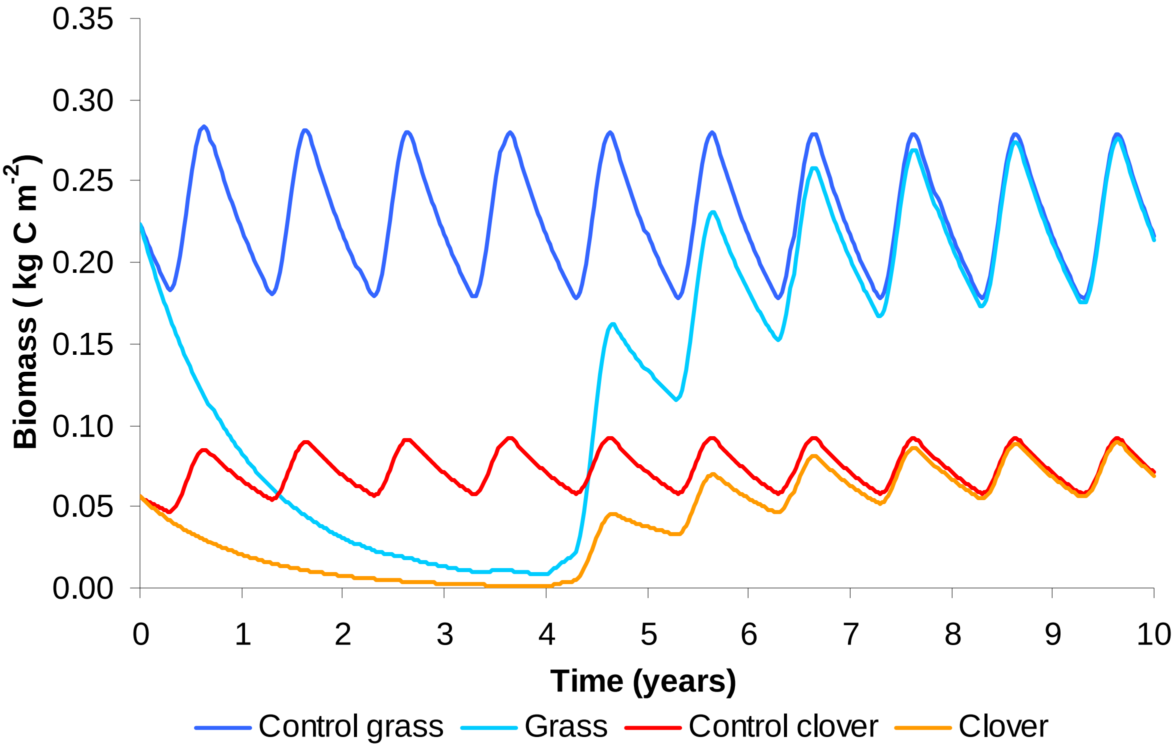

Figure 21 Comparison of biomass between grass and clover with (0.1 l/min) and without injection

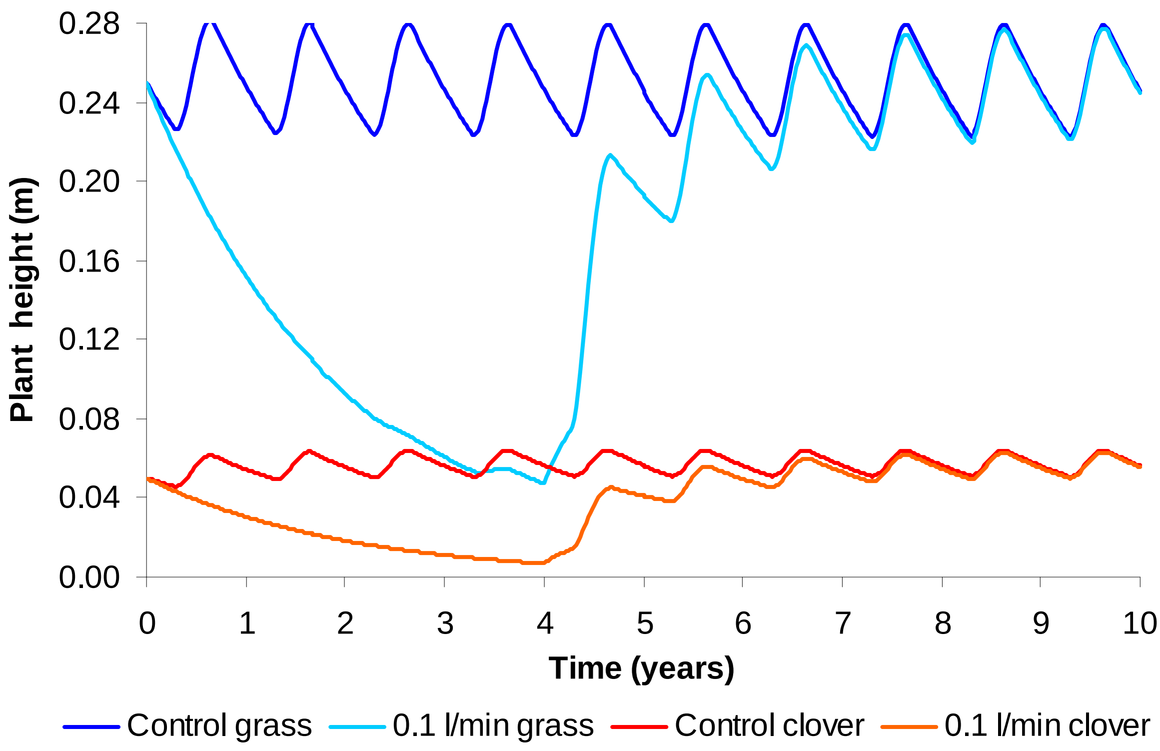

Figure 22 Comparison in height change between grass and clover with (0.1 l/min) and without injection

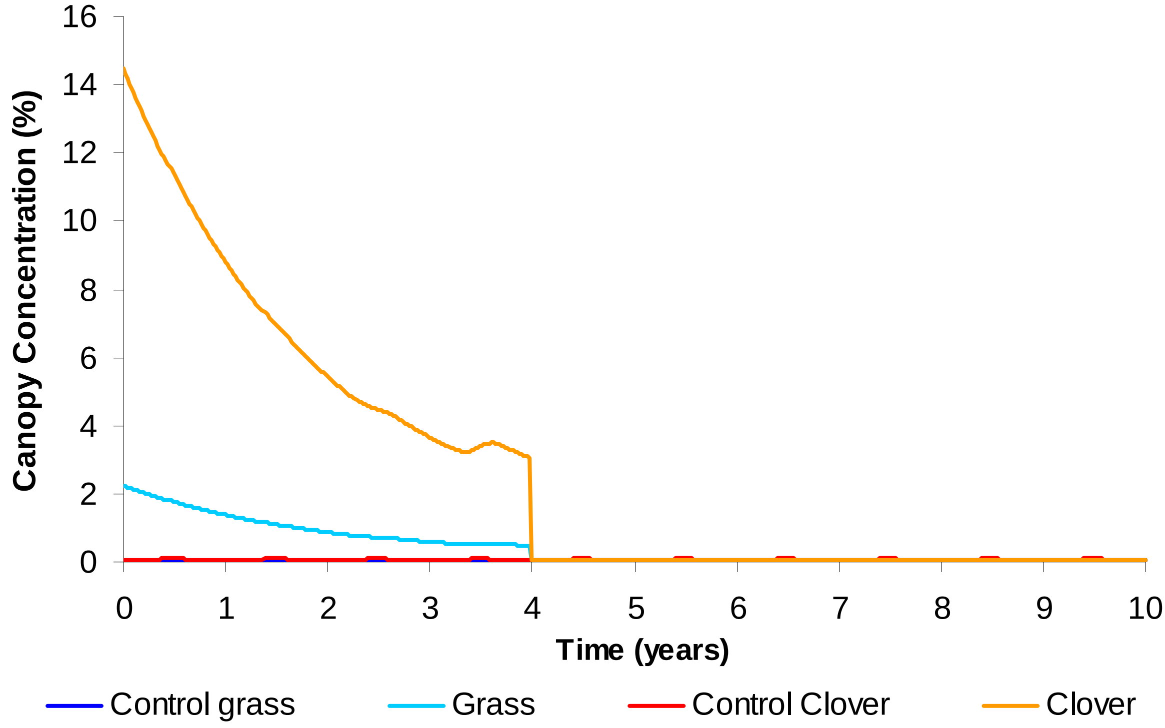

Figure 23 Comparison of CO_2 concentration in the canopy between grass and clover with (0.1 l/min) and without injection

In practice the aim would be to identify any amount of leakage from a storage site. Depending on the rate, this might lead to partial reduction or even an increase in biomass. A range of smaller injection rates are consequently investigated.

Grass shows insignificant effects at an injection rate of 0.0001 l/min, which corresponds to a 25% increase in the background flux (Figure 24). Fertilisation effects are calculated at 0.001 l/min, and at 0.01 l/min a decline in biomass is calculated. In comparison, clover shows considerable biomass reduction at 0.001 l/min (Figure 25). The effects at 0.01 l/min are as severe as for 0.1 l/min, suggesting that the worst effect is noticed at lower leakage rates than for grass. The most significant difference between the two plant species is at 0.01 l/min when the remaining biomass for grass and clover after 3.46 yrs, which corresponds to peak growth season, is 73% and 4% respectively (Table 4).

The Player output can be shown as a time series of percentage of biomass reduction for different leakages rates (Figure 26). This relationship could then be used in combination with remote sensing data to identify and quantify leakages from a storage site (Bateson et al., 2008). The need to have physical installations throughout the site could then be minimised.

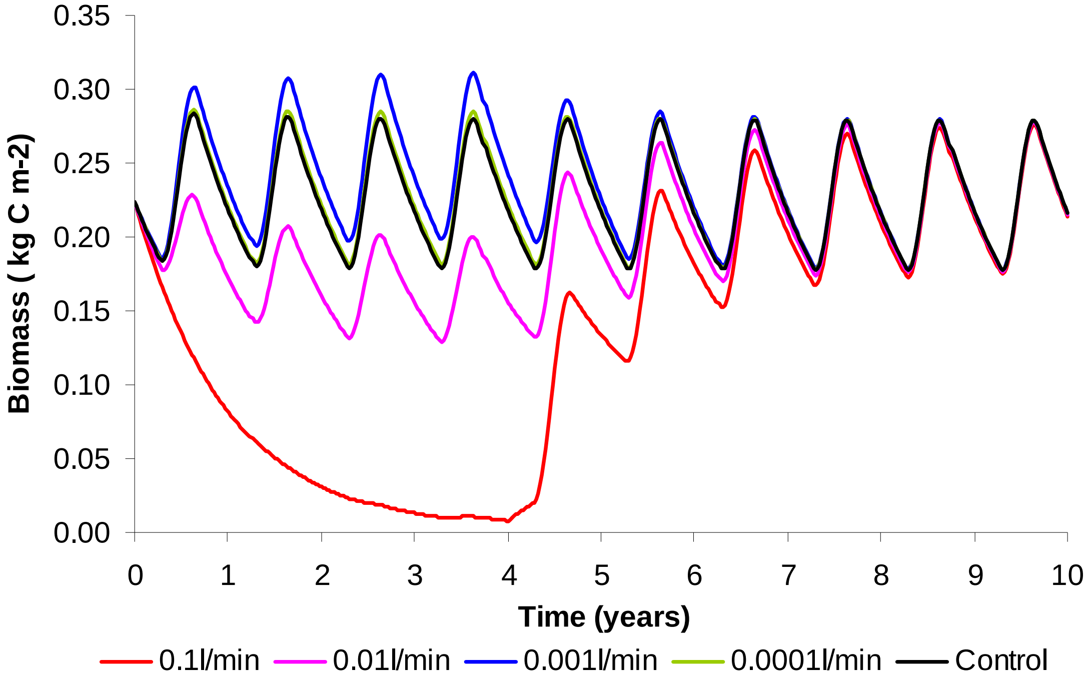

Figure 24 Impact of different injection rates on the biomass of grass.

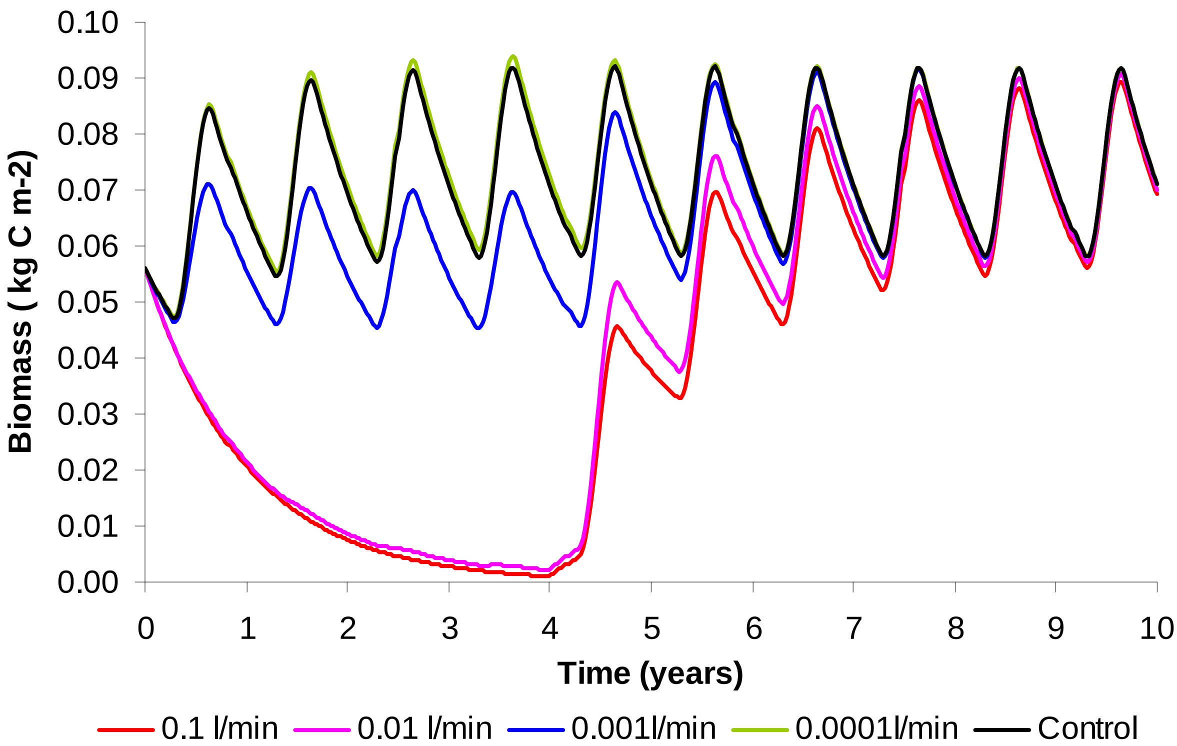

Figure 25 Impact of different injection rates on the biomass of clover

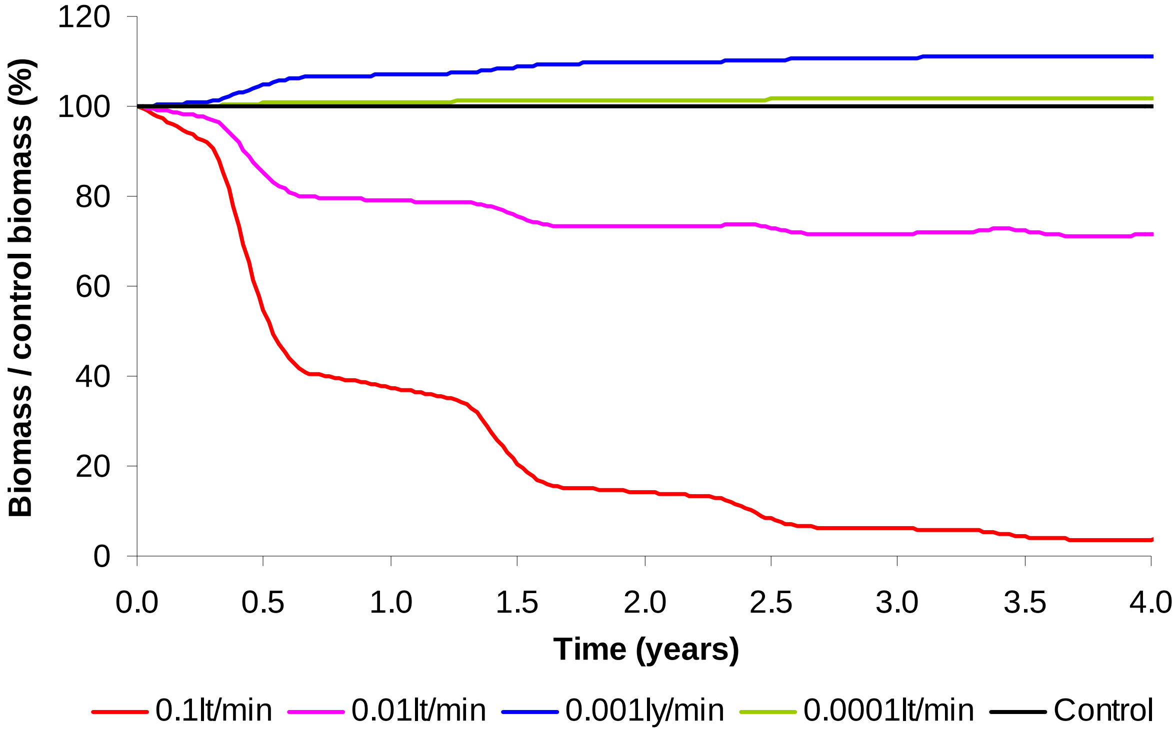

Figure 26 Standing biomass of grass as a percentage of biomass under no injection

Table 4 Model Output for biomass and biogenic flux for various injection rates after 3.46 years (high growth season)

Injected Flux	Biogenic Flux	Biogenic over Injected flux	Grass Biomass	Grass Biomass ratio	Clover Biomass	Clover Biomass ratio	$[CO_2]$ root Zone	$[CO_2]$ Canopy clover	$[CO_2]$ Canopy grass	$CO_2]$ above Canopy
l/min CO_2	l/min CO2	%	kg C m^{-2}	%	kg C m^{-2}	%	%	%	%	%
0	0.00042	NA	0.226	100.0	0.074	100.0	0.42	0.097	0.048	0.0385
0.0001	0.00043	4.26	0.229	101.6	0.076	102.4	0.52	0.111	0.050	0.0386
0.001	0.00043	0.43	0.250	110.9	0.057	77.6	1.35	0.259	0.072	0.0387
0.01	0.00029	0.03	0.164	72.7	0.003	4.1	9.10	1.613	0.232	0.0390
0.1	0.00015	0.00	0.010	4.6	0.002	2.4	75.94	3.348	0.530	0.0394

6 Future development of the ASGARD Player

6.1 AIM OF THE UPDATED PLAYER

The updated Player will aim to simulate the movement of CO_2 below the rooting zone in addition to the initial aim of representing the effect of CO_2 on plants. The data suggest that two thirds of the gas injected moves laterally and possibly downwards to the bedrock. This could explain why CO_2 concentrations above background were detected in the control plots. Data are available to calibrate the model.

6.2 MODEL CHANGES AND CONCEPTUAL MODEL

The proposed changes are the following:

- **Near surface processes**: inclusion of the QPAC near surface processes model
- **Model structure**
    - **a.** increase the modelled area to include all the BGS plots (G1-G10)
    - **b.** Modify how the user specifies the location of CO_2 injection. An import option from an ascii file might be the solution
- **Modification of the soil-plant model**
    - **a.** addition of bare earth as a third "species" in the input file for plant coverage
    - **b.** enable the more tolerant species to take over the space of the less sensitive species when this one dies
    - **c.** addition of advective flow in the rooting zone

The near surface processes will be initially modelled using a multiphase flow model. Once the processes are well understood, a simplified model will be created.

7 Input to discussions on the experimental design at ASGARD for the RISCS project

The QPAC Player is a valuable tool that can simulate the effect of CO_2 on plants. Within the RISCS project, the model could be improved and ultimately it could be applied to other sites as a prediction tool at storage sites contributing to the improvement of risk assessment. It will be necessary to calibrate the model and to understand better how CO_2 affects different parts of plants. While studies have shown that some species are more tolerant than others and have established concentration values above which plant die-off is observed, there is limited knowledge on which form of the CO_2 (gas or in solution) and which plant parts are more vulnerable. Controlled experiments are thus needed.

For this purpose, the following issues are relevant when establishing the experimental design at ASGARD for the RISCS project.

.

<u>Biomass/ Height measurements</u>

The Player calculates the effect of CO_2 on plants as biomass and height change. It is therefore necessary to measure the biomass or/and height of the species present on the field site.

Frequency of measurements
Data collected at more regular intervals, e.g. weekly, would allow the user/modeller to define the effect of CO_2 on plants in more detail.

Plant species of grassed plots
From the experiment it was possible to establish CO_2 concentrations above which plant die-off was observed. However, this was from limited samples and it was hard to quantify the differences between species. Such a relationship could be defined by controlling the plant species. For example, there could be three sets of plots, each set containing either clover, grass or mixed pasture. Where modifying the plant species is not an option, the difference in plant species response could be established if the CO_2 distribution at the surface was uniform. This would necessitate a different type of injection than currently installed at ASGARD, such as a circular slotted tube.

Injection rates
Small injection rates can lead to fertilisation or a slight decrease in plant biomass without plant die-off. Hence it would be useful to develop a relationship between CO_2 flux/concentration and effect on plants that could be achieved by injecting at different rates. An example of the possible experimental layout is shown below. If this is not possible, a relationship could still be established in single or two species plots, where a full range of CO_2 values can be observed.

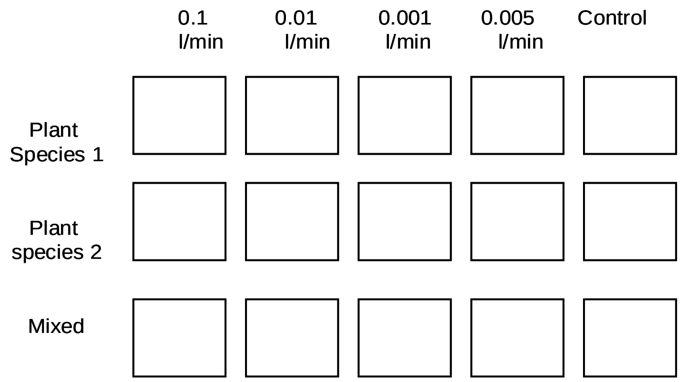

Figure 27 Example of possible experimental layout

Botanic measurement techniques
Where the CO_2 concentration at the surface is not uniform throughout a plot, it is recommended to collect the different types of data, such as botanic and CO2 concentration, based on the same sub-plotting method.

Distance between plots/ Vertical barriers
The migration of CO_2 from gassed to control plots should be avoided. This could be achieved by installing vertical barriers or potentially by increasing the distance between the plots. The latter has the following disadvantages a) it would use more space from the already limited size of the site and b) it will not prevent CO_2 from migrating laterally at the current site where there is a preferential lateral movement. Vertical barriers extending to the Mercia mudstone could deal with both of these issues and has the following added benefits: a) they would allow for CO_2 budget calculations within the soil zone and b) they could result in a more uniform or larger area with elevated CO_2 levels at the surface as the gas will be forced to move upward. Vertical barriers were used at ZERT, a similar experimental facility in the USA (Spangler et al, 2009), and expertise from that project could be sought.

Herbicide treatment

The application of herbicide on experimental plots should depend on what is represented. The application would be expected on plots aimed at replicating conditions on agricultural land, while it might not be necessary on plots representing pasture. The type of research will also influence the application or not of herbicides; microbiological studies might be constrained depending on the effect of the herbicide on the microbes.

Plot size

In plots that will remain as mixed pasture with a variety of plant species, the size of the plots should be big enough for the overall plant composition between plots to be similar. This would increase the confidence when comparing gassed and control plots. It would also allow CO_2 concentration to drop to background concentration at the edges of the plot.

Other parameter measurement

One key parameter in the model is soil moisture. This is currently assumed to be constant throughout the experiment, when in reality it is not. It is recommended to measure soil moisture content at various depths. This would allow more detailed modelling of plant growth and the effects of elevated levels of CO_2.
Other measurements that would be useful for the model calibration are concentration of CO_2 at the canopy and at the surface.

Lab experiment

For better control over some of the parameters, it might be necessary to conduct lab experiments. The CO_2 can, for example, be directly delivered to the plant and thus toxicity and fertilisation parameters more accurately calculated.

Appendix 1

Table 5 List of parameters within the soil-plant model.

[To be added]

References

British Geological Survey holds most of the references listed below, and copies may be obtained via the library service subject to copyright legislation (contact libuser@bgs.ac.uk for details). The library catalogue is available at: http://geolib.bgs.ac.uk.

BATESON L, VELLICO L, BEAUBIEN, SE, PEARCE, JM, ANNUNZIATELLIS, A, G. CIOTOLI, G, COREN, F, LOMBARDI, S and MARSH, S. 2008. The application of remote-sensing techniques to monitor CO2-storage sites for surface leakage: Method development and testing at Latera (Italy) where naturally produced CO2 is leaking to the atmosphere. *International Journal of Greenhouse Gas Control*, Vol. 2, 388-400.

BEAUBIEN, S E, CIOTOLI, G, COOMBS, P, DICTOR, M C, KRUGER, M, LOMBARDI, S, PEARCE, J M, and WEST, J M. 2008. The impact of a naturally occurring CO2 gas vent on the shallow ecosystem and soil chemistry of a Mediterranean pasture (Latera, Italy). *International Journal of Greenhouse Gas Control*, Vo. 2, Issue 3, 373-387.

INTERGOVERNMENTAL PANEL ON CLIMATE CHANGE (IPCC), B. Metz, O..Davidson, J.C. de Coninck, M. Loos, M. and L. A. Meyer, (eds.) (2005) IPCC Special Report on Carbon Dioxide Capture and Storage, *Cambridge University Press, Cambridge, UK and New York, USA*. 442pp.

LIMER, L M C, MAUL, P R, and THORNE, M C 2008. A Soil-plant Model for the Latera Site. Quintessa Report QRS-1220B-2 version 1.0.

MAUL, P, BEAUBIEN, S E, BOND, A, LIMER, L, LOMBARDI, S, PEARCE, J, THORNE, C, and WEST, J. 2009. Modelling the fate of carbon dioxide in the near-surface environment at the Latera natural analogue site. *Energy Procedia*, Vol 1, 1879-1885.

MAUL, P, BOND, A, LIMER, L and THORNE, M. 2008. System-Level Modelling for the Latera site: Final Report. *Quintessa Report* QRS-1320B-3 version 1.0.

SPANGLER, L H, DOBECK, L M, REPASKY, K, NEHRIR, A, HUMPHRIES, S, BARR, J, KEITH, C, SHAW, J, ROUSE, J, CUNNINGHAM, A, BENSON, S, OLDENBURG, C M, LEWICKI, J L, WELLS, W, DIEHL, R, STRAZIZAR, B, FESSENDEN, J, RAHN, T, AMONETTE, J, BARR, J, PICKLES, W, JACOBSON, J, SILVER, E, MALE, E, RAUCH, H, GULLICKSON, K, TRAUTZ, R, KHARAKA, Y, BIRKHOLZER, J and WIELOPOLSKI, L. 2009. A controlled field pilot for testing near surface CO_2 detection techniques and transport models. *Energy Procedia*, Vol. 1, 2143-2150.

WEST, J M, PEARCE, J M, COOMBS, P, FORD, J R, SCHEIB, C, COLLS, J J, SMITH, K L and STEVEN, M D. 2009. The impact of controlled injection of CO2 on the soil ecosystem and chemistry of an English lowland pasture. *Energy Procedia*, Vol 1, 1863-1870.

WEST, J M. (Ed.). 2007. Ecosystem responses to CO_2 leakage–Model approach. Final Report: Feasibility study to set up European Test Facilities for studying impacts on Terrestrial and Marine Ecosystems and on Human Health (Joint Research Activity 4). IA-4 Joint Research Development Deliverable Report. *CO_2 GeoNet Report.*