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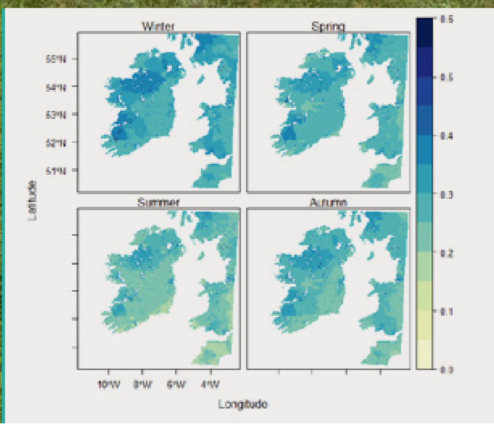
epa Research

SoMoSAT – Soil Moisture Estimates from Satellite-based Earth Observations

Authors: Rowan Fealy, Tim McCarthy, Rafale De Andrade Moral, Ajay Sathiyan Nair, Dazhi Li, Kazeem Ishola, Reamonn Fealy and Lilian O'Sullivan



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Rialtas na hÉireann
Government of Ireland

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2. Office of Environmental Enforcement
3. Office of Evidence and Assessment
4. Office of Radiation Protection and Environmental Monitoring
5. Office of Communications and Corporate Services

The EPA is assisted by advisory committees who meet regularly to discuss issues of concern and provide advice to the Board.

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Identifying pressures

In spite of the recognised importance of soil moisture interactions for climate, and their relevance for understanding hydrological, agricultural and ecological processes, there is a paucity of soil water observations globally. Even at the regional and country scale, only limited observations are available, and many of these are limited in duration and/or extent. As a consequence, alternative techniques have been developed to derive estimates of soil moisture, including water balance-based approaches, the use of remotely sensed information and the application of land surface modelling techniques. Water balance-based approaches are typical at the catchment scale, while remote sensing and land surface modelling techniques have been employed to generate global/regional soil moisture estimates. While remote sensing-based methods offer potential for monitoring, significant uncertainties remain concerning retrieval algorithms and monitoring locations with dense vegetation cover and organic soils. At present, they are also limited to a daily temporal resolution. Machine learning techniques, which can address issues around the use of single sensor-based approaches, have been successfully employed to derive high-resolution soil moisture estimates and represent a novel approach to complement existing techniques.

Informing policy

Soil moisture is classified as an essential climate variable and is an essential parameter for use in a range of applications, including groundwater resource estimation, catchment-scale rainfall run-off and flood estimation/management, ecosystem productivity, nutrient transport management and modelling, crop production, and land surface and climate modelling. Nationally, this research will inform policy development and implementation in support of catchment monitoring and management, groundwater resource estimation and catchment-scale nutrient or contaminant modelling. More broadly, the research will also support the wider research and stakeholder community through the provision of a gridded soil moisture product for Ireland. A key output from the research was the deployment of a number of *in situ* soil moisture sensors, which will support a national initiative to deploy an integrated network of soil moisture sensors across Ireland – coordinated through the Irish Soil Moisture Observation Network.

Developing solutions

The research addresses a number of shortcomings associated with the use of existing remote sensing derived soil moisture estimates. A machine learning technique, random forest, was employed to downscale the European Space Agency's Climate Change Initiative combined data product, representing both active and passive sensors, to derive a harmonised soil moisture product for Ireland. While the combined global soil moisture product represents the current state of the art in generating a global-scale soil moisture product, the resolution of the data, ~25 km, is too coarse for most applications. The machine learning model was found to largely reproduce the available soil moisture measurements, based on independent tests of the model. A land surface model was also employed to generate estimates of soil moisture for Ireland, using forcing data obtained from the European Centre for Medium-Range Weather Forecast. A key advantage of the land surface model is its ability to generate model estimates of soil moisture over various soil depths, in contrast to satellite-derived estimates, which are limited to the top 2–5 cm. Consideration should be given to the operational deployment of both models for use in generating soil moisture estimates in near real time.

EPA RESEARCH PROGRAMME 2021–2030

SoMoSAT – Soil Moisture Estimates from Satellite-based Earth Observations

(2019-CCRP-MS.66)

EPA Research Report

Prepared for the Environmental Protection Agency

by

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This report is based on research carried out/data from June 2020 to October 2022. More recent data may have become available since the research was completed.

The EPA Research Programme addresses the need for research in Ireland to inform policymakers and other stakeholders on a range of questions in relation to environmental protection. These reports are intended as contributions to the necessary debate on the protection of the environment.

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Executive Summary

Soil moisture is classified as an essential climate variable and is an essential parameter for use in a range of applications, including groundwater resource estimation; catchment-scale rainfall run-off and flood estimation/management; habitat mapping and ecosystem productivity estimation; nutrient transport management and modelling; and crop production and land surface and climate modelling. In spite of its importance, direct observations of soil moisture are very limited globally – those that exist are typically of limited duration and spatial extent. Consequently, alternative approaches for estimating soil moisture have been developed, including water balance models, the use of remotely sensed information (e.g. from the European Space Agency/Copernicus) and the application of land surface modelling techniques. While spaceborne methods and methods based on land surface modelling offer significant potential for monitoring and modelling soil moisture at national and sub-national scales, their resolution is currently in the order of tens of kilometres. The research outlined here sought to develop a novel data platform to ingest, analyse and fuse multi-thematic and multi-temporal Earth observation data streams, to derive high-spatial-resolution estimates of soil moisture for Ireland. The methodology incorporates spaceborne, geospatial and *in situ* data using novel machine learning techniques to derive a single harmonised product suitable for use in a range of applications.

Outputs from this research will inform the strategic development of a national monitoring programme and generate a harmonised high-resolution soil moisture product to underpin applications in a range of areas, including catchment management and sustainable land use management. The research will help Ireland to meet its international reporting obligations under the United Nations Framework Convention on Climate Change, through improved land use and soil respiration modelling, and support the development and implementation of other national policies in line with, for example, the EU Water Framework Directive and the Nitrates Directive. The outputs could also support the development of indicators for Ireland’s national Land Use Review.

1 Introduction

1.1 Context

Understanding the interactions and feedback between the land surface and the atmosphere is a focus of international research efforts; much of the recent effort has been directed towards developing a more comprehensive understanding of the role of soil moisture in modulating climate variability on various spatial and temporal scales. Water retained on, or within, the land surface as soil moisture – defined as the total amount of water, including water vapour, in an unsaturated soil (AMS, 2022) – acts to limit evaporation, and therefore the subsequent partitioning of available energy, into sensible and latent heat (Bowen ratio) (e.g. Ishola *et al.*, 2020), and of moisture into evaporated moisture and run-off. The partitioning of energy received at the surface directly influences the development and stability of the atmospheric boundary layer (deep/well mixed; shallow, moist). The importance of soil moisture in limiting evaporation is particularly evident during periods of prolonged high or extreme temperatures experienced over soil moisture-limited regimes; available energy is preferentially channelled into sensible heat, which can act to amplify the initial temperature response (moisture-limited regime). This is in contrast to a well-watered site, where available energy is primarily dissipated from the surface through latent heat exchanges (energy-limited regime). Depending on the initial perturbation, for example a wet or dry anomaly, soil moisture can also retain a "memory" of past weather events and can therefore lead to persistence in the climate system (Seneviratne *et al*., 2010). Soil moisture also influences the partitioning of precipitation into run-off and evaporation, with consequences for river discharge and, in particular, flooding and timing of peak flow.

Over vegetated land surfaces, the transfer of soil water to the atmosphere is primarily through transpiration or evaporation of water from leaves through plant stomata. Plants regulate water (and carbon) transfer through their stomatal apertures. Stomata close during times of water stress, but, when there is a plentiful supply of water and plants are growing, the stomata are open and gases (including water vapour and CO_2) are exchanged in the process of photosynthesis. Consequently, plant CO_2 uptake is directly related to soil moisture. High temperatures, when coupled with reduced soil moisture availability, have a significant impact on ecosystem productivity, primarily reflected by reduced primary production (Ciais *et al*., 2005; Bastos *et al*., 2014), with impacts on plant and soil (autotrophic and heterotrophic) respiration and the carbon balance (Reichstein *et al*., 2013).

Regions can also switch between moisture-limited and energy-limited regimes over the course of a year or depending on land cover (Seneviratne *et al*., 2010); for example, Ireland has a maritime temperate climate with ample year-round precipitation, yet frequently experiences seasonal soil moisture deficits typically associated with those locations defined as having well-drained soil characteristics (and seasonally water limited). Climate change is likely to result in increased sensitivity (drying, altered energy balance, etc.) in locations that already experience seasonal soil moisture deficits and result in new areas becoming exposed (Seneviratne *et al*., 2010). While Ireland does not experience the extremes in temperature associated with continental Europe, it is subject to the occurrence of rainfall extremes, particularly droughts (Noone *et al.*, 2017), the frequency and magnitude of which are also projected to increase globally by the end of the century (Seneviratne *et al*., 2012). These changes, if realised (e.g. Fealy *et al*., 2018), will have consequences for ecosystems in Ireland, with the role of drought stress, rather than heat stress, having been highlighted as the primary factor in limiting ecosystem productivity (De Boeck *et al.*, 2011).

In spite of the recognised importance of soil moisture interactions for climate, and the relevance of these interactions for understanding hydrological, agricultural and ecological processes, there is a paucity of soil water observations globally (Figure 1.1). This is for a variety of reasons: soil moisture often falls between administrative boundaries (meteorology and hydrology); the cost and maintenance requirements of instrumentation; and the heterogeneity of soil moisture, which makes it difficult to obtain representative measurements (point versus areal), etc. Outside of

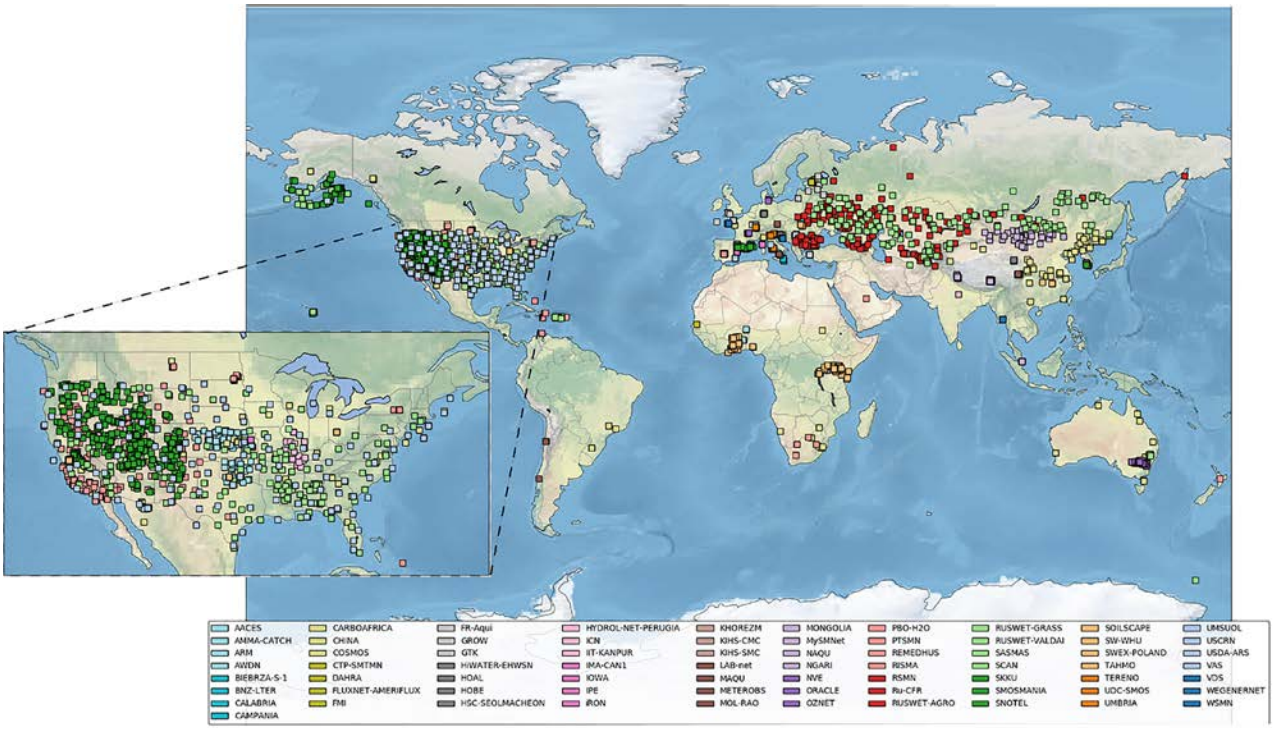

Figure 1.1. Sites listed in the International Soil Moisture Network. Reproduced from Dorigo *et al*. (2021); licensed under CC BY-NC-ND 4.0 DEED (https://creativecommons.org/licenses/by-nc-nd/4.0/).

a handful of countries, including the USA and the UK, few have established soil moisture monitoring networks; where data are available, they are often limited in duration and/or extent. Citizen science or crowdsourcing efforts have attempted to fill this gap – for example, the GROW Observatory is a citizen science initiative that aims to establish a network of low-cost sensors across Europe. Similar initiatives have been developed in the USA (the GLOBE Programme), Iran (e.g. Karamouz *et al*., 2021), Ethiopia (Rigler *et al*., 2022) and elsewhere. While such initiatives are very positive in terms of engaging citizens, they can also generate a large volume of data. In an analysis of the GROW Observatory data, Xaver *et al*. (2020) found that, while good agreement existed between the low-cost sensors and data from more costly, scientific instruments across a range of metrics, the temporal stability of the low-cost probes was found to be lower.

In response to the paucity of *in situ* soil moisture measurements, a variety of approaches have been developed to acquire, or derive estimates of, soil moisture data, including satellite-based measurements (e.g. Soil Moisture Active Passive (SMAP), Advanced Microwave Scanning Radiometer 2 (AMSR2), Soil Moisture and Ocean Salinity (SMOS), Advanced Scatterometer (ASCAT)) (e.g. Dorigo *et al*., 2017); empirical or process-based water balance approaches (e.g. soil moisture deficit model; Schulte *et al*., 2005); soil–vegetation–atmosphere transfer models (e.g. Kurnik *et al*., 2014); and land surface modelling techniques (e.g. Santanello *et al*., 2016) (Table 1.1). Water balance-based approaches are typical at the catchment scale, where the catchment represents a bounded box with measurable inputs (e.g. rainfall) and outputs (e.g. evapotranspiration; streamflow), while remote-sensing and land surface modelling techniques have been employed to generate global, continental or regional datasets (satellite-based measurements: surface soil moisture 0–5 cm; land surface modelling: soil profile over soil layers), typically at coarse spatial and/or temporal resolutions (Table 1.1). While spaceborne methods offer good potential for monitoring (e.g. drying/wetting), significant uncertainties remain with regard to retrieval algorithms and in locations with dense vegetation cover and organic soils (Dorigo *et al*., 2017). At present, these methods are also typically limited to a daily temporal resolution. While land surface models (LSMs) provide an opportunity to simulate soil moisture at sub-daily temporal resolution through the soil column, the accuracy of these approaches has been found to be

Table 1.1. Selection of global soil moisture products (direct retrieval, merged, modelled) covering up to the present day

Institution or reference	Product	Technique	Spatial resolution	Temporal resolution
NASA	SMAP	Satellite direct retrieval	3, 9, 36 km	1–2 days
NASA	SMAP and Sentinel-1	Satellite direct and merged	1–3 km	1–2 days
BEC	SMOS	Satellite direct retrieval	25 km	Daily
EUMETSAT	ASCAT	Satellite direct retrieval	12.5, 25, 50 km	1–2 days
NASA	AMSR2	Satellite direct retrieval	25 km	Daily
ESA	CCI SM product	Merged active and passive sensors	~25 km (0.25°)	Daily
NOAA	SMOPS	Derived from multi-satellites and sensors	~25 km (0.25°)	6 hourly
NASA	GLDAS	Data assimilation with LSM	~25 km (0.25°)	3 hourly
Sungmin and Orth (2021)	SoMo.ml	Machine learning trained on *in situ* data, scaled using ERA5	~25 km (0.25°)	Daily

This is not an exhaustive list of soil moisture products. See Karthikeyan *et al.* (2017a), Liu *et al.* (2020) and Peng *et al.* (2021) for a more detailed listing and review of soil moisture products.

BEC, Barcelona Expert Centre; CCI SM, Climate Change Initiative Soil Moisture; ESA, European Space Agency; EUMETSAT, European Organisation for the Exploitation of Meteorological Satellites; GLDAS, Global Land Data Assimilation System; NOAA, National Oceanic and Atmospheric Administration; SMOPS, Soil Moisture Operational Products System.

dependent on the quality of the boundary or forcing meteorological datasets and the physical descriptors of the landscape employed (e.g. soil hydraulic parameters). The assimilation of remotely sensed soil moisture estimates into an LSM has been identified as one potential way to overcome the limitations in both approaches and increase the skill of the model in land data assimilation estimates of soil moisture (e.g. Liu *et al.*, 2011; Albergel *et al.,* 2017).

To achieve any skill increase, reliable satellite soil moisture estimates are essential for assimilation into the LSM. To address the coarser spatial resolution, and other issues, associated with satellite-derived products, Carlson *et al.* (1994) exploited the relationship between surface soil water content and satellite-derived thermal data and Normalised Difference Vegetation Index (NDVI) data (e.g. Taktikou *et al.*, 2016; Zhang and Zhou, 2016). More recently, high-resolution (10 m^2) data from the Sentinel-1 platform of the European Space Agency (ESA) have been employed in a number of studies (e.g. Pulvirenti *et al.*, 2018; Greifeneder *et al.*, 2019), including in combination with NDVI data and information on thermal/brightness (e.g. Alexakis *et al.*, 2017) and land surface features, including surface topography and roughness. While high-resolution Sentinel data are valuable for a spatial evaluation of soil moisture, revisit times are > 1 day. The use of statistical and data-driven approaches (e.g. Rodriguex-Fernandex *et al.*, 2015) to combine data from both active (e.g. scatterometer) and passive (e.g. radiometers) satellite sensors to derive soil moisture estimates of high spatial and/or temporal resolution (e.g. Kolassa *et al.*, 2017) has become increasingly more widespread. These combined or merged data products can address the complexity and issues associated with the use of a single satellite or sensor and have been shown to generally outperform single-sensor-based approaches (e.g. Dorigo *et al.*, 2017). Satellite downscaling techniques (regionalisation), using machine learning (ML), have also been employed (e.g. Mohanty, 2013) to estimate sub-grid-scale soil moisture, and their use has become widespread in recent years for estimating soil moisture at global (e.g. Sungmin and Orth, 2021), regional and local scales (e.g. Zappa *et al.*, 2019; Kovačević *et al.*; 2020; Liu *et al.*, 2020), as they have been found to perform as well as or better than other techniques (Sabaghy *et al.*, 2018) (Chapter 2).

1.2 Research Objectives

Here, we sought to evaluate, and subsequently utilise, a suitable approach or approaches for employing the available large number of multi-thematic and multi-temporal Earth observation data and available *in situ* data to derive high-resolution spatial estimates of soil moisture for Ireland.

To achieve this, the following key objectives were identified:

- Undertake a review and assessment of existing and potential new methodologies (e.g. artificial intelligence (AI)/ML; land surface modelling) for use in deriving high-resolution soil moisture estimates, recognising challenges in terms of soil, climate, topography and vegetation.
- Review and collate relevant Earth observation, meteorological and land cover data and available soil moisture measurements.
- Implement and evaluate the selected methodological approaches.
- Develop a user-friendly web-based portal to provide easy access to the model outputs.

A number of challenges existed in this regard. Ireland does not currently have an *in situ* network for monitoring soil moisture akin to the comprehensive meteorological or hydrological networks that exist in this country and elsewhere; soil moisture measurements that do exist have typically been obtained as part of short-term (~< 3–5 years) eddy covariance measurements from specific land cover types (e.g. grass, arable land). Consequently, soil moisture measurements that are available are limited in extent, representation (e.g. land cover, soil type) and duration. In addition, the availability of suitable optical and thermal satellite-based information is limited by cloud coverage in Ireland, restricting the type of study (e.g. time-limited spatial evaluation over available scenes; reliance on products derived from optical-based satellite platforms) or satellite platform (e.g. use of satellite-based cloud-penetrating radar). However, the availability of merged active and passive microwave satellite data products (e.g. the ESA Climate Change Initiative (CCI) Soil Moisture (SM) product), which are insensitive to cloud cover, provides a potential way forward.

In recognition of the importance of soil moisture measurements and the absence of such a network in Ireland, a number of initiatives have been developed for deploying soil moisture instruments. For example, Terrain-AI, a strategic partnership programme funded through Science Foundation Ireland and Microsoft, deployed a number of time domain reflectometer (TDR) soil moisture probes, which are co-located with the existing meteorological or National Agricultural Soil Carbon Observatory (NASCO) flux tower networks funded by the Department of Agriculture, Food and the Marine (DAFM). Similarly, University College Dublin and Met Éireann, as part of the Joint Working Group on Applied Agricultural Meteorology (AGMET) community and funded by DAFM, have deployed cosmic ray neutron sensor (CRNS) instruments for determining spatial estimates of soil moisture based on the sensor footprint. As part of the research outlined here, TDR sensors were deployed to complement the growing network of *in situ* soil moisture sensors. While each of these deployments is being undertaken as part of separate funded research initiatives, the siting of instruments is being coordinated between the various projects, to ensure that an optimum network design can be implemented (e.g. the Irish Soil Moisture Observation Network (ISMON); Daly *et al*., 2021) (Figure 1.2). The intent is that the sensors deployed will continue beyond the lifetime of the individual funded projects and ultimately contribute to establishing a long-term soil moisture monitoring network in Ireland.

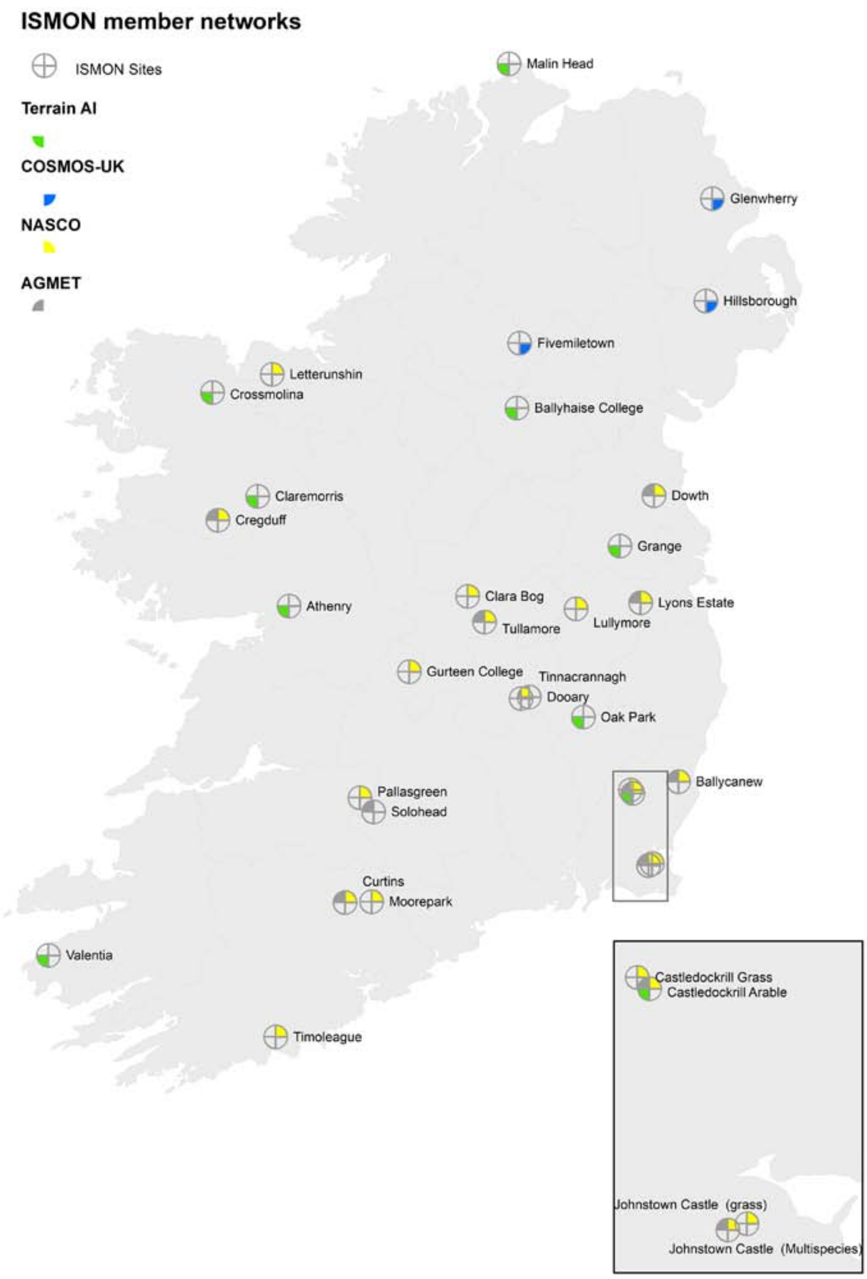

Figure 1.2. Map of soil moisture sensors deployed by Terrain-AI/EPA SoMoSAT, AGMET and NASCO, including the UK Cosmic-ray Soil Moisture Monitoring Network (COSMOS-UK) sites for Northern Ireland, and operating under the ISMON umbrella. Source: Daly *et al*. (2021); figure produced by S. Green.

2 Review

2.1 Context

Earth observation data, and in particular spaceborne satellite data, can provide an essential contribution to and complement the *in situ* monitoring of essential climate variables because of the large area/swath coverage and overpass times. While such data are not a replacement for direct *in situ* observations, if suitably evaluated, they are complementary and offer the potential to deliver outputs suitable for use in a wide range of applications. A variety of approaches exist in this regard, ranging from the use of optical and thermal data to microwave data or the combination of both optical and radar data. Petropoulos *et al*. (2015), in their review, provided a comprehensive synthesis of 20 years of efforts to utilise Earth observation data from satellite platforms to estimate surface soil moisture, including optical, passive and active microwave and combined methods. In general, while optical methods were found to provide good spatial resolution and benefit from the potential to employ multiple satellite platforms, their use can be compromised by issues related to cloud cover, high vegetation cover and atmospheric attenuation. Similar issues, related to cloud and vegetation cover, can affect thermal infrared-based approaches, which have the added limitation of lower revisit times and consequently lower temporal resolution.

The use of passive (radiometer) and active (radar) microwave-based approaches offers a number of advantages: the backscatter or brightness temperature is directly related to soil moisture, and these approaches are not limited by cloud cover. Algorithms employed for both passive and active microwave sensors, required to convert the signal (e.g. brightness temperature from passive sensors; radar backscatter from active sensors) into a surface soil moisture response, are directly influenced by the soil's dielectric properties, which provides a direct proxy for surface soil moisture (Engman and Chauhan, 1995; Karthikeyan *et al*., 2017a). However, microwave-based approaches are subject to attenuation by the atmosphere and vegetation, particularly at higher frequencies, and by interference from human microwave sources (Peng *et al*., 2021). Rainfall events can also make it difficult or impossible to separate the 'soil moisture' signal from noise (Karthikeyan *et al*., 2017a). While the temporal resolution of both passive and active microwave sensors is typically low, there is a marked difference in the spatial resolution between passive and active sensors. For example, the current spatial resolution of passive sensors employed for estimating soil moisture is in the order of 25 km or greater, whereas the ESA Sentinel-1 synthetic aperture radar (SAR) data have a spatial resolution in the order of 20 m (C Band SAR).

2.2 Overview of Methods

2.2.1 Triangle method

In an early application of satellite data to estimate surface soil moisture, Carlson *et al*. (1994) employed a soil–vegetation–atmosphere transfer (SVAT) model with surface radiant temperature and NDVI data, derived from the NOAA-11 satellite operated by the National Oceanic and Atmospheric Administration, over an agricultural watershed in Pennsylvania, USA. Following the removal of cloudy pixels and selection of low-relief areas, their analysis was confined to two dates in July (7 and 18 July 1990). They found that the model generated outputs that were "qualitatively realistic" in terms of the spatial distribution but highlighted the impact of high fractional vegetation amounts. This approach, which is referred to as the trapezoid or triangle method, is based on an interpretation of the relationship between a remotely sensed vegetation index and surface temperature, which when plotted resembles a triangle. The triangle method has been widely applied to estimate soil moisture; however, the approach has a number of recognised limitations.

More recent efforts have focused on the use of the physically based Optical Trapezoid Model (OPTRAM), proposed by Sadeghi *et al*. (2017), which employs shortwave infrared transformed reflectance and NDVI data to estimate soil moisture. OPTRAM was developed to address limitations with the trapezoid or triangle model, which requires satellite-based thermal data and calibration for each observation date.

OPTRAM has been validated with data from a range of satellite platforms, including Landsat-8, Moderate Resolution Imaging Spectroradiometer (MODIS) and Sentinel-2, and for different climate conditions (Babaeian *et al.*, 2019). Babaeian *et al.* (2019) utilised OPTRAM, but replaced NDVI with the Soil Adjusted Vegetation Index, to estimate soil moisture at the field scale. The OPTRAM outputs, which were compared with outputs from TDR soil probes, were found to largely reproduce the measured values and spatial variation in soil moisture, attributed to the high-resolution imagery employed.

2.2.2 Water Cloud Model

The Water Cloud Model, originally developed by Attema and Ulaby (1978), is a widely used semi-empirical model applied to estimate soil moisture over vegetated areas (Figure 2.1). It employs vegetation descriptors, such as the NDVI or Leaf Area Index (LAI), to account for the impact of vegetation on radar backscatter and assumes that only soil moisture varies in the period of interest; all other parameters, such as vegetation water content and soil surface roughness, are assumed to be sufficiently time invariant. However, agricultural practices associated with vegetation dynamics, ploughing and rainfall events smoothen soil roughness and the vegetation dielectric constant, which led Sabaghy *et al*. (2018) to conclude that obtaining soil moisture estimates from radar backscatter remains challenging. Moreover, satellite data can be used to estimate soil moisture in only the first few centimetres of the soil layer.

2.2.3 Regionalisation or downscaling approaches

A variety of statistical and ML-based approaches have been developed to downscale or regionalise the various coarse-resolution soil moisture products (e.g. Table 1.1) to higher spatial resolutions. Conceptually, statistical downscaling approaches have a long history of development and have found widespread application in the environmental sciences, particularly in climate science, where a range of techniques have been developed to downscale coarse-resolution information from global climate models to the regional or local scale. Methods,

Figure 2.1. Modified Water Cloud Model framework based on ESA Sentinel-1 SAR and Landsat-8 Optical Land Imager data. This figure was published in *International Journal of Applied Earth Observation and Geoinformation*, Vol 72, Bao *et al.*, Surface soil moisture retrievals over partially vegetated areas from the synergy of Sentinel-1 and Landsat 8 data using a modified water-cloud model, Pages 76–85, Copyright Elsevier (2018).

which include those from ordinary linear regression to ML-based neural networks, are predicated on the assumption that a relationship can be established between a coarse-scale predictor and the regional- or local-scale phenomenon of interest. For soil moisture estimation, the inclusion of ancillary predictor variables that characterise the local or site-specific geographical context (e.g. elevation, slope, soil texture, etc.) has been highlighted as important (e.g. Werbylo and Niemann, 2014; Peng *et al*., 2017). Ultimately, the selection of a parsimonious suite of predictors or covariates, selected on the basis of representing physical processes and/or having statistical relevance, is a pragmatic choice when downscaling. In the context of downscaling soil moisture from coarse-scale estimates of soil moisture, the relationship can be expressed as follows:

$$\text{Soil moisture}_{\textit{in situ}} = f_{(\text{Soil moisture (coarse), Meteorology (high res.), Topography (high res.), Vegetation (high res.), Soil texture (high res.), ...})} \quad (2.1)$$

where Soil moisture$_{\textit{in situ}}$ is the measured response variable of interest; Soil moisture (coarse) represents the resolution of the gridded soil moisture product to be downscaled or regionalised; and high res. (or high resolution) is the common resolution of the ancillary covariates and represents the required spatial resolution of the downscaled soil moisture. Schematically, the method is represented as shown in Figure 2.2.

A variety of statistical techniques can be used to quantify the relationship between the measured *in situ* soil moisture and a suite of covariates; statistical ML methods have been found to outperform many other techniques (Zappa *et al*., 2019; after Sabaghy *et al*., 2018). While numerous ML methods can be used for prediction or classification, of these the random forest (RF) method (Breiman, 2001) is one of the most popular and widespread method employed because of its ability to model non-linear relationships and minimise the potential for overfitting (Zappa *et al*., 2019).

2.2.4 Land surface modelling

As an alternative to the satellite-based methods, catchment-based hydrological models and LSMs have found widespread application in estimating soil moisture. While hydrological models typically simulate the water balance on the catchment or response-unit scale, based on a prescribed set of forcings, LSMs dynamically resolve the energy and water fluxes on a discretised grid, and can be point, catchment, landscape or global in scale. Fundamentally, the governing equations employed to estimate the water balance in both approaches are similar (Brocca *et al*., 2017). In the absence of globally observed soil moisture datasets, LSMs informed by observed meteorology (including reanalysis data) were employed to fill the observation gap (Senevirante *et al*., 2010). This led to the development of initiatives such as the Global Land Data Assimilation System (GLDAS). While outputs from GLDAS remain coarse (1°; 0.25°), the project has generated an archive of long-term simulated soil moisture datasets, including a suite of land surface fluxes, from a variety of different LSMs, including NOAH, community land model (CLM),

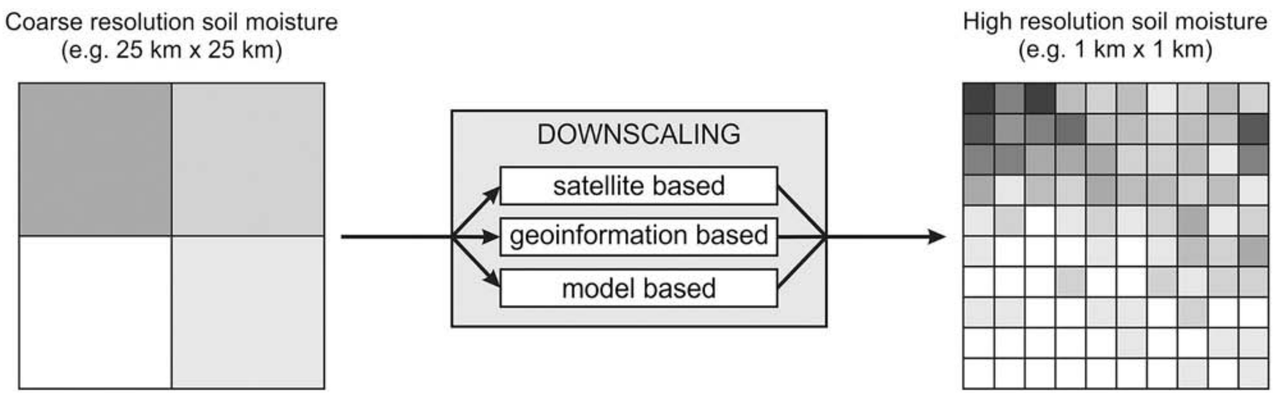

Figure 2.2. Schematic overview of downscaling coarse-resolution soil moisture data to generate high-resolution products. Reproduced from Peng *et al*. (2017); licensed under CC BY-NC-ND 4.0 DEED (https://creativecommons.org/licenses/by-nc-nd/4.0/).

variable infiltration model (VIC) and Mosaic. Koster *et al*. (2009) highlighted that model-based estimates of soil moisture are largely dependent on the model employed (Wei, 1995); when model dependencies were accounted for, the models were found to produce similar temporal variations in soil moisture across a range of climates.

2.2.5 Data assimilation

To address limitations in both satellite-derived and LSM-simulated estimates of soil moisture, significant efforts have focused on converging both approaches through data assimilation techniques. Following the recommendations of Wei (1995) with regard to the need for a more integrated approach, encompassing the then newly emerging satellite data for monitoring soil moisture, modelling and *in situ* measurements, Houser *et al*. (1998) employed a four-dimensional data assimilation technique to integrate data from a passive microwave satellite sensor into a hydrological land surface scheme (TOPMODEL-based Land–Atmosphere Transfer Scheme (TOPLATS)) and estimate soil moisture over an experimental watershed in the USA. The use of data assimilation techniques has been shown to improve LSMs' estimation of deeper layer soil moisture and surface fluxes. Consequently, the use of data assimilation techniques to ingest single variables or more than one variable into LSMs has become more widespread, particularly over the past 10 years. While a number of challenges remain, with regard to method, pre-processing, computational cost and uncertainty assessment, the benefits of data assimilation appear to be very promising.

2.3 New Data Products Relevant to Research

As no single platform or sensor can meet the variety of needs (accuracy, temporal/spatial resolution, longevity) of the end-user community (e.g. weather forcing, climate modelling, agriculture, water management, etc.) (Sabaghy *et al*., 2018), approaches that seek to optimise the information obtained from a range of satellite platforms and sensors have been developed. Such combined approaches, which include the use of thermal and optical sensors (e.g. Carlson *et al*., 1994), passive and active microwave sensors (e.g. Liu *et al*., 2012a) and microwave and optical sensors (e.g. Huang *et al*., 2020; Tong *et al*. 2020), can address a number of the limitations associated with a single platform or sensor type. One such initiative is the ESA CCI SM project, which developed, and continues to refine and improve, algorithms to merge active, passive and combined active and passive microwave sensors, to produce a long-term harmonised and quality-controlled global daily soil moisture product at 0.25° resolution (Gruber *et al*., 2019) (Figure 2.3).

Karthikeyen *et al*. (2017b) undertook an assessment of the performance of the available remotely sensed soil moisture products with respect to temporal coverage and spatial and temporal performance. They evaluated data from eight passive sensors, namely the Scanning Multichannel Microwave Radiometer, the Special Sensor Microwave – Imager, the microwave imager of the Tropical Rainfall Measuring Mission, the WindSat mission sensor, the Advanced Microwave Scanning Radiometer – Earth Observing System (AMSR-E), the AMSR2 mission sensor, the SMOS mission sensor and the SMAP mission sensor; and two active sensors, namely the European Remote Sensing (ERS-1 and ERS-2 missions) satellites and ASCAT from MetOP-A/B; and the combined active and passive data produced by the ESA CCI SM project. Their evaluation was based on an assessment of these data against data from >1000 *in situ* monitoring sites, distributed across the contiguous US region, obtained from the International Soil Moisture Network. Their findings indicate that, while systematic differences were evident between the different datasets, the temporal performance of the ESA CCI was comparable to that of the other products. Interestingly, higher correlations were found for all products for spatial performance, with respect to the measurement network, than for temporal performance.

Zhu *et al*. (2019) found that the ESA CCI combined data product (e.g. active and passive sensors) outperformed both the active-only and passive-only products in their analysis over test sites distributed across China, Spain and Canada. They recommended that the combined data product be used in subsequent climatological and hydrological research. These findings are consistent with those of Xu *et al*. (2020) in their analysis of the ESA CCI data over the Great Lakes in the USA.

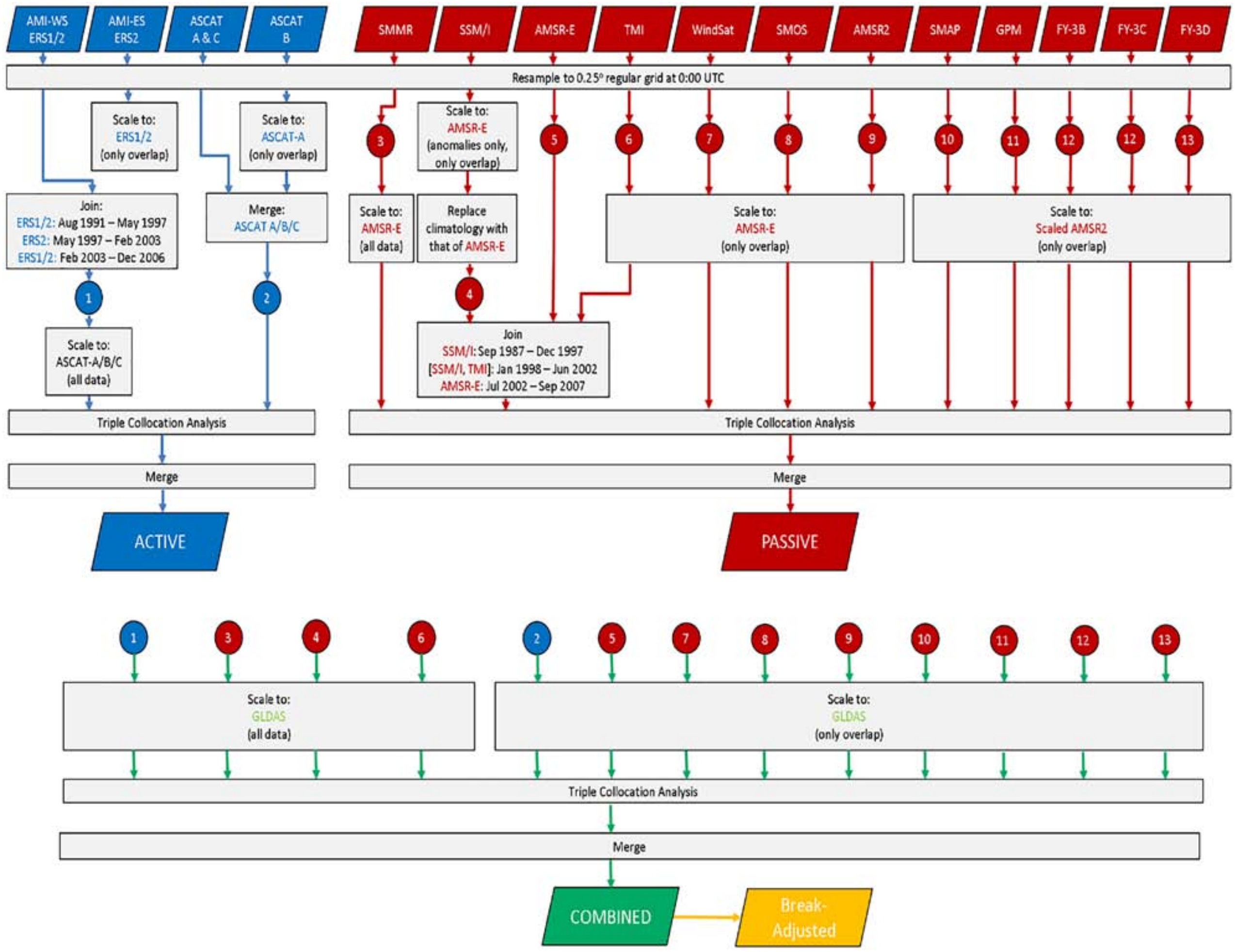

Figure 2.3. Scheme employed by the ESA to merge data from active, passive, and active and passive microwave sensor platforms. Source: https://esa-soilmoisture-cci.org (accessed 28 February 2023).

2.4 Conclusion

The combined global soil moisture product from ESA CCI represents a significant development in deriving harmonised long-term estimates of soil moisture. However, a number of limitations remain. These centre around gaps in the data, the fact that satellite-derived soil moisture estimates represent the signal from only the top 2–5 cm of the surface layer and, perhaps the most limiting, the fact that the spatial resolution of satellite-derived soil moisture data remains too coarse for many applications (Sabaghy *et al*., 2018).

Kovačević *et al*. (2020) applied a gap-filling procedure, to generate a continuous temporal and spatial coarse-resolution soil moisture product, which provided the input to their downscaling approach using the RF method. They evaluated the method over California during 2016 and concluded that, while additional improvements were necessary, the methodology could successfully generate high-resolution estimates of soil moisture. Brocca *et al*. (2011) employed the semi-empirical approach of Wagner *et al*. (1999) to derive Soil Water Index (SWI) values, to provide an estimate of root-zone soil moisture based on the known surface soil moisture. More recently, Grillakis *et al*. (2021) employed ML techniques along with physical descriptors of the soil, vegetation and climate to estimate *in situ* root-zone soil moisture. They found good agreement between the estimated root-zone soil moisture, using the ESA CCI soil moisture data and modelled data derived from the European Centre for Medium-Range Weather Forecasts (ECMWF) ERA5-Land dataset and NASA's Famine Early Warning Systems Network (FEWS NET) Land Data Assimilation System (FLDAS) reanalysis data.

3 Data and Methods

3.1 Data

3.1.1 In situ *data*

Figure 3.1 illustrates the UK Centre for Ecology and Hydrology (UKCEH) COMOS-UK CRNS site network, with *in situ* measurements of soil moisture being available for the period 2013–2019. Daily data were obtained from the UKCEH Environmental Information Data Centre and comprised information on sites, instrumentation data, and processing and quality control data. They also included the date, site name, CRNS-derived volumetric water content

Figure 3.1. Location of COSMOS-UK sites. Source: adapted from Cooper *et al*. (2021); licensed under CC BY 4.0 (https://creativecommons.org/licenses/by/4.0/).

(VWC) (%) and the D86_75M parameter (cm), which is the effective sensing depth (D86) within the source area footprint (75 m radius), following the method of Köhli *et al*. (2015). For a detailed description of the CRNS data and their processing, see Boorman *et al*. (2020). In addition, metadata for each site were also obtained, outlining the soil type (e.g. mineral, organic, calcareous), altitude, recorded land cover type and bulk density (Boorman *et al*., 2020). Table 3.1 provides a list of relevant *in situ* and site-recorded variables. Daily aggregated values from the CRNS network, obtained from the UKCEH, were derived from the daily averaging of sensor counts and not the hourly estimated VWC values (Stanley *et al*., 2019).

3.1.2 Gridded data

Daily 1-km gridded data for maximum and minimum temperature and precipitation (HadUK-Grid v1.1.0.0) were obtained from the UK Meteorological Office and were accessible from the CEDA Archive, which is part of the Natural Environmental Research Council Environmental Data Service. The daily data, which are available from 1960 to 2021, were interpolated from *in situ* meteorological observations from across the UK (Hollis *et al*., 2018). The data are available as climate- and forecast-compliant network common data form (netCDF) files on the British National Grid (EPSG: 27700).

Daily 1-km gridded data for maximum and minimum temperature and precipitation, covering Ireland, were also obtained from the Irish meteorological agency, Met Éireann. The data are provided in comma-separated variable (csv) format on TM65/ Irish National Grid (EPSG: 29902) – with northing and easting associated with each point. The csv data were converted to gridded netCDF files using the ncdf4 (Pierce, 2023) and raster (Hijmans, 2023) packages in R (R Core Team, 2021).

Daily mean temperatures were calculated from the available maximum and minimum temperatures for both the HadUK-Grid and Met Éireann gridded data. All gridded meteorological data were subsequently reprojected to the World Geodetic System 1984 (WGS84) (EPSG: 4326).

Table 3.1 provides a description of the available *in situ* measurements from the UKCEH's Cosmic-ray Soil Moisture Monitoring Network (COSMOS-UK) and candidate predictor variables used in the training dataset for the ML-based approach, covering the UK and Ireland.

Gridded data on soil textural properties, including bulk density, clay, sand and silt, were obtained from SoilGrids of the World Soil Information Service (Poggio *et al*., 2021). SoilGrids provides global soil information at 250 m and 1 km resolution at six depth layers. Global maps were derived using ML statistical methods to estimate soil properties based on soil observations from almost 240,000 locations. Data from the soil layer representative of the 5–15 cm depth were subsequently employed in the ML model, as this layer had the highest the frequency of CRNS returns.

In addition to the predictor variables employed in the ML-based approach (Table 3.1), 3-hourly reanalysis data from the ECMWF were obtained from the ERA5-Land model (Muñoz Sabater, 2019) as initial and boundary/forcing conditions for the LSM-based approach. ERA5-Land provides global coverage of a range of near-surface and sub-surface meteorological variables at 0.1° resolution (~9 km). The meteorological forcing variables included 2-m temperature and specific humidity, 10-m U wind and V wind, surface pressure, precipitation and both shortwave and longwave radiation. In addition, the following variables were required to initialise the model: soil temperature, surface skin temperature, canopy water and snow water equivalent. Data for all variables were obtained for the period 2009–2022.

3.1.3 Satellite-derived data

Gridded (0.25°) satellite-derived soil moisture data were obtained from the ESA CCI SM product. Data version 05.2 was originally obtained but subsequently replaced by version 07.1, the latest release. Version 07.1 employs an intra-annual bias correction method for the harmonisation of sensor data, with improved temporal and spatial coverage, and data are available from 1978 to 2021. Data from the combined active and passive (Figure 2.3) sensors were obtained for the period from 2010 to 2021, as the temporal and spatial coverage prior to this period is relatively poor.

Elevation data were obtained from the European Digital Elevation Model (EU-DEM) (version 1.0), a hybrid digital elevation model, based on NASA's Shuttle Radar Topography Mission (SRTM) and

Table 3.1. List of available *in situ* measurements from UKCEH COSMOS-UK sites and candidate predictor variables for the training dataset covering the UK and Ireland for the ML-based approach

Name of index	Source	Spatial resolution	Input type	Description
ID	COSMOS-UK UKCEH		*In situ*	Identification number of site
Date				Model time range
Location	COSMOS-UK UKCEH	Point	*In situ*	Location of the site/area of interest
Latitude	COSMOS-UK UKCEH	Point	*In situ*	Latitude of the site/area of interest
Longitude	COSMOS-UK UKCEH	Point	*In situ*	Longitude of the site/area of interest
Altitude	COSMOS-UK UKCEH	Point	*In situ*	Altitude in meters
Land cover	COSMOS-UK UKCEH	Areal	*In situ*	Recorded land cover at site
Soil Moisture	COSMOS-UK UKCEH	Areal	*In situ*	VWC from COSMOS UK locations derived from CRNS network
D86_75M	COSMOS-UK UKCEH	Areal	*In situ*	Effective depth; D86 at 75 m distance from CRNS
CCI SM	ESA CCI SM	25 km	Satellite	Soil moisture from 25 km resolution; ESA CCI SM combined data
MODIS NDVI	MOD13A1	500 m	Satellite	Normalised difference vegetation index
MODIS EVI	MOD13A1	500 m	Satellite	Enhanced vegetation index
MODIS Land Cover Type	MCD12Q1	500 m	Satellite	Land cover type
MODIS Land Surface Temperature	MOD11A1	1 km	Satellite	Land surface temperature
EU-DEM		500 m	Satellite	EU digital elevation model, 500 m resolution
Aspect		500 m	Derived	Aspect refers to the compass direction that a hillside or slope faces, with the value in degrees; four neighbouring cells
Slope		500 m	Derived	Slope represents the rate of change of elevation; four neighbouring cells
Roughness		500 m	Derived	Roughness is the degree of irregularity of the surface – calculated as the difference between the maximum and the minimum value of a cell and its eight surrounding neighbours
TPI		500 m	Derived	Topographic position index – difference between the value of a cell and the mean value of its eight surrounding neighbours
TRI		500 m	Derived	Topographic ruggedness index – mean of the absolute differences between the value of a cell and the value of its eight surrounding neighbours
TWI		500 m	Derived	Topographic wetness index
General Curvature		500 m	Derived	General curvature of the landscape
Bulk Density	SoilGrids	250 m	Soil	Bulk density of the fine earth fraction (5–15 cm depth)
Clay	SoilGrids	250 m	Soil	Proportion of clay particles (< 0.002 mm) in the fine earth fraction (5–15 cm depth)
Sand	SoilGrids	250 m	Soil	Proportion of sand particles (> 0.05 mm) in the fine earth fraction (5–15 cm depth)
Slit	SoilGrids	250 m	Soil	Proportion of silt particles (≥ 0.002 mm and ≤ 0.05 mm) in the fine earth fraction (5–15 cm depth)
Maximum Temperature	HadUK-Grid; Met Éireann	1 km	Weather	Daily maximum air temperature measured between 09:00 UTC on day D and 09:00 UTC on day D + 1 (°C), interpolated to a 1-km grid
Minimum Temperature	HadUK-Grid; Met Éireann	1 km	Weather	Daily minimum air temperature measured between 09:00 UTC on day D – 1 and 09:00 UTC on day D (°C) interpolated to 1-km grid
Precipitation	HadUK-Grid; Met Éireann	1 km	Weather	Daily precipitation (mm) interpolated to a 1-km grid

ASTER Global Digital Elevation Map (GDEM), that has been fused, using a weighted averaging approach. The data, available at a spatial resolution of 500 m, were obtained through the Copernicus Land Monitoring Service. The tile locations covering the UK and Ireland were obtained, merged and reprojected to WGS84 (EPSG: 4326). Landscape morphometry data were derived from the elevation data, including slope, aspect, roughness, Topographic Position Index (TPI) and Topographic Wetness Index (TWI) data, and general curvature was derived using the Cran R (R Core Team, 2021) raster package (Hijmans, 2023).

MODIS land cover and vegetation indices were obtained from the Application for Extracting and Exploring Analysis Ready Samples (AppEEARS) service provided by NASA Earthdata services. The following data were derived from Terra and Aqua combined Moderate Resolution Imaging Spectroradiometer (MODIS): NDVI (MOD13A1) version 6.1 (Didan, 2021), Enhanced Vegetation Index (MOD13A1) version 6.1, land cover type (MCD12Q1) version 6 (Friedl and Sulla-Menashe, 2022) and land surface temperature (MOD11A1) (Wan *et al*., 2021) data. Data from the vegetation indices were available at 16-day intervals. Following visual inspection of the data, values were subsequently filtered on the basis of the quality code. Remaining outliers in the data were removed using the time series outliers (tsoutliers) function (Hyndman, 2021) following the method of Chen and Liu (1993), implemented in R (R Core Team, 2021). A Savitzky–Golay smoothing filter, using the Signal package (Signal Developers, 2013), was subsequently applied to the vegetation indices to smooth and temporally interpolate the data to match the resolution of the meteorological and soil moisture data.

In addition to the MODIS land cover data employed for the RF-based approach, the 100-m raster CORINE Land Cover (CLC) data for 2018 were obtained and used as input for the NOAH LSM. The 44 CLC classes were initially reclassified into 21 categories to match MODIS categories (Table 3.2), with particular emphasis placed on the “permanent wetlands” reclassification. This resulted in a total of 12 land cover classes relevant for the geographical domain included in the NOAH model simulations (see Figure 3.10). The data were then resampled to 250 m. To generate the required geographical files for input to NOAH, the CLC 2018 data were converted to binary format, and were then used as input to the Weather, Research and Forecasting model Pre-Processing System (WPS). The WPS generates the gridded geographical information required to run the NOAH model.

3.2 Methods

3.2.1 Machine learning-based approach

The RF statistical method has been widely employed to downscale soil moisture from coarse-resolution satellite-derived soil moisture estimates and has a number of advantages. The RF method utilises an

Table 3.2. Categorisation of the CLC 2018 categories into MODIS equivalent categories

MODIS land cover class	IGBP name	CLC class
1	Evergreen needleleaf forests	312
4	Deciduous broadleaf forests	141/311
5	Mixed forests	313
7	Open shrublands	322/324
10	Grasslands	231/321
11	Permanent wetlands	411/412/421/423
12	Croplands	211
13	Urban and built-up lands	111/112/121/122/123/124/131/132/133/142
14	Cropland/natural vegetation mosaics	222/242/243
16	Barren or sparsely vegetated	331/332/333/334
17	Water	523
21	Lakes	511/512/521/522

Only relevant classes are shown in the table (see Figure 3.10).
IGBP, International Geosphere-Biosphere Programme.

ensemble of decision trees to generate predictions or probabilities of observations belonging to a particular category. Predictions generated from decision trees typically change significantly when small changes are made to the dataset or when new predictors are included. Depending on different decision tree-growing algorithms, decision trees are prone to overfitting the data, unless they are pruned adequately. Using the RF method provides a way of solving these issues. Since each decision tree within an RF is allowed to use only a random subset of the predictors, overfitting is attenuated and there is no need for tree pruning. Moreover, since the predictions are then an average of the predictions generated by each tree within the RF, the variability is also smaller when changes are made to the data or when predictors are added and/or removed. Therefore, RFs are an extension of decision trees that are less prone to overfitting and present less variability. Interpretability is still possible by looking at "variable importance", which can be calculated as the decrease in explained variability if a particular variable is removed from the analysis. The variables/predictors that yield a greater decrease in explained variability are, therefore, the most important for predicting the response variable. A Bayesian framework for RFs is called the Bayesian Additive Regression Trees (BART) framework (Chipman *et al*., 2010). In this framework, prior information on tree structure is incorporated into a Bayesian estimation approach, and favours shallow trees, such that each tree contributes a small amount of the explanatory response.

An initial examination of a number of statistical (e.g. linear regression) and ML (RF, BART) approaches and transformations of the response variable (e.g. logit-transformed versus raw values for soil moisture range of 0–1) was undertaken. Following this initial evaluation, the RF method was selected because of its better performance.

Figure 3.2 provides a schematic of the workflow. To generate the training dataset, temporally varying (e.g. meteorological data, vegetation indices, land cover) and static (e.g. elevation, soil properties) data were extracted for each COSMOS-UK CRNS site location for the period from 2013 to 2021, with 2013 marking the start of good/improved station coverage. Prior to training the model, the extracted data were compared with the site information obtained from the UKCEH, where comparable measurements were available. Site information and locations were also assessed using a visual assessment with Google Maps. A number of issues were identified at this point. For example, one of the sites had incorrect site coordinates, which was subsequently rectified. A more significant issue was identified with regard to the recorded land cover and the land cover extracted from the MODIS land cover data, specifically where site-recorded land cover data did not match satellite-derived information. Consequently, land cover data were obtained from a number of different sources, including through the visual assessment of historical imagery from Google Earth, the Global Land Cover (2015–2019) and CLC (2018) datasets, and the EU Land Use and Land Cover Survey (LUCAS) (2013 and 2015). While land cover classes were not directly comparable between the different datasets, it was possible to subjectively map the different definitions across the land cover classes. Following this preliminary assessment, MODIS land cover data were employed; this was also the most pragmatic choice for applying the model to the Irish domain.

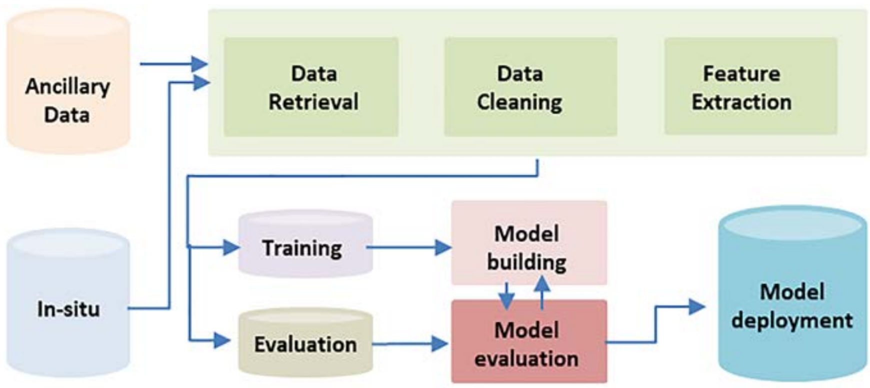

Figure 3.2. Schematic of the workflow employed.

In addition, a number of site locations were excluded from the training data. Due to the spatial resolution of the ESA CCI SM data (0.25°), any CCI grids that overlaid a site location less than 12.5 km from the coast were excluded, to limit the impact of sea grids on the estimation of soil moisture. A number of sites were also excluded based on a visual assessment of the measured data. Excluded sites included Redmere, Harwood Forest, Moreton Morrell and Plynlimon. This resulted in a total of 36 sites being available for inclusion in the training data. The screening of time periods was also undertaken, to remove the contamination effect of snow cover on satellite-derived soil moisture estimates. A pragmatic approach was taken to exclude dates based on days that recorded a mean temperature of less than 0°C and where rainfall had been recorded. Prior screening of the potential covariates was undertaken to obtain a parsimonious suite of predictors for use in the model training. Screening involved standard tests of the statistical significance of association between variables (Figure 3.3), principal components analysis to identify families of related predictors and the evaluation of relevance from a physical process point of view.

An extensive assessment of training and evaluation periods and candidate predictors was undertaken. Initially, much of the focus on model training was

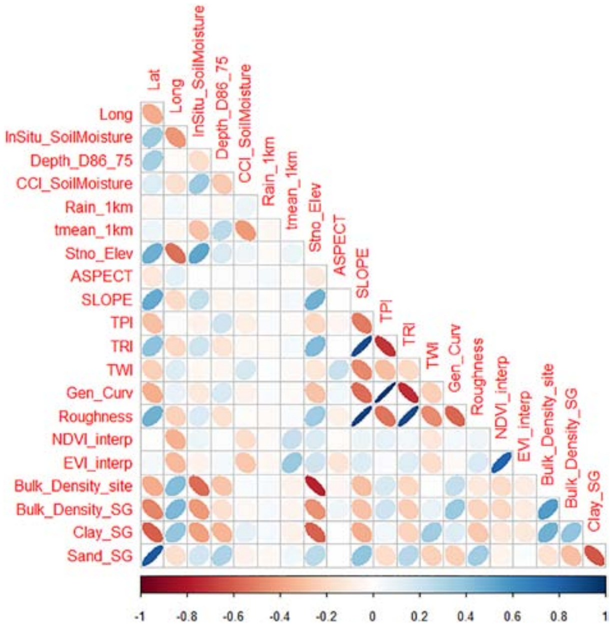

Figure 3.3. Correlation matrix showing Pearson's *R* values between the CRNS sites *in situ* and candidate predictors.

on the period 2013–2018, with data from outside this period withheld from model evaluation and the selection of the mtry parameter, a model-tuning parameter. The R package CAST (Meyer *et al*., 2023) was used to evaluate the selection of different space and time folds (e.g. leave time out; leave location out (LLO)). Employing a split sample (2013–2018; 2019) resulted in high modelled *R*-squared values, the metric used to quantify the model, for the training period. Similarly, high *R*-squared values were obtained for the independent evaluation of the model for 2019. However, when the RF model was applied to an equivalent suite of predictors for a site withheld from the model training, the model did not perform well (Figure 3.4).

On a visual assessment of the importance of the predictors in the RF model, the effective depth (D86_785M) covariate was found to be the dominant variable of importance, higher than the ESA CCI SM and meteorological variables (Figures 3.5 and 3.6). Following investigation, it was determined that the D86_75M variable is not an independent variable and, in fact, that the calculation of effective depth is a function of the total soil water content; hence, the predictive ability of the model is high when *in situ* estimates of effective depth are available, and, conversely, the model has no or low predictive ability when an effective depth is specified for an independent site. As the CRNS returns are variable-depth measurements, and thus require a control, we made the necessary assumption that the effective depth was a characteristic of the instrument and site and that each site had a mean effective depth based on which the CRNS returns or counts were obtained. Both the NDVI and EVI were also evaluated for inclusion as covariates. When included, the relative importance of the variables altered and, interestingly, a vegetation index was not selected during the forward feature selection (FFS) tests.

Performing the FFS test is akin to performing forward stepwise regression in multiple linear regression analysis, in that predictors are added in descending order of importance until the addition of a new variable results in no/dis improvement in the model. The FFS algorithm with LLO (*k*-fold = 20) identified 12 covariates as optimum (Figure 3.7). Values for mtry and the number of trees were also evaluated using the grid search (expand.grid) option. Values from 1 to 15

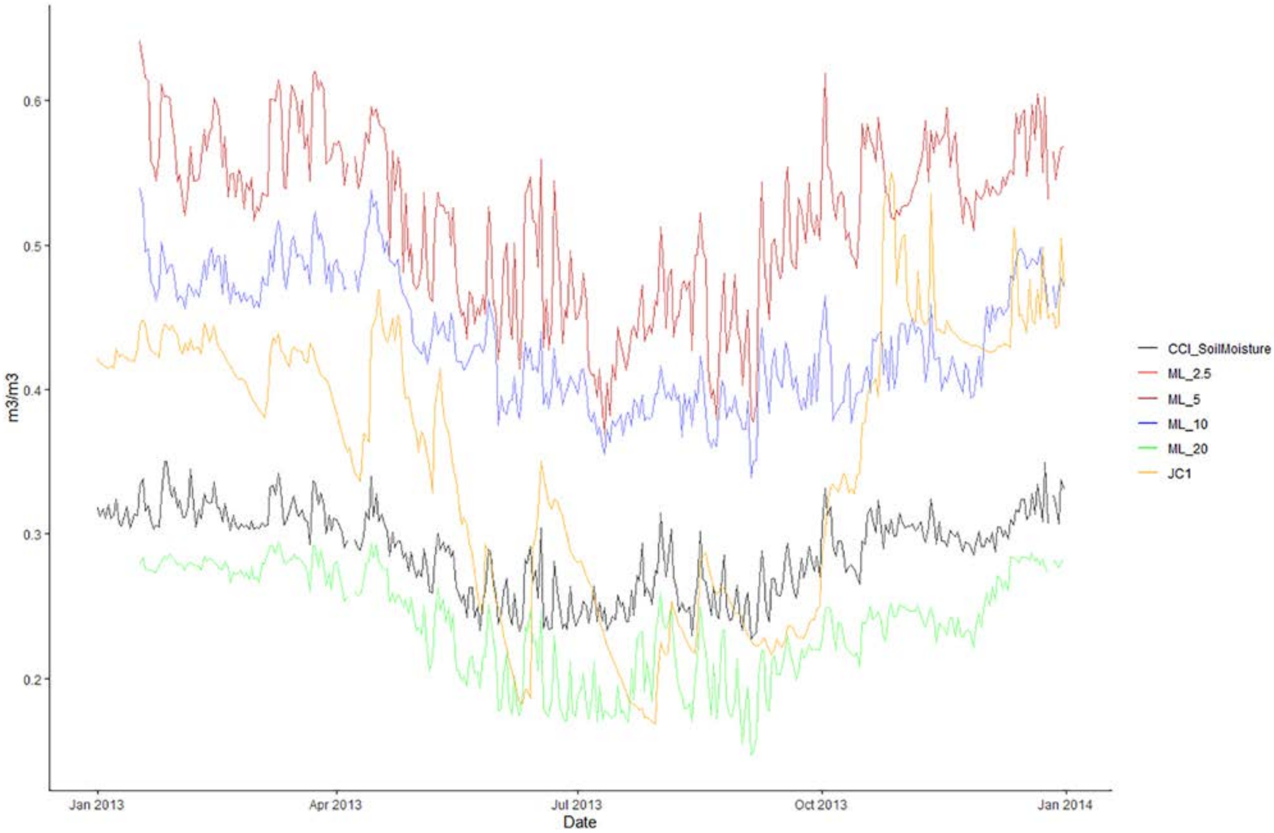

Figure 3.4. Evaluation of the initial RF model against an independent measurement site. ML_2.5, ML_5, ML_10 and ML_20 indicate RF model-estimated soil moisture values at various depths (2.5, 5, 10 and 20 cm, respectively); CCI_SoilMoisture shows the ESA CCI SM-estimated soil moisture values; and JC1 shows *in situ* data (5 cm depth) from a site withheld from the model training.

were evaluated for mtry, and 500, 100 and 1500 were evaluated for the number of trees. This resulted in the final section of mtry equal to 5 and 500 trees. The *k*-fold value was set to the number of sites. The final suite of covariates employed in the model is outlined in Table 3.3. While the models trained with and without NDVI did not differ significantly, NDVI was considered important to include in the final model from a physical process point of the view (Figure 3.8). Based on the training period (2013–2018), the root-mean-square error (RMSE) was 0.073, the mean absolute error (MAE) was 0.061 and the *R*-squared value was 0.582.

3.2.2 *Machine learning model evaluation – in situ data for Ireland*

Only limited *in situ* data were available from a number of sites in Ireland, and these were generally collected as part of the monitoring of surface fluxes associated with eddy covariance measurements. Data were obtained either directly from site owners, as in the case of Johnstown Castle (Teagasc) and the Carlow Grassland (Trinity College Dublin), or through the European Fluxes Database Cluster (http://www.europe-fluxdata.eu/) for Dripsey and Donoughmore (Table 3.4). Critically, the lack of coherent and/or consistent metadata associated with the limited available *in situ* data (instrument type; placement and measurement depth; site relocation) means that the subsequent analysis was limited. For example, the *in situ* measurements from the two sensors at Johnstown Castle appeared to be consistent during 2013; however, following a site relocation, the measurements differed between the two sensors (Figure 3.9). A comparison of the ML model outputs with data from the GROW Observatory was also undertaken, but the findings are not reported on here because of issues related to the length and reliability of the GROW time series.

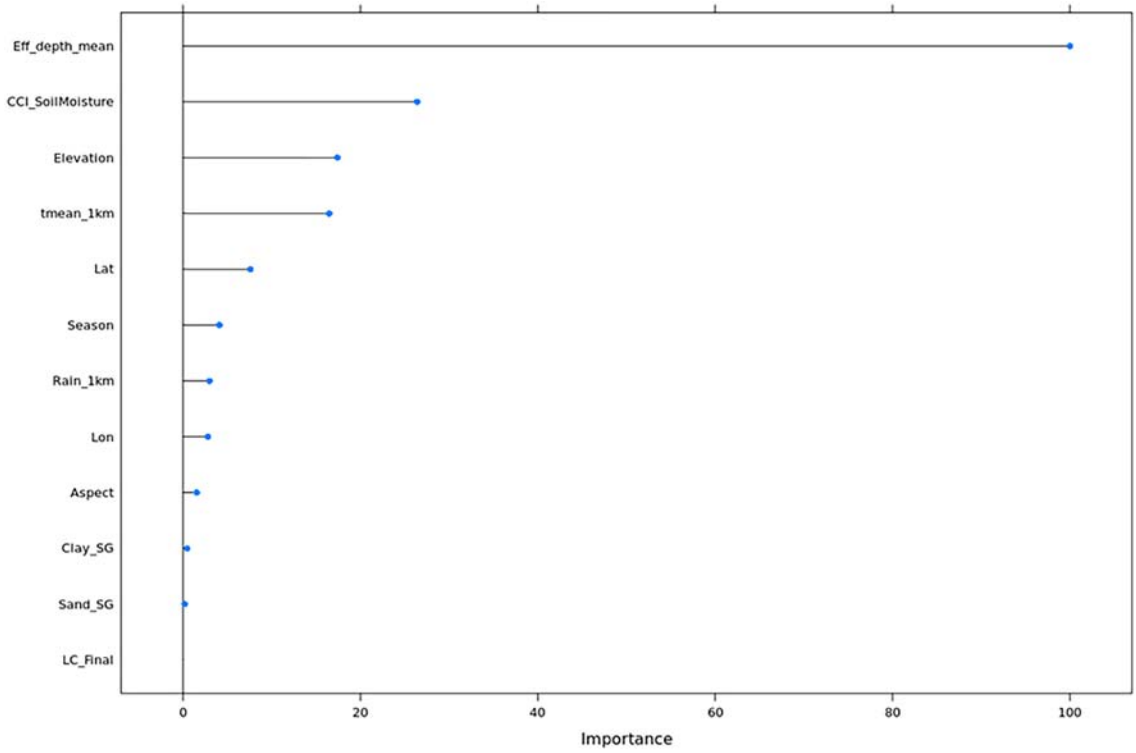

Figure 3.5. Importance of the predictor covariates identified in the initial model building. CCI_ SoilMoisture, CCI soil moisture; Clay_SG, clay (soil grids); Eff_depth_mean, mean effective depth; Lat, latitude; LC_Final, land cover; Lon, longitude; Rain_1km, rainfall (1-km grid); Sand_SG, sand (SoilGrids); tmean_1km, temperature (1-km grid).

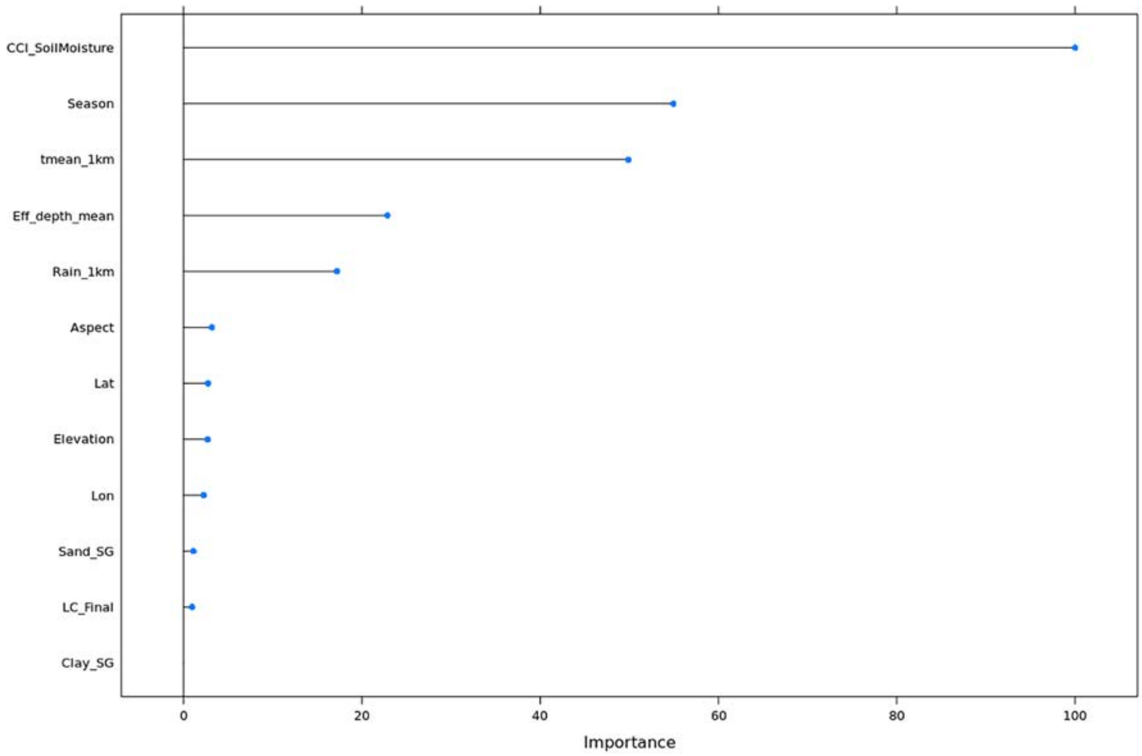

Figure 3.6. Importance of the predictor covariates employed in the model following the use of a site effective depth variable (Eff_depth_mean). CCI_SoilMoisture, CCI soil moisture; Clay_SG, clay (soil grids); Eff_depth_mean, mean effective depth; Lat, latitude; LC_Final, land cover; Lon, longitude; Rain_1km, rainfall (1-km grid); Sand_SG, sand (soil grids); tmean_1km, temperature (1-km grid).

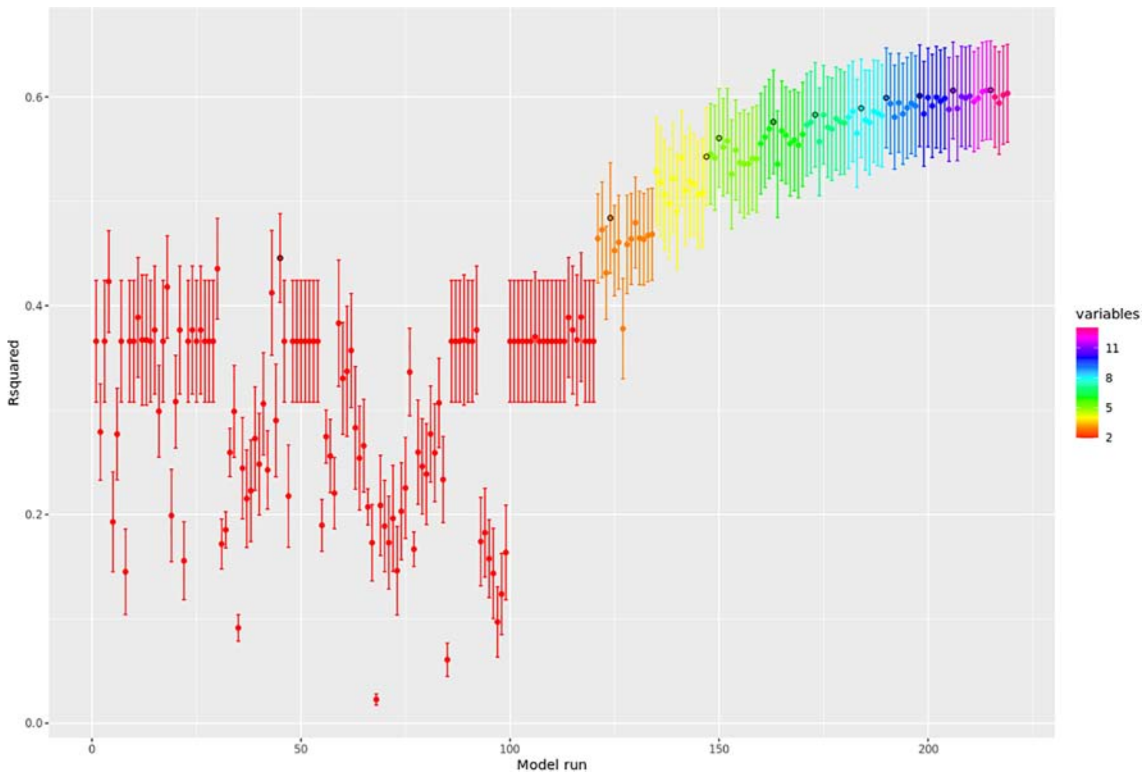

Figure 3.7. Change in *R*-squared values resulting from the addition of covariates in the FFS.

Table 3.3. List of covariates employed in the RF model to estimate soil moisture without and with NDVI, selected based on the independent training period 2013–2018

Name of index	Description	Variable importance without NDVI (%)	Variable importance with NDVI (%)
Latitude	Latitude of the site/area of interest	4.5	5.65
Longitude	Longitude of the site/area of interest	3.8	3.42
Season	Categorical variable: DJF [1], MAM [2], JJA [3] and SON [4]	51.4	49.17
D86_75M (mean)	Site mean effective depth D86 at 75 m	26.7	22.41
CCI SM	25 km ESA CCI SM	100	83.52
NDVI	Normalised difference vegetation index	–	100
MODIS Land Cover Type	Land cover type	0.3	0.00
Digital Elevation Model	EU DEM 500 m	5.1	5.21
Aspect	Aspect based on four neighbouring cells	2.9	3.64
Clay	Proportion of clay particles (5–15 cm depth)	0.0	2.26
Sand	Proportion of sand particles (5–15 cm depth)	2.7	5.68
Mean Temperature	Calculated from the max. and min. gridded temperature grids	65.1	54.62
Precipitation	Daily gridded precipitation (mm)	29.4	42.37

DJF, December, January, February; JJA, June, July August; MAM, March, April, May; SON, September, October, November.

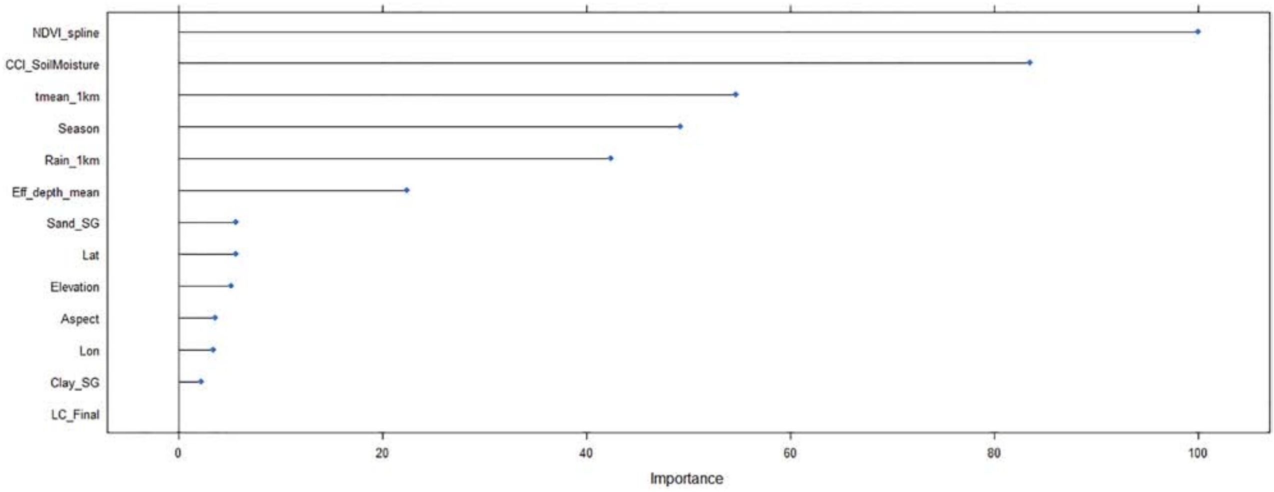

Figure 3.8. Importance of the predictor covariates employed in the final model following the use of a site effective depth variable and the inclusion of the NDVI. CCI_SoilMoisture, CCI soil moisture; Clay_SG, clay (soil grids); Eff_depth_mean, mean effective depth; Lat, latitude; LC_Final, land cover; Lon, longitude; Rain_1km, rainfall (1-km grid); Sand_SG, sand (soil grids); tmean_1km, temperature (1-km grid).

3.2.3 NOAH land surface model

The NOAH LSM (Niu *et al.*, 2011) was set up over a domain covering the island of Ireland and included a portion of the west coast of Great Britain (Figure 3.10). The model projection was set to Lambert Conformal Conic, appropriate for mid-latitude locations. The domain is represented by 591 grids from east to west and 611 grids from north to south, with a spatial resolution of 1000 m. The model default geographical data were employed for the portion of Great Britain included in the domain; for the island of Ireland, the CLC 2018 dataset, reclassified to MODIS, was used to represent land cover (Figure 3.10). The default soil texture information based on dominant textural class, available at a resolution of ~5 km and obtained from the hybrid STATSGO/FAO dataset for the top layer and bottom layer soil (FAO, 2023), was employed in the NOAH LSM (Figure 3.11). In general, default model settings and parameters were employed, with the exception of the stomatal resistance option, which was set to the empirical-based Jarvis scheme (Table 3.5). The model was run with a time step of 30 minutes, and model outputs were saved every hour. The computational time required to run the model equated to approximately 15 hours of wall time per model-year on a 32-core machine.

Table 3.4. List of available *in situ* soil moisture measurements collected as part of various projects

Site	Owner/source	Land cover	Measurement (No. sensors × time)	Period	Soil
Johnstown Castle	Teagasc	Grass	2 × 30 min SWC	2013, 2018–2021	Imperfect drainage; sandy loam
Carlow	TCD	Grass	30 min SWC (% volume)	2003	
Dripsey	UCC/European Fluxes Database Cluster (Kiely *et al.*, 2008)	Grass	3 × 30 min SWC (% volume) – 5 cm 1 × 30 min	2003–2007 2002–2012	Poorly drained/reclaimed; organic topsoil
Donoughmore	UCC /European Fluxes Database Cluster (Kiely *et al.*, 2008)	Broadleaf forest	30 min SWC (% volume)	2009–2012	Poorly drained; organic soil

Data presented were collected as part of the following projects: CarboEuropeIP; EPA funded (Kiely *et al.*, 2018); European Fluxes Database Cluster (Papale *et al.*, 2006). The measurement column indicates the number of sensors and time resolution and, where known or reported, depth. The SWC is measured as percentage volume of water to the unit volume of soil.

SWC, soil water content; TCD, Trinity College Dublin; UCC, University College Cork.

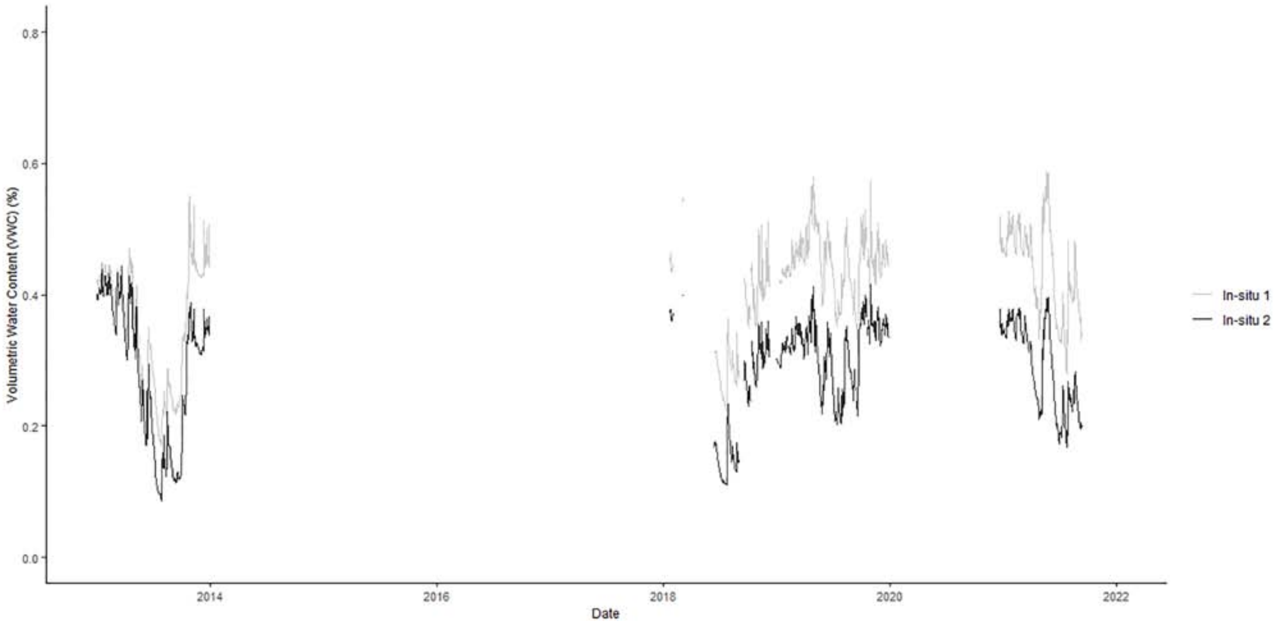

Figure 3.9. ***In situ*** **measurements from the two sensors (In-situ 1 and In-situ 2) located at Johnstown Castle for 2013, 2018–2019 and 2021.**

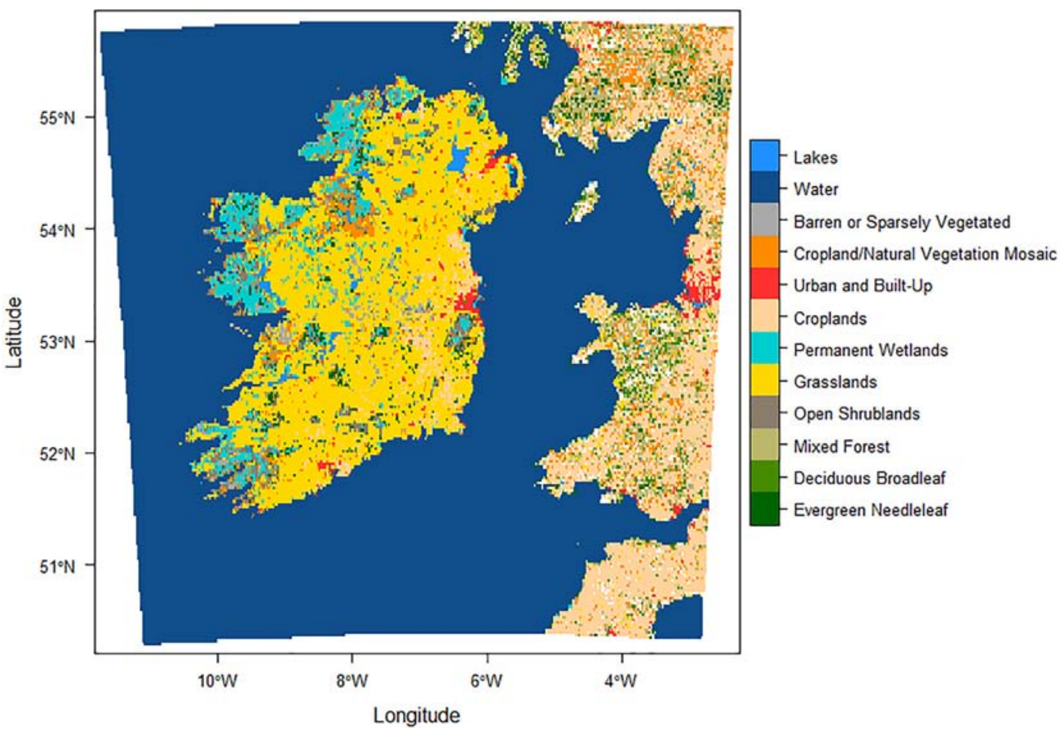

Figure 3.10. CLC 2018 dataset employed in the NOAH LSM. Land cover categories are classified as MODIS categories for use in NOAH, based on the CORINE data resampled from 250 m to 1000 m in the WPS based on a majority rule.

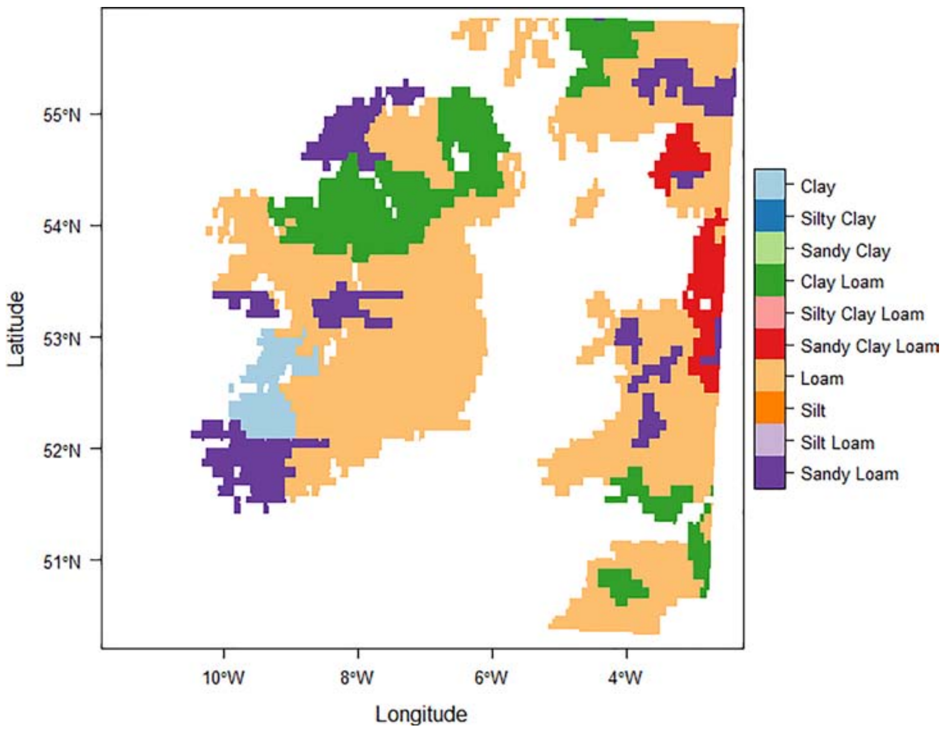

Figure 3.11. Dominant soil textural class based on default STATSGO/FAO soil data.

Table 3.5. Selected model options/schemes and soil layer information

NOAH-MP schemes	Model selection
Dynamic vegetation	Off; table LAI (default)
Canopy stomatal resistance	Jarvis
Radiative transfer	Two-stream applied to vegetated fraction (default)
Surface resistance	Sakaguchi and Zeng (2009) (default)
Soil thickness (m)	0.07; 0.21; 0.72; 1.89
Soil depth (m)	0.0–0.07; 0.7–0.28; 0.28–100; 100–189

LAI, Leaf Area Index; MP, multiparameterisation.

Prior to running the model, the ERA5-Land meteorological inputs were initially used to derive a 3-hourly average meteorological year or "climatology" for the period 2009–2021. Model spin-up was then carried out with this climatology forcing for a period of 10 model-years. This was undertaken to bring the relevant model stores (e.g. soil moisture; soil temperature) to an assumed equilibrium with the climate over this period. The model was then run with the ERA5-Land 3-hourly meteorological forcing data, with the model stores based on the outputs of the spin-up runs. The first year of the run, 2009, was discarded.

4 Results

4.1 Machine Learning Evaluation

In the absence of significant *in situ* soil moisture measurements from Ireland, the RF model was initially evaluated against the COSMOS-UK CRNS data for 2019, which represent data for an independent time period withheld from the model training period (2013–2018). At site level, Pearson's *R* values ranged from a minimum of 0.284 to a maximum of 0.931. In general, the model performed best for the cropland land cover class and poorest for the evergreen forest class (Table 4.1). The model also appears to perform well over the broadleaf forest and open shrubland land cover types, but this is based on a single site for each of these land cover types (Table 4.1). The good model performance over cropland is not unexpected based on the fact that 15 sites were classified as "arable and horticulture" in the training data. Similarly, the poorer performance over the evergreen needleleaf forest site (Harwood Forest) is likely to be associated with the impact of dense vegetation on the satellite returns and the soil moisture conditions of the underlying organic soils. This site displays the highest mean VWC across all the sites and years (Figure 4.1).

Table 4.1. Pearson's *R* values summarised by MODIS land cover class

MODIS land cover class	Pearson's *R*	*n*
1. Evergreen needleleaf forest	0.413	1
4. Deciduous broadleaf forest	0.828	1
7. Open shrubland (woody perennials)	0.814	1
9. Savanna (tree cover 10–30%)	0.627	3
10. Grassland	0.718	28
12. Cropland	0.781	15

Table 4.2 shows the Pearson's *R* values summarised according to the different soil types, as classified at the measurement sites and provided in the site metadata. The model appears to display the lowest skill in estimating soil moisture over organic soils (Pearson's $R = 0.50$), while, for mineral and mineral composite soils, the model appears to have good skill. Typically, organic soils are associated with higher VWCs (%) and display a greater range in values than mineral soils (Figure 4.2). Figure 4.3 shows the RF model-estimated VWC for the independent evaluation period (2019) at Glensaugh, characterised by MODIS as the savanna land cover type (tree cover 10–30%; canopy > 2 m) and on organic soil. Also included in Figure 4.3 are the ESA CCI SM-estimated VWC values for the co-located grid. The ESA CCI SM values significantly underestimate the measured values for this site, which could be partly or wholly explained by

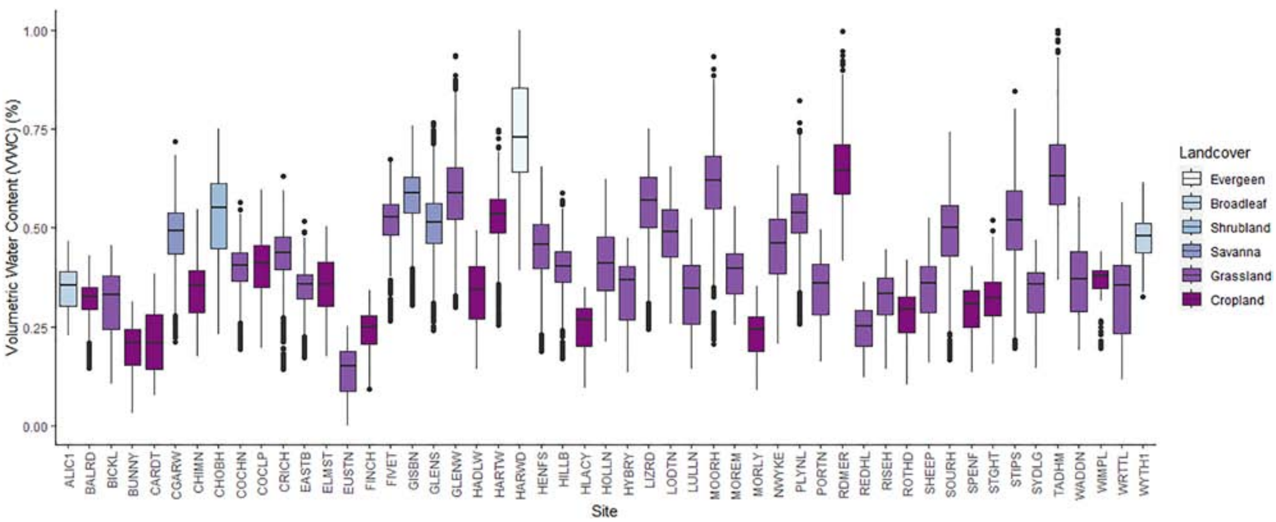

Figure 4.1. Box plots of the VWC (%) for the COSMOS-UK CRNS sites selected for model training (2013–2018) and evaluation (2019) over the period 2013–2019. Sites are colour coded according to their respective MODIS land cover class.

Table 4.2. Pearson's *R* values summarised by soil data as classified at site

Soil type	Pearson's *R*	*n*
Mineral soil	0.733	33
Calcareous mineral soil	0.861	9
Organic soil over mineral soil	0.814	1
Organic soil	0.500	6

the grid resolution (0.25°). While the RF model does not perform as well for organic soils as for other soil types, the RF-estimated values lie close to the mean of the measured values and do appear to capture some of the temporal variability evident at this site (Pearson's $R = 0.536$).

Figure 4.4 shows the RF model-estimated VWC for 2019 at Holme Lacy, characterised as cropland land cover overlying mineral soils (Pearson's $R = 0.882$). Also included in Figure 4.4 are the ESA CCI SM-estimated VWC values for the co-located grid. For this site, the ESA CCI SM values provide a much closer match to the measured values. Extensive areas of similar land cover are likely to be better represented by the ESA CCI SM product than more

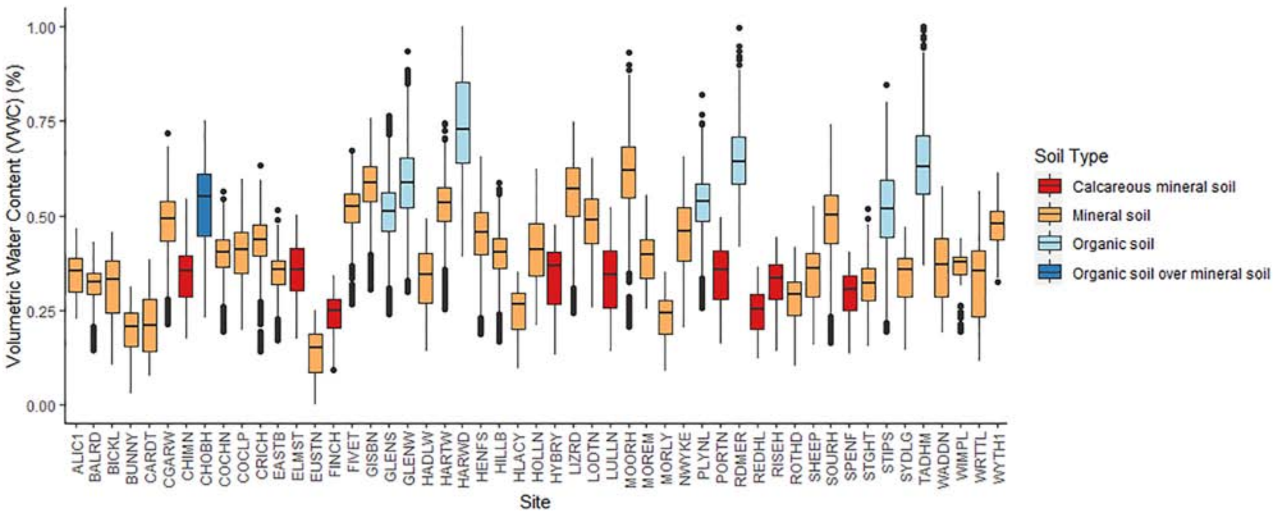

Figure 4.2. VWC (%) for the COSMOS-UK CRNS sites selected for model training (2013–2018) and evaluation (2019) over the period 2013–2019. Sites are colour coded according to their soil type classification.

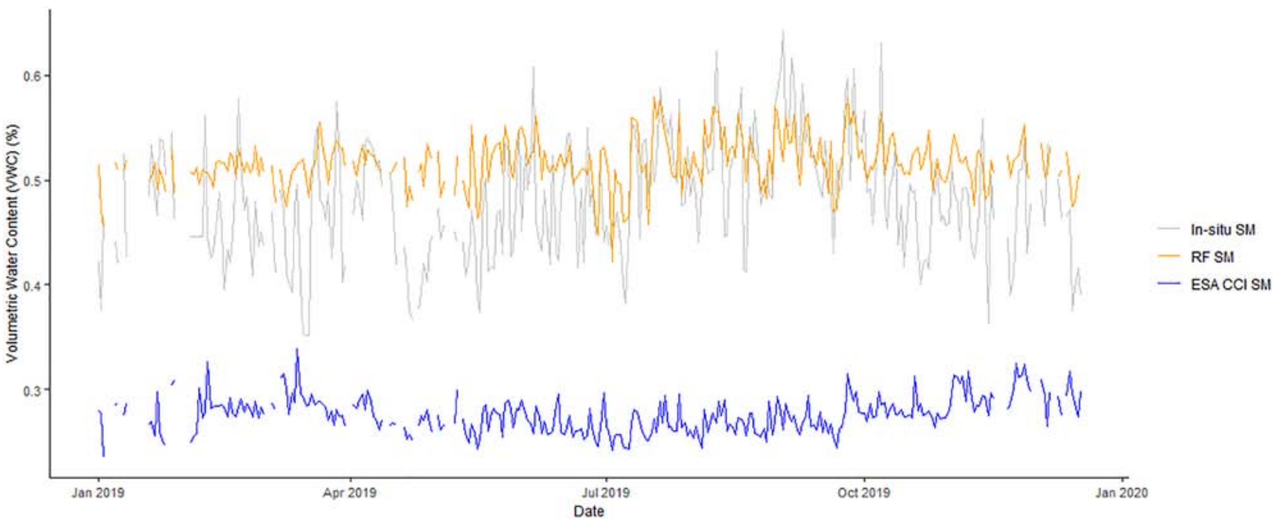

Figure 4.3. VWC (%) for Glensaugh, classified as savannah land cover and located on organic soil, for the independent evaluation period of 2019 (In-situ SM; grey). The RF-estimated VWC values (RF SM) are shown in orange and the ESA CCI SM-estimated values in blue.

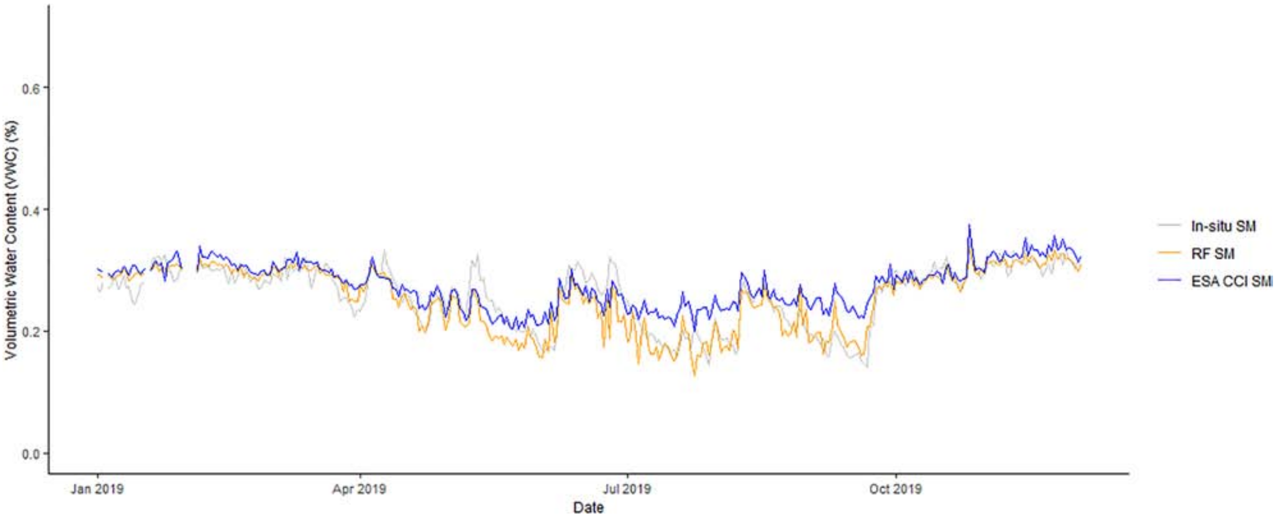

Figure 4.4. VWC (%) for Holme Lacy, classified as arable and horticulture on mineral soil, for the independent evaluation period of 2019 (In-situ SM; grey). The RF-estimated VWC values (RF SM) are shown in orange and the ESA CCI SM-estimated values in blue.

heterogeneous landscapes are, as the return for the latter will be an integrated response from surfaces with different moisture retention properties. While the model generally performed well for cropland sites on mineral soils, the lowest Pearson's *R* value (Pearson's $R=0.284$) was associated with a site that had these characteristics (Figure 4.5). This site, Balruddery, is located close to the mouth of a large river/estuary on the River Tay and was not included in the model training because of its proximity to the coast; however, the ESA CCI SM values are close to the *in situ* values at this site, suggesting that the ESA values were not overly impacted by the returns from the river/sea surface. Based on the RF model, the modelled soil water content is overestimated particularly during the winter months, most likely because of either too much rain or insufficient evapotranspiration in the model. As Balruddery lies on the east coast of Scotland (see Figure 3.1), in the rain shadow of the Scottish Highlands, it is possible that the interaction between latitude, longitude and rainfall and temperature in the RF model resulted in the overestimation, particularly evident during the winter and autumn months, at this location.

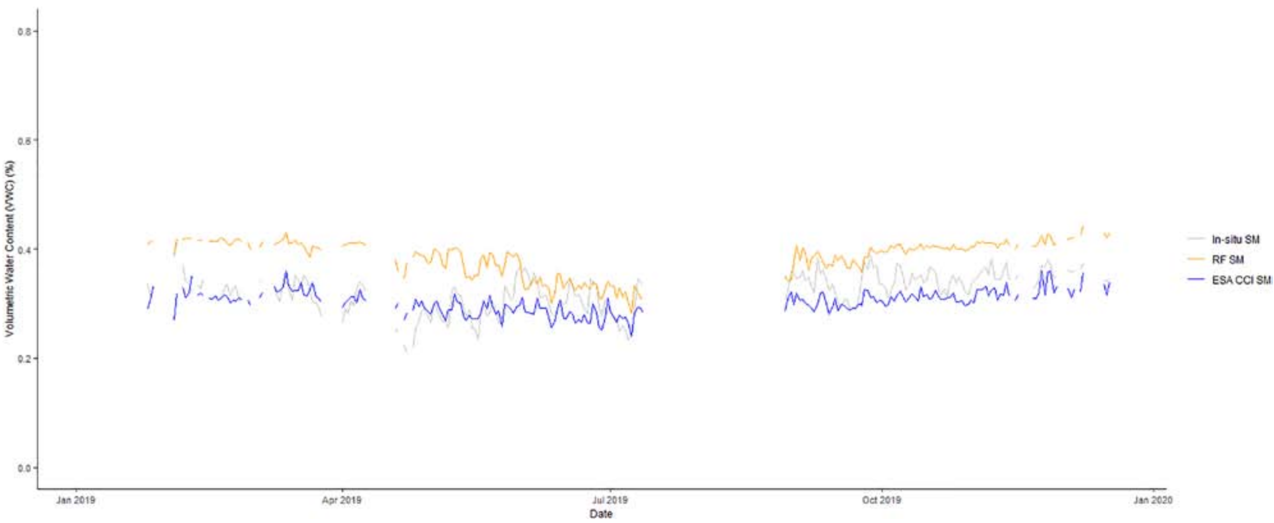

Figure 4.5. VWC (%) for Balruddery, classified as arable and horticulture on mineral soil, for the independent evaluation period of 2019 (In-situ SM; grey). The RF-estimated VWC values (RF SM) are shown in orange and the ESA CCI SM-estimated values in blue.

In general, the model appears capable of estimating soil moisture across the majority of sites (Figure 4.6), across different land cover types (Figure 4.7) and on different soil types, based on an evaluation of the RF model for the independent period. Overall, the model was found to perform better for cropland and grassland cover types and for mineral soils. The model also appears capable of estimating soil moisture in organic soils, but less skilfully than for mineral soils.

Following the evaluation of the RF model with the COSMOS-UK CRNS data for 2019, the trained model was employed in conjunction with an equivalent suite of covariates (see Table 3.3) obtained for Ireland. The model was employed to estimate soil moisture at four specified depths, namely 7.5, 15, 20 and 45 cm. The specified depths were employed as constants in the model and replaced the site mean effective depth parameter (D86_75M) employed to train the model.

4.2 Machine Learning Evaluation for Available Sites in Ireland

Figures 4.8 and 4.9 show the comparison between the *in situ* measurements at Johnstown Castle for 2013 (Figure 4.8; Table 4.3) and for 2018, 2019 and 2021 (Figure 4.9; Table 4.3), the RF-estimated values at 7.5 cm and the ESA CCI SM values. The Pearson's *R* values between the measured and

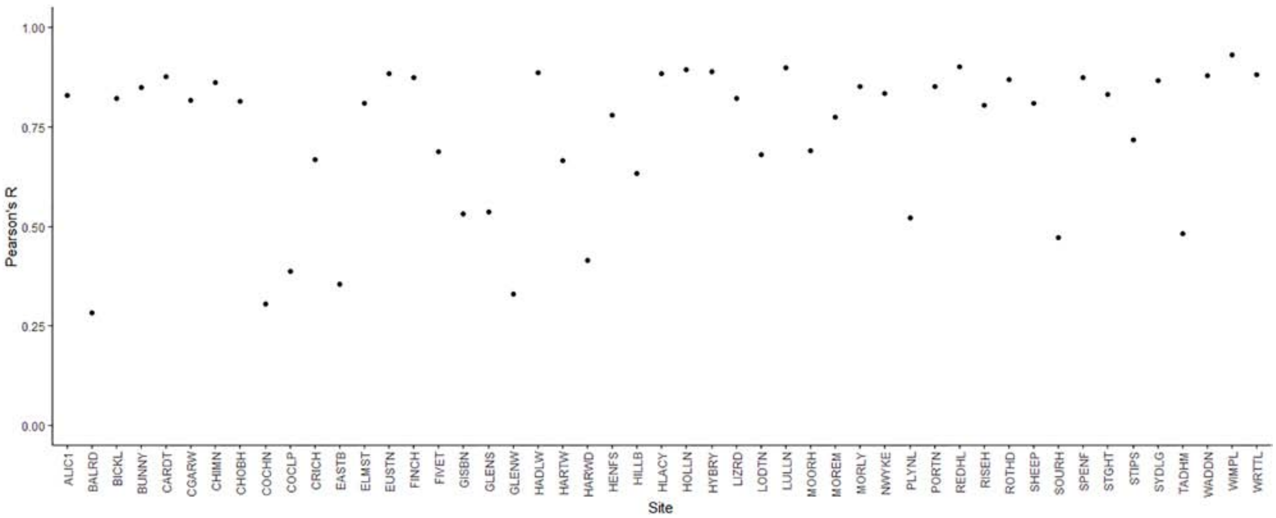

Figure 4.6. Pearson's *R* values for each of the COSMOS-UK CRNS sites and RF-estimated soil moisture values for the independent evaluation period (2019).

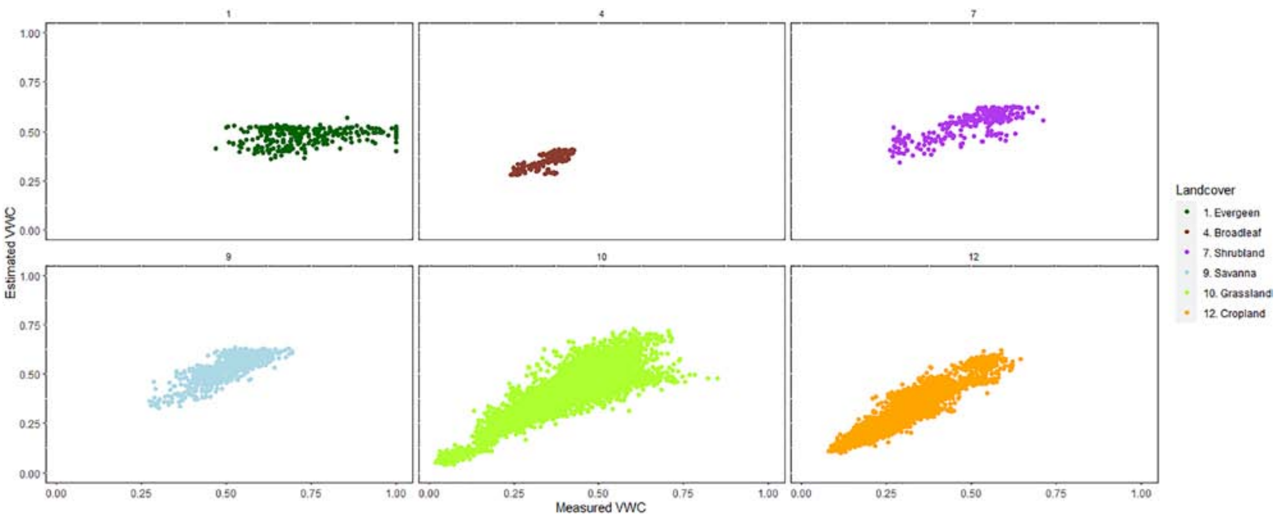

Figure 4.7. Scatterplots of measured VWC (%) and RF model-estimated VWC (%) by MODIS land cover type for the independent evaluation period (2019).

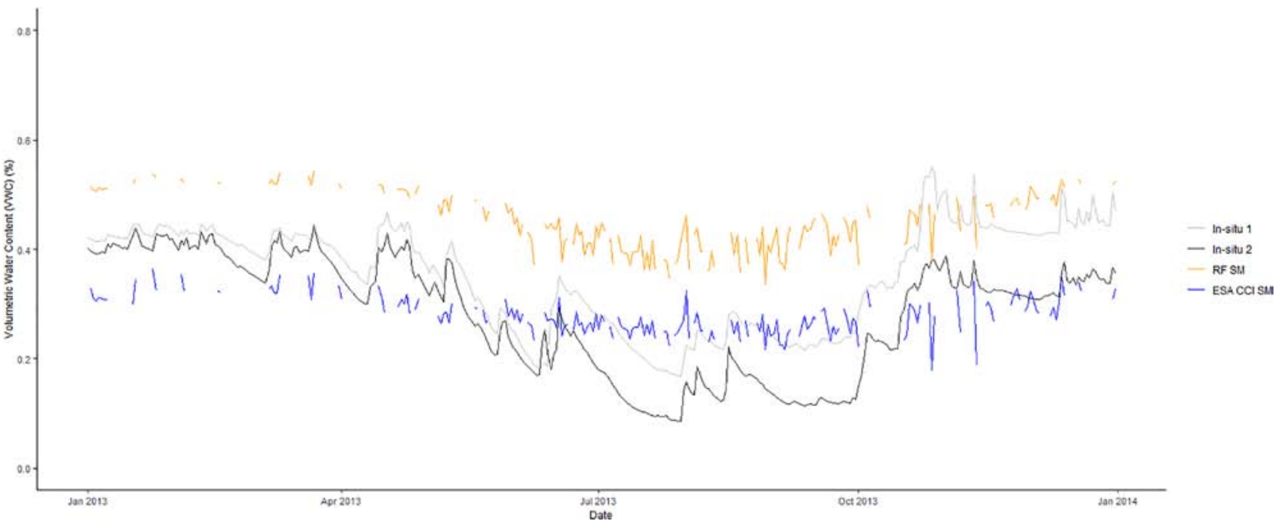

Figure 4.8. *In situ* soil moisture measurements from Johnstown Castle (In-situ 1 and In-situ 2; 5 cm depth), RF model-estimated soil moisture values (RF SM; 7.5 cm) and ESA CCI SM-estimated values for 2013.

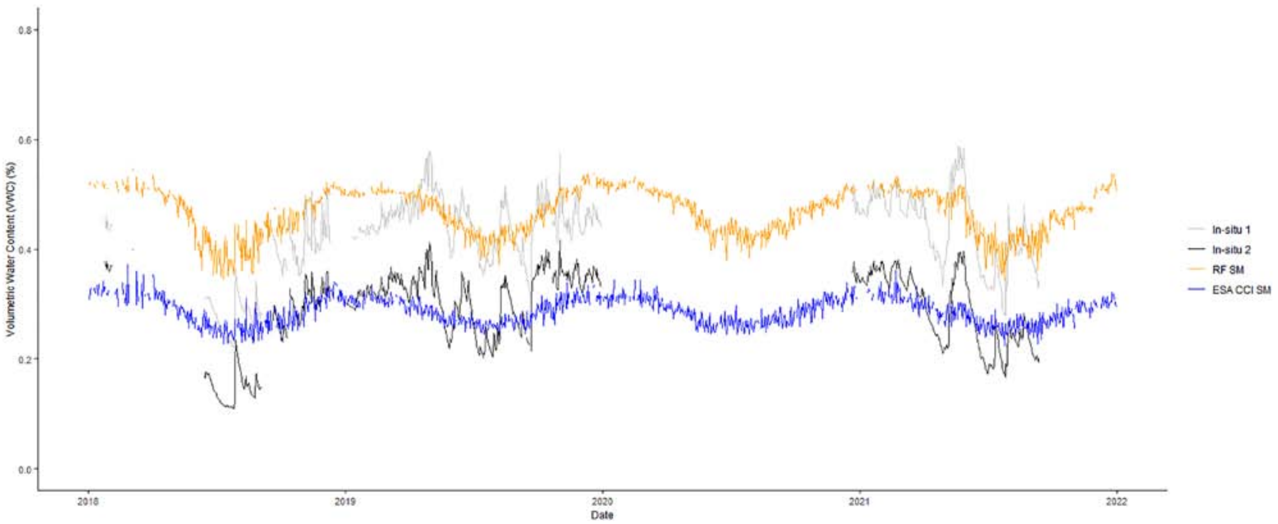

Figure 4.9. *In situ* soil moisture measurements from Johnstown Castle (In-situ 1 and In-situ 2; 5 cm depth), RF model-estimated soil moisture values (RF SM; 7.5 cm) and ESA CCI SM-estimated values for 2018–2021.

RF-estimated soil moisture for 2013 are 0.74 and 0.82 for *in situ* sensors 1 and 2, respectively. While *in situ* sensor 2 displays a higher Pearson's *R* value, MAE and RMSE values are higher for this sensor (MAE 0.2, RMSE 0.21) than for *in situ* sensor 1 (MAE 0.13, RMSE 0.14). These findings are consistent with those for the period 2018–2021, with Pearson's *R* values of 0.7 (MAE 0.05, RMSE 0.07) and 0.8 (MAE 0.18, RMSE 0.18) for *in situ* sensors 1 and 2, respectively. Figure 4.10 shows the scatterplots for each of the available years of *in situ* measurements.

Figures 4.11 and 4.12 show the comparison between the *in situ* measurements at Dripsey for the period 2003–2007 and RF-estimated soil moisture for two depths, 7.5 cm (Figure 4.11) and 15 cm (Figure 4.12), and ESA CCI SM values. The Pearson's *R* value between *in situ* sensor 1 and the RF-estimated soil moisture value at 7.5 cm is 0.68 (MAE 0.1, RMSE 0.13), while for *in situ* sensor 2 and RF-estimated soil moisture at this depth the Pearson's *R* value is 0.71 (MAE 0.02, RMSE 0.03).

Table 4.3. Pearson's *R* values between the ESA CCI SM, RF and NOAH LSM soil moisture estimates and available *in situ* measurements for available time periods

	ESA CCI SM product	RF model			NOAH LSM		
Site	Pearson's *R*	Pearson's *R*	MAE	RMSE	Pearson's *R*	MAE	RMSE
Johnstown Castle							
2013	0.57; 0.66	0.74; 0.82	0.13; 0.2	0.14; 0.21	0.78	0.11	0.13
2018–2021	0.62; 0.75	0.7; 0.8	0.05; 0.18	0.07; 0.18	0.85	0.05	0.05
Dripsey							
2003–2007	0.54; 0.52	0.66; 0.71	0.1; 0.02	0.13; 0.03	–	–	–
2010–2012	0.52	0.62	0.06	0.07	0.83	0.13	0.14
Carlow: 2003	0.66; 0.57	0.55; 0.46	0.09; 0.06	0.11; 0.07	–	–	–
Donoughmore: 2009–2012	0.49	0.61	0.05	0.06	0.86	0.11	0.11

Model results represent independent sites not included in model training. The values are shown for the available sensors at each site.

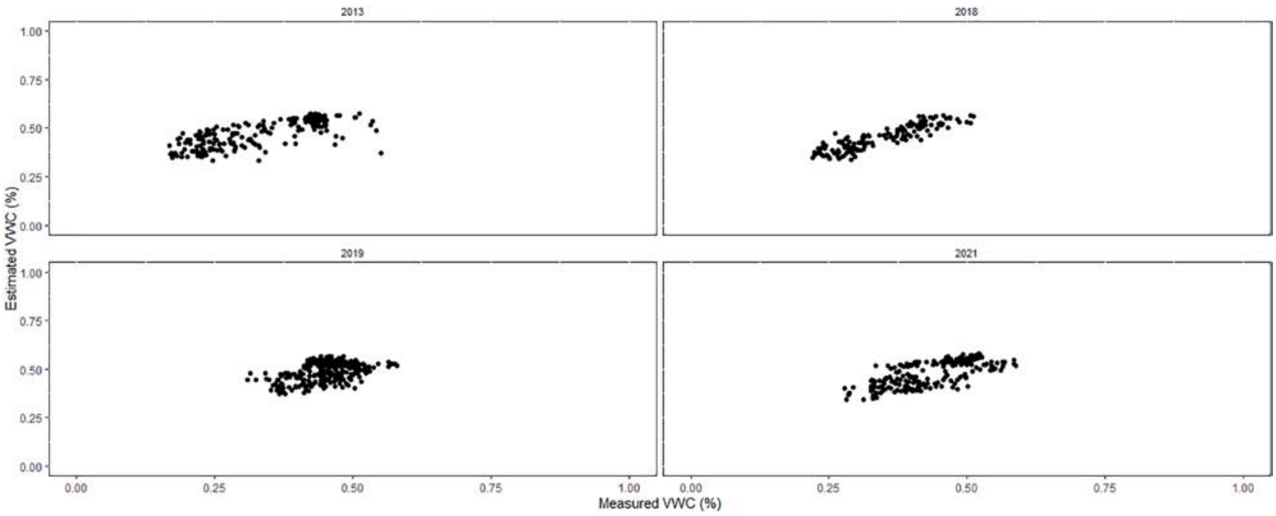

Figure 4.10. Scatterplot of measured and RF-estimated volumetric soil moisture from Johnstown Castle for 2013, 2018, 2019 and 2021.

Data from 1 year, 2003, were available from a grassland experiment at Oakpark, County Carlow, for two sensors, at reported depths of 20 and 40 cm. RF-estimated soil moisture values for model depths of 7.5, 15 and 20 cm were averaged for comparison with the *in situ* measurements from 20 cm and values for model depths of 7.5, 15, 20 and 45 cm were averaged for comparison with the *in situ* measurements from 40 cm. The Pearson's *R* value between the measured and *in situ* sensor value at 20 cm was 0.55 (MAE 0.09, RMSE 0.11) and the *R* value was 0.46 (MAE 0.06, RMSE 0.07) for the *in situ* sensor at 40 cm (Figure 4.13).

In situ soil moisture data for a deciduous broadleaf forest located near Donoughmore, County Cork, and in close proximity to the Dripsey grassland site were obtained for the period from 2009 to 2012 (Kiely *et al.*, 2018). The site was previously under grassland. Figure 4.14 shows the comparison between the *in situ* measurements, RF-estimated soil moisture values at 15 cm and the ESA CCI SM values. The Pearson's *R* value for this site was 0.61 (MAE 0.05, RMSE 0.06).

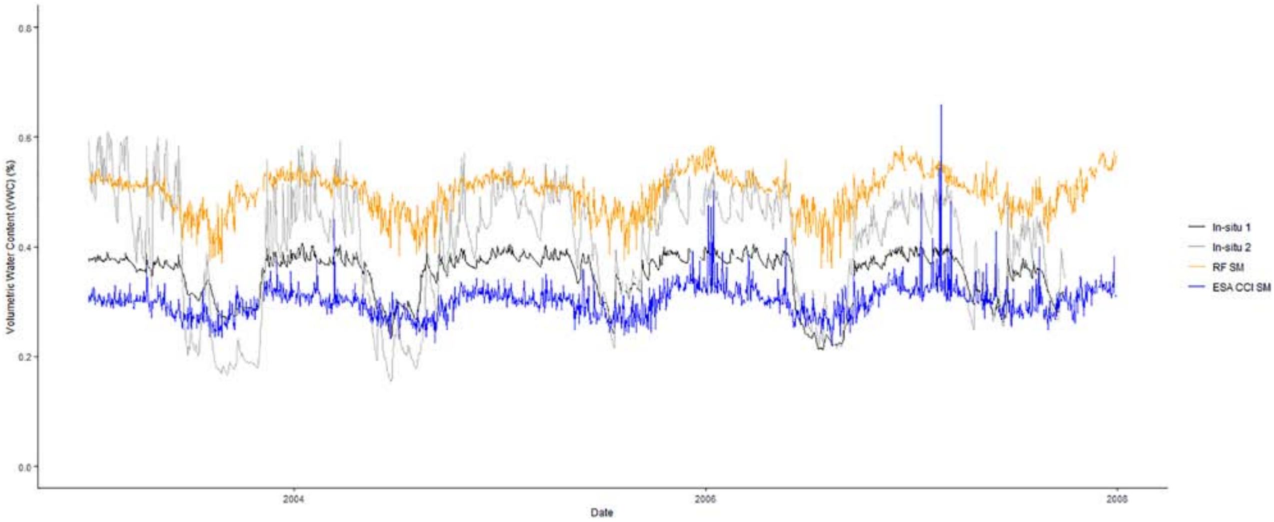

Figure 4.11. *In situ* soil moisture measurements from Dripsey (In-situ 1 and In-situ 2; 5 cm depth), RF model-estimated soil moisture values (7.5 cm) and ESA CCI SM-estimated values for 2003–2007. *In situ* sensor 3 values are not shown, as they are similar to those of *in situ* sensor 1 (In-situ 1).

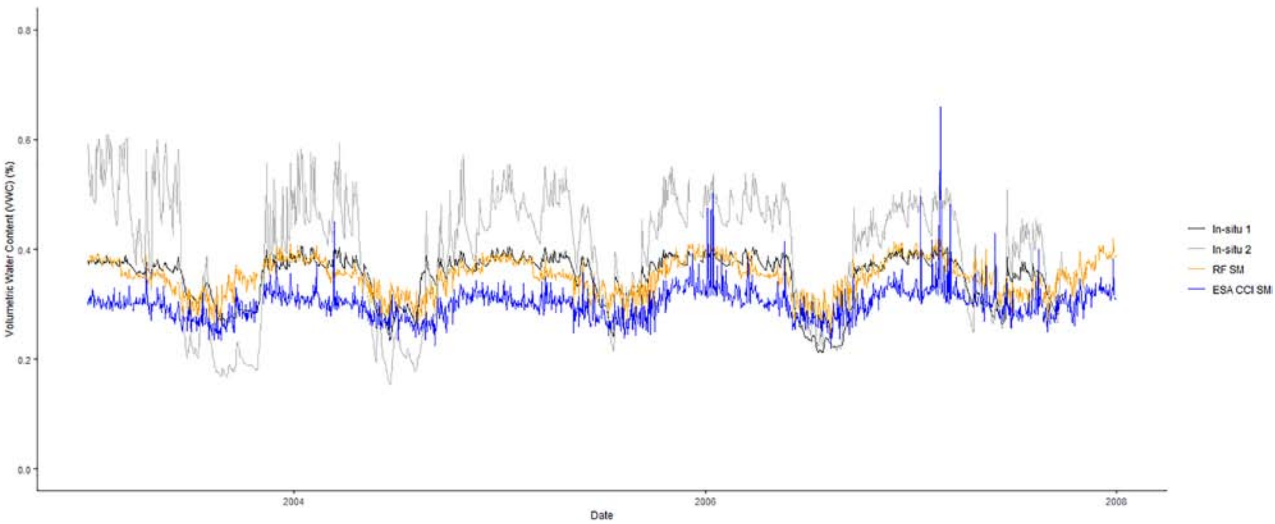

Figure 4.12. *In situ* soil moisture measurements from Dripsey (In-situ 1 and In-situ; 25 cm depth), RF model-estimated soil moisture values (15 cm) and ESA CCI SM-estimated values for 2003–2007. *In situ* sensor 3 values are not shown, as they are similar to those of *in situ* sensor 1 (In-situ 1).

4.3 NOAH Land Surface Model

An evaluation of the NOAH LSM against available *in situ* measurements for the period from 2010 to 2021 is described below. Figures 4.15 and 4.16 show the comparison between the NOAH LSM at 3.5 and 17.5 cm depths (mid-points of soil layers) and the *in situ* measurements at Johnstown Castle for 2013 (Figure 4.15) and 2018–2021 (Figure 4.16). The Pearson's *R* values were 0.78 (MAE 0.11, RMSE 0.13) for 2013 and 0.85 (MAE 0.05, RMSE 0.05) for the period 2018–2021 for the NOAH LSM-estimated soil moisture values at 3.5 cm depth.

Similarly, for Dripsey, the Pearson's *R* value between the *in situ* measurements for the period 2010–2012 and NOAH LSM-estimated soil moisture values at 3.5 cm was 0.83 (MAE 0.13, RMSE 0.14) (Figure 4.17). At the broadleaf site, Donoughmore, the Pearson's *R* value was 0.86 (MAE 0.11, RMSE 0.11) between the *in situ* soil moisture measurements and the NOAH LSM-estimated soil moisture values at 17.5 cm (Figure 4.18).

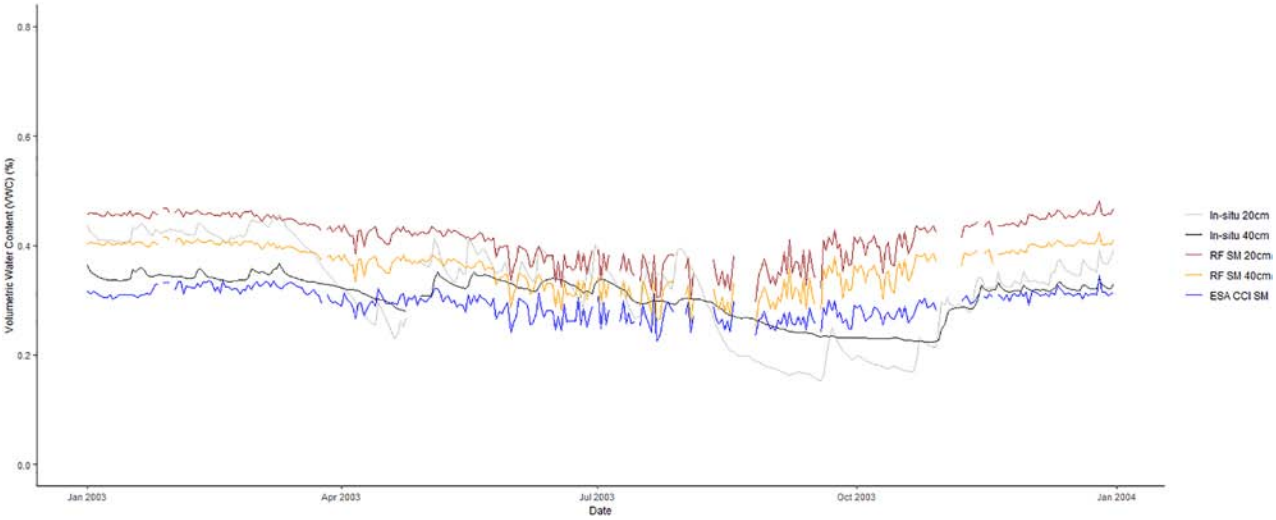

Figure 4.13. ***In situ*** **soil moisture measurements from Carlow (In-situ 20 cm and In-situ 40 cm), RF model-estimated soil moisture values at 20 cm (RF SM 20 cm; mean of 7.5, 15 and 20 cm values), RF model-estimated soil moisture values at 40 cm (RF SM 40 cm; mean of 7.5, 15, 20 and 45 cm values) and ESA CCI SM-estimated values for 2003.**

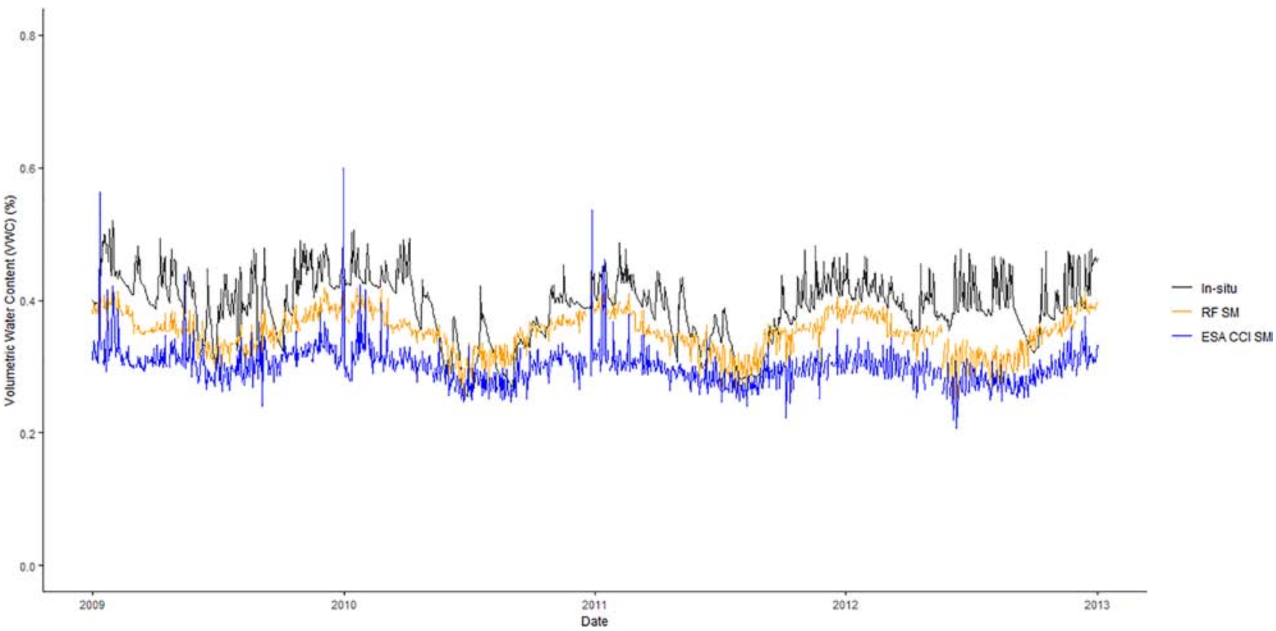

Figure 4.14. ***In situ*** **soil moisture measurements from Donoughmore (deciduous broadleaf forest) (In-situ), RF model-estimated soil moisture values at 15 cm (RF SM) and ESA CCI SM-estimated values for the period 2009–2012.**

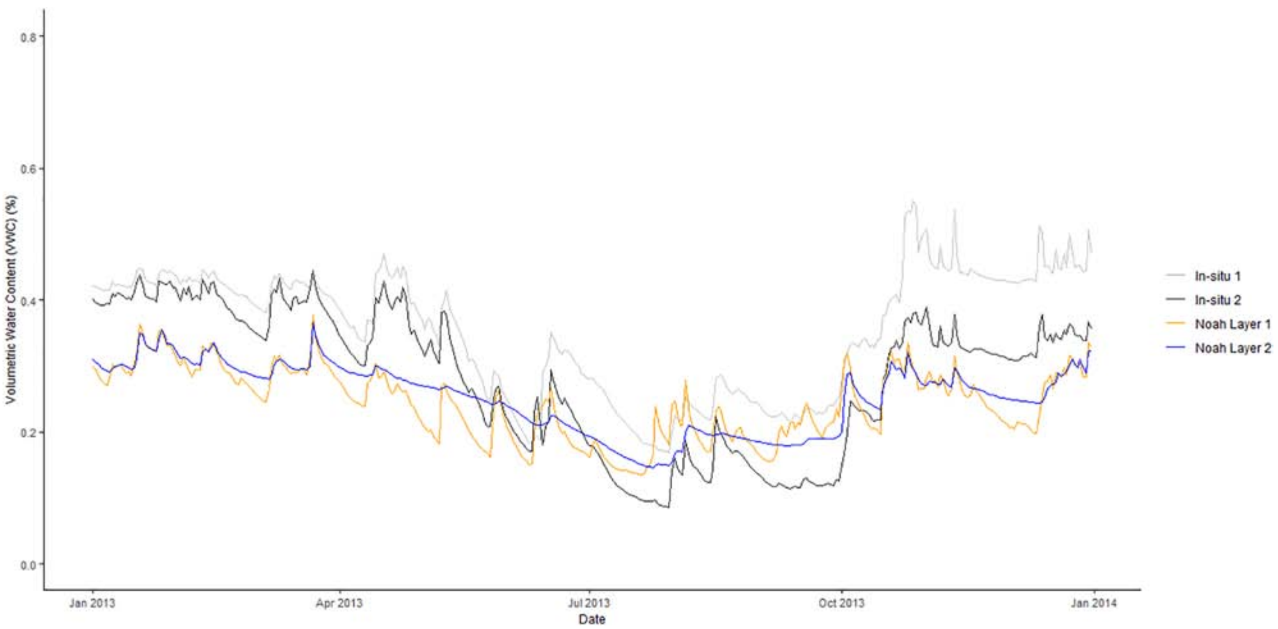

Figure 4.15. ***In situ*** **soil moisture measurements from Johnstown Castle (In-situ 1 and In-situ 2; 5 cm depth) and NOAH LSM-estimated soil moisture values at 3.5 cm (NOAH Layer 1) and 17.5 cm (NOAH Layer 2) for 2013.**

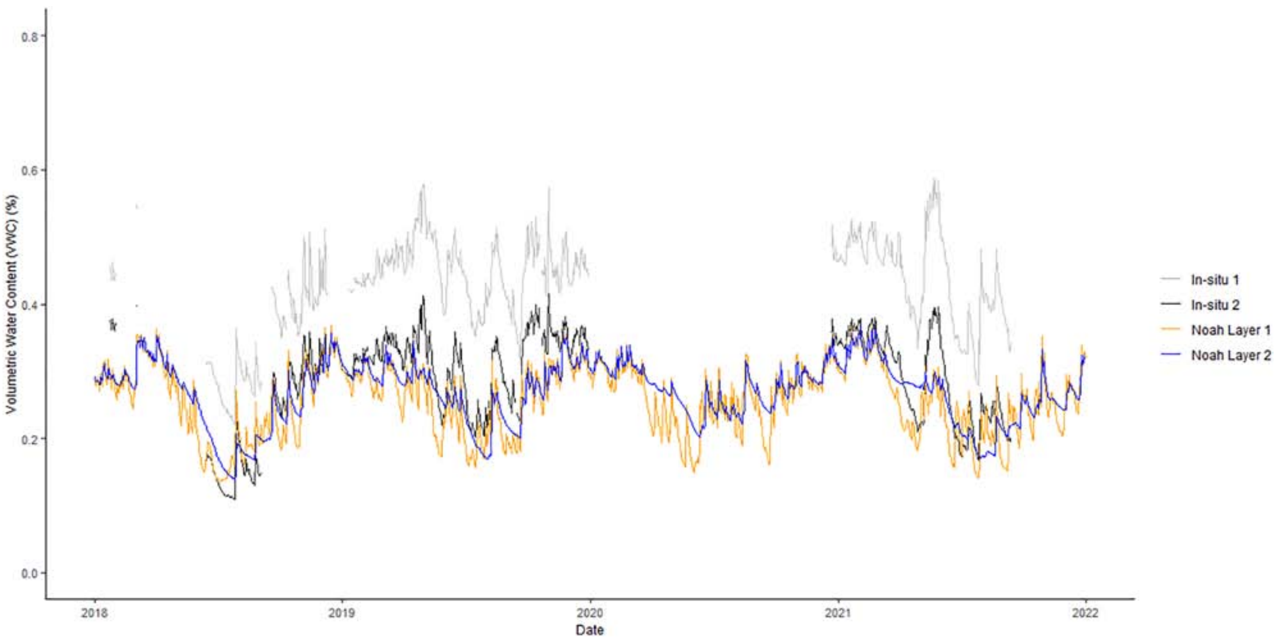

Figure 4.16. ***In situ*** **soil moisture measurements from Johnstown Castle (In-situ 1 and In-situ 2; 5 cm) and NOAH LSM-estimated soil moisture values at 3.5 cm (NOAH Layer 1) and 17.5 cm (NOAH Layer 2) for the period 2018–2021.**

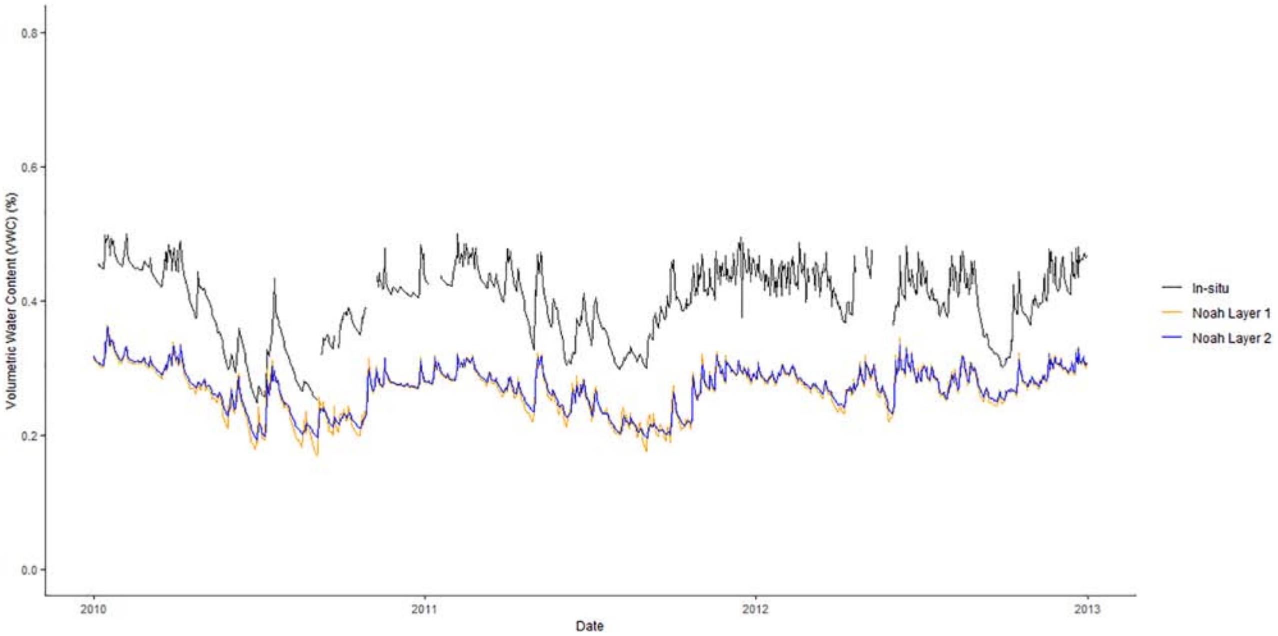

Figure 4.17. ***In situ*** **soil moisture measurements from Dripsey (In-situ) and NOAH LSM-estimated soil moisture values at 3.5 cm (NOAH Layer 1) and 17.5 cm (NOAH Layer 2) for the period 2010–2012.**

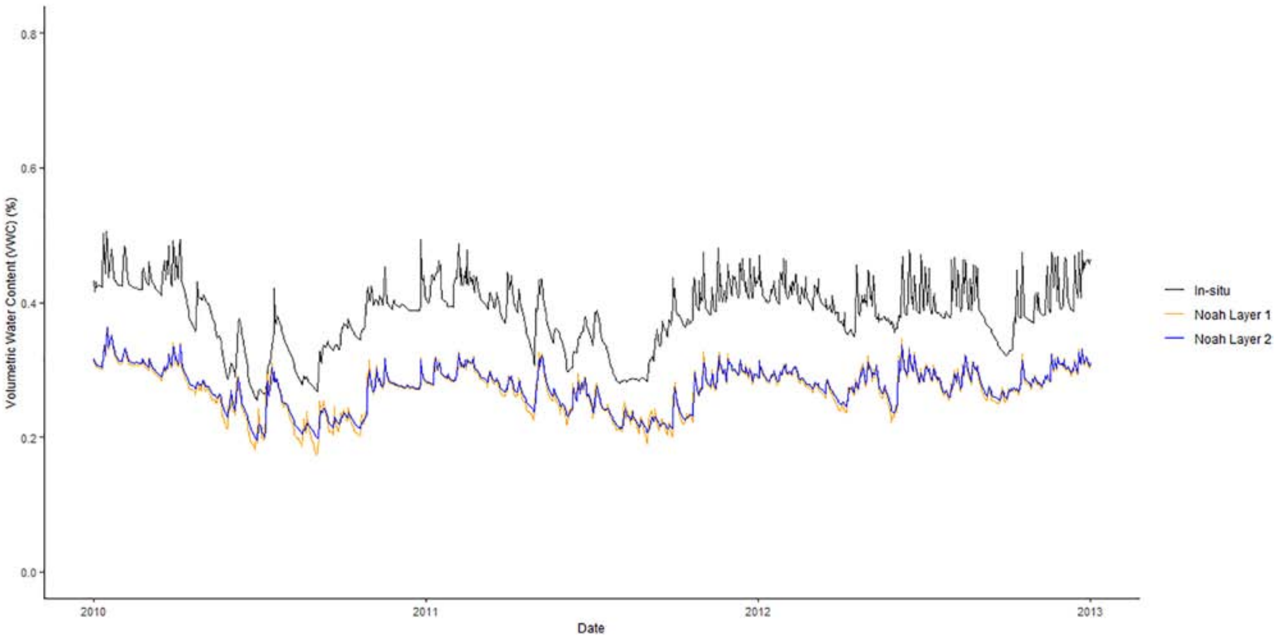

Figure 4.18. ***In situ*** **soil moisture measurements from Donoughmore (In-situ) and NOAH LSM-estimated soil moisture values at 3.5 cm (NOAH Layer 1) and 17.5 cm (NOAH Layer 2) for the period 2010–2012.**

5 Discussion

It is important to highlight that the comparisons of both the RF model and the NOAH LSM with the *in situ* data are between areal (spatial, gridded) and point data and that the representation of processes may differ between these spatial scales. In spite of this, both modelling approaches demonstrate capability in estimating soil moisture at sites where *in situ* measurements are available. The performance of the RF model, which was trained on data from COSMOS-UK sites, was the same as or better than the independent evaluation period when applied to the limited number of sites from Ireland. This indicates that the RF model is not likely to be overparameterised and is reasonably robust. While the RF model was shown to have lower performance over organic soils than other soil types for the evaluation period with the COSMOS-UK data, it was found to perform reasonably well at both Dripsey and Donoughmore, which are sites with poorly or impeded drainage on organic soil (see Table 3.4). With the exception of Carlow, the RF model displays better performance at all sites than the original ESA CCI SM product does. This is not unexpected, based on the resolution of the ESA CCI soil moisture dataset, which is ~25 km, and, therefore, the ESA CCI estimated values are reflective of aggregate processes across a larger sensor footprint.

Figure 5.1 shows the seasonal mean VWC (%) for the 7.5-cm layer from the RF model for the period 2010–2021. For the 7.5-cm layer, soil moisture shows clear seasonality in Ireland, with the winter months (December, January and February) displaying the highest VWC (0.53 $m^3 m^{-3}$) and the summer months (June, July and August) the lowest (0.44 $m^3 m^{-3}$), when averaged across the domain. During the summer months, drier regions along the east and south coasts are evident. These locations are subject to seasonal soil moisture deficits due to a combination of low precipitation, higher atmospheric water demand associated with higher temperature and freer draining soils.

Table 4.3 also shows a summary of Pearson's R correlations between the NOAH LSM estimates and the available *in situ* data. In general, the NOAH LSM-estimated values display higher Pearson's R values than the RF model estimates, but with higher MAE and RMSE values, with the exception of the 2018–2021 period at Johnstown Castle. This is evident from the figures in Chapter 4 (Figures 4.16, 4.18 and 4.19), where NOAH is shown to underestimate soil moisture based on the comparisons with measured *in situ* values at both Dripsey and Donoughmore. The reported field capacity (FC) for Johnstown Castle is 32% (Ishola *et al*., 2020), which lies close to the FC employed in the NOAH LSM (Figure 5.2) and derived from the default soil information. This FC value of 32% is also consistent with the measurements from the second *in situ* sensor at Johnstown Castle (see Figure 4.16). In contrast to the reported FC value at Dripsey of 32% (Liu *et al*., 2012b), which lies close to the model-prescribed FC value (0.329%; see Figure 5.2) for this location, the measured *in situ* data (see Figures 4.12 and 4.16) would indicate a higher FC than that reported or employed in the model. To

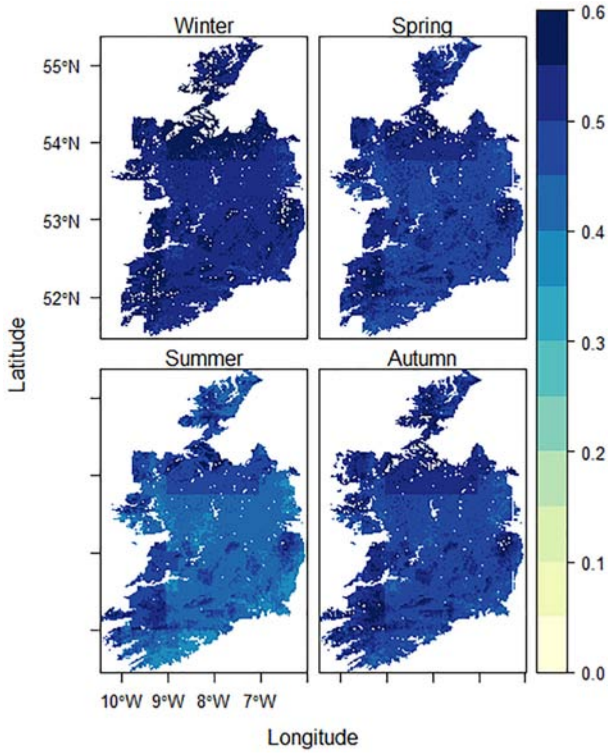

Figure 5.1. Seasonal mean VWC at 7.5 cm estimated by the RF model for the period 2010–2021.

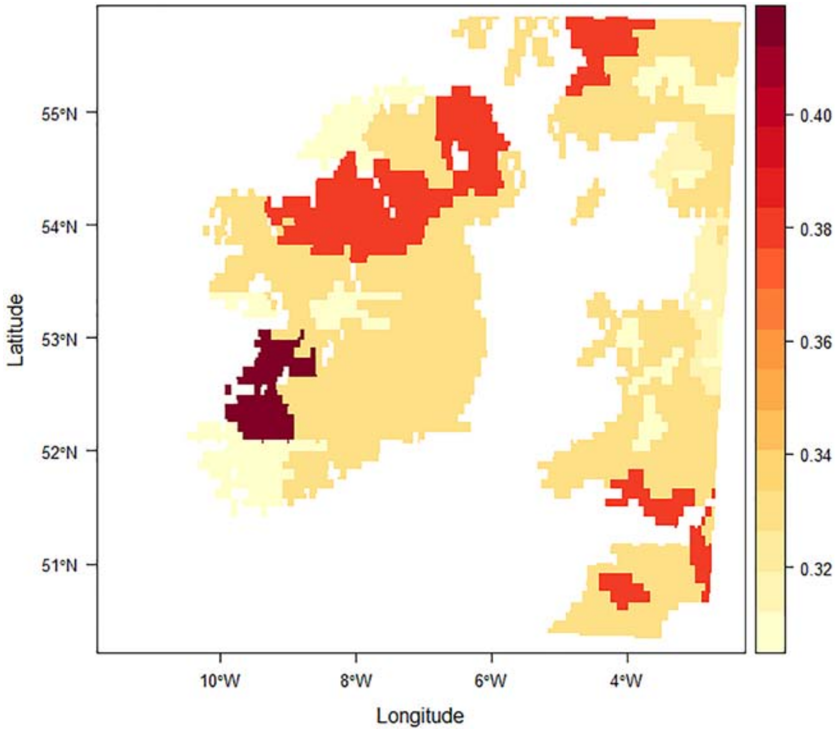

Figure 5.2. FC values taken from the default soil parameter table for the associated soil textural class employed in the NOAH LSM.

illustrate the importance of model-prescribed FC values for the estimation of soil moisture, a model grid location with an FC value of 0.41% and under similar synoptic forcing (proximally located on the Kerry–Cork–Limerick border) was extracted and compared with the *in situ* measurements from Dripsey (Figure 5.3). It is clear that the higher FC value gives rise to a higher model-estimated soil moisture content value. While direct measurements of the water capacity of the soil can be made at different pressures, FC is a conceptual measure defined as the water retained in the soil at –33 $\mathrm{J\,kg^{-1}}$ (equivalent to –0.33 bar), and it plays a central role in many hydrological models that simulate soil–plant–water interactions, the estimation of which relies on having good soil information.

Figure 5.4 shows the seasonal mean VWC ($\mathrm{m^3\,m^{-3}}$) for the 0–7 cm layer from the NOAH LSM for the period 2010–2021. While the spatial distribution is evidently similar to that of the RF approach (see Figure 5.1), the NOAH LSM-estimated values are lower. The spatial distributions of the default soil textures (see Figure 3.11) and associated prescribed FC values (Figure 5.2) are also evident in the seasonal soil moisture estimates.

To ensure that the outputs from this research can be used to inform and support new research in the area, we developed an *in situ* dashboard, to enable users to access *in situ* measurements from the instruments deployed as part of this funding (Figures 5.5 and 5.6). In addition, we developed the R-shiny online app, to facilitate access to the model output data (Figure 5.7), available at https://terrain-ai.shinyapps.io/Irish-Soil_Moisture/. Through the R-shiny app, users can select a location and specify a soil depth and time period of interest and download data from the RF model and NOAH LSM as a comma-delimited text file that can be read in any subsequent software package.

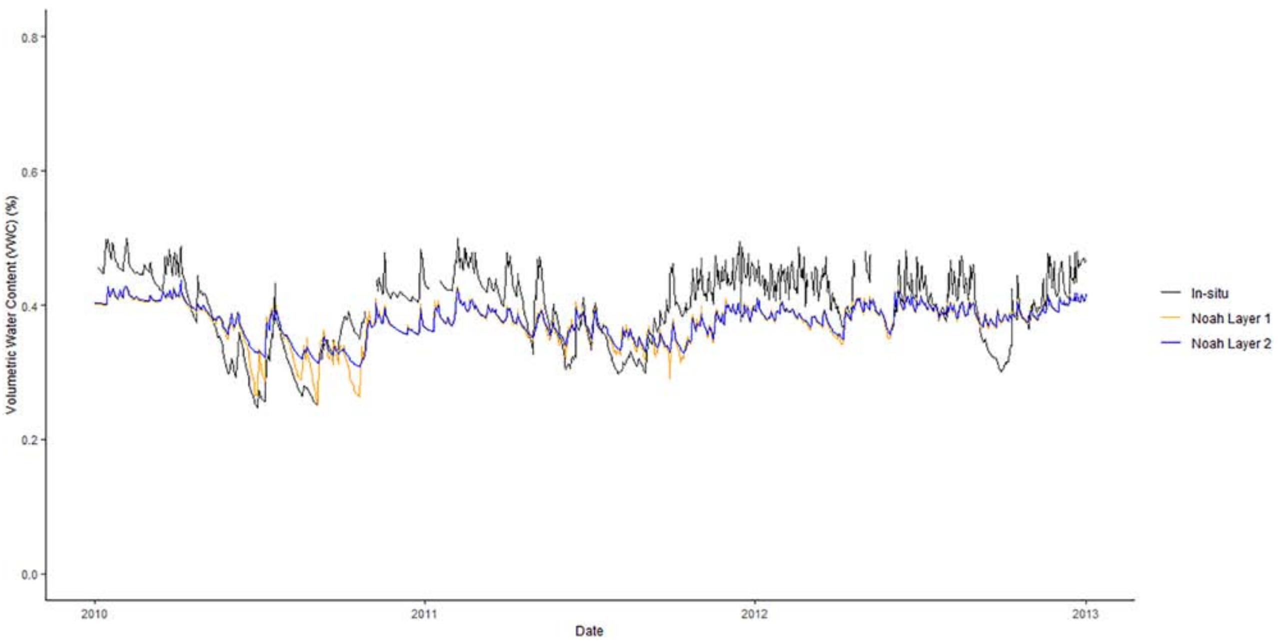

Figure 5.3. NOAH LSM-estimated soil moisture values for the 0–7 cm layer (NOAH Layer 1) and 7–21 cm layer (NOAH Layer 2) obtained from a proximal grid location experiencing similar synoptic-scale forcing but with a high FC value (0.412) relative to the published FC value (0.32) and model-specified FC value (0.329).

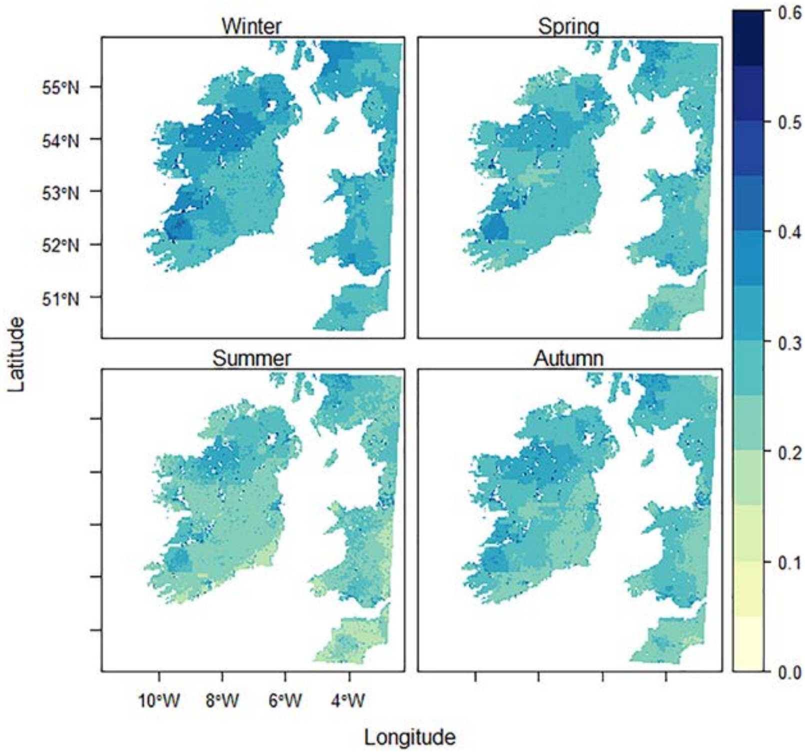

Figure 5.4. Seasonal mean VWC for the 0–7 cm layer from the NOAH LSM, calculated for the period 2010–2021.

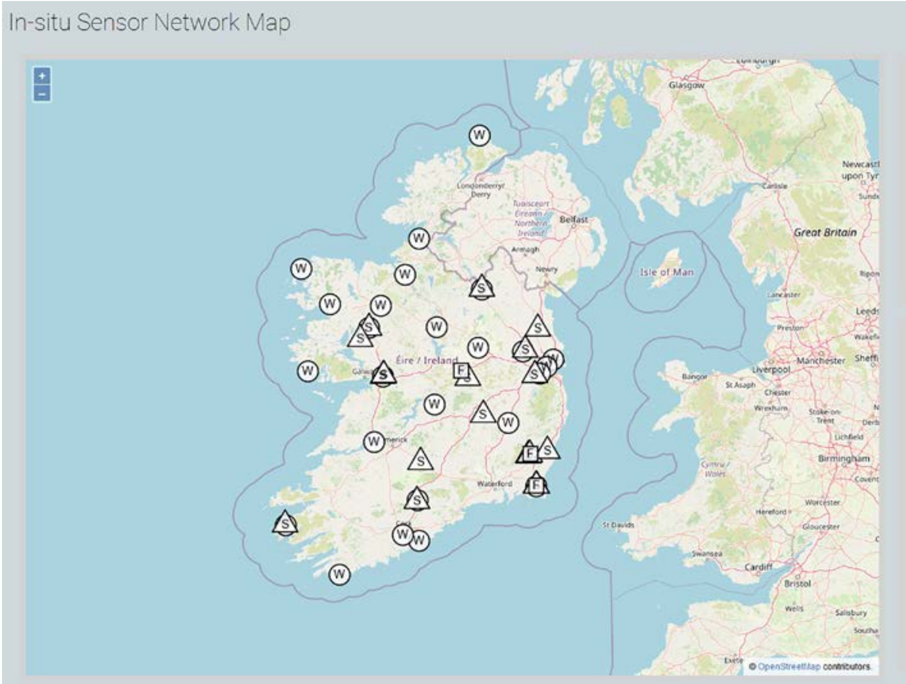

Figure 5.5. ***In situ*** **sensor map access interface.**

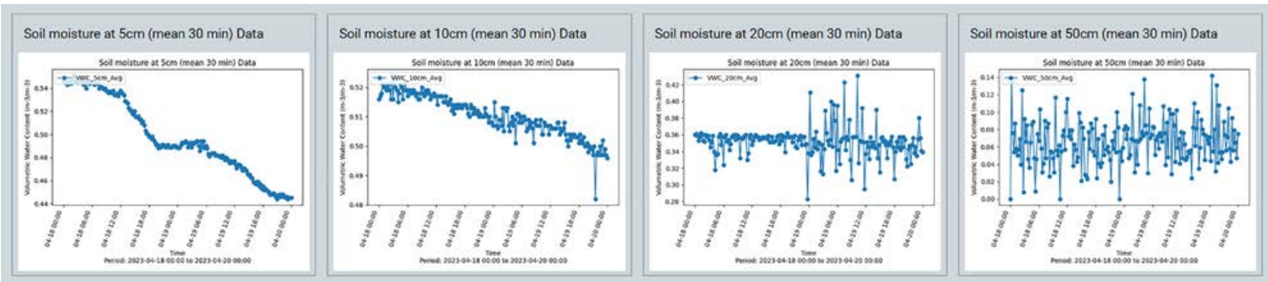

Figure 5.6. Access to real-time soil moisture data for a selected site.

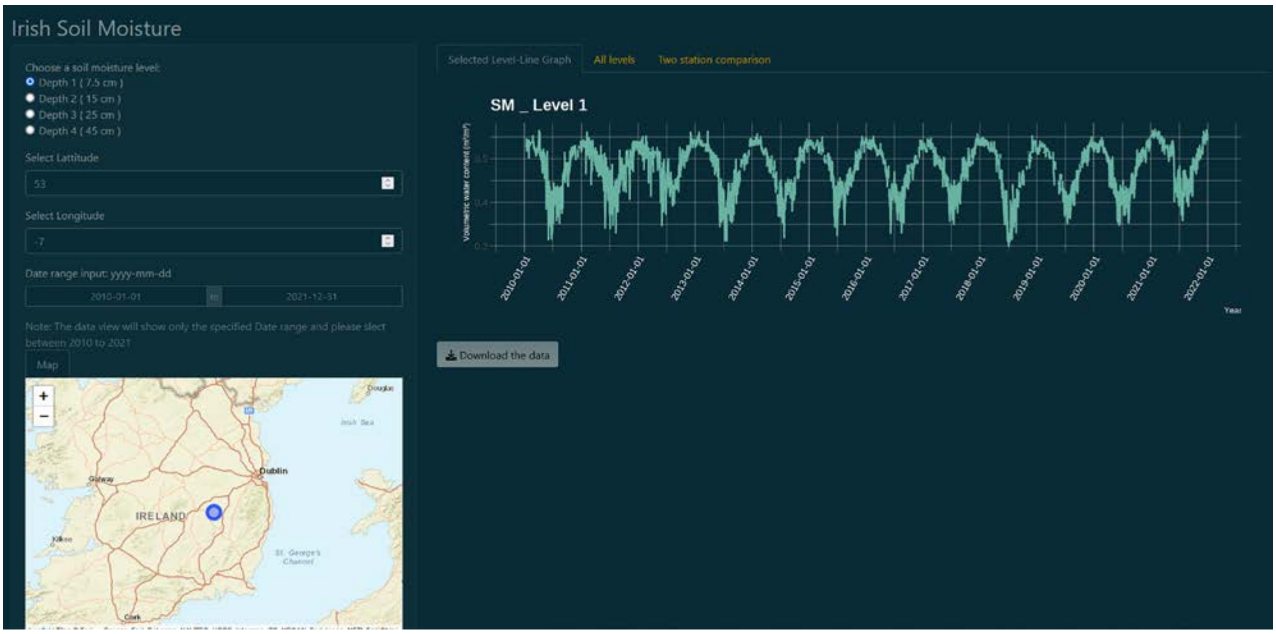

Figure 5.7. R-shiny app for selecting a location and downloading a comma delimited text file of soil moisture data for selected depths and time periods.

6 Conclusions

Soil moisture has been identified as an essential climate variable, and information on soil moisture plays a central role in understanding and modulating soil–plant–atmosphere interactions. It is also important to measure and monitor soil moisture conditions for agriculture, to support on-farm decision-making and assess the potential for drought conditions. Information on soil moisture is also important for many hydrological applications and is of critical importance for understanding the role of extreme climate events. Yet, in spite of the recognised importance of understanding soil moisture, many countries, including Ireland, lack the integrated monitoring infrastructure necessary for measuring soil moisture. There is an urgent need to address this from a policy perspective. While remote sensing can support the monitoring of soil moisture, it is not a replacement for *in situ* measurements. In addition to a comprehensive and distributed network of soil moisture sensors, an operational LSM that can utilise remotely sensed and *in situ* measurements is also required.

A key objective of the current research was to evaluate, and subsequently utilise, a suitable approach for employing the available and existing large number of multi-thematic and multi-temporal Earth observation data in combination with available *in situ* data to derive estimates of soil moisture for Ireland. To achieve this, we employed two approaches, namely a statistical ML approach using the RF classification method and a dynamic LSM. While both approaches were found to have value, more research is needed to develop national monitoring and modelling capacity in this important area.

A key limitation of the research was the fact that Ireland does not have a centrally administered and maintained soil measurement network akin to the meteorological and hydrological networks operated by Met Éireann and the Office of Public Works; only fragmented and limited-duration *in situ* data are available from a small number of sites. In recognition of this shortcoming, DAFM provided funding to support the deployment of CRNS instruments, maintained by University College Dublin and Met Éireann. Terrain-AI, funded by the Science Foundation Ireland through a strategic partnership with Microsoft, has also deployed soil moisture sensors; additional sensors were deployed as part of the research reported on here. These represent community-led initiatives – and require oversight and investment if the monitoring programme is to be consolidated and expanded.

In spite of the lack of a centrally administered and maintained soil measurement network, both modelling approaches were demonstrated to be capable of estimating soil moisture, based on available *in situ* observations. Future work should focus on the potential to integrate satellite information directly into the land surface modelling framework, through data assimilation techniques, and integrate the RF model outputs into a dynamical modelling approach.

More generally, environmental data, in Ireland and elsewhere, remain very fragmented and are distributed across numerous national and international data owners and providers. Ireland also lacks a centralised data catalogue, with associated metadata information. Consequently, researchers spend a significant amount of time sourcing and obtaining permissions to use data collected through previous, and often publicly funded, research. Significant benefits could be delivered, to both the research community and wider society, through the development of a coordinated national research infrastructure to support and foster environment-related research activities, generate new knowledge and support improved policy implementation. This would also support the integration of existing, and new, monitoring networks that are maintained and managed by different organisations, often with different purposes in mind.

Key recommendations:

- Develop a centrally administered and maintained distributed network of soil moisture sensors. Ideally, these sensors would be co-located with existing meteorological instrumentation, to understand the drivers and processes associated with soil moisture.
- Undertake a national soil survey that can provide detailed and high-resolution soil information, including soil textural information and information

on soil properties (porosity, saturated hydraulic conductivity and derived information such as FC). This is critical to the success of an *in situ* network and a modelling framework.

- Develop a comprehensive modelling framework that can integrate a range of different Earth observation data to support the operational modelling and forecasting of soil moisture. This would also support high-resolution hydrological monitoring and modelling similar to the National Water Model in the USA or the Global Flood Awareness System.
- Develop a national environmental research infrastructure, underpinned by existing and new monitoring networks, computational resources and storage, workflows and modelling tools, to support and foster research and innovation and provide support to enable the development of improved policies and policy implementation.
- Support the development of national capacity building beyond typical funded project lifetimes, to ensure that core expertise can be retained and developed.

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Abbreviations

AGMET	Joint Working Group on Applied Agricultural Meteorology
AI	Artificial intelligence
AMSR2	Advanced Microwave Scanning Radiometer 2
ASCAT	Advanced Scatterometer
CCI	Climate Change Initiative
CCI SM	Climate Change Initiative Soil Moisture
CLC	CORINE Land Cover
CLM	Community land model
COSMOS-UK	UK Cosmic-ray Soil Moisture Monitoring Network
CRNS	Cosmic ray neutron sensor
csv	Comma-separated variable
DAFM	Department of Agriculture, Food and the Marine
ECMWF	European Centre for Medium-Range Weather Forecasts
ESA	European Space Agency
FC	Field capacity
FFS	Forward feature selection
GLDAS	Global Land Data Assimilation System
ISMON	Irish Soil Moisture Observation Network
LAI	Leaf Area Index
LLO	Leave location out
LSM	Land surface model
MAE	Mean absolute error
ML	Machine learning
MODIS	Moderate Resolution Imaging Spectroradiometer
NASCO	National Agricultural Soil Carbon Observatory
NDVI	Normalised Difference Vegetation Index
netCDF	Network common data form
OPTRAM	Optical Trapezoid Model
RF	Random forest
RMSE	Root-mean-square error
SAR	Synthetic aperture radar
SMAP	Soil Moisture Active Passive
SMOS	Soil Moisture and Ocean Salinity
TDR	Time domain reflectometer
UKCEH	UK Centre for Ecology and Hydrology
VIC	Variable infiltration model
VWC	Volumetric water content
WGS84	World Geodetic System 1984
WPS	Weather, Research and Forecasting model Pre-Processing System

An Ghníomhaireacht Um Chaomhnú Comhshaoil

Tá an GCC freagrach as an gcomhshaol a chosaint agus a fheabhsú, mar shócmhainn luachmhar do mhuintir na hÉireann. Táimid tiomanta do dhaoine agus don chomhshaol a chosaint ar thionchar díobhálach na radaíochta agus an truaillithe.

Is féidir obair na Gníomhaireachta a roinnt ina trí phríomhréimse:

Rialáil: Rialáil agus córais chomhlíonta comhshaoil éifeachtacha a chur i bhfeidhm, chun dea-thorthaí comhshaoil a bhaint amach agus díriú orthu siúd nach mbíonn ag cloí leo.

Eolas: Sonraí, eolas agus measúnú ardchaighdeáin, spriocdhírithe agus tráthúil a chur ar fáil i leith an chomhshaoil chun bonn eolais a chur faoin gcinnteoireacht.

Abhcóideacht: Ag obair le daoine eile ar son timpeallachta glaine, táirgiúla agus dea-chosanta agus ar son cleachtas inbhuanaithe i dtaobh an chomhshaoil.

I measc ár gcuid freagrachtaí tá:

Ceadúnú

- Gníomhaíochtaí tionscail, dramhaíola agus stórála peitril ar scála mór;
- Sceitheadh fuíolluisce uirbigh;
- Úsáid shrianta agus scaoileadh rialaithe Orgánach Géinmhodhnaithe;
- Foinsí radaíochta ianúcháin;
- Astaíochtaí gás ceaptha teasa ó thionscal agus ón eitlíocht trí Scéim an AE um Thrádáil Astaíochtaí.

Forfheidhmiú Náisiúnta i leith Cúrsaí Comhshaoil

- Iniúchadh agus cigireacht ar shaoráidí a bhfuil ceadúnas acu ón GCC;
- Cur i bhfeidhm an dea-chleachtais a stiúradh i ngníomhaíochtaí agus i saoráidí rialáilte;
- Maoirseacht a dhéanamh ar fhreagrachtaí an údaráis áitiúil as cosaint an chomhshaoil;
- Caighdeán an uisce óil phoiblí a rialáil agus údaruithe um sceitheadh fuíolluisce uirbigh a fhorfheidhmiú
- Caighdeán an uisce óil phoiblí agus phríobháidigh a mheasúnú agus tuairisciú air;
- Comhordú a dhéanamh ar líonra d'eagraíochtaí seirbhíse poiblí chun tacú le gníomhú i gcoinne coireachta comhshaoil;
- An dlí a chur orthu siúd a bhriseann dlí an chomhshaoil agus a dhéanann dochar don chomhshaol.

Bainistíocht Dramhaíola agus Ceimiceáin sa Chomhshaol

- Rialacháin dramhaíola a chur i bhfeidhm agus a fhorfheidhmiú lena n-áirítear saincheisteanna forfheidhmithe náisiúnta;
- Staitisticí dramhaíola náisiúnta a ullmhú agus a fhoilsiú chomh maith leis an bPlean Náisiúnta um Bainistíocht Dramhaíola Guaisí;
- An Clár Náisiúnta um Chosc Dramhaíola a fhorbairt agus a chur i bhfeidhm;
- Reachtaíocht ar rialú ceimiceán sa timpeallacht a chur i bhfeidhm agus tuairisciú ar an reachtaíocht sin.

Bainistíocht Uisce

- Plé le struchtúir náisiúnta agus réigiúnacha rialachais agus oibriúcháin chun an Chreat-treoir Uisce a chur i bhfeidhm;
- Monatóireacht, measúnú agus tuairisciú a dhéanamh ar chaighdeán aibhneacha, lochanna, uiscí idirchreasa agus cósta, uiscí snámha agus screamhuisce chomh maith le tomhas ar leibhéil uisce agus sreabhadh abhann.

Eolaíocht Aeráide & Athrú Aeráide

- Fardail agus réamh-mheastacháin a fhoilsiú um astaíochtaí gás ceaptha teasa na hÉireann;
- Rúnaíocht a chur ar fáil don Chomhairle Chomhairleach ar Athrú Aeráide agus tacaíocht a thabhairt don Idirphlé Náisiúnta ar Ghníomhú ar son na hAeráide;
- Tacú le gníomhaíochtaí forbartha Náisiúnta, AE agus NA um Eolaíocht agus Beartas Aeráide.

Monatóireacht & Measúnú ar an gComhshaol

- Córais náisiúnta um monatóireacht an chomhshaoil a cheapadh agus a chur i bhfeidhm: teicneolaíocht, bainistíocht sonraí, anailís agus réamhaisnéisiú;
- Tuairiscí ar Staid Thimpeallacht na hÉireann agus ar Tháscairí a chur ar fáil;
- Monatóireacht a dhéanamh ar chaighdeán an aeir agus Treoir an AE i leith Aeir Ghlain don Eoraip a chur i bhfeidhm chomh maith leis an gCoinbhinsiún ar Aerthruailliú Fadraoin Trasteorann, agus an Treoir i leith na Teorann Náisiúnta Astaíochtaí;
- Maoirseacht a dhéanamh ar chur i bhfeidhm na Treorach i leith Torainn Timpeallachta;
- Measúnú a dhéanamh ar thionchar pleananna agus clár beartaithe ar chomhshaol na hÉireann.

Taighde agus Forbairt Comhshaoil

- Comhordú a dhéanamh ar ghníomhaíochtaí taighde comhshaoil agus iad a mhaoiniú chun brú a aithint, bonn eolais a chur faoin mbeartas agus réitigh a chur ar fáil;
- Comhoibriú le gníomhaíocht náisiúnta agus AE um thaighde comhshaoil.

Cosaint Raideolaíoch

- Monatóireacht a dhéanamh ar leibhéil radaíochta agus nochtadh an phobail do radaíocht ianúcháin agus do réimsí leictreamaighnéadacha a mheas;
- Cabhrú le pleananna náisiúnta a fhorbairt le haghaidh éigeandálaí ag eascairt as taismí núicléacha;
- Monatóireacht a dhéanamh ar fhorbairtí thar lear a bhaineann le saoráidí núicléacha agus leis an tsábháilteacht raideolaíochta;
- Sainseirbhísí um chosaint ar an radaíocht a sholáthar, nó maoirsiú a dhéanamh ar sholáthar na seirbhísí sin.

Treoir, Ardú Feasachta agus Faisnéis Inrochtana

- Tuairisciú, comhairle agus treoir neamhspleách, fianaise-bhunaithe a chur ar fáil don Rialtas, don tionscal agus don phobal ar ábhair maidir le cosaint comhshaoil agus raideolaíoch;
- An nasc idir sláinte agus folláine, an geilleagar agus timpeallacht ghlan a chur chun cinn;
- Feasacht comhshaoil a chur chun cinn lena n-áirítear tacú le hiompraíocht um éifeachtúlacht acmhainní agus aistriú aeráide;
- Tástáil radóin a chur chun cinn i dtithe agus in ionaid oibre agus feabhsúchán a mholadh áit is gá.

Comhpháirtíocht agus Líonrú

- Oibriú le gníomhaireachtaí idirnáisiúnta agus náisiúnta, údaráis réigiúnacha agus áitiúla, eagraíochtaí neamhrialtais, comhlachtaí ionadaíocha agus ranna rialtais chun cosaint chomhshaoil agus raideolaíoch a chur ar fáil, chomh maith le taighde, comhordú agus cinnteoireacht bunaithe ar an eolaíocht.

Bainistíocht agus struchtúr na Gníomhaireachta um Chaomhnú Comhshaoil

Tá an GCC á bainistiú ag Bord lánaimseartha, ar a bhfuil Ard-Stiúrthóir agus cúigear Stiúrthóir. Déantar an obair ar fud cúig cinn d'Oifigí:

1. An Oifig um Inbhunaitheacht i leith Cúrsaí Comhshaoil
2. An Oifig Forfheidhmithe i leith Cúrsaí Comhshaoil
3. An Oifig um Fhianaise agus Measúnú
4. An Oifig um Chosaint ar Radaíocht agus Monatóireacht Comhshaoil
5. An Oifig Cumarsáide agus Seirbhísí Corparáideacha

Tugann coistí comhairleacha cabhair don Ghníomhaireacht agus tagann siad le chéile go rialta le plé a dhéanamh ar ábhair imní agus le comhairle a chur ar an mBord.

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