

## AGRO-CLIMATIC CHANGE AND EUROPEAN SOIL SUITABILITY: REGIONAL MODELLING AT MONTHLY TIME-STEPS

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**A b s t r a c t.** This paper describes the development of ACCESS-I (Agro-Climatic Change and European Soil Suitability), a model that will simulate the soil water balance and crop growth, for soil map units within regions, under conditions of climate change. ACCESS-I has been developed for spatial application over large geographic areas, and so its data input requirements have been kept to a minimum. These include the use of meteorological data with monthly time-steps, and the estimation of soil hydraulic properties from simple soil survey data (particle size distribution, organic carbon content and bulk density) using pedotransfer functions.

The soil water balance component of ACCESS-I considers evaporation and transpiration separately, as well as defining root front development and root density. Biomass accumulation is estimated using the concept of water use efficiency, and crop yields (for wheat, maize, sunflower and soybean) are calculated from the total biomass, using a crop dependent harvest index. The model considers the influence of atmospheric CO<sub>2</sub> concentrations on crop yields through the water use efficiency. ACCESS-I also contains a sub-model to assess soil workability, a major constraint to crop production in northern latitudes. A spreadsheet validation protocol has been developed for ACCESS-I in which experimental datasets can be compared directly with simulation output files in the same format. Comparison of observed and modelled data from central England have shown ACCESS-I to be able to simulate the soil water balance and biomass accumulation to acceptable levels of accuracy.

**K e y w o r d s:** model, land use evaluation, soil water balance, crop phenology, agro-climate

### INTRODUCTION

This paper reports on the development, validation procedures and spatialisation of the

model known as ACCESS-I (Agro-Climatic Change and European Soil Suitability). ACCESS-I is a composite model including agro-climatic indices, soil water balance and crop production modules (Table 1). The main characteristics of ACCESS-I are:

- plant growth and the soil water balance are calculated monthly;
- crop-specific modules are used for calculation of crop development, whereas a single module is used for biomass accumulation based on water use efficiency;
- a single simulation run can encompass a full rotation involving several crops, years and sites;
- the soil is divided into two layers of varying thickness, each of which is allocated a separate set of physical properties;
- the water balance is driven by the soil matric potential;
- model runs are for soil map units, using pedotransfer functions to derive soil datasets.

The development of ACCESS-I has drawn on earlier modelling approaches, notably SI-BIL [27], for the physical principles of the soil water balance and biomass accumulation, and AFRCWHEAT [19] for the crop phenology of winter wheat.

**Table 1.** Basic crop-climate parameters for ACCESS-I

Parameter	Crop				Reference
	Maize	Soybeans	Sunflower	Winter wheat	
<i>Tbase</i> (°C)	10/6	5/10	5/6	0	Driessen, Konijn [10]; INRA Toulouse
<i>Topt</i> (°C)	25/22.5	25	25	15/13	Sharpley, Williams [25]; INRA Toulouse
<i>ETSm</i>	1600/1950	1750/1400	1700/1680	1600/2150	Driessen, Konijn [10]; INRA Toulouse
<i>RDSroot</i>	0.7	0.61	0.6	0.56	Driessen, Konijn [10]
<i>RERmax</i>	1.5/1.2	1.2	1.2	1.2	Boons-Prins <i>et al.</i> [1]; Crop 41*
<i>RDmax</i>	100/75.0	120	150	125	Boons-Prins <i>et al.</i> [1]; Crop 41
<i>WUE</i>	C4	C3	C3	C3	Crop 41
<i>SLA</i>	0.0035/ 0.0014	0.0023/ 0.0015	0.0030/ 0.0025	0.0024/ 0.0016	Driessen, Konijn [10]
<i>LAImax</i>	5	5/6	5/6	8/7	Sharpley, Williams [25], INRA Toulouse
<i>HI</i>	0.35/050	0.35/0.31	0.30/0.25	0.40/0.42	Driessen, Konijn [10]; Sharpley, Williams [25]

Note: \* crop-climate database developed by the Agricultural University, Wageningen, The Netherlands.

#### THE MECHANISMS OF THE MODEL

##### Accumulated temperature (AT)

This is the integrated excess of temperature above a fixed base value (*Tbase*), over an extended period such as a month or a year. When calculated over the growing season, it is regarded as a reasonable guide to energy input, and has been shown to correlate with crop potential and vegetative growth. Accumulated temperatures above 0 °C and 5.6 °C are useful for assessing the suitability of land for different types of agriculture. There are other *AT* isotherms which correlate well with agricultural practice. For example, most arable areas have more than 1250 day-degrees above 0 °C, and 850 day-degree isotherms define areas where low temperature precludes virtually any agricultural activity [17]:

$$AT = \sum_1^n (T_{mean} - T_{base}) \text{ for } T_{mean} > T_{base}. \quad (1)$$

##### Humidity index

The ratio precipitation/potential evapo-

transpiration (*P/ETo*) is a convenient indicator of available moisture. This index is, in effect, the same as Thornthwaite's 'moisture index' [30], although Thornthwaite used the index in percentage rather than in ratio form. A value of 1.0 indicates that precipitation and potential water loss through evapotranspiration are equal. Values above 1.0 indicate a potential water surplus and values below 1.0 a potential water deficit [16]:

$$HUI = P/ETo. \quad (2)$$

Using this humidity index it is possible to develop a climatic classification [30], with different climatic zones being identified on the basis of a monthly, seasonal, or annual humidity index [16].

##### Growing period

Under European conditions, equal attention should be given to moisture and temperature criteria. In Mediterranean areas the growing season will be limited mainly by the summer moisture deficit, while at high altitudes in the north of Europe low winter temperatures will be the major factor reducing the

growing period [36]. The FAO approach was adapted in ACCESS-I, in which the growing period (*GP*) is defined as the time (days) in the year during which precipitation exceeds  $0.5 ETo$  (potential evapotranspiration calculated by the modified Penman method), extended by the time that a maximum available water content (*AWC*) of 100 mm (or less if not available) in the soil has been depleted. In addition, this growing period is interrupted by the time that mean air temperatures are below  $6.5^{\circ}\text{C}$ . A normal growing period must exhibit a humid period, i.e., a period with an excess of precipitation over potential evapotranspiration [11].

### The soil water balance

This is based on a 'piston' type model in which the soil profile is divided using two independent criteria (Fig. 1): the 'intrinsic' soil physical properties (topsoil and subsoil); and, the presence of the crop root system (root zone and no-root-zone).

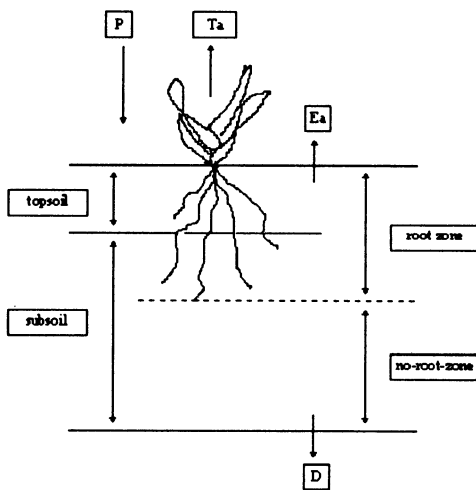


Fig. 1. Basic compartments of the soil-plant system for ACCESS-I.

The boundary between topsoil and subsoil is fixed by the user from a knowledge of the soil types in the region. The boundary between 'root zone' and 'no-root-zone' changes with time according to root system development. Therefore, the percentage of topsoil and subsoil in the 'root zone' also changes with time.

A monthly soil water balance is calculated only for the root zone. The 'no-root-zone' is regarded, over the period of simulation, as having the same soil matric potential (water content) as at the beginning of the simulation (initial condition). The root zone is considered homogeneous with respect to soil physical properties and root system development. Therefore, in the root-zone, the soil water content for given values of soil matric potential is the weighted average of the water contents in the topsoil and those in the subsoil. The weighting factors are derived from the percentage of topsoil and subsoil depths in the root-zone.

### Maximum evaporation

In the presence of a crop, the maximum evaporation rate ( $Em$ ) is always lower than the potential evaporation rate, even if the rate of water supply from below does not limit the rate of evaporation. Ritchie [20] suggested the following relationship to account for the reduction in the rate of evaporation due to shading of the soil surface under a crop canopy [8,35]:

$$Em = e^{-keLAI} ETo \quad (3)$$

where,  $ke$  is the light extinction coefficient and  $LAI$  is the leaf area index ( $\text{m}^2\text{m}^{-2}$ ). In order to determine  $LAI$ , an estimation of the actual transpiration rate is necessary. As a first approach, the model considers that the actual transpiration equals potential evapotranspiration multiplied by the ratio of  $ETo$  to precipitation. Using this approach the values of  $LAI$  are slightly overestimated, but the consequences of this for subsequent computations are not great.

### Actual evaporation

The model considers that for a number of days ( $PEdays$ ) after a significant rainfall event the actual evaporation rate ( $Ea$ ) equals the maximum,  $Em$ . The dependence of the parameter  $PEdays$  on the site and month can be calculated for an 'average' climatic year from

analysis of recorded meteorological data. The value  $PEdays$  can also be provided by more accurate simulation models. For all other days the value of  $Ea$  is zero. The number of days with rain is given for each month of simulation as an input parameter:

$$Ea = Em Rdays PEdays \quad (4)$$

where,  $PEdays$  is the number of days with potential evapotranspiration after each rainfall event and  $Rdays$  is the number of rain-days in the month.

### Potential transpiration

The potential transpiration rate ( $TRm$ ) is found by subtracting soil evaporation ( $Em$ ) from the potential evapotranspiration ( $Eto$ ) [35]:

$$TRm = (1 - e^{-keLAI}) ETo \quad (5)$$

### Root density

As in the case of the estimation of the potential evaporation and transpiration, it is necessary to have a forecast of the average value of the root biomass for the simulation month. The estimation is similar to that for the leaf area index. The values for root volume ( $Vr$ ) and root density ( $Lr$ ) can easily be estimated from the root system biomass using the assumption that roots are cylindrical tubes with uniform radii:

$$Vr = Qroot / 0.27 \quad (6)$$

where,  $Vr$  is the rooting volume ( $\text{cm}^3$  roots  $\text{cm}^{-3}$  soil),  $Qroot$  is the estimated root biomass ( $\text{g cm}^{-3}$ ) and 0.27 represents the root density ( $\text{g dry matter cm}^{-3}$  fresh root). In the final step rooting density ( $\text{cm-roots cm}^{-3}\text{-soil}$ ) is derived from the rooting volume by assuming an average root radius:

$$Lr = Vr / (\pi ARR^2) \quad (7)$$

where,  $ARR$  is the average root radius which varies between 0.05 and 0.07 mm with 0.06 mm being a good estimate [13].

### Root sink term

The soil water extraction rate  $Sr$  ( $\text{cm}^3\text{-water cm}^{-3}\text{-soil day}^{-1}$ ) is determined by climatological and soil conditions. The meteorologically determined root sink ( $Sr$ ) is calculated from potential transpiration and root front depth:

$$Sr = TRm / RD \quad (8)$$

The soil determined root sink ( $Sr_{\psi}$ ) is calculated according to the following equation [29]:

$$Sr_{(\psi)} = 0.012566 / \log 2(1 - Vr) Lr K_{(\psi)} \psi / (\eta - 1) \left[ 1 - (\psi / \psi WP)^{\eta - 1} \right] \quad (9)$$

where,  $0.012566 / \log 2(1 - Vr)$  is a geometric constant,  $1 - Vr$  is the volume of soil not filled by roots ( $\text{cm}^3 \text{cm}^{-3}$ ),  $Lr$  is the effective root length ( $\text{cm-root cm}^{-3}\text{-soil}$ ),  $K$  is the hydraulic conductivity ( $\text{cm day}^{-1}$ ),  $\psi$  is the soil matric potential (bar),  $\eta$  is the pore size distribution index [3], and  $\psi WP$  is the soil matric potential at the wilting point (bar). The power exponent  $\eta$  is estimated, together with the soil water retention curve and hydraulic conductivity, using pedotransfer functions.

The soil water extraction rate is reduced under limited soil aeration with a threshold value of  $0.1 \text{ cm}^3 \text{cm}^{-3}$  gas porosity. Below this value the water extraction rate is decreased linearly to a factor of 0.01 at values below  $0.03 \text{ cm}^3 \text{cm}^{-3}$  gas porosity [12].  $Sr(\psi)$  is estimated for topsoil and subsoil. The actual  $Sr(\psi)$  value is related to the root zone and is obtained using the same weighted averages as for the soil water retention curve.

### Actual transpiration

An essential part of the model is the estimation of monthly values of actual transpiration ( $TRa$ ). The basic hypothesis is that the amount of water accessible for transpiration is supplied by two independent sources: soil available water and rainfall. The soil available

water pool uses the relationship between the root sink term and the soil matric potential. A root sink term characteristic curve (Fig. 2) is calculated for the same values of the soil matric potential as those used in the estimation of pedotransfer functions [28]. For given values of the soil matric potential, root system development and potential transpiration, the root sink term is [29]:

$$S(\psi) = \min \left\{ TRm / RD \right. \\ \left. 0.01256 / \log(2(1 - Vr)) Lr K(\psi) \psi / \right. \\ \left. (\eta - 1) \left[ 1 - (\psi / \psi W P)^{\eta - 1} \right] \right\} \quad (10)$$

where, *TRm* is the potential transpiration (cm day<sup>-1</sup>), *RD* is the root front depth, and other terms are as in Eq. (9).

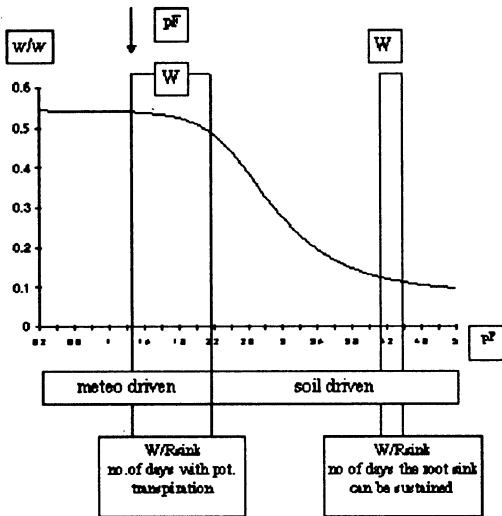


Fig. 2. The soil water store in ACCESS-I.

If the soil determined root sink is greater than the meteorological root sink, the number of days are calculated for which potential transpiration of the crop can be supported. If, however, the root sink term is less than the meteorological sink, or if the root sink term falls below the meteorological root sink, a stepwise reduction in soil matric potential (in increments of 0.2 pF units) is used to determine the time in days, that the root sink term can

be sustained for the associated water content. Thereby, it is possible to derive a stepwise relationship between time and the root sink term, considering the soil matric potential computed from the water balance of the previous month to be starting value. Based on such a relationship, it is possible to estimate the amount of water transferred from the soil available water pool as crop transpiration.

The model considers that the water from rainfall is intercepted by the crop root system in order to fulfil the weather-induced transpiration demands. Therefore, the water from the rainfall pool is added to the amount of water that is passed from the soil available water pool. If this total amount of water exceeds the value of the potential transpiration then actual transpiration equals potential transpiration, otherwise it represents the actual transpiration.

### Drainage

The model assumes free drainage (*D*) with a water flux equal to the unsaturated hydraulic conductivity for topsoil or subsoil (depending on the position of the root front) at the initial value of the soil matric potential. This is modified by precipitation (*P*) and hydraulic conductivity (*K*) according to:

$$D = 0.9 P \quad \text{for } K > P \\ D = K \quad \text{for } K < P. \quad (11)$$

### Root-zone water balance

A simple water balance is computed for the root zone for each month of simulation. The input elements of the water balance are precipitation (*P*), and the soil water added through the development of the root system. The output elements of the water balance are actual transpiration (*TRa*, in cm), actual evaporation (*Ea*, in cm) and the freely-drained water (*D*, in cm):

$$\theta = P - Ea - TRa - D. \quad (12)$$

The resulting value of water content  $\theta$  is compared with the soil water characteristic curve of the root zone (weighted average between

topsoil and subsoil curves) in order to estimate the new starting value of the soil matric potential in the root zone for the next month.

### Crop phenology

Many studies have shown that germination and other phenological stages of plant development may only proceed following a certain accumulation of temperature, either between development stages or during the growing season. One measure of this accumulation is the effective temperature sum (*ETS*), also variously known as accumulated temperature, thermal time, growing degree days and (erroneously) heat units. They are defined as the accumulation of temperatures above a given threshold temperature, commonly the temperature at which significant growth begins [7,17,22].

Because crop phenology not only determines the start of distinct phases in crop development, but also determines the mass fraction for the partitioning of dry matter, a monthly time step was considered to be inappropriate. Therefore a cubic spline interpolation of minimum and maximum monthly temperature values is used to provide 'daily' time steps for the calculation of crop phenology. In the model, crop development is expressed in relative terms from 0 to 1 according to the following formula:

$$RDS = ETS / ETS_m \quad (13)$$

where, *RDS* is the relative development stage, *ETS* is the effective temperature sum, and *ETS<sub>m</sub>* is the total temperature sum required for maturity.

### The temperature remainder index Model (TRIM)

The Temperature Remainder Index Model [22] calculates accumulated temperature (°C days) by:

$$ETS = \sum_1^n \delta (T_{mean} - T_{base})$$

$$\delta = 0, \quad ETS = 0 \quad (14)$$

where,  $\delta$  is 1 for  $T_{mean} > T_{base}$ , and 0 for

$T_{mean} < T_{base}$ . This calculation of thermal time is appropriate for predicting plant development if several conditions are met [21]:

- the temperature response of the development rate is linear over the range of temperatures experienced;
- the daily temperature does not fall below  $T_{base}$  for a significant part of the day;
- the daily temperature does not exceed an upper threshold temperature for a significant part of the day;
- the growing season of the plant has the same mean temperature as  $T_{mean}$ .

### Corn Heat Units

The model uses a separate function for maximum and minimum temperatures and this has become known as the Corn Heat Unit model. The function for minimum temperature is linear with a threshold at 4.4 °C, and that for maximum temperature is quadratic with a threshold at 10 °C and an optimum of 30 °C. Combining these two functions gives the daily rate of crop development [6]:

$$ETS_{max} = 3.33(T_{max} - 10) - 0.084(T_{max} - 10)^2$$

$$T_{max} < 10, \quad ETS_{max} = 0$$

$$ETS_{min} = 1.8(T_{min} - 4.4)$$

$$T_{min} < 4.4, \quad ETS_{min} = 0$$

$$ETS = 0.5(ETS_{max} + ETS_{min}). \quad (15)$$

### Soybean development units

Brown and Chapman [4] derived a similar equation to that of Corn Heat Units for soybeans. The numerical values provided by this equation were called Soybean Development Units:

$$ETS = \sum_1^n 3.258 (T_{mean} - 10.0) - 0.08195(T_{mean} - 10.0)^2 \quad (16)$$

where,  $T_{mean}$  is the daily mean temperature (°C).

## AFRC Wheat

The development procedures for winter wheat were adapted from the AFRCWHEAT 2 phenological routines [19]. The model takes thermal time, vernalisation and photoperiod into account and provides the occurrence of emergence, double ridge, terminal spikelet, anthesis, grain fill and maturity stages:

$$ETS = \sum_1^n Tt Fp Fv \quad (17)$$

where,  $Tt$  is the thermal time ( $^{\circ}\text{C}$  days),  $Fp$  is the photoperiod factor (dimensionless) and  $Fv$  is the vernalisation factor (dimensionless).

### Thermal time

Temperature is assumed to vary sinusoidally through the day between maximum ( $T_{max}$ ) and minimum ( $T_{min}$ ), and the increment of the thermal time ( $T_t$ ) for 1 day is approximately the sum of eight 3 hour periods ( $T_h$  in  $^{\circ}\text{C}$ ):

$$T_t = 1/8 \sum_{r=1}^{r=8} (T_h - T_{base}) \quad (18)$$

where,

$$T_h = T_{min} + pr (T_{max} - T_{min}) \quad (19)$$

and,

$$pr = 1/2 \left[ 1 + \cos(\pi(2r-1)/8) \right] \quad (20)$$

### Photoperiod factor

This is calculated according to:

$$\begin{aligned} F_p &= 0 && \text{if } P_h < P_b \\ &= (P_h - P_b) / (P_{opt} - P_b) && \text{if } P_b < P_h < P_{opt} \\ &= 1 && \text{if } P_h > P_{opt} \end{aligned} \quad (21)$$

where,  $P_h$  is photoperiod-effective hours,  $P_b$  is the minimum photoperiod (hours) and  $P_{opt}$  an optimum photoperiod (hours) beyond which development rate is not sensitive to photoperiod.

### Vernalisation factor

This factor ( $F_v$ ) depends on the accumulation of vernalising days ( $V_{DD}$ ), and these in turn depend on the vernalising effectiveness

factor ( $V_{eff}$ ) of the ambient temperature each day:

$$\begin{aligned} V_{eff} &= 1 && \text{if } 3 < T < 10 \text{ } ^{\circ}\text{C} \\ &= (T+4)/7 && \text{if } -4 < T < 3 \text{ } ^{\circ}\text{C} \\ &= (17-T)/7 && \text{if } 10 < T < 17 \text{ } ^{\circ}\text{C}. \end{aligned} \quad (22)$$

The mean value for  $V_{eff}$  for each day is determined assuming a sinusoidal temperature variation, and  $V_{DD}$  (days) is the accumulated value of  $V_{eff}$  since sowing.  $F_v$  is defined as:

$$\begin{aligned} F_v &= 0 && \text{if } V_{DD} < 8 \text{ days} \\ &= (V_{DD}-8)/25 && \text{if } 8 < V_{DD} < 33 \text{ days} \\ &= 1 && \text{if } V_{DD} > 33 \text{ days}. \end{aligned} \quad (23)$$

## Biomass accumulation

Biomass accumulation is based on the water-use efficiency ( $WUE$ ) concept, which is defined as the amount of biomass (kg dry matter) synthesised per unit area (ha) and per unit crop transpiration (cm). It is a crop-dependent function which allows for the following growth constraints:  $\text{CO}_2$ , air temperature and crop water stress.

### Potential water use efficiency

There is a distinct difference in water use efficiency for species with different photosynthetic pathways. Assimilation rate and transpiration rate are the main determinants for this variable, which is roughly twice as great for C4 as for C3 plants, irrespective of the level of solar radiation. In the ACCESS model, the average potential water use efficiency is set at  $500 \text{ kg ha}^{-1} \text{ cm}^{-1}$  for C3 plants, and  $1000 \text{ kg ha}^{-1} \text{ cm}^{-1}$  for C4 plants [15].

### $\text{CO}_2$ concentration

To represent the overall effect of  $\text{CO}_2$ -induced growth in the model, the concept of the biotic growth factor  $\beta$  is used, which modifies growth rate as follows [14]:

$$Gn = Go(1 + \beta \ln(C/Co)) \quad (24)$$

where,  $Gn$  is net water use efficiency,  $Go$  is the gross  $WUE$  rate,  $Co$  is the present  $CO_2$  concentration (340 ppmv),  $C$  is the future  $CO_2$  concentration (ppmv), and  $\beta$  - the biotic growth factor - has a value of 0.7 under good nutrient supply, dropping to about half this value with nitrogen shortage and to zero with phosphorus deficiency.

### Temperature

The air temperature dependence of water use efficiency ( $\delta T$ ) is calculated using a similar approach to that proposed by Feddes *et al.* [12], in which the water use efficiency is assumed to decrease linearly from the potential value, 1, at an optimum temperature (18-20 °C) to 0 at a threshold temperature (0-4 °C):

$$\sigma T = T_{mean} / T_{opt} \quad (25)$$

where,  $\delta T$  is the temperature dependence,  $T_{mean}$  is the mean temperature (°C) and  $T_{opt}$  a crop-dependent optimum temperature (°C).

### Relative transpiration deficit

The relative transpiration deficit ( $RTD$ ) is used as a measure of the degree of moisture stress experienced by the plant. It is defined as the difference between potential transpiration ( $TTm$ , in cm) and actual transpiration ( $TRa$ , in cm), as a fraction of the potential transpiration ( $TRm$ ) [18,33,34]:

$$RTD = (TRm - TRa) / TRm. \quad (26)$$

### Cumulative transpiration deficit

The value of  $RTD$  divided by a time constant (buffer time in days, the resistance of the plant against water stress) is integrated to yield the cumulative relative transpiration deficit ( $CTDT$ ). Since it is unlikely that a mild degree of water stress has any lasting effect on plant performance, the value is only accumulated when it exceeds 0.4. The value of the cumulative transpiration deficit is constrained between 0 and 1, by multiplying its rate of accumulation by 1.0 minus its own value [18,33,34]. In the ACCESS-I model, water-use

efficiency starts to deteriorate when  $CTDT$  exceeds 0.55.

### Actual water use efficiency

The crop water-stress influence on water-use efficiency is related to the cumulated transpiration deficit ( $\sigma$ ) [33,34], which is estimated on a monthly time-step. The water use efficiency as affected by the water stress is [27]:

$$Ga = Gn(1 - \sigma)^b \quad \text{if } \sigma > \sigma_o \quad (27)$$

where,  $Ga$  is the water-stress affected crop water-use efficiency ( $kg\ ha^{-1}\ cm^{-1}$ ),  $Gn$  net water-use efficiency, and  $b$  and  $\sigma_o$  are crop dependent parameters. In the model,  $\sigma_o$  is set to 0.55 and  $b$  to 0.2 for all crops. These are empirical values derived from experimental data from Romania and Poland.

### Biomass accumulation

The new synthesised biomass in a month ( $Q$ ) is then:

$$Q = Ga \sigma T TRa \quad (28)$$

where,  $Q$  is the biomass (kg),  $Ga$  is the actual water use efficiency ( $kg\ ha^{-1}\ cm^{-1}$ ),  $\sigma T$  is the temperature dependence, and  $TRa$  is the actual transpiration ( $cm\ month^{-1}$ ).

### Dry-matter distribution

The partition of the new synthesised biomass ( $Q$ ) to plant organs (leaves and roots) is based on the phenologically dependent mass fraction,  $fr(org)$ :

$$Q_{org} = Q fr(org). \quad (29)$$

The  $LAI$  is calculated from leaf biomass using a phenology-dependent specific leaf area index ( $SLA$ ):

$$LAI = Q_{leaf} SLA_{min} - (SLA_{max} - SLA_{min}) RDS \quad (30)$$

where,  $Q_{leaf}$  is the leaf biomass (kg),  $SLA$  is the specific leaf area index ( $ha\ kg^{-1}$ ), and  $RDS$  is the relative development stage.



Crop yield ( $Y_{crop}$ ) is obtained from total biomass using a crop dependent harvest index ( $HI_{crop}$ ):

$$Y_{crop} = Q HI_{crop}. \quad (31)$$

**ROOT FRONT DEVELOPMENT**

Maximum rooting depth is a crop dependent input parameter, modified by maximum soil depth according to:

$$RD_{max} = \min \{RD_{max} (crop), SD_{max}\}. \quad (32)$$

The duration of root development ( $RD_{period}$ ) is specified in terms of a relative development stage, at which root development stops. Root front development can be modelled using three different techniques: linear, non-linear, and based on penetration resistance:

$$RDS_{root} = ETS / (RD_{period} ETS_m) \quad (33)$$

where,  $RDS_{root}$  is the relative development stage for roots,  $ETS$  is accumulated day degrees,  $RD_{period}$  is the relative development stage at which root growth ceases, and  $ETS_m$  is day degrees to maturity. The length of the root-growth period is a crop dependent parameter. For most annual crops the moment when the root system ceases to develop occurs between about 0.6 and 0.7 of the time from emergence to maturity.

**Linear root development**

A linear root development is assumed between sowing and the end of root development:

$$RD = RD_m RDS_{root} \quad (34)$$

where,  $RD$  is the rooting depth (cm) and  $RD_m$  is the maximum rooting depth (cm).

**Non-linear root development**

A non-linear root development function was developed by Borg and Grimes [2] based on 135 field observations of 48 crop species. The rooting depth is a function of the maximum rooting depth and time, expressed as relative crop development from sowing to maturity:

$$RD = RD_m \left[ 0.5 + 0.5 \sin \left( 3.03 \frac{ETS}{ETS_m} - 1.47 \right) \right]. \quad (35)$$

**Root development based on penetration resistance**

The consequence of the assumptions in a piston-type model is that, during the growth period, the root front develops in a soil layer having the same value of the soil matric potential ( $\psi_o$ ) as that at the beginning of the simulation. The actual root elongation rate ( $v_{root}$ ), as affected by the soil matric potential and soil resistance to penetration, is estimated using the theory of root growth mechanics [9]:

$$v_{root} = v_{pot} \left[ \frac{\psi_o}{\psi_w} + \exp(-0.6931(Q_p / Q_{l2})) \right] \quad (36)$$

where,  $v_{pot}$  is the potential elongation rate (cm day<sup>-1</sup>),  $\psi_o$  is the soil matric potential (bar),  $\psi_w$  is the wilting point water potential of the crop (bar),  $Q_r$  is a crop dependent constant, and  $Q_p$  is the soil resistance to penetration (MPa), calculated for topsoil or subsoil conditions depending on the position of the root-front tip, for the soil matric potential value  $\psi_o$ . The monthly advance of the root-front depth ( $RD$ ) is the product of  $v_{root}$  and the number of days with root growth.

**MACHINERY WORK-DAYS**

Workability is an important factor in land suitability, especially in the highly mechanised farming systems of northern Europe [23,24]. A model has been developed to estimate the time during a month when mechanised field operations can be performed. The algorithm uses the soil water routing technique with daily time-steps from the EPIC model [25]. In order to adopt the procedure for a monthly time-step, the total monthly rainfall is divided into consecutive one-day events. The amount of rainfall in each event is the difference between the water content in the top layer at total porosity, and that at the threshold

value corresponding to soil workability. Rain is added to the day when the soil water content in the top layer equals, or is less than, the threshold value for workability. The procedure stops when all the monthly rainfall has been added and the topsoil water content reaches the threshold value for workability. The algorithm returns the number of days required to reach this condition. The difference between the number of days in the month and the output of the algorithm is the number of workable days.

The travel time through a layer is computed from a linear storage equation:

$$TT_l = \frac{PO_l - FC_l}{Ksat_l} \quad (37)$$

where,  $TT_l$  is the travel time through layer  $l$  (h),  $PO_l$  is the porosity (mm),  $FC_l$  is the water content at field capacity (mm),  $Ksat_l$  is saturated hydraulic conductivity ( $\text{mm h}^{-1}$ ). Daily percolation can be computed by taking the difference between soil water content at the start of the computation ( $SW_{ol}$ ), and the soil water content at field capacity ( $FC_l$ ):

$$O_l = (SW_{ol} - FC_l) [1.0 - \exp(-\Delta t / TT_l)] \quad (38)$$

where,  $O_l$  is the percolation rate for layer  $l$  ( $\text{mm day}^{-1}$ ), and  $\Delta t$  is the time interval (24h). The threshold value of soil matric potential for workability, in the topsoil, is a user defined parameter. Preliminary tests indicate that this threshold value is associated with the soil matric potential value corresponding to the inflection point of the derivative of the soil water retention curve.

## SPATIALISATION

### Soil and site data

The site information required for the model consists of a location description, latitude and longitude (decimal format). The soil data comprise the reference code of the soil, the number of measurement layers and their genetic symbols. For each layer, the upper and lower boundary must be specified, as must the stone, sand and clay contents (%), the bulk density ( $\text{g cm}^{-3}$ ), and the organic carbon con-

tent (%). In addition, the water content at saturation (mass basis), the residual water content (mass basis); the 'van Genuchten' parameters  $\alpha$  and  $n$  [28], and the saturated hydraulic conductivity ( $Ksat$ ,  $\text{cm day}^{-1}$ ) are required.

### Climate data

The model operates with a monthly meteorological time-step. Input data comprise a year and month code, the mean monthly maximum and minimum temperature ( $^{\circ}\text{C}$ ), rainfall (cm), potential evapotranspiration (cm), and the average number of days with rainfall.

### Crop data

A data file is required for each crop describing the following parameters: crop generic name; the water use efficiency, optimum temperature, base temperature and the total day-degrees required to maturity. The rooting system is described by the maximum root elongation rate, the maximum rooting depth, and the period, in relative development stages, during which roots develop. Specific maximum and minimum leaf area, and dry matter distribution coefficients for leaves and roots, are also specified according to the relative development stages.

### Soil water retention curve

The soil water retention curve and the relative unsaturated hydraulic conductivity are calculated from the closed-form equation developed by van Genuchten [32], using the 'Mualem-type' relationship between power coefficients. The parameters  $\alpha$  and  $n$  of the model are estimated from particle-size distribution and bulk density data [28] on a regional basis.

$$\frac{\theta - \theta_r}{\theta_s - \theta_r} = \left[ (1 + \alpha \psi)^n \right]^{-m} \quad m = 1 - 1/n \quad (39)$$

$$\frac{K(\theta)}{K_{sat}} = \left( \frac{\theta - \theta_r}{\theta_s - \theta_r} \right)^{0.5} \left( 1 - \left[ 1 - \left( \frac{\theta - \theta_r}{\theta_s - \theta_r} \right)^{\frac{1}{\alpha}} \right]^m \right)^2 \quad (40)$$

$$I = \sum i_m = \sum \left( \frac{T_{mean}}{5} \right)^{1.5} \quad \text{for } m = \text{months } 1 \dots 12 \quad (42)$$

and the exponent, *a*, is calculated (to 2 significant figures) from:

$$a = 6.710^{-7} I^3 - 7.710^{-5} I^2 + 1.810^{-2} I + 0.449 \quad (43)$$

where,  $\theta$  is the soil water content (m/m) at pressure head  $\psi$ ,  $\theta_r$  is the residual soil water content (m/m),  $\theta_s$  is the water content at saturation (m/m),  $\alpha$ ,  $n$  and  $m$  are equation parameters,  $K(\theta)$  is the hydraulic conductivity at soil water content  $\theta$  and  $K_{sat}$  is the saturated hydraulic conductivity (cm day<sup>-1</sup>).

**Soil water content**

Soil water contents are estimated using van Genuchten’s equation for topsoil and subsoil at given values of soil matric potential, the values of which range from saturation (1.0 in pF units) to ‘standard’ wilting point (4.2 in pF units) in steps of 0.2 pF units.

**Soil penetration resistance**

The values of soil penetration resistance, at the same soil matric potentials used in the estimation of the soil water retention curve, were calculated using clay content, bulk density and soil water content using a semi-empirical model [5].

**Potential evapotranspiration**

If no potential evapotranspiration ( $ET_o$ ) data are available, Thornthwaite’s formula is used to calculate potential evapotranspiration on a monthly basis. The formula is based mainly on temperature, and the method has a latitude adjustment factor based on day length [26]:

$$ET_o = 16 Nm \left( \frac{10 T_{mean}}{I} \right)^a \quad (41)$$

where,  $Nm$  is the monthly adjustment factor related to hours of daylight,  $T_{mean}$  is the monthly mean temperature (°C), and  $I$  is the heat index for the year, given by:

For latitudes greater than 50° North and South, the day-length value at 47.5° was used, as recommended by Thornthwaite [30]; this allowing for the fact that energy receipt at high latitudes is increasingly small, despite long daylight hours. Where the mean monthly temperature exceeds 26.5°C,  $ET_o$  is determined directly from temperature, i.e. the relationship between temperature and  $ET_o$  in very hot months is independent on the overall warmth or coolness of the annual climate. Where mean monthly temperature is below zero,  $ET_o$  is also zero, implying insufficient energy to evaporate water [16], thus:

$$ET_o = -415.85 + 32.244 T_{mean} - 0.43253 T_{mean}^2 \quad (44)$$

In very cold climates, with temperatures in most months below zero and one or two months with small positive temperatures, the annual heat index takes a very small value. Very large values of  $ET_o$  result. Since the Thornthwaite method was not designed for very cold climates, a cut-off can be applied where the annual heat index is <10 (generally northwards of about 65°N), and no  $ET_o$  estimate is made for any month [16].

**Initial soil matric potential**

Initial values for soil matric potential are difficult to obtain in a spatial context. To overcome this problem, an iterative procedure was adopted as outlined by Thornthwaite and Mather [31]. Modifying this approach, the climatic water balance ( $P-ET_o$ ) is combined with

soil water characteristics to estimate initial soil pF values. The procedure starts at the beginning of the first month when  $P-ET_o$  is negative. Adding the total negative  $P-ET_o$  value to this estimate, and converting the result into a value of soil moisture retention, one obtains an estimated value of moisture stored in the soil at the end of the period of negative  $P-ET_o$ . Adding the total positive  $P-ET_o$  values now provides an estimate of the moisture retention at the end of the period of recharge. Converting this value into potential water loss one again obtains a value of potential deficiency at the beginning of the period with negative  $P-ET_o$  values. Repeating this process results in an ever closer approximation to the value of potential deficiency, with which to begin the accumulation of the negative  $P-ET_o$ , and subsequently for the whole year. The inverse of the soil water retention curve can then be used to obtain the relevant pF values associated with each monthly value.

#### MODEL OPERATION

ACCESS operates within the Microsoft WINDOWS™ environment using a front-end to integrate the different input file types, i.e., control files, region files, soil files, climate files, crop diary files, crop parameter files, climate perturbation files and options files. ACCESS-I generates three output files (a monthly summary file, a land use summary file and a simulation summary file) containing all the simulation results, as summarised in Table 2.

#### VALIDATION

A validation protocol for ACCESS-I has been established in the form of a Microsoft EXCEL™ spreadsheet. Whilst the spreadsheet was kept as universal as possible, it should be stressed that modifications will be needed to accommodate different validation sites. For a comprehensive validation of the model, laboratory determined soil water retention data, field soil moisture measurements, field soil matric potential, rooting depth and biomass accumulation are required. The fol-

lowing steps are implemented in the spreadsheet.

#### Soil water retention curve - laboratory data

The van Genuchten parameters for each layer must be defined from laboratory determined water retention data by means of curve fitting routines such as RETC (U.S. Salinity Laboratory, Riverside), or SOLVER in Microsoft EXCEL™. The water content at saturation ( $Wqs$ ) should be set to total porosity and  $m=1-1/n$ . The van Genuchten parameters  $Wqs$  and  $Wres$  are corrected for coarse fragments, and two additional correction factors can be introduced at this stage. The first is to adjust for a possible difference between calculated soil water content at 15 bar using the van Genuchten function, and the measured value at 15 bar, the second is to compare the water retention curves obtained from laboratory measurements with those obtained from the experimental values of soil water content and soil matric potential from field measurements

#### Soil water content - field measurements

Soil water content measurements from neutron probe data or TDR measurements (M/M - fraction) are used to construct soil water retention curves from field measurements. These are then compared to the laboratory derived water retention curve, and adjustments can be introduced if substantial differences occur. In the presence of stones these data should also be corrected for coarse fragments (M/M - fraction).

#### Relative water content - field measurements

Relative water content is calculated using coarse fragment corrected total porosity to inspect data integrity, i.e., to search for abnormalities in the data due to measurement errors. These calculations are not used further in the validation exercise. In the final steps of the procedure, the van Genuchten function is used to calculate the water content for each layer as a function of the matric potential. The values derived by these

Table 2. ACCESS-I output data

Monthly summary file	Land use file	Simulation summary file
year	'Fallow'	<b>Input files</b>
month	period	control file
mean temperature (°C)	$\Sigma$ precipitation (cm)	region file
$\Sigma$ precipitation (cm)	$\Sigma$ potential evapotranspiration(cm)	perturbation file
$\Sigma$ potential evapotranspiration (cm)	$\Sigma$ potential evaporation (cm)	crop diary file
$\Sigma$ maximum evaporation (cm)	$\Sigma$ potential transpiration (cm)	options file
$\Sigma$ maximum transpiration (cm)	$\Sigma$ actual evaporation (cm)	path for soil files
$\Sigma$ actual evaporation (cm)	$\Sigma$ actual transpiration (cm)	path for climate files
$\Sigma$ actual transpiration (cm)	$\Sigma$ drainage (cm)	<b>Output files</b>
$\Sigma$ drainage (cm)	$\Sigma$ water balance (cm)	simulation summary file
water balance (cm)		monthly summary file
$\Sigma$ water balance (cm)	OR	landuse file
relative development stage		model parameters
root front depth (cm)	crop	Length of simulation
leaf area index	period	CO <sub>2</sub> concentration
biomass - leaves (kg ha <sup>-1</sup> )	yield (kg ha <sup>-1</sup> )	days with potential evaporation
biomass - total (kg ha <sup>-1</sup> )	$\Sigma$ precipitation (cm)	initial matric potential
AT/PT	$\Sigma$ potential evapotranspiration (cm)	precedent crop root depth
	$\Sigma$ potential evaporation (cm)	<b>Options</b>
	$\Sigma$ potential transpiration (cm)	ET <sub>o</sub> data
	$\Sigma$ actual evaporation (cm)	root development model
	$\Sigma$ actual transpiration (cm)	initial soil matric potential
	$\Sigma$ drainage (cm)	
	$\Sigma$ water balance (cm)	

procedures are then adjusted for the rooting depth to obtain an average water content over the rooting zone. These data are then used in a look-up table to derive the pF values associated with the neutron probe measurements averaged over the same rooting depth.

### Graphical comparisons

Model output of soil matric potential can be included at this stage for a graphical comparison of simulated with experimental values for the validation of the soil water balance. In addition, a graph is set up for the comparison of simulated with experimental values of biomass. Examples of the graphical output are given in Figs 3 and 4, which show the relationship between observed and measured va-

lues of the soil water balance, and biomass accumulation, respectively.

### LIMITATIONS OF ACCESS-I

Because ACCESS-I is designed to operate for relatively large spatial applications, i.e., at the regional level, a number of assumptions have been made that could influence the model outputs. These include:

- the monthly time step for physical and physiological processes does not allow accurate simulation of processes having a smaller time resolution;
- free drainage is assumed as the lower boundary condition, which is not always realistic, e.g., in the presence of ground water or impermeable horizons;

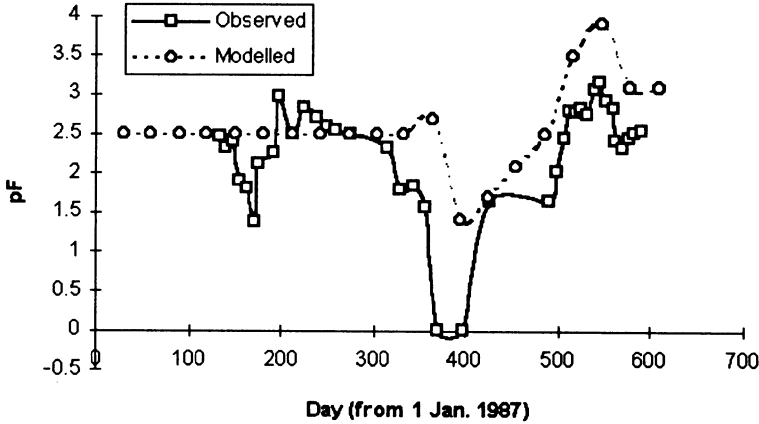


Fig. 3. Observed and modelled soil water balance data for a Cuckney soil under winter wheat in Central England.

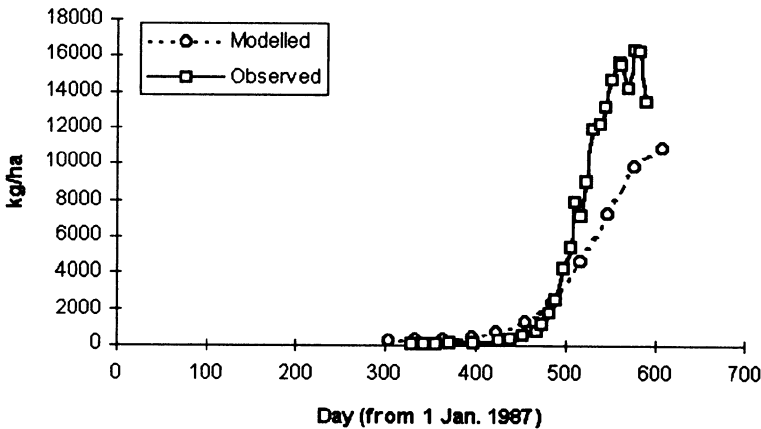


Fig. 4. Observed and modelled biomass accumulation for winter wheat in Central England on a Cuckney soil.

- the soil matric potential below the rooting zone is assumed to be constant for the simulation period;
- the amount of water available for transpiration is supplied by two independent sources: soil available water and rainfall;
- leaf interception of rainfall, surface run-off, lateral water transfer, capillary rise and preferential water flow through macropores are not considered;
- no growth limiting factors other than light, temperature, or water are considered, and for the sake of simplicity the interactions between these

- factors are not taken into account;
- the model considers that the influences of temperature and crop water stress on the water-use efficiency are independent.

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