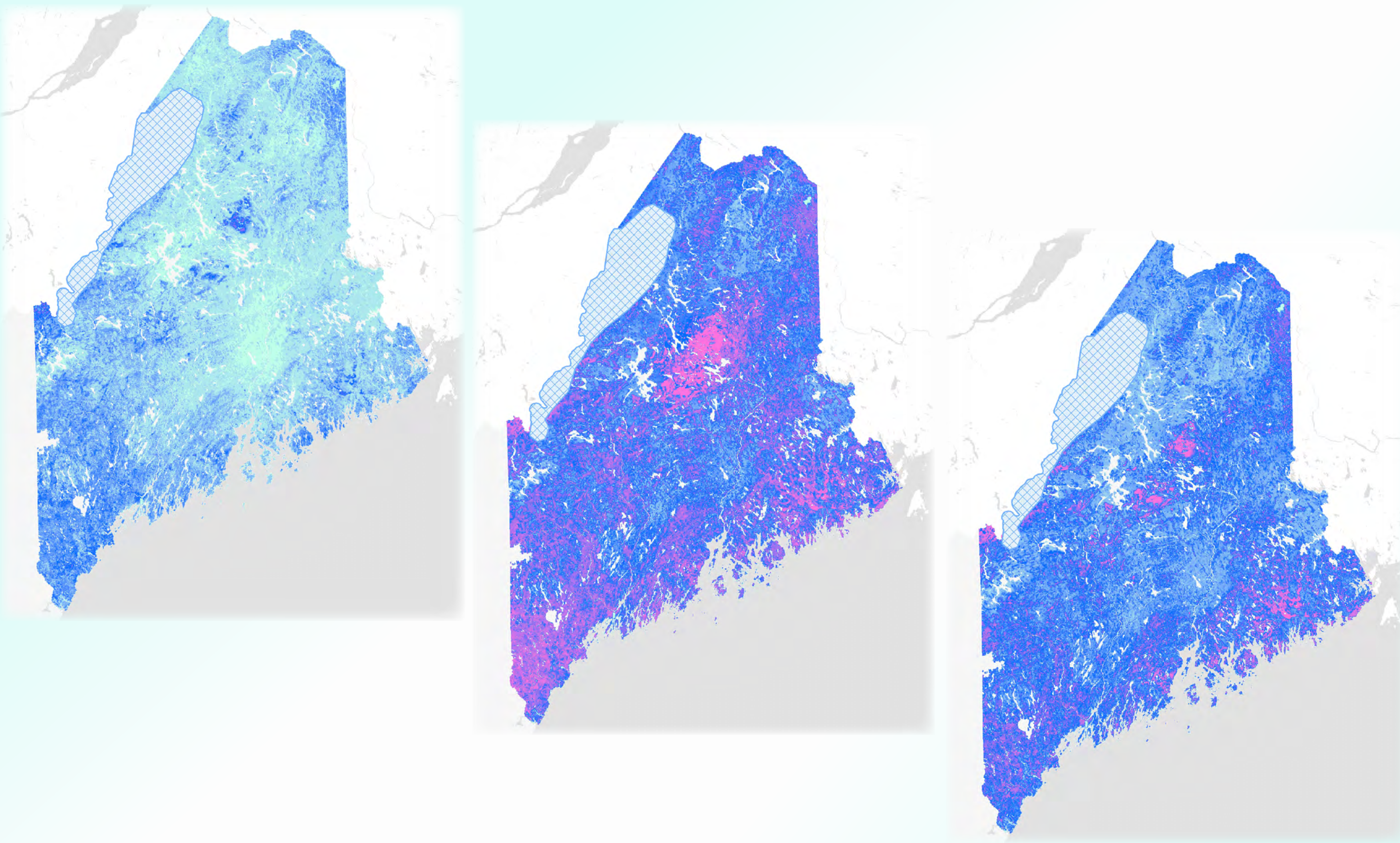
Prepared in cooperation with the Maine Geological Survey

Groundwater Recharge Estimates for Maine Using a Soil-Water-Balance Model—25-Year Average, Range, and Uncertainty, 1991 to 2015



Scientific Investigations Report 2019–5125

U.S. Department of the Interior
U.S. Geological Survey

Cover. Base map of figures 17 (left), 18 (middle), 16 (right) from this report.

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By Martha G. Nielsen and Stephen M. Westenbroek

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U.S. Department of the Interior
DAVID BERNHARDT, Secretary

U.S. Geological Survey
James F. Reilly II, Director

U.S. Geological Survey, Reston, Virginia: 2019

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Suggested citation:
Nielsen, M.G., and Westenbroek, S.M., 2019, Groundwater recharge estimates for Maine using a Soil-Water-Balance model—25-year average, range, and uncertainty, 1991 to 2015: U.S. Geological Survey Scientific Investigations Report 2019–5125, 56 p., https://doi.org/10.3133/sir20195125.

Associated data for this publication:
Nielsen, M.G., 2019, Soil-Water-Balance (SWB) model archive used to simulate potential annual recharge in Maine, 1991–2015: U.S. Geological Survey data release, https://doi.org/10.5066/P9GRP7DH.

Nielsen, M.G., and Westenbroek, S.M., 2019, Simulated 25-year median potential recharge datasets for Maine, 1991–2015: U.S. Geological Survey data release, https://doi.org/10.5066/P9052ULY.

ISSN 2328-0328 (online)

Contents

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Conversion Factors

U.S. customary units to International System of Units

Multiply	By	To obtain
	Length	
inch (in.)	2.54	centimeter (cm)
foot (ft)	0.3048	meter (m)
mile (mi)	1.609	kilometer (km)
	Area	
square mile (mi^2)	259.0	hectare (ha)
square mile (mi^2)	2.590	square kilometer (km^2)
	Flow rate	
cubic foot per second (ft^3/s)	0.02832	cubic meter per second (m^3/s)
inch per year (in/yr)	25.4	millimeter per year (mm/yr)
	Hydraulic conductivity	
foot per day (ft/d)	0.3048	meter per day (m/d)

Temperature in degrees Fahrenheit (°F) may be converted to degrees Celsius (°C) as

$$°C = (°F - 32) / 1.8.$$

Datum

Horizontal coordinate information is referenced to the North American Datum of 1983 (NAD 83).

Abbreviations

Φ	phi
AWC	available water capacity
FAO56	Food and Agriculture Organization of the United Nations Drainage and Irrigation Paper 56
gSSURGO	gridded Soil Survey Geographic Database
K_{cb}	plant growth coefficient
MAE	mean absolute error
MELCD	Maine Land Cover Dataset
netCDF	Network Common Data Format
NRCS	Natural Resources Conservation Service
p-value	probability
PEST	Parameter ESTimation
PPCC	probability plot correlation coefficient
r	correlation coefficient
RMSE	root mean square error
SSEBop	operational Simplified Surface Energy Balance
SVD	singular value decomposition
SWB	Soil-Water-Balance
USDA	U.S. Department of Agriculture
USGS	U.S. Geological Survey

Groundwater Recharge Estimates for Maine Using a Soil-Water-Balance Model—25-Year Average, Range, and Uncertainty, 1991 to 2015

By Martha G. Nielsen and Stephen M. Westenbroek

Abstract

To address the lack of information on the spatial and temporal variability of recharge to groundwater systems in Maine, a study was initiated in cooperation with the Maine Geological Survey to use the U.S. Geological Survey Soil-Water-Balance model to evaluate annual average potential recharge across the State over a 25-year period from 1991 to 2015. The Maine Soil-Water-Balance model was calibrated using annual observations of recharge, runoff, and evapotranspiration for 32 calibration watersheds in the State during 2001–12 (902 total observations). Observations of recharge, runoff, and evapotranspiration were developed for each watershed to reduce the possibility of nonunique combinations of model parameters during the calibration. The Maine Soil-Water-Balance model was run using an optional evapotranspiration calculation method that provides more control for calibration than the standard method. The model was calibrated using the Parameter ESTimation software suite.

The overall mean model error (average of all annual residuals for recharge, runoff, and precipitation) was 0.39 inches. The mean of the absolute value of the residuals, or the mean absolute error, was 2.32 inches. The root mean squared error for the calibrated model overall was 3.14 inches. Statistical tests indicated that the model residuals are normally distributed. To determine the potential uncertainty in the median annual potential recharge that results from uncertainty in the parameters as they relate to information contained in the observations, 300 alternate model realizations were run, and the standard deviation of the median potential recharge value at every pixel was calculated.

Simulated 25-year median potential recharge across the State is widely variable; this variability closely follows patterns of precipitation, with additional variability contributed by the patchwork nature of the combinations of land-use class and hydrologic soil group inputs, and distribution of available water capacity in the soil across the State. Overall, the 25-year median annual potential recharge across the State is 7.5 inches, ranging from a low of about 5 inches to over 30 inches. The statewide range in the 25-year minimum values is from just over 2 inches to just over 20 inches. The statewide range in the 25-year maximum potential recharge is between 15 and 48 inches per year.

The model areas with the highest simulated median potential recharge include areas underlain by type A soils (sandy and well drained), particularly those that also have land uses with low or little vegetation (blueberry barrens, developed, open space, scrub/shrub, and cropland, for example). The potential recharge values for these areas are similar to previously published values for comparable soil types.

The 25-year average potential recharge grids were compared to recharge evaluated through groundwater-flow models or other methods in four hydrogeologic settings at six study areas in the State. A key factor in the ability of the Soil-Water-Balance model to reproduce the earlier study results was whether the available water-capacity data were an appropriate match for the hydrologic soil groups. The Maine Soil-Water-Balance model does a good job in representing an accurate potential recharge under circumstances where the surficial mapped soils extend below the surface to the water-table aquifer and where the available water-capacity data are in an appropriate range for the hydrologic soil group. One hydrogeologic setting that was challenging for the model was where a silt and clay layer was below a shallow soil unit that did not have available water-capacity data that were appropriate for the hydrologic soil group. In these cases, typically the available water-capacity data were very low, not accounting for the impedance of water flow provided by the underlying soil. The model also does not simulate well areas where bedrock surfaces are above the water table but below the plant rooting zone.

The data products accompanying this report are intended to be used to provide first-cut estimates of recharge for geographic areas no smaller than the smallest watersheds used in the calibration of the model—or about 1.5 square miles. It is recommended that the grids are used to calculate an area-wide average potential recharge for any given area of study, and an uncertainty around the mean should be calculated from the standard deviation grid at the same time.

Introduction

A small amount of groundwater recharge (or potential recharge) information exists for the State of Maine. Groundwater recharge is one of the most difficult components of the water cycle to determine, yet it is important for determining water availability for almost any purpose (for example, irrigation or drinking-water withdrawals, and in-stream flows for aquatic resources). Few site-specific recharge estimates in the State, either from calibrated groundwater-flow models or other analytical studies, have been published, and all the estimates published to date cover small geographic areas. Most groundwater used in Maine falls under three general categories: domestic private-well usage, crop irrigation, and public-water supply. Groundwater availability varies greatly across the State: productive sand and gravel aquifers (many of which are narrow valley-fill aquifers) are spatially discontinuous and cover a relatively small percentage of the landscape, and less productive glacial till and bedrock areas cover most of the State.

The largest limiting factors to sustainable groundwater use are the ability of an aquifer to store and transmit water and the amount of recharge to aquifers. Recharge is also highly variable—published values range from 2 to over 27 inches per year (in/yr) —and the physical characteristics of the soil and material above the underlying aquifers contribute greatly to the amount of recharge in any given location. Recharge also varies year-by-year depending on climate conditions, such as temperature and the amount and timing of rainfall and snowmelt.

To increase the ability of managers to understand the spatial and temporal variability of recharge to groundwater systems across the State of Maine and to analyze water budgets across the landscape, a study was initiated by the U.S. Geological Survey (USGS), in cooperation with the Maine Geological Survey to use the USGS Soil-Water-Balance (SWB) model to evaluate annual average potential recharge across the State. This study constructed and calibrated an SWB model of annual potential recharge over a 25-year period (1991 to 2015). Results are presented as 25-year annual average potential recharge (mean and median), the range of annual potential recharge (minimum and maximum) over the same time period, and the standard deviation of the mean 25-year average potential recharge, which was calculated using Monte Carlo methods (for a description of this method applied in groundwater modeling, see Anderson and others, 2015, p. 471).

Purpose and Scope

The purpose of this report is to document the construction and calibration of the SWB model for the State of Maine, and to describe the average (mean and median), minimum, and maximum annual potential recharge for the State from 1991 to 2015 and the uncertainty of those calculations. The SWB model archive is available in an accompanying data release (Nielsen, 2019). This study provides a baseline of information on potential recharge rates for the State of Maine. The methods and a summary of the project results are presented in this report; detailed data in the form of geospatial layers of average annual, minimum, and maximum potential recharge and model uncertainty are made available in an accompanying data release (Nielsen and Westenbroek, 2019).

Previous Studies

Few data are available from published studies on groundwater recharge rates in Maine. Although consultants and State agencies have constructed numerous small groundwater-flow models for the analysis of groundwater availability for public drinking-water supplies and for the delineation of wellhead protection zones, the recharge rates used in those models are not available publicly and have not been published. A compilation of recharge rates for many typical soil types across the State was published in 1996 by the Geological Society of Maine (Gerber and Hebson, 1996) using results from several calibrated groundwater models conducted by consulting companies in the early 1990s, but that was the last published summary of available data and included relatively few studies primarily in southern Maine. Recharge rates for glaciomarine silt/clay soils ranged from 2 to 12 in/yr, rates for sandy glacial outwash were reported as high as 27 in/yr, and recharge to bedrock units ranged from 2 to 6 in/yr. The USGS has published a limited number of groundwater studies with recharge analyses (Morrissey, 1983; Tepper and others, 1990; Nielsen, 2002; Nielsen and Locke, 2012, 2015), but these are limited in geographic coverage and report recharge values within the same range as earlier studies. To date (2019), there have not been any previous attempts at providing even a general statewide average of recharge rates for various aquifers, soil types, or both across the whole State.

Use of the Soil-Water-Balance Model for Regional-Scale Recharge Estimation

In recent years, the USGS has made frequent use of a computer code called the Soil-Water-Balance (SWB) Model (Westenbroek and others, 2010, 2018) to generate spatial datasets of potential recharge for large geographic areas such as the State of Minnesota (Smith and Westenbroek, 2015) and the glaciated terrain across the northern United States (Trost and others, 2018). The SWB method of recharge estimation calculates potential recharge to groundwater using inputs of precipitation, temperature, land cover, and soil information, and estimates of potential and actual evapotranspiration (ET). The calculations done using this method traditionally have been used in the agricultural sector to estimate crop water demands, but they also can be used to provide estimates of excess soil moisture, which is the source of recharge to groundwater (Westenbroek and others, 2010). Using independent data on recharge for a particular study area, others have calibrated the SWB output for long-term (annual to multiyear average annual) recharge in Minnesota (Smith and Westenbroek, 2015), Rhode Island (Friesz and Stone, 2014), the Lake Michigan Basin (Feinstein and others, 2010), the North Atlantic Coastal Plain (Masterson and others, 2013), the Appalachian Plateau (McCoy and others, 2015), and the USGS glacial aquifers study area (Trost and others, 2018). Long-term base flow from unregulated USGS streamgages has been used by many of these studies to represent spatially averaged watershed recharge as a calibration target dataset for SWB models. A thorough summary of the use of base-flow-derived recharge estimated by various methods of hydrograph separation used as a calibration target dataset for large SWB models is given in Trost and others (2018). For the Maine SWB model, streamflow data from 32 unregulated watersheds were used for the recharge and runoff calibration targets (fig. 1; table 1).

Although the SWB software simulates other components of the overall water budget, including direct runoff and actual ET, few SWB model calibrations to date have used more than observed recharge values to calibrate the model. The SWB model software includes many potential adjustments that control ET and runoff, and the values chosen for these parameters cascade through the calculations to impact potential recharge as well. None of the previous examples of calibrated SWB recharge models reviewed for this study constrained the calibration using ET data, which could result in a nonunique and possibly inappropriate fit of the model parameters. The Maine SWB recharge model presented in this report was calibrated using all available water-balance terms (recharge, direct runoff, and ET), which should result in a more robust and better constrained model. Furthermore, none of the SWB model studies published to date have attempted to quantify the uncertainty in the results, possibly because of the long run times for a large SWB model; this study conducted a robust calculation of the uncertainty in the modeled potential recharge across the State of Maine.

Description of Study Area

The Maine SWB recharge model was applied to the near-surface soils and shallow aquifers across the State of Maine, where soil data to run the model were available. The model was run for all soil types in the State, regardless of whether they constituted a significant water-bearing unit or not. The surficial soils in Maine are all derived from the action of glaciers on the landscape, either as depositional units directly from the melting of the glaciers, or a later reworking of the glacial deposits. Some areas are now devoid of what would be a typical soil because the advance and retreat of glaciers and subsequent erosion has exposed the underlying bedrock at the land surface. These, too, are mapped and classified within the study classification scheme, and model output is reported.

A few areas of the State were excluded from the model because soil data have not been mapped and published in these areas. The White Mountain National Forest in western Maine does not have published soil data, nor does the former Brunswick Naval Air Station in the southern part of the State. The soil information necessary to run the SWB model is lacking over surface-water bodies as well. No calculations were done in any of these areas.

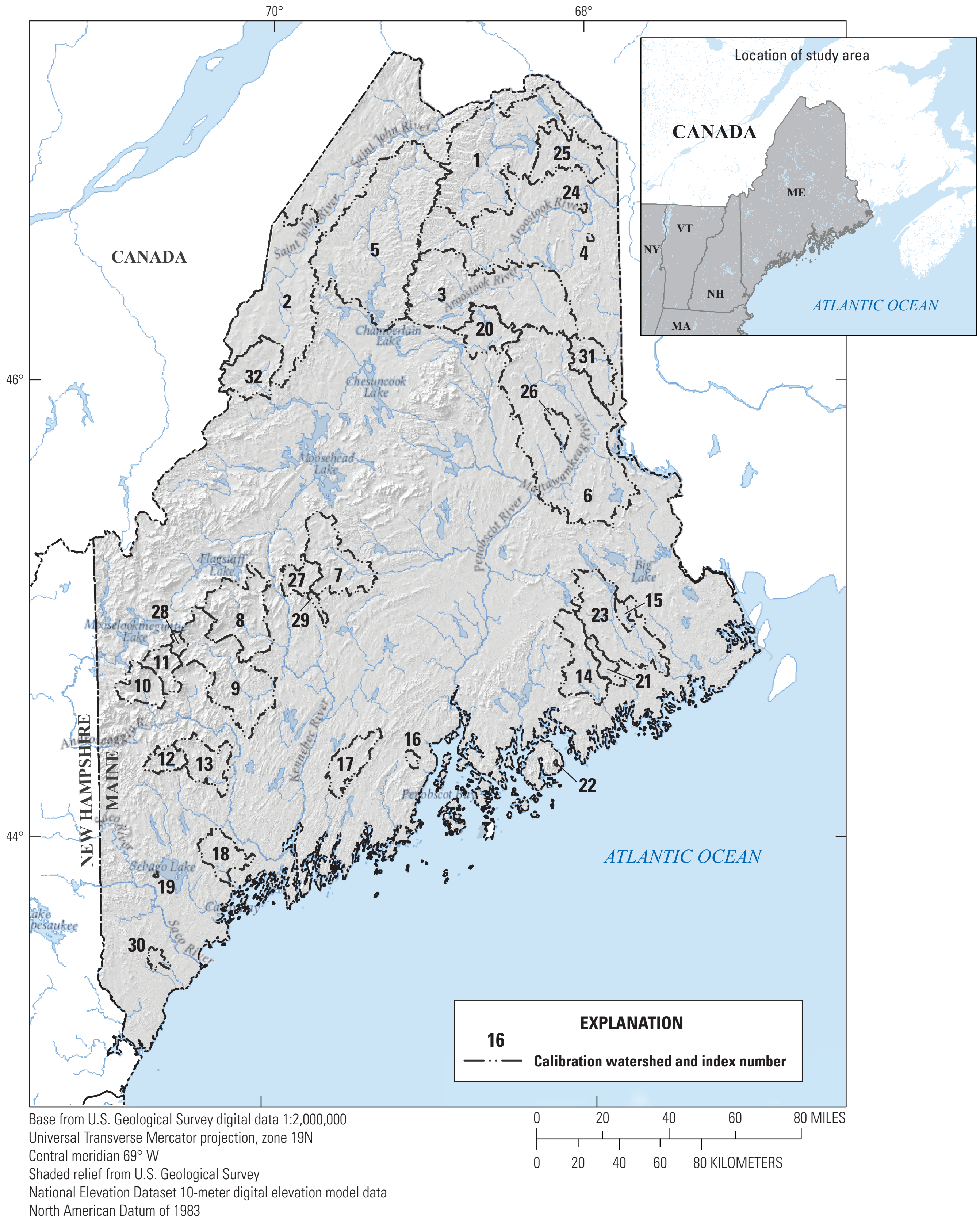


Figure 1. Calibration watersheds used in the Maine Soil-Water-Balance model and location of the study area.

Table 1. Calibration watersheds used in the Maine Soil-Water-Balance model and associated streamgage information.

[mi^2, square mile]

Calibration watershed index number (fig. 1)	Watershed observation name	Watershed area (mi^2)	Streamgage station name (with station number)
1	Fish River	867.1	Fish River near Fort Kent, Maine (01013500)
2	St. John River	1,339.0	St. John River at Ninemile Bridge, Maine (01010000)
3	Aroostook River	895.1	Aroostook River near Masardis, Maine (01015800)
4	Williams Brook	3.9	Williams Brook at Phair, Maine (01017550)
5	Allagash River	1,229.6	Allagash River near Allagash, Maine (01011000)
6	Mattawamkeag River	1,420.3	Mattawamkeag River near Mattawamkeag, Maine (01030500)
7	Piscataquis River	297.3	Piscataquis River near Dover-Foxcroft, Maine (01031500)
8	Carrabassett River	352.7	Carrabassett River near North Anson, Maine (01047000)
9	Sandy River—Mercer	516.1	Sandy River near Mercer, Maine (01048000)
10	Ellis River	130.4	Ellis River at South Andover, Maine (01054300)
11	Swift River	96.8	Swift River near Roxbury, Maine (01055000)
12	Little Androscoggin River	73.9	Little Androscoggin River near South Paris, Maine (01057000)
13	Nezinscot River	168.5	Nezinscot River at Turner Center, Maine (01055500)
14	Narraguagus River	227.0	Narraguagus River at Cherryfield, Maine (01022500)
15	Old Stream	29.8	Old Stream near Wesley, Maine (01021480)
16	Ducktrap River	15.0	Ducktrap River near Lincolnville, Maine (01037380)
17	Sheepscot River	144.9	Sheepscot River at North Whitefield, Maine (01038000)
18	Royal River	141.0	Royal River at Yarmouth, Maine (01060000)
19	Stony Brook	1.6	Stony Brook at East Sebago, Maine (01063310)
20	Seboeis River	172.7	Seboeis River near Shin Pond, Maine (01029200)
21	Pleasant River	61.1	Pleasant River near Epping, Maine (01022260)
22	Otter Creek	1.3	Otter Creek near Bar Harbor, Maine (01022840)
23	Machias River	457.7	Machias River at Whitneyville, Maine (01021500)
24	Hardwood Brook	5.7	Hardwood Brook below Glidden Brook near Caribou, Maine (01017060)
25	Little Madawaska River	234.1	Little Madawaska River at Caribou, Maine (01017290)
26	Wytopitlock Stream	48.6	Wytopitlock Stream near Wytopitlock Maine (01030350)
27	Austin Stream	90.6	Austin Stream at Bingham, Maine (01046000)
28	Sandy River—Madrid	25.3	Sandy River near Madrid, Maine (01047200)
29	East Branch Wesserunsett Stream	19.4	East Branch Wesserunsett Stream near Athens, Maine (01048220)
30	Kennebunk River	26.4	Kennebunk River near Kennebunk, Maine (01067950)
31	Meduxnekeag River	170.6	Meduxnekeag River near Houlton, Maine (01018000)
32	North Branch Penobscot River	223.5	North Branch Penobscot River near Pittston Farm, Maine (01027200)

Soil-Water-Balance Modeling Approach

The SWB model was chosen for this study because it uses readily available datasets that cover the entire State. The model can thus estimate an average annual potential recharge rate for areas in the State that are relatively inaccessible and have not before had any hydrogeologic investigations to evaluate recharge. The final dataset produced by the model is not uniformly precise, however, and the use of automatic model calibration using parameter estimation allows for evaluating the uncertainty contributed by variability in the match of the model output to a large set of calibration data (observations) and the uncertainty in model parameters in the final datasets.

Model Theory

The SWB model (Westenbroek and others, 2010) calculates potential recharge using a modified Thornthwaite-Mather soil-water accounting method (Thornthwaite and Mather, 1957). Water-budget calculations are performed on each model cell for each day of the simulation, where recharge is the excess of the sources of water to each cell (precipitation and snowmelt) minus the sinks (interception, runoff, and ET), adjusted for changes in soil moisture (Westenbroek and others, 2010). Precipitation during the winter when the average daily temperature is below freezing is stored as snowpack, which the SWB model allows to melt during days when at least part of the day is above freezing. Direct runoff is controlled using the curve-number method (Cronshey and others, 1986), which accounts for soil types, land use, the soil-surface condition, and antecedent runoff conditions. Runoff curve numbers are set initially and allowed to vary during the simulation period in relation to the degree of soil saturation and whether the ground is frozen (Westenbroek and others, 2010). Water that could infiltrate the soil given the results of the curve-number method calculations but exceed the maximum infiltration capacity of the soil are represented as "rejected recharge" and are part of the overall runoff term. ET is calculated using one of several possible methods (see below in this section), and when potential ET is less than or equal to the amount of water available in the soil for use, actual ET equals potential ET. If the amount of water available is less than the potential ET, SWB calculates the amount of water that can be readily extracted for actual ET using Thornthwaite-Mather retention curves (Westenbroek and others, 2010). SWB calculates a daily residual soil moisture surplus (potential recharge), the net change in soil moisture, and the daily ending soil moisture value, used to compute the water balance for the next day (fig. 2).

The SWB software uses two types of inputs: climate and physical data covering the simulation area; and tabular data (model parameters) that control the calculations of potential recharge, runoff, and ET. Gridded climate data were used as model inputs and include daily precipitation, and daily minimum and maximum temperature. The physical datasets for the model include a grid of available water-capacity (AWC) values and hydrologic soil groups (available from the Natural Resources Conservation Service [NRCS] soils data; Soil Survey Staff, 2016) and land-use classes, which are available from a variety of sources.

The SWB software (Westenbroek and others, 2010, version 1.2) provides two basic options for calculating ET: the Thornthwaite-Mather approach (Thornthwaite and Mather, 1957) or the Food and Agriculture Organization of the United Nations Drainage and Irrigation Paper 56 (FAO56) approach (Allen and others, 1998). According to the SWB user manual, "Thornthwaite and Mather's work was motivated by a need to estimate the surplus and deficit of soil water for irrigation needs, and may not necessarily represent ideal values for the purposes of groundwater-recharge estimation" (Westenbroek and others, 2010, p. 16). The FAO56 approach (Allen and others, 1998) also is widely applied for agricultural purposes but provides more explicit calculations of ET based on plant-growth water demand and ET from the soil surface between plants. The plant-growth water demand calculations are based on plant-growth coefficients (K_{cb} values) that compare the ability of a type of vegetation to transpire water from the root zone compared to a reference crop (well-watered grass) during different phases of the growing season. Settings that control the soil surface ET (bare soil readily evaporable water and total evaporable water) can be adjusted to simulate soil covered with a layer of leaf litter, as is typically found in forested areas of New England. The implementation of the FAO56 calculations in SWB version 1.2 (and SWB version 2.0) are discussed in Westenbroek and others (2018).

The general approach to performing the model calculations is illustrated in figure 2, showing the overall inputs, use of datasets and variable parameters, and model outputs for each day. The cycle starts with a daily precipitation amount, daily minimum and maximum temperatures, and any residual soil moisture and snowpack; the various components of the water budget are calculated in steps. The amount available for net infiltration (potential recharge) is the second-to-last water-budget component that is calculated for each day. The final daily calculation is the residual soil moisture and residual snowpack (in cold months), which is then carried over as input to the next day's calculations. All of these calculations are performed on each gridded cell of the model.

Model Area

The model area for this study encompasses land areas within the State of Maine. The active model domain excludes areas where soils data are not available, including surface-water bodies, the White Mountain National Forest, and former Brunswick Naval Air Station (for which soil data are not published).

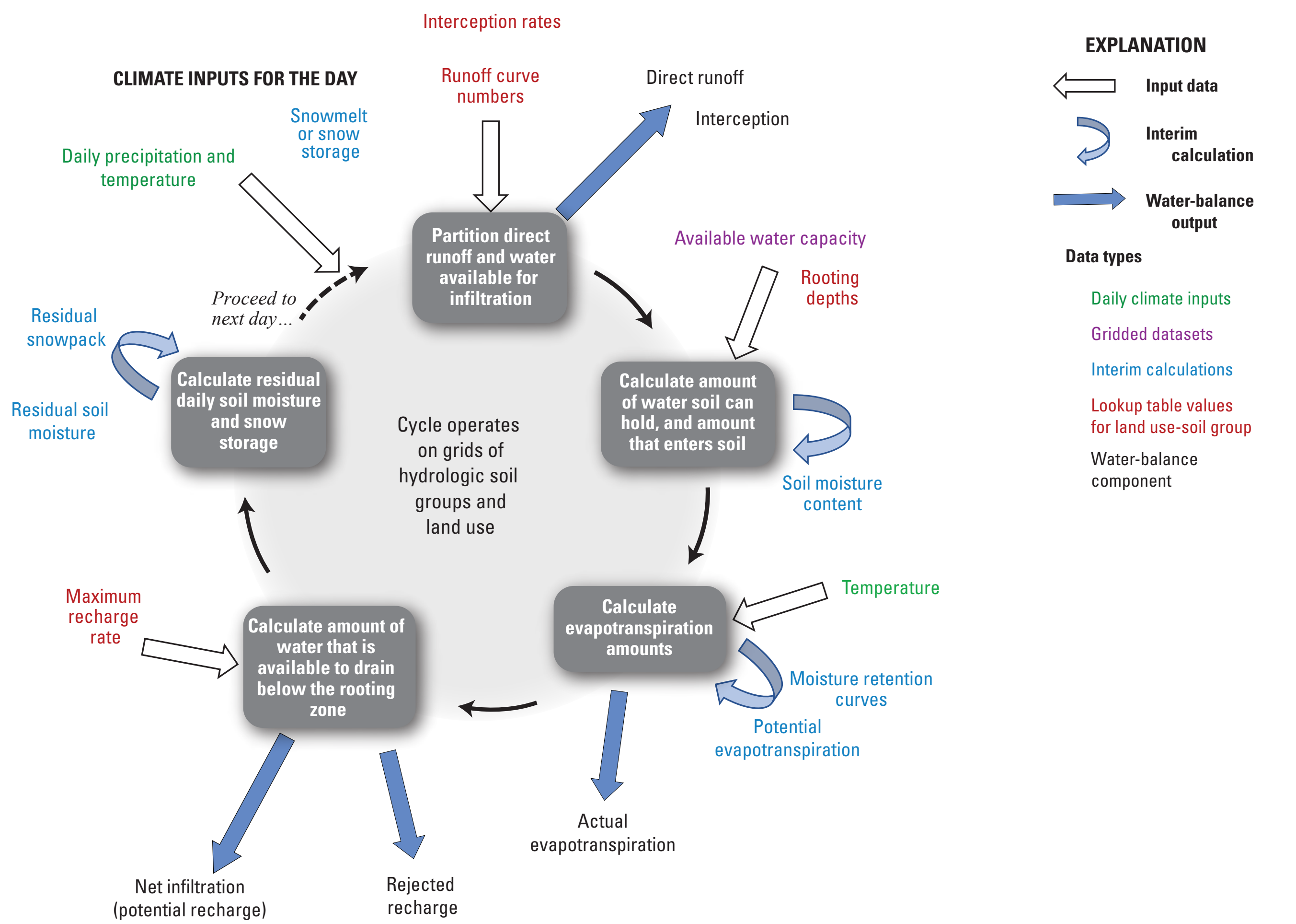


Figure 2. Operation of daily Soil-Water-Balance calculations and water-balance output.

Model Limitations and Assumptions

The SWB model provides a useful method to calculate spatially varying potential recharge to groundwater on monthly to yearly time periods. However, there are some limitations to the model and assumptions that the user must consider. Westenbroek and others (2010) and Trost and others (2018) discuss the limitations and assumptions of the SWB method in detail. An abbreviated discussion of the most important considerations is presented below:

1. The SWB model calculates potential recharge as infiltration below the root zone. The results are not a substitution for recharge determined by detailed site-specific studies, such as a groundwater-flow model, where the timing and exact magnitude of groundwater recharge are needed to answer water-resource management questions.

2. The validity of the results requires that the input data (hydrologic soil groups, AWC, and land use) are known. Uncertainty from inaccurate soil data cannot be quantified in the analysis of uncertainty in the model calibration. In some areas of Maine, the soils data are the result of interpolation between soil units that are mapped based on aerial photography, and in some remote areas the soils data are not highly accurate (L. Hodgeman, NRCS, oral commun., 2015). The model does not calculate recharge over open surface-water bodies.

3. The SWB model does not account for lag times in the movement of water infiltrated below the rooting zone to the actual water table. Therefore, model results should not be used for periods of less than 1 year, and yearly estimates of potential recharge should only be presented as approximate and should most appropriately be used to represent ranges of potential recharge (Hunt and others, 2008; Trost and others, 2018).

4. The SWB model does not track the depth to water table in the simulations and does not represent conditions of very shallow water tables explicitly. Areas with abundant wetlands may not be simulated well, and some major processes of groundwater-surface water interaction in these areas are not accounted for (Westenbroek and others, 2010; Trost and others, 2018).

5. The curve-number method has limitations in its ability to track water flow, and is best applied at the watershed scale, so the SWB output is best applied at scales of watersheds and not individual land parcels. It has also been suggested that curve numbers themselves vary by precipitation events and that the methods to account for this in the SWB model only capture some of this variability (Westenbroek and others, 2010).

6. Interception in the SWB model is accounted for in a “bucket” approach, where the volume is taken out of the direct precipitation available for infiltration. But the interception volume, which subsequently evaporates after the event is done, is not used in the ET calculations in SWB version 1.2. Using high interception numbers in the SWB model may result in the ET of interception water being counted twice in the model. Interception was turned off in the Maine SWB model to correct for this artifact.

Model Calibration Approach

Automated parameter estimation was used to calibrate the Maine SWB model, using the Parameter ESTimation (PEST) software (Doherty and Hunt, 2010). The method of calculating excess soil moisture (potential groundwater recharge) in the SWB model uses many adjustable parameters contained in the lookup tables (appendix tables 1.2 and 1.3, available for download at https://doi.org/10.3133/sir20195125). The values in the lookup tables together control how SWB divides up input to the hydrologic system into daily fractions of direct runoff, plant interception, soil infiltration, ET, soil moisture storage, rejected recharge, and infiltration of excess soil moisture to the water table (potential recharge), which are summed over a monthly or annual timestep. Some of these parameters have nonunique combinations that can produce the same amount of potential recharge for a given period. For example, an increase in the runoff curve number will generally increase direct runoff and make less water available for recharge. But decreasing the plant rooting depth can offset this by also reducing the amount of water available for transpiration after water has entered the rooting zone. Decreasing the runoff curve number to decrease runoff can be offset by an increase in the plant rooting depth, resulting in the same net recharge.

At the end of a timestep (monthly or annual), all the SWB output can be put into the general water-budget categories of runoff, infiltration of water beneath the root zone (potential recharge), actual ET, and storage of water in the soil or snowpack. For the Maine SWB model, an annual timestep was chosen to sum the SWB outputs.

To reduce the nonuniqueness of the calibration, three types of calibration targets were used: runoff, potential recharge, and ET. Runoff and potential recharge were derived from hydrograph separation, and ET was derived from satellite data. Direct runoff, as a component of hydrograph-separation calculations, is analogous to the sum of the SWB calculations of “runoff outside” (direct runoff during a precipitation event, or Hortonian overland flow; Chow and others, 1988) and “rejected recharge” (water that initially infiltrates the soil zone during a precipitation event but cannot infiltrate through the soil zone because of limitations in the maximum infiltration capacity of the soil, or saturation overland flow; Chow and others, 1988). Base flow is often assumed to represent long-term discharge from groundwater, which should equal groundwater recharge if ET from the water table is negligible and the groundwater and surface-water watersheds are coincident (Healy, 2010).

The calibration was conducted in stages, first by using a subarea of the model for an initial calibration (using 4 watersheds) and then finalizing the calibration with the whole State and 32 calibration watersheds (table 2). Because of the numerical burden of the number and speed of SWB runs needed for the calibration, the calibration was done using a 500-m grid-cell size, which runs four times faster than the final model spatial discretization of 250-m grid-cell size. Details of the calibration data, procedure, and results are presented below.

Table 2. Land-use classes for the Maine Soil-Water-Balance model.

Land-use code	Land-use class (fig. 3)	Percentage
2	Developed—High intensity	0.3
3	Developed—Moderate	0.3
4	Developed—Low intensity	0.5
5	Developed—Open space	0.5
6	Cultivated crops	2.4
7	Pasture/hay	2.1
8	Grassland	0.2
9	Deciduous forest	15.1
10	Evergreen forest	20.3
11	Mixed forest	35.2
12	Scrub/shrub	10.3
13	Wetland forest	3.7
14	Wetlands from soils	4.2
15	Wetlands	1.3
16	Roads/runways/bare rock	1.4
20	Bare land	0.1
21	Open water	1.6
22	Blueberry barrens	0.3
27	Alpine/tundra	<0.1
30	Gravel pits	0.1

Processing of Calibrated Model Output

After the Maine SWB model calibration was completed, the model was run for a 26-year simulation period (1990–2015) using the final best-fit values for both lookup tables used in the simulation (appendix tables 1.2 and 1.3). Running the model for 26 years allows for a spin-up year that sets up the soil moisture and snow storage properly for the first year of the desired simulation (1991). The initial year of the run (1990) was not used in any of the subsequent processing steps. The final model runs used a finer model grid-cell size (250 m) than the calibration runs (500 m).

The 25 annual recharge grids were run through several postprocessing steps to obtain the final model results. The first step was to do statistical analysis on the 25 annual grids—calculating the 25-year minimum, mean, median, and maximum values for each pixel in the model domain. This was done using the ArcGIS version 10.6 software. Further postprocessing of the calculated grids included removing data from an exclusion zone in northwestern Maine (see the “Groundwater Recharge Estimates for Maine, 1991–2015” section, below) and screening out anomalously high values, which can arise from slightly misaligned original input grids. The top 0.25 percent of calculated values were reassigned to the 99.75-percentile value. In the following discussion, the 99.75-percentile value is termed the “maximum” for each grid. A final postprocessing step was to apply a low-pass filter (3 by 3 cells), which smoothed out the impact of single pixels that had values that were very dissimilar to their local neighborhood of values, which generally was a result of slightly misaligned input grids. The low-pass filter also smoothed out abrupt boundaries between zones of very different simulated potential recharge. Although a slight loss of information results from the smoothing process, the resulting grids better reflect the scale of landscape variability in the State and reduce the potential for misuse of the potential grids that could arise from assuming pixel-scale variability is reflective of actual conditions. Further discussion of the model outputs refers to the grids with the low-pass filter applied, unless otherwise noted. These steps were carried out using a combination of ArcGIS data manipulation and python-based raster analysis.

Model Uncertainty Representation

One of the goals of this investigation was to be able to portray the uncertainty inherent in the estimated values of potential recharge. Current numerical methods for evaluating the uncertainty of a model calibrated using PEST (Doherty and Hunt, 2010) limit the analysis to uncertainty in the overall model results that arise from uncertainties in the values of the parameters that are used in the model. No measure currently (2017) exists for incorporating uncertainty from the model input data (such as the soil grids or climate data) into this analysis, unfortunately. Portraying the uncertainty in the results of the SWB modeling exercise is difficult because the study result is not a prediction of a change in some measurable volume or measurement of interest but rather a surface across the entire State. Techniques of uncertainty analyses using linear-based first-order, second-moment methods to analyze model response to specific conditions at a particular time and place (see White and others, 2016) are not readily applicable to this kind of output. No published SWB model has shown the spatial uncertainty in the modeled potential recharge to date (2019).

The null-space Monte Carlo method of Tonkin and Doherty (2009) was used to spatially represent the uncertainty in the potential recharge grids. Because of the complexity of the analysis, the uncertainty calculations were run using only one of the final grids: the median potential recharge grid. Because the mean potential recharge grid differs only a small percentage (about 2 percent) from the median grid, the uncertainty for the mean grid should not be substantially different from that for the median grid.

The Monte Carlo analysis was performed using many potential alternate realizations of the suite of model parameter values (Tonkin and Doherty, 2009) used in the calibration. The pyEUM software (White and others, 2016) was used to generate the 300 unique parameter sets needed to run the analysis. Each realization of the set of parameter values was generated by sampling a normal distribution of values around the calibration best-fit value for each modeled parameter (even if they were not specifically estimated using PEST), using an assumed possible range of values of plus or minus 3 sigma (σ). The upper and lower bounds of the ranges for each parameter were first obtained from the PEST calibration upper and lower bounds, which were adjusted after the calibration for this purpose to create balanced upper and lower reasonable ranges of values around the calibration value. For computational efficiency, the Monte Carlo runs were done using the 500-m grid-cell size used in the calibration. Simultaneous model runs were controlled and organized using the HTCondor computer cluster at the T.C. Chamberlin computing center at the USGS Wisconsin office of the Upper Midwest Water Science Center.

Maine Soil-Water-Balance Model Description and Calibration

The SWB software (Westenbroek and others, 2010), version 1.2, was used for the simulation of recharge and other components of the water budget for Maine. The Maine SWB model used two scales of input and output data. The model was calibrated at a 500-m grid-cell size using 12 years of simulation to make the run times for the model reasonable enough to allow for thousands of model runs per calibration run. Once the lookup table values were calibrated, the model was run for the final time for a 25-year period using a 250-m grid-cell size. The model domain includes 678,384 500-m grid cells and 2.713 million 250-m grid cells.

Model Input Data Summary

The input required for running the Maine SWB model consists of (a) grids describing the study domain (land use, hydrologic soil types, and soil AWC); (b) gridded daily climate data; (c) tabular values (parameters) that control the water balance calculations, including runoff curve numbers, maximum potential infiltration rates, rooting depths, and information on how interception is handled for each combination of land-use class and hydrologic soil type (these are sent to the SWB software in a tab-delimited text file called the land-use lookup table); and (d) another set of tabular values in a lookup table for implementing the FAO56 ET calculations, called the irrigation lookup table. Gridded data from all data sources except the climate data were resampled to the Maine SWB model scales of 250 and 500 m (see the “Gridded Model Data” section below).

Gridded Model Data

Land-use data for the Maine SWB model were based on the Maine Land Cover Dataset (MELCD; Maine Office of Geographic Information Systems, 2006; see appendix 1). The MELCD data are based on Landsat Thematic Mapper 5 and 7 imagery from 1999 and 2000 and have a spatial resolution of 5 m. Land-use classes from the MELCD were condensed into 19 categories (table 2; fig. 3). Some modifications to water, wetland areas, and gravel pits were made using the NRCS soils data so that these areas did not conflict between the soil classes and land uses. The resampling to 250- and 500-m grid resolution was done by calculating the most prevalent land use in each larger grid cell. A test was done to determine whether resampling to coarser grid cells changed the overall distribution of land uses in the study area. When the 5-m MELCD data were resampled to 250 and 500 m, the overall percentage of each land use was the same as the original, to within 0.2 percent.

The other two data inputs for SWB (hydrologic soil groups and AWC) were produced for this study using gridded soil survey data from 2016 (NRCS gridded Soil Survey Geographic Database [gSSURGO] data, Soil Survey Staff, 2016). The data format is a raster of soil map-unit keys with a 10-m resolution. The map-unit keys link the raster cells to many attribute tables, including (among others) hydrologic soil groups, drainage classes, soil-unit descriptions, parent material, and AWC. The gridded data were resampled to 250 and 500 m for the Maine SWB model.

The hydrologic soil groups (U.S. Department of Agriculture [USDA], NRCS, 2007) are used in SWB alongside land use to classify the landscape into combinations of land use/vegetation and soil texture that are assumed to transmit water similarly through the rooting zone and unsaturated zone to the water table under the same climatic conditions (Westenbroek and others, 2010). Previous studies using the NRCS hydrologic soil groups as the basis for the soil type data in SWB have generally used the standard seven hydrologic soil groups as defined by the NRCS (A, A/D, B, B/D, C, C/D, and D), where the soils in groups A, B, C, and D range from being able to transmit water very freely (group A soils) to soils that do not transmit water well at all, especially when saturated (group D soils). The groups A/D, B/D, and C/D refer to soils that transmit water differently when saturated and often apply to areas with shallow water tables (wetland areas; USDA, NRCS, 2007).

An initial evaluation of the use of SWB in Maine for this study determined that the group D soils include a range of soil types that ranges, on one end, from tight clay deposits on coastal lowlands, to areas that have thin (0–6 in.) soils over exposed bedrock in mountainous areas with high slopes. Because the process of generating runoff and recharge from incoming precipitation in these areas is quite different, the group D soils for Maine were subdivided into three subgroups based on the soil drainage class for each soil unit: “D–Ex” are the D soils that are also excessively drained (primarily shallow soils over bedrock, often steep slopes); “D–SoEx” (somewhat excessively drained D soils) are primarily soils in subdued hilly areas and often are composed of glacial till; “D–Poor” (poorly and somewhat poorly drained D soils) are a group of several poorly drained soil types, including glacial clay deposits, silt loam soils (farmable but not peats), silt-loams, and silty clay loams and silt loams (no plant material or peat mentioned). Some are tidal marshes or upland areas of poor drainage (forested). The nine hydrologic soil groups used in the Maine SWB model are listed in table 3, and their distribution is shown in figure 4.

The model calculates potential recharge based on each cell’s individual land-use class and hydrologic soil group. Considering all the possible combinations of land-use class and hydrologic soil groups in the model area, there are 171 possible categories created by the intersection of these two datasets (table 4). Many of the categories have near zero area across the landscape. The 35 most-abundant categories (named using the format of “land-use class:hydrologic soil group”) together represent 86 percent of the State (fig. 5). Maine is primarily a forested State—13 of the 15 most-abundant categories include mixed, evergreen, deciduous, or wetland forest land-use classes. The other two most abundant categories are scrub/shrub:D–Poor and scrub/shrub:C/D, which largely cover areas in northern and northwestern Maine that were recovering from heavy logging operations in the 1990s. The mixed forest:D–poor, evergreen forest:D–poor, mixed forest:C/D, mixed forest:C, mixed forest:D–SoEx combined account for 37.9 percent of the model area.

The AWC in the soil horizon is defined as the number of inches of water that can be held per foot of soil thickness (see the NRCS Soil Survey Manual [Ditzler and others, 2017] for a complete description of the derivation of these data). The AWC is used by SWB to calculate the maximum amount of soil-water storage that can be held in a model grid cell. SWB calculates the total amount of potential soil moisture storage as the AWC times the rooting zone depth for each model cell, where the rooting zone depths are adjusted for each land-use

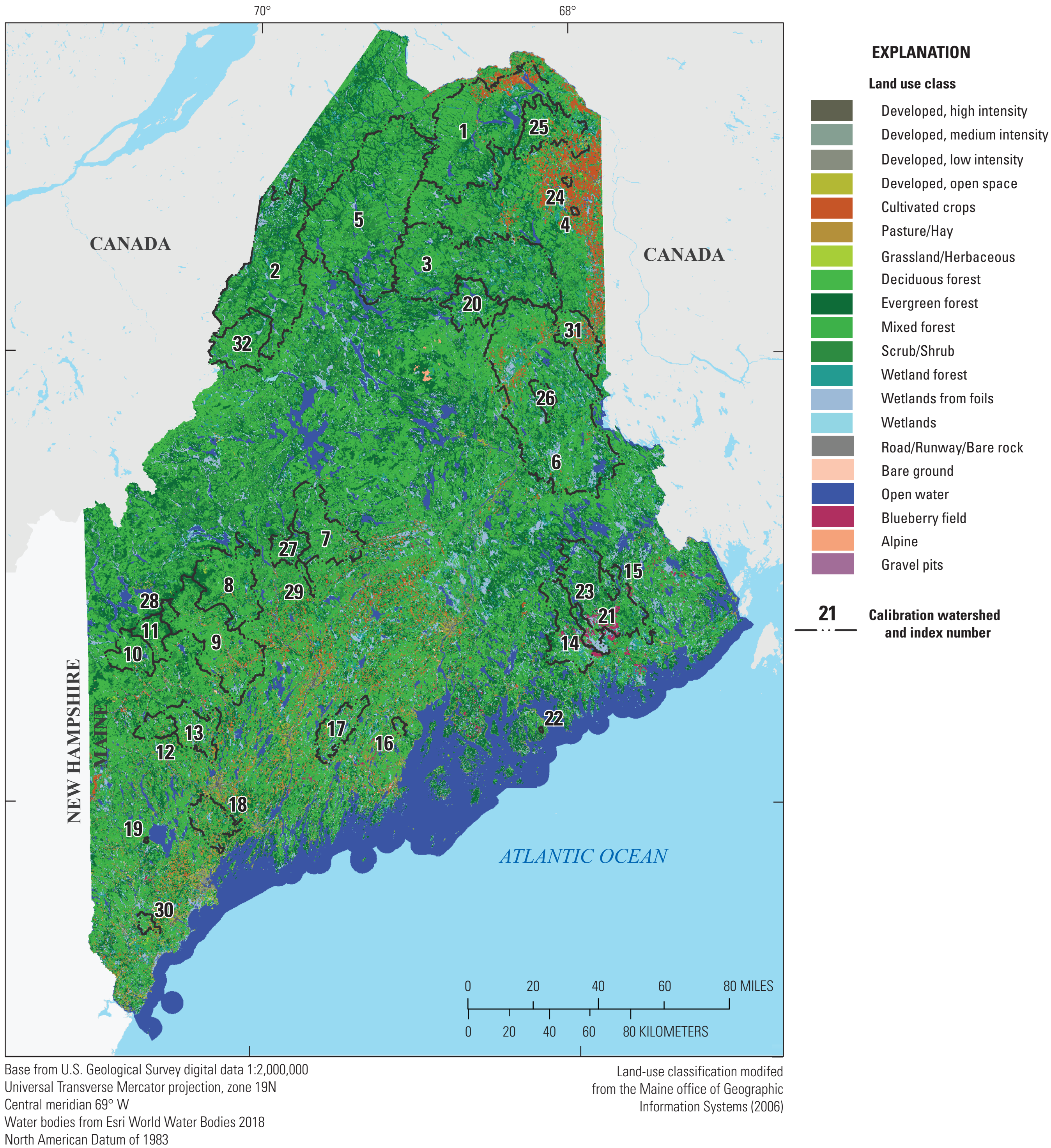


Figure 3. Land use for the Maine Soil-Water-Balance model and calibration watersheds.

Table 3. Hydrologic soil groups used in the Maine Soil-Water-Balance model.

Soil group number	Hydrologic soil group (fig. 4)	Description	Percentage of model area
1	A	Low runoff potential when wet; water is transmitted freely through the soil	7.6
2	A/D	High water transmission rates; water table <60 centimeters from the surface (often wetlands)	4.2
3	B	Moderately low runoff potential when wet; water transmission is unimpeded	4.3
4	B/D	Moderate water transmission rates; water table <60 centimeters from the surface (often wetlands)	2.0
5	C	Moderately high runoff potential when wet; water transmission is somewhat restricted	15.9
6	C/D	Moderately low water transmission rates; water table <60 centimeters from the surface (often wetlands)	18.4
7	D–Ex	High runoff potential; water movement is restricted; excessively drained (primarily thin soils over shallow bedrock)	2.0
8	D–SoEx	High runoff potential when wet; water movement is restricted; somewhat excessively to moderately drained	12.6
9	D–Poor	High runoff potential when wet; water movement is restricted; typically clayey textures; somewhat poorly to poorly drained	32.9

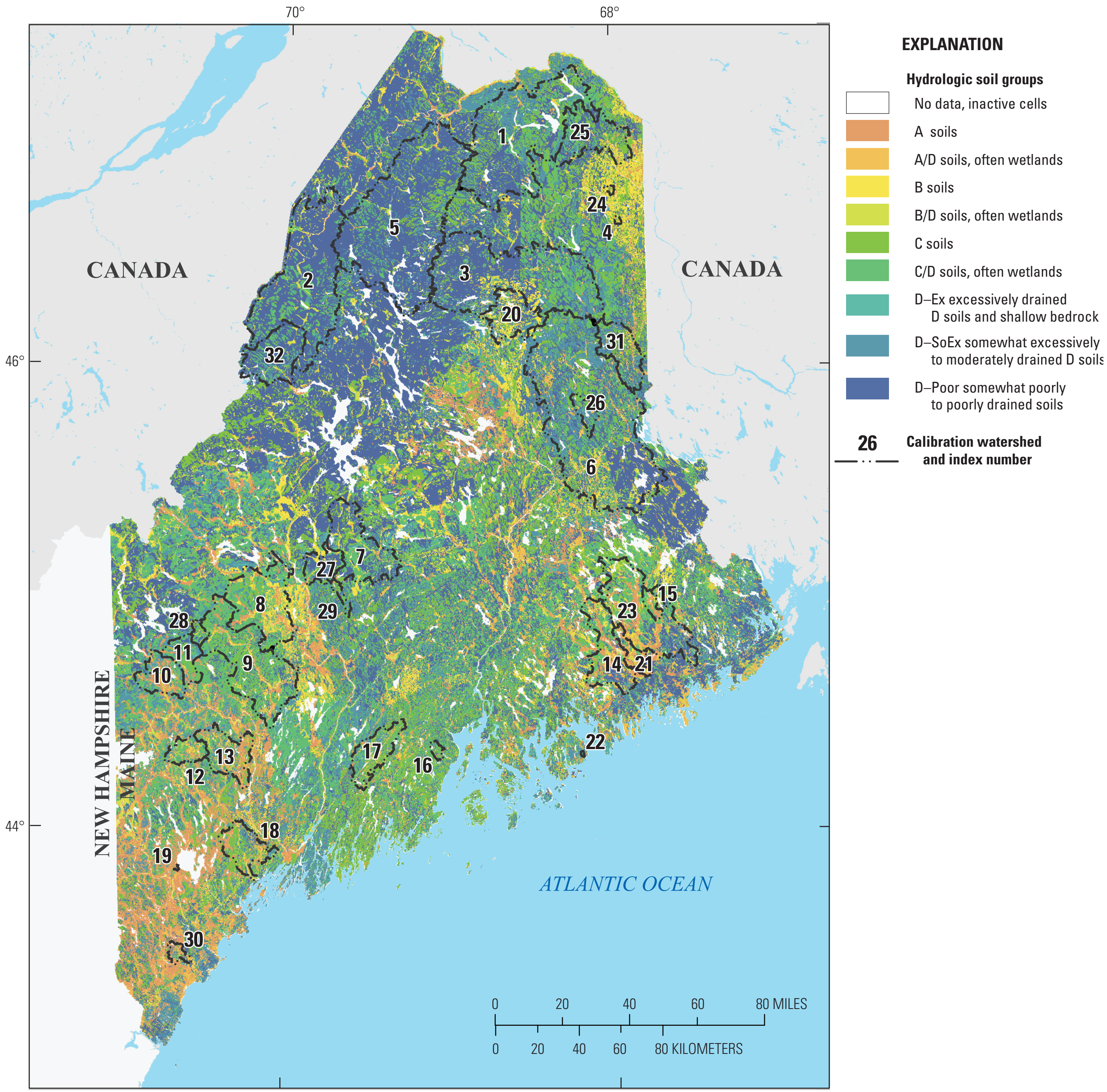
class:hydrologic soil group category using the SWB lookup table (see the "Lookup Tables and Control File" section below). The available water-capacity grid for Maine (fig. 6) was obtained from the gSSURGO data (Soil Survey Staff, 2016), and modified for areas of missing data (appendix 1).

Although the AWC of the soil, or the amount of water that a soil can hold under saturated conditions, could be thought of as a component of the soil's hydrologic description, there is not a strong relation between the hydrologic soil groups and the AWC for Maine soils, as illustrated in figure 7. The AWC for hydrologic soil groups A and D–Ex are distinctive in that there is a higher proportion of cells with less than 3 in. of storage per foot than in the other categories, which would be appropriate for very sandy soils (generally describing group A), or thin soil over bedrock (D–Ex). And the amount of water-holding capacity generally increases as the soil group's capacity to transmit water gets lower, which would be appropriate for finer-grained soils that can hold more water than coarse-grained sandy soils. However, the graphs (fig. 7) illustrate that sometimes the AWC for a soil group does not match the description well—for example, the A/D soil group generally represents wet areas that are poorly drained, and the lack of drainage could increase the amount of water that the soil will hold dramatically as compared to the same soil that has free drainage. The way that SWB calculates infiltration below the rooting depth in a case where the AWC is low does not consider the lack of drainage, however, and could result in more calculated recharge than would otherwise seem reasonable.

The DayMet (version 3) daily climate data from the Oak Ridge National Laboratory (Oak Ridge, Tennessee; Thornton and others, 2018) were the source of the daily minimum and maximum temperature and daily precipitation data used in the Maine SWB model. These data, which are available in the Network Common Data Form (netCDF) format, have a spatial resolution of 1 kilometer. The DayMet data are derived from an algorithm that models daily temperature and precipitation based on ground-surface observations, elevation, and incident solar radiation (Thornton and others, 2018).

Precipitation is a major driver of potential recharge. Typically, the annual precipitation for Maine falls between 40 and 50 in. (fig. 8), with higher amounts at higher elevations and in some of the coastal areas and lower amounts in the rain shadow behind the northern end of the Appalachian Mountains and in northern Maine.

Another source of modeled precipitation data for the Nation are the Parameter-elevation Regressions on Independent Slopes Model (PRISM) data from Oregon State University (PRISM Climate Group, Oregon State University, 2012): annual "normal" precipitation from 1981 to 2010 (fig. 9). These data are available as monthly and annual data, with a spatial resolution of 800 m. These data do not have the spatial or temporal granularity of the DayMet data and cannot be used with the SWB model, but the overall spatial pattern of annual precipitation for Maine should be comparable for both datasets. A gross comparison of the DayMet annual average (fig. 8) and the PRISM data (fig. 9) indicates general agreement in the overall patterns and amounts of annual precipitation, except for the area along the northwestern border with Canada, generally in the area covered by calibration watersheds numbers 2 (St. John River) and 32 (North Branch Penobscot River; and part of 5 [Allagash River]), extending south along the border towards New Hampshire (see fig. 8). This discrepancy is assumed to be an artifact of the interpolation method used by DayMet and the available weather stations between Maine and adjacent areas



Base from U.S. Geological Survey digital data 1:2,000,000
Universal Transverse Mercator projection, zone 19N
Central meridian 69° W
Water bodies from Esri World Water Bodies 2018
North American Datum of 1983

Hydrologic soil group data modified from Soil Survey staff (2016)

Figure 4. Hydrologic soil groups of the Maine Soil-Water-Balance model and calibration watersheds.

Table 4. Percentage of Maine Soil-Water-Balance model and calibration watersheds covered by each combination of land-use class and hydrologic soil group.

[Values in **bold text** cover more than 0.5 percent of the total]

Land-use code	Land-use class (fig. 3)	Percentage of model area by hydrologic soil group (fig. 4)									Total for each land use (percent)
		A	A/D	B	B/D	C	C/D	D–Ex	D–SoEx	D–Poor	
	Maine Soil-Water-Balance model										
2	Developed–High intensity	0.07	0.02	0.02	0.01	0.07	0.03	<0.01	0.04	0.05	0.31
3	Developed–Moderate	0.07	0.02	0.02	0.00	0.06	0.03	0.01	0.04	0.04	0.29
4	Developed–Low intensity	0.12	0.03	0.03	0.01	0.10	0.06	0.01	0.07	0.08	0.51
5	Developed–Open space	0.11	0.03	0.04	0.01	0.12	0.05	0.01	0.08	0.10	0.54
6	Cultivated crops	0.19	0.03	**0.60**	0.07	**0.59**	0.39	0.01	0.23	0.26	2.37
7	Pasture/hay	0.24	0.04	0.14	0.05	**0.58**	0.35	0.02	0.23	0.41	2.06
8	Grassland	0.02	0.01	0.01	0.00	0.03	0.03	0.01	0.03	0.04	0.18
9	Deciduous forest	**0.93**	0.18	**0.63**	0.07	**3.37**	**3.80**	0.44	**2.67**	**3.04**	15.14
10	Evergreen forest	**1.61**	**0.74**	**0.73**	0.36	**2.47**	**3.04**	**0.54**	**2.52**	**8.30**	20.32
11	Mixed forest	**2.54**	**0.86**	**1.32**	0.42	**5.98**	**7.25**	**0.55**	**4.64**	**11.67**	35.24
12	Scrub/shrub	**0.51**	0.17	0.36	0.08	**1.40**	**1.84**	0.14	**1.27**	**4.57**	10.33
13	Wetland forest	0.21	0.34	0.09	0.25	0.25	0.46	0.03	0.18	**1.85**	3.67
14	Wetlands from soils	0.29	**1.49**	0.08	0.40	0.23	0.33	0.05	0.13	**1.21**	4.20
15	Wetlands	0.12	0.12	0.05	0.17	0.11	0.15	0.02	0.07	0.50	1.30
16	Roads/runways/bare rock	0.15	0.04	0.08	0.02	0.30	0.25	0.03	0.15	0.31	1.35
20	Bare land	0.03	0.00	0.01	0.00	0.01	0.02	0.00	0.01	0.03	0.12
21	Open water	0.21	0.11	0.10	0.07	0.20	0.19	0.14	0.21	0.40	1.63
22	Blueberry barrens	0.14	0.03	0.01	0.00	0.04	0.06	0.01	0.01	0.02	0.32
27	Alpine/tundra	<0.01	0.00	0.01	0.00	0.00	0.01	0.01	0.01	0.00	0.03
30	Gravel pits	0.04	0.01	<0.01	0.00	0.01	<0.01	0.00	<0.01	0.01	0.06
All	Total for each soil group:	7.61	4.25	4.32	1.99	15.92	18.36	2.01	12.62	32.89	99.98
	Calibration watersheds										
2	Developed–High intensity	0.02	0.00	0.01	0.00	0.02	0.01	<0.01	0.01	0.00	0.07
3	Developed–Moderate	0.02	0.00	0.01	0.00	0.02	0.02	0.00	0.01	0.01	0.09

Table 4. Percentage of Maine Soil-Water-Balance model and calibration watersheds covered by each combination of land-use class and hydrologic soil group.—Continued

[Values in **bold text** cover more than 0.5 percent of the total]

Land-use code	Land-use class (fig. 3)	Percentage of model area by hydrologic soil group (fig. 4)									Total for each land use (percent)
		A	A/D	B	B/D	C	C/D	D–Ex	D–SoEx	D–Poor	
					Calibration watersheds—Continued						
4	Developed–Low intensity	0.03	0.00	0.01	0.00	0.03	0.03	0.00	0.02	0.02	0.14
5	Developed–Open space	0.03	0.00	0.01	0.01	0.05	0.02	0.00	0.02	0.02	0.17
6	Cultivated crops	0.09	0.01	0.19	0.03	0.27	0.41	0.00	0.20	0.38	1.59
7	Pasture/hay	0.14	0.02	0.09	0.04	0.24	0.29	0.01	0.18	0.16	1.15
8	Grassland	0.01	0.00	0.00	0.00	0.01	0.03	0.00	0.02	0.02	0.10
9	Deciduous forest	**0.61**	0.12	0.49	0.05	**2.13**	**5.70**	0.21	**3.27**	**3.14**	15.71
10	Evergreen forest	**0.98**	0.47	0.48	0.36	**1.33**	**3.41**	0.07	**10.30**	**2.64**	20.04
11	Mixed forest	**1.37**	0.47	**0.91**	0.38	**4.19**	**9.67**	0.17	**14.22**	**5.80**	37.19
12	Scrub/shrub	0.27	0.09	0.25	0.09	**0.95**	**2.68**	0.05	**6.32**	**1.73**	12.42
13	Wetland forest	0.15	0.21	0.06	0.28	0.15	**0.53**	0.00	**2.48**	0.25	4.11
14	Wetlands from soils	0.21	**1.05**	0.05	**0.58**	0.14	0.26	0.01	**1.42**	0.09	3.82
15	Wetlands	0.08	0.08	0.03	0.17	0.05	0.12	0.00	0.46	0.06	1.06
16	Roads/runways/bare rock	0.09	0.02	0.04	0.02	0.15	0.26	0.00	0.25	0.15	0.99
20	Bare land	0.01	0.00	0.00	0.00	0.01	0.03	0.00	0.02	0.01	0.08
21	Open water	0.10	0.07	0.04	0.06	0.06	0.10	0.01	0.28	0.06	0.76
22	Blueberry barrens	0.29	0.08	0.01	0.00	0.01	0.05	0.00	0.02	0.01	0.48
27	Alpine/tundra	<0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.01
30	Gravel pits	0.02	0.00	<0.01	0.00	0.00	<0.01	0.00	<0.01	0.00	0.03
All	Total for each soil group:	4.52	2.69	2.69	2.08	9.80	23.62	0.54	39.48	14.57	100.00

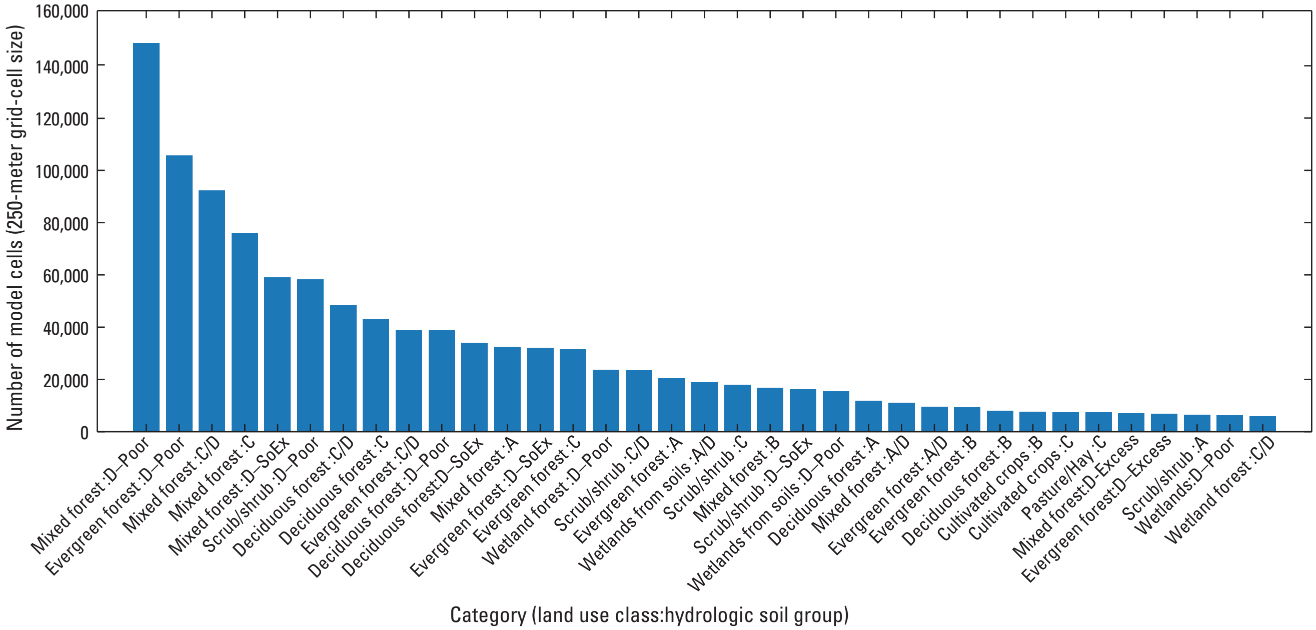


Figure 5. Abundance of land use class:hydrologic soil group categories for the top 35 categories in the Maine study area.

in Canada. Impacts of this zone on the modeled SWB potential recharge are discussed in the "Simulated Recharge for Maine, 1990–2015" section.

Lookup Tables and Control File

The Maine SWB model uses two lookup tables to calculate the water balance terms: the primary land-use lookup table, and a second irrigation lookup table, which was used for the ET calculations using the FAO56 ET method (Westenbroek and others, 2018; Allen and others, 1998), which gives much greater control over the ET simulation as compared to the default Thornthwaite-Mather method (Thornthwaite and Mather, 1957. The primary land-use lookup table contains values for runoff curve numbers, maximum daily recharge, and rooting depths for each combination of land-use class and hydrologic soil group in the model (example shown in table 5; see full table, appendix table 1.2). With 19 land-use classes and 9 hydrologic soil groups, the Maine SWB model has 171 different values for each of these categories. Lookup values for interception (if used) vary with land use and growing season and are also included in the SWB land-use lookup table. The irrigation land-use table (see example in table 6; see full table, appendix table 1.3) includes plant growth settings such as crop coefficients (K_{cb} values for onset of growth, plant maturity, and senescence), growing-season lengths, and bare soil evaporation settings for every land-use class.

Calibration of Maine Soil-Water Balance Model

The model calibration used an automated parameter estimation approach, using highly parameterized inversion and PEST software (Doherty and Hunt, 2010; Welter and others, 2015) to fit the curve number, maximum daily recharge, and rooting depth values in the SWB lookup table and several parameters that control the ET calculations using the FAO56 method (Allen and others, 1998). The land-use lookup table values, as well as irrigation table lookup table values and multipliers for groups of irrigation table lookup values were treated as model parameters and adjusted during the calibration (appendix tables 1.2 and 1.3). The PEST software orchestrates the running of several hundred model runs, adjusting parameter values in an iterative fashion, until the objective function is satisfactorily minimized, and further changes in parameter values do not provide substantial improvements in the overall model fit.

Calibration targets included all three major components of the water budget: recharge, direct runoff, and ET. Initial attempts at model calibration using only the recharge and direct runoff water-budget components for calibration targets resulted in a fairly good model fit, but once the ET calculations were compared to known values, the misfit was unacceptably large. These initial attempts used the Thornthwaite and Mather (1957 ET calculations that the SWB software uses by default. Switching to the FAO56 method (Allen and others, 1998) and adding ET observations and parameters that control the ET calculation helped achieve a more wholistic model fit.

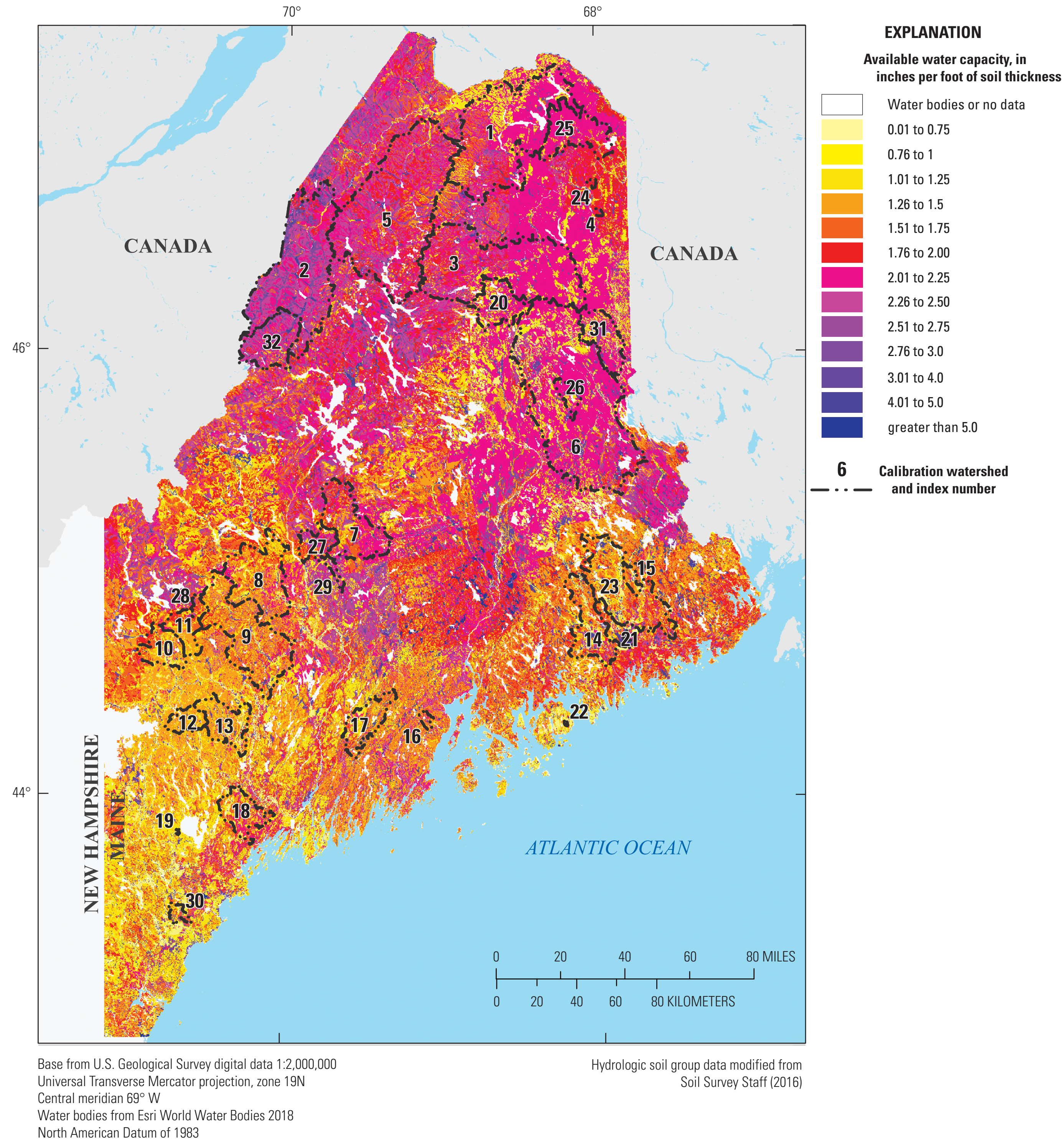


Figure 6. Available water capacity of the Maine Soil-Water-Balance model and calibration watersheds.

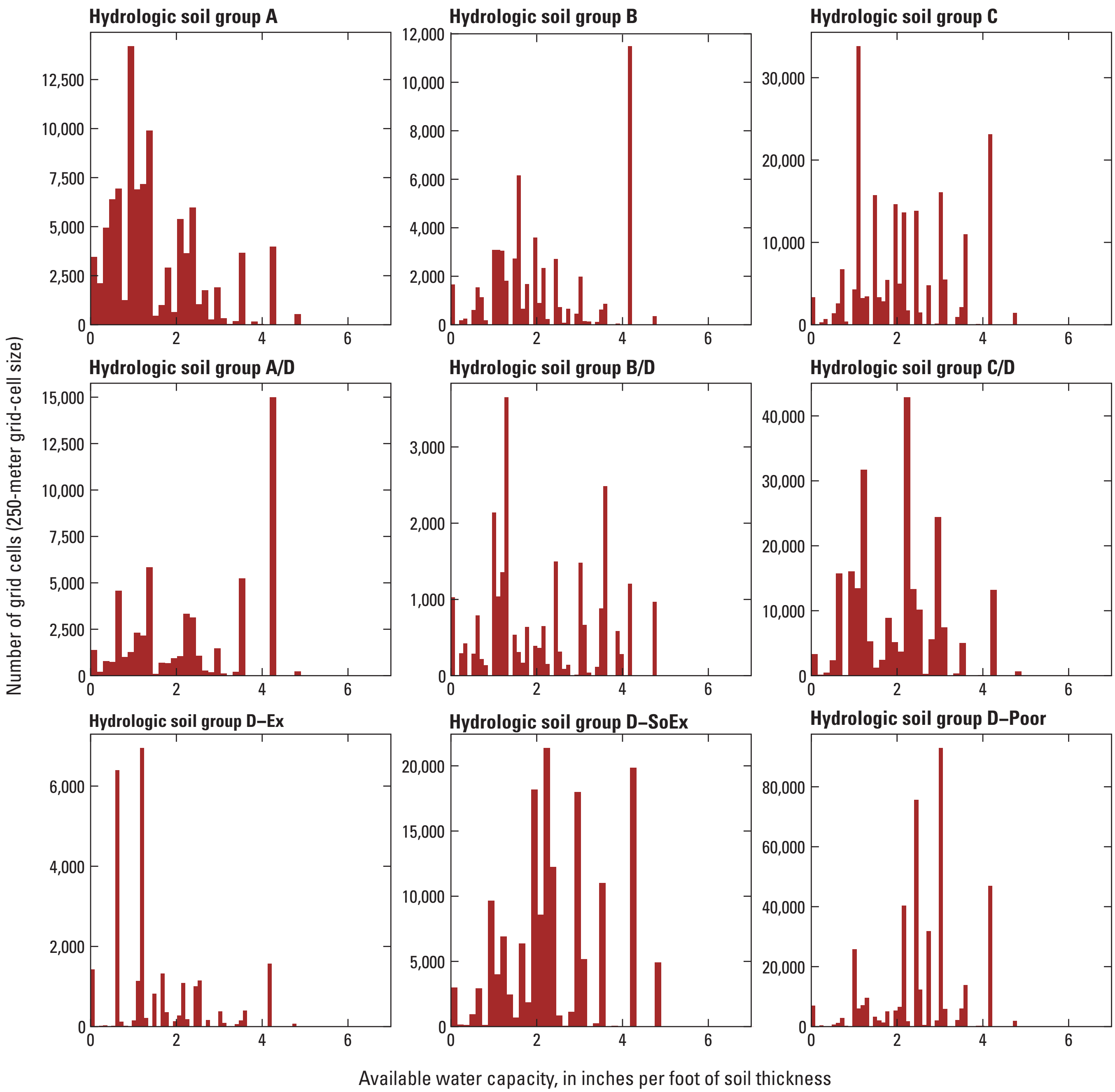
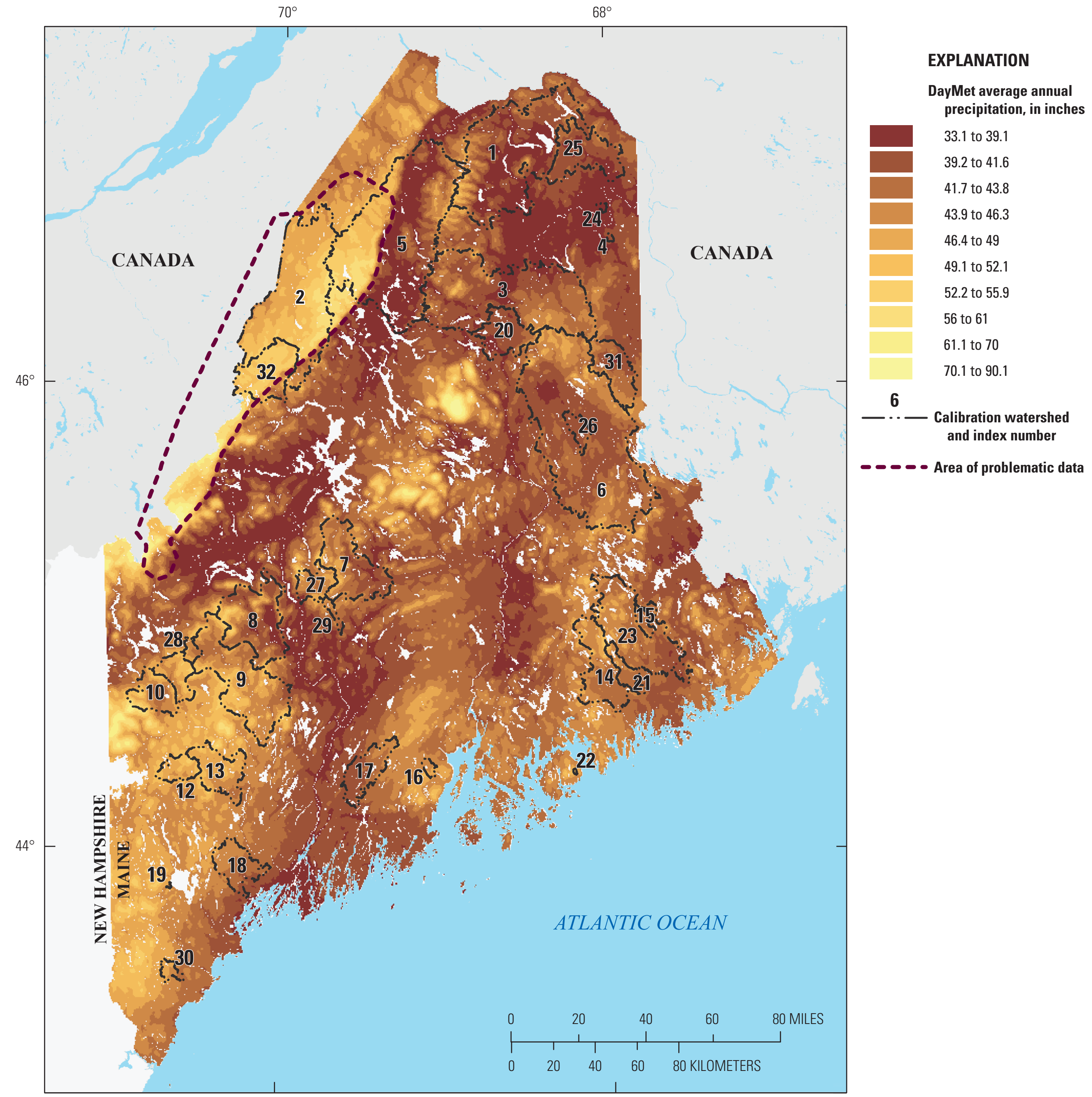


Figure 7. Distribution of available water capacity values for each hydrologic soil group in the Maine Soil-Water-Balance model.



Base from U.S. Geological Survey digital data 1:2,000,000
Universal Transverse Mercator projection, zone 19N
Central meridian 69° W
Water bodies from Esri World Water Bodies 2018
North American Datum of 1983

Precipitation data from Thornton and others (2018)

Figure 8. DayMet average annual precipitation, 1991 to 2015, for the Maine Soil-Water-Balance model and calibration watersheds.

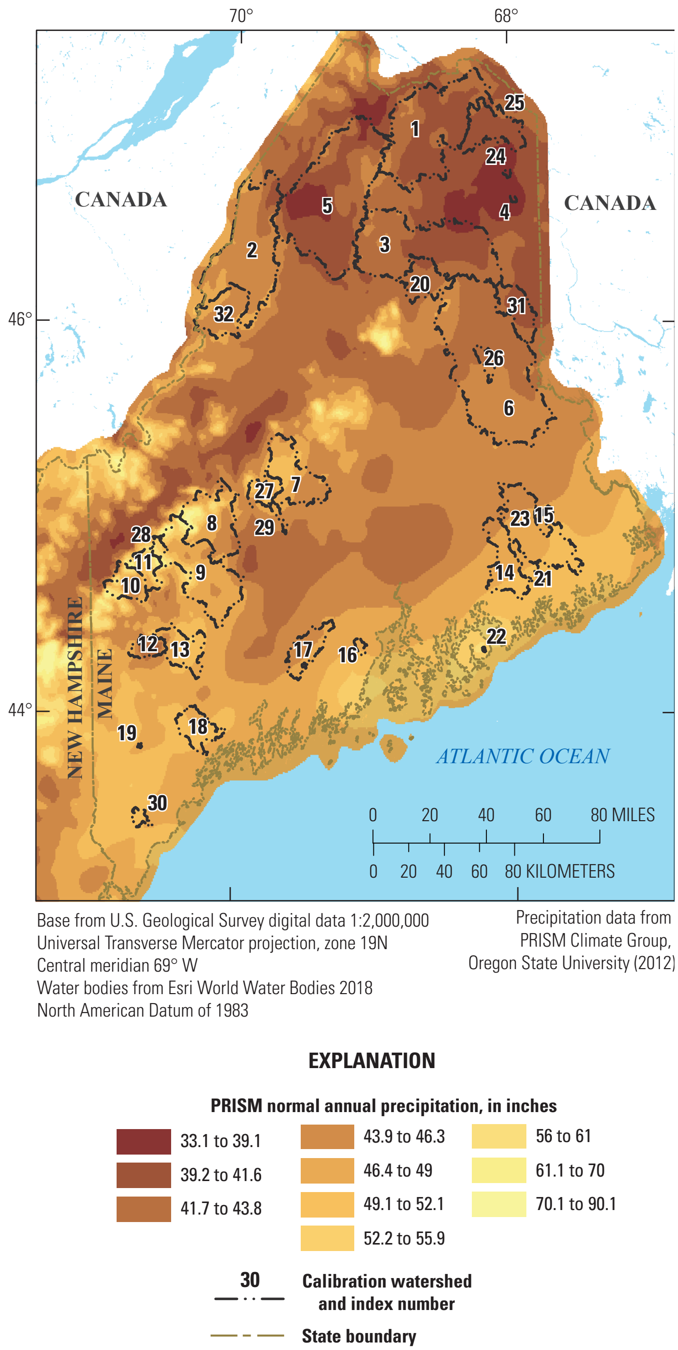


Figure 9. Parameter-elevation Regressions on Independent Slopes Model (PRISM) normal annual precipitation 1981 to 2010, for the Maine Soil-Water-Balance model and calibration watersheds.

Parameterization

PEST's use of highly parameterized inversion allows for the use of hundreds of model parameters, while not introducing problems of parameter insensitivity and correlation. The primary parameter set for the Maine SWB model consisted of values in the land-use lookup table: 515 parameters for runoff curve numbers, maximum daily recharge, and rooting depths. The interception values were fixed at zero and not used as parameters. The irrigation lookup table accounted for another 28 parameters that controlled the ET calculations: 13 K_{cb} values and 15 multipliers for bare-soil evaporation applied across sections of the table (543 total parameters; see appendix 2, tables 2.1 and 2.2, available for download at https://doi.org/10.3133/sir20195125, for complete lists).

To reduce the number of parameters from the lookup table evaluated during parameter estimation, a threshold of 0.1 percent of the domain (1,200 model cells) was set so that values for combinations of land-use class and hydrologic soil group that were not widespread in the model (and would provide little value to the overall calibration) were not adjusted during the parameter estimation runs. Initial values for the lookup table were based on pilot calibration exercises for small subset areas of the Maine SWB model. The final parameter estimation runs used 223 adjustable parameters.

SWB model runs and the calibration were performed on a Linux-based operating system, with a Windows 10 emulator, and on a Windows 10 operating system. Parallel processing of the calibration runs was conducted through HTCondor on a dedicated cluster of several hundred computer cores.

PEST uses singular value decomposition during the iteration runs to group parameters into super-parameters, which reduces potential parameter correlation issues that can plague other parameter-estimation procedures.

Calibration Targets and Weights

In total, 3 sets of calibration targets for 32 calibration watersheds (fig. 1; table 1) were used as input to the parameter-estimation runs, which used 13 years of data (2000–12). (The first year [2000] is a model spin-up year; the actual calibration time period is from 2001 to 2012 [12 years].) A shortened period (as compared to the 1991 to 2015 total time period) for calibration was used for increased overall efficiency and to avoid excessively long calibration run times. The 2000–12 time period was chosen because it includes periods of low flows (2001–3) and periods of high flows (2005 and 2008). The watersheds selected for inclusion in the calibration met the following criteria: flows at the streamgage location represented natural conditions and were unregulated. Four of the watersheds that were used are above the optimal size for hydrograph separation (500 square miles); consequently, the observations from these watersheds were weighted lower than the others. A minimum was not placed on the number of years of streamflow record for the watersheds, which had between 4 and 12 years of record for the calibration.

Table 5. Example land-use lookup table for runoff curve numbers, maximum recharge rate, interception, and rooting zone depths used by the Soil-Water-Balance model.

[See descriptions of hydrologic soil groups (A, B, D–SoEx, and D–Poor) in table 3. Hydrologic soil groups A/D, B/D, C, C/D, and D–Ex are not included in this example table (see appendix table 1.2, available for download at https://doi.org/10.3133/sir20195125, for the full table); in/d, inch per day; ft, foot]

Land-use code	Land-use class	Runoff curve numbers				Maximum potential recharge rate (in/d)				Interception storage		Rooting-zone depth (ft)			
		A	B	D–SoEx	D–Poor	A	B	D–SoEx	D–Poor	Growing season	Non-growing season	A	B	D–SoEx	D–Poor
2	Developed—High intensity	69.2	85.0	80.0	80.0	1.20	1.50	0.48	0.15	0	0	1.02	1.59	1.17	0.94
3	Developed—Moderate	89.6	85.0	80.0	80.0	1.70	1.54	0.45	0.19	0	0	2.36	1.79	1.12	0.97
4	Developed—Low intensity	59.5	59.3	80.0	80.0	4.00	1.56	0.35	0.13	0	0	1.50	1.70	0.55	0.52
5	Developed—Open space	59.9	60.0	80.0	80.0	4.00	2.47	0.25	0.10	0	0	1.50	2.00	0.51	1.00
6	Cultivated crops	30.0	66.7	67.6	68.4	3.00	2.18	2.43	0.10	0	0	1.50	2.06	1.00	1.00
7	Pasture/hay	34.8	40.0	69.3	66.9	3.00	2.13	0.50	0.10	0	0	1.24	2.02	1.00	1.00
8	Grassland	34.9	40.0	69.2	67.7	3.06	2.55	0.40	0.20	0	0	1.72	2.31	2.71	0.60
9	Deciduous forest	40.0	45.9	65.0	75.0	5.00	3.00	0.60	0.25	0	0	7.00	7.07	5.00	5.00
10	Evergreen forest	40.0	45.3	65.0	70.0	5.00	3.00	0.60	0.25	0	0	7.00	7.10	5.00	5.00
11	Mixed forest	40.0	45.4	65.0	70.0	5.00	3.00	0.60	0.25	0	0	7.00	7.21	5.00	5.00
12	Scrub/shrub	40.0	40.3	75.0	60.0	5.00	3.00	0.50	0.20	0	0	5.00	5.02	5.00	5.00
13	Wetland forest	47.7	58.5	66.6	40.0	1.00	0.50	1.50	0.27	0	0	7.05	5.15	3.00	2.51
14	Wetlands from soils	31.6	40.0	68.5	44.7	1.00	1.44	1.50	0.25	0	0	3.00	5.91	0.52	0.75
15	Wetlands	51.3	62.8	68.8	41.8	4.00	0.87	0.96	0.25	0	0	3.00	1.68	1.01	0.75
16	Roads/runways/bare rock	70.0	70.0	75.0	70.0	0.04	0.03	0.12	0.04	0	0	0.20	0.38	1.75	0.30
20	Bare land	72.0	80.0	80.0	71.3	3.01	2.00	0.25	0.21	0	0	0.76	0.75	0.75	0.71
21	Open water	100.0	100.0	100.0	100.0	0.00	0.00	0.00	0.00	0	0	0.00	0.00	0.00	0.00
22	Blueberry barrens	23.6	50.0	71.0	66.0	3.30	2.00	0.25	1.50	0	0	0.50	0.50	1.00	0.88
27	Alpine/tundra	90.0	90.0	90.0	90.0	0.25	0.25	0.25	0.25	0	0	0.50	0.50	0.50	0.50
30	Gravel pits	49.6	52.0	70.0	75.0	3.00	2.00	0.25	0.22	0	0	0.29	0.28	0.28	0.28

[See descriptions of hydrologic soil groups (A, B, D–SoEx, and D–Poor) in table 3. Hydrologic soil groups A/D, B/D, C, C/D, and D–Ex are not included in this example table (see appendix table 1.3, available for download at https://doi.org/10.3133/sir20195125, for the full table); ft, foot; in., inch; K_{cb}, transpiration crop coefficient; mm/dd, month/day]

Land-use code	Land-use class	Maximum crop height (ft)	Plant growth settings									Bare soil evaporation settings							
			Crop coefficient (K_{cb})				Planting/ growth initiation date (mm/dd)	Growing season lengths (days)				Readily evaporable water (in.)				Total evaporable water (in.)			
			Initial	Middle	Late	Minimum		Initial	Deviation	Middle	Late	A	B	D–SoEx	D–Poor	A	B	D–SoEx	D–Poor
2	Developed–High intensity	5	0.3	0.5	0.5	0.15	05/01	20	20	90	30	0.089	0.056	0.075	0.196	0.126	0.062	0.09	0.235
3	Developed–Moderate	5	0.3	0.8	0.5	0.15	05/01	20	20	90	30	0.089	0.056	0.075	0.196	0.126	0.067	0.09	0.235
4	Developed–Low intensity	5	0.3	1	0.7	0.15	05/01	20	20	90	30	0.089	0.056	0.175	0.196	0.21	0.067	0.21	0.235
5	Developed–Open space	5	0.3	0.8	0.7	0.15	05/01	20	20	90	30	0.089	0.056	0.175	0.196	0.21	0.112	0.21	0.235
6	Cultivated crops	2.75	0.15	0.8	0.2	0.15	06/01	10	20	60	20	0.089	0.056	0.175	0.196	0.354	0.112	0.222	0.555
7	Pasture/hay	3.5	0.4	0.85	0.5	0.2	05/01	20	30	80	35	0.089	0.056	0.175	0.196	0.21	0.112	0.21	0.235
8	Grassland	3.5	0.4	0.85	0.5	0.2	05/01	20	30	80	35	0.089	0.056	0.175	0.196	0.21	0.112	0.21	0.235
9	Deciduous forest	35	0.35	1	0.6	0.15	05/01	20	10	90	30	0.089	0.056	0.075	0.196	0.126	0.067	0.09	0.235
10	Evergreen forest	35	0.65	0.9	0.65	0.3	04/15	20	10	100	50	0.089	0.056	0.075	0.196	0.126	0.067	0.09	0.235
11	Mixed forest	35	0.45	1	0.65	0.25	05/01	20	10	90	30	0.089	0.056	0.075	0.196	0.126	0.067	0.09	0.235
12	Scrub/shrub	10	0.2	0.7	0.45	0.1	05/15	20	10	70	30	0.089	0.056	0.075	0.196	0.126	0.067	0.09	0.235
13	Wetland forest	30	0.3	1.25	0.75	0.2	05/01	10	20	90	30	0.089	0.056	0.075	0.196	0.126	0.067	0.09	0.235
14	Wetlands from soils	10	0.3	1.25	0.75	0.2	05/01	10	20	90	30	0.089	0.056	0.075	0.196	0.126	0.112	0.09	0.235
15	Wetlands	3.28	0.3	1.25	0.75	0.3	05/01	10	20	90	30	0.089	0.056	0.075	0.196	0.354	0.169	0.222	0.555
16	Roads/runways/bare rock	1	0.3	0.3	0.3	0.15	05/01	10	20	90	20	0.089	0.056	0.075	0.075	0.126	0.062	0.09	0.09
20	Bare land	2	0.3	0.3	0.3	0.1	04/15	20	70	90	30	0.089	0.056	0.175	0.196	0.354	0.112	0.222	0.555
21	Open water	1	0.15	1.05	1.05	0.1	04/15	20	70	90	30	0.089	0.056	0.175	0.196	0.21	0.169	0.21	0.235
22	Blueberry barrens	1	0.3	0.7	0.5	0.15	05/01	10	30	80	20	0.089	0.056	0.075	0.075	0.09	0.067	0.09	0.09
27	Alpine/tundra	2	0.4	0.7	0.5	0.15	06/15	20	10	30	20	0.038	0.019	0.075	0.075	0.09	0.022	0.09	0.09
30	Gravel pits	1	0.3	0.3	0.3	0.1	04/15	20	70	90	30	0.089	0.056	0.175	0.196	0.354	0.112	0.222	0.555

Development of Observation Values

As noted earlier, the observations used for the calibration included evaluations of annual recharge and direct runoff from base-flow separation analysis for 32 watersheds and annual ET data from a national ET gridded dataset (Reitz and others, 2017) for the same watersheds. Although some of the watersheds had less than the 13 years of streamflow data for the 2000–12 period, the ET data were used for all years in all watersheds.

Many methods exist for base flow-separation analysis to divide streamflow records into base flow (recharge) and direct runoff components. A common means of determining recharge and (or) runoff for a gaged watershed is by performing a hydrograph analysis, either using base-flow separation or other techniques, such as recession-curve displacement. The recession-curve displacement method was explicitly developed to determine episodic recharge from a hydrograph (Rutledge, 2007). Base flow-separation techniques use the base-flow component of the hydrograph as an approximation of groundwater discharge and, by conservation of mass, groundwater recharge (assuming that the surface-water and groundwater basin boundaries are coincident for a measurement point). The non-base flow component of the hydrograph is the direct runoff component. Base flow-separation methods assume that recharge and groundwater discharge is a continuous process, whereas the recession-curve displacement method analyzes the hydrograph assuming that recharge is an episodic event in response to precipitation events (Rutledge, 2007; Healy, 2010; Barlow and others, 2015) This study used nine methods (see appendix 2 for details) to evaluate the streamflow records (each method divides the total streamflow into a base-flow and direct runoff component), and the median of the nine calculation outputs was used as the calibration target for annual recharge (base flow) and annual runoff observations.

The ET observations were extracted from the Reitz and others (2017) data, which are national datasets of monthly estimates of ET, modeled using a modification of the operational Simplified Surface Energy Balance (SSEBop) approach. Watershed data were extracted from the monthly grids, averaged across each watershed for each month, and the monthly data summed to get an annual ET observation for each year over each watershed.

The base flow-separation analysis provided 315 recharge observations and 315 runoff observations for the 12-year calibration period. Although not all watersheds had the full 12 years of streamflow data, ET data were available for the full 12 years for every watershed, resulting in 416 ET observations.

Weights on Observations

Parameter estimation methods require that observations each be given a weight, which establishes its relative influence in the calibration process. One method of calculating weights of an observed value is to estimate the error or variance of the measurement used as the observation (Hill and Tiedeman, 2007; Anderson and others, 2015). Because the recharge and runoff observations were each calculated from a population of nine possible values, the variance (σ^2) was used for each of the observations, with some modifications, as discussed later in this section. The initial weight of each observation was set at $1/\sigma^2$.

Variances on recharge and runoff were generally lower during years of relative drought (2001–2), and higher during wet years (2005 and 2008). Also, some watersheds generally had higher variances than others, especially smaller ones with flashier runoff (calibration watersheds 15 [Old Stream], 22 [Otter Creek], 26 [Wytopitlock Stream], 16 [Ducktrap River], and 29 [East Branch Wesserunsett Stream]; fig. 1; table 1).

Initial weights on the ET observations were calculated from the variance of the ET across all years of the calibration. This method gave each watershed's ET observation the same weight across all years and made the weight proportional to the year-to-year variability of the ET estimates at a given location.

While attempting to make the observation weights as objective as possible, the modeler may make adjustments to balance the weights in the model. This will create a set of weights that best fulfills the purpose of the model (Anderson and others, 2015). Some adjustments were made to the Maine SWB observation weights to balance the influence of some outliers, to reduce the influence of very large watersheds that stretch the recommended limits on base flow-separation methods, and to reduce the influence of watersheds on the northwest border with Canada that fell in the zone of anomalous precipitation patterns (calibration watersheds 2 [North Branch Penobscot River] and 32 [St. John River]; fig. 1; table 1). Finally, after the analysis of preliminary calibration runs, it was determined that watershed 19 (Stony Brook) may have significant groundwater underflow beyond the streamgage; thus, the runoff and recharge observations for that watershed were given zero weight in the final calibration. The ET weights as initially calculated were scaled to be proportionate with the final weights for the recharge and runoff observations so that the model considered each set of observations fairly equally during the calibration.

The final dataset of observations used in the calibration included 268 weighted recharge and runoff observations (each) and 366 weighted ET observations, for a total of 902 weighted observations. The final observed values and weights on each observation are given in appendix 2 (table 2.6, available for download at https://doi.org/10.3133/sir20195125).

Parameter Estimation

Parameter estimation refers to the use of software to find the best fit solution of parameter values to reduce the model error, or lack of agreement between the measured and the model simulated values for each observation. The residual (measured value minus the simulated value) for each observation is multiplied by the observation weight, squared (making each value a positive number), and summed (Anderson and others, 2015). The model objective function, or phi (Φ), is the sum of the squared residuals for the model. The combination of parameter values with the lowest possible objective function thus constitutes the best-fit model. The PEST software (Doherty and Hunt, 2010; Doherty, 2004) was used in the calibration of the Maine SWB model. PEST uses information about the model parameters that are set up to run thousands of model runs to find the best fit model. The model runs were controlled and organized using the HTCondor computer cluster at the T.C. Chamberlin computing center at the Wisconsin USGS office.

The modeler controls which parameters will be adjustable during the estimation runs and how much to allow parameters to vary. The upper and lower bounds, within which PEST is allowed to test alternative values, are set for all the parameters in the model. Upper and lower bounds used for the runoff curve numbers, maximum potential recharge, and plant rooting depths used by the SWB lookup table were set using the modeler's best judgement and values used in other SWB models. Upper and lower bounds for the adjustable parameters for the FAO56 ET lookup table were set after a literature search on the possible ranges of values that would be reasonable for Maine. The complete list of parameters used, whether they were adjustable in the model, and the upper and lower bounds are provided in appendix 2 (tables 2.1 and 2.2).

Initial estimation runs were done that allowed PEST to use the full range of the parameter bound in the best-fit calculations. However, this resulted in some parameters being estimated at their furthest possible limits, not at a most "reasonable" value. PEST allows the modeler to use their knowledge of the system to further reign in the parameter adjustments, so the final values are as close as possible to values the modeler thinks are most reasonable. Tihkonov regularization is a process that can be used in PEST to find the best fit of parameters with a penalty to moving the parameters too far away from a "preferred" value (Anderson and others, 2015). This method prevents highly parameterized models from becoming over-fit, which may result in smaller model error but may not represent reality well (Anderson and others, 2015). The model error of a model using regularization will not be as small as one without but should result in a more parsimonious model. The final Maine SWB runs were done using Tihkonov regularization, after evaluating the parameter values of the initial runs.

The PEST parameter estimation also made use of singular value decomposition (SVD) to reduce the problems that can be introduced in a highly parameterized model of highly correlated parameters and insensitive parameters. SVD groups parameters into super parameters during the estimation runs and uses these super parameters to reduce the correlation and insensitive parameter issues. A more detailed discussion on the use of SVD can be found in Anderson and others (2015).

Model Fit—Comparison to Observations

The model calibration process compared 902 weighted observations of recharge, runoff, and ET to the model output for 2001–12. The model fit for the final calibrated parameters is evaluated by comparing the observed values of recharge, direct runoff, and ET to the model output values and to the residuals. The overall mean model error (average of all residuals) was 0.39 in. The mean of the absolute value of the residuals, or the mean absolute error (MAE), was 2.32 in. The root mean squared error (RMSE) for the calibrated model overall is 3.14 in. For the recharge observations only, the overall mean model error was 0.03 in., the MAE was 2.64 in., and the RMSE was 3.43 in. The runoff observations are not as well fit: the overall mean model error was 1.06 in., the MAE was 2.75 in., and the RMSE was 3.78 in. The ET observations have a smaller range in values and a smaller range in errors: the RMSE for ET observations was 2.27 in., and the MAE for ET observations was 1.77 in., whereas the mean overall model error for ET was 0.16 in.

Figure 10*A* illustrates the total model error, showing the observed and simulated values, as compared to the 1:1 line and a fitted line that represents the actual mathematical relation between the observed and simulated values. In a perfectly calibrated model that reproduced all observations precisely, all the points would line up with a 1:1 relation between the observed and simulated values. The Nash-Sutcliffe efficiency (NSE) test (Nash and Sutcliffe, 1970) is a normalized statistic that indicates how well the observed versus simulated values fits the 1:1 line (Moriasi and others, 2007; Trost and others, 2018). A Nash-Sutcliffe efficiency value of 1.0 would indicate a perfectly calibrated model; the value for the Maine SWB model is 0.75. The simulated model results line up closely to the 1:1 line, indicating a relatively accurate model where the residuals do not deviate significantly from the line in one direction or another. Figure 10*B* shows the plot of residuals. The probability plot correlation coefficient (PPCC) test (Helsel and Hirsch, 1992) evaluates the normality of the residuals. The PPCC test for the Maine SWB model indicated a normal distribution of residuals across the 1:1 line (PPCC value=0.98401, probability [*p*-value] less than 0.0001). In other words, the residuals for the overall model are not very skewed. Another common statistic used to determine the fit of the model is the correlation coefficient squared (r^2). The r^2 value for the simulated versus observed values for the Maine SWB model is 0.76.

The use of Tihkonov regularization, as discussed earlier, prevents an "overfit" model, where a closer model fit is obtained at the expense of keeping parameter values close to the modeler's judgment of most reasonable values. A larger r^2

and smaller RMSE could have been obtained without using regularization, but this could have led to model overfitting and unreasonable parameter values.

Considering each type of observation separately (fig. 11) shows that the observations for recharge (fig. 11*A*, *D*) fall most closely to the 1:1 line, but the residuals (fig. 11*D*) are somewhat skewed (the NSE for the recharge observations alone was 0.58, and the PPCC test indicated normality of the residuals, *p*-value=0.0065). At the high end of observed recharge (more than 25 in/yr) the model underpredicts potential recharge, shown by having a positive residual. At low amounts of observed recharge (less than 15 in/yr), the model overpredicts some of the values, shown by having a negative residual. Between 15 and 25 in/yr, the model does not consistently over- or under-predict the potential recharge. The runoff simulated values have the greatest degree of deviation from the observed values (fig. 11*B*), and the residuals (fig. 11*E*) deviate more from the observed values for watersheds and years with high amounts of runoff (NSE=0.52, PPCC indicated normality of the residuals, *p*-value<0.001). This indicates that the model has difficulty partitioning sufficient water into the runoff part of the water budget when overall runoff is quite high (over 20 in. of observed runoff). The Maine SWB model performs better for runoff when the modeled runoff is less than 20 in/yr.

The ET observations (fig. 11*C*) are equally balanced across the 1:1 line, but the residuals (fig. 11*F*) are quite skewed between lower and higher observations (NSE=0.26, PPCC test indicated non-normal residuals at alpha [α]=0.05). The model estimates more ET than the SSEBop observations at the lower range of observed values and too little at the higher range of ET observed values. Comparisons of SSEBop ET estimates to ET flux towers (Reitz and others, 2017; Kim, 2017) have shown that at low ET measurements, the SSEBop method underestimates ET, and at higher ET measurements, the SSEBop method overestimates ET. The estimation bias for the SSEBop method could account for at least some of the skewness in the SWB model results because the errors are in the same direction as they are when comparing actual ET measurements to the SSEBop estimates.

Another graphical approach to evaluating the model performance is a comparison of the observed and simulated three major water-budget components by year for individual watersheds. Six calibration watersheds distributed across the State were selected to illustrate the model performance on a watershed basis (fig. 12). The calibration watersheds, in a clockwise order around the State from north to southwest (fig. 1; table 1), are watersheds 5 (Allagash River; fig. 12*A*), 31 (Meduxnekeag River; fig. 12*B*), 14 (Narraguagus River; fig. 12*C*), 17 (Sheepscot River; fig. 12*F*), 12 (Little Androscoggin River; fig. 12*E*), and 8 (Carrabassett River; fig. 12*D*). All but the Meduxnekeag River watershed have 12 years of complete observations; watershed 31 has more limited recharge and runoff observations, spanning 2004–12. The bars for simulated and observed ET and recharge are just about identical in several years for every watershed. The bars for the observed and simulated runoff are the most unequal, and some watersheds seem to have a consistent bias—in the Allagash River watershed, the modeled runoff is generally higher than observed (and the recharge lower), which could be an artifact of the base flow-separation methods used to calculate the observations (this watershed has a relatively high amount of surface-water storage, and the hydrograph-separation techniques

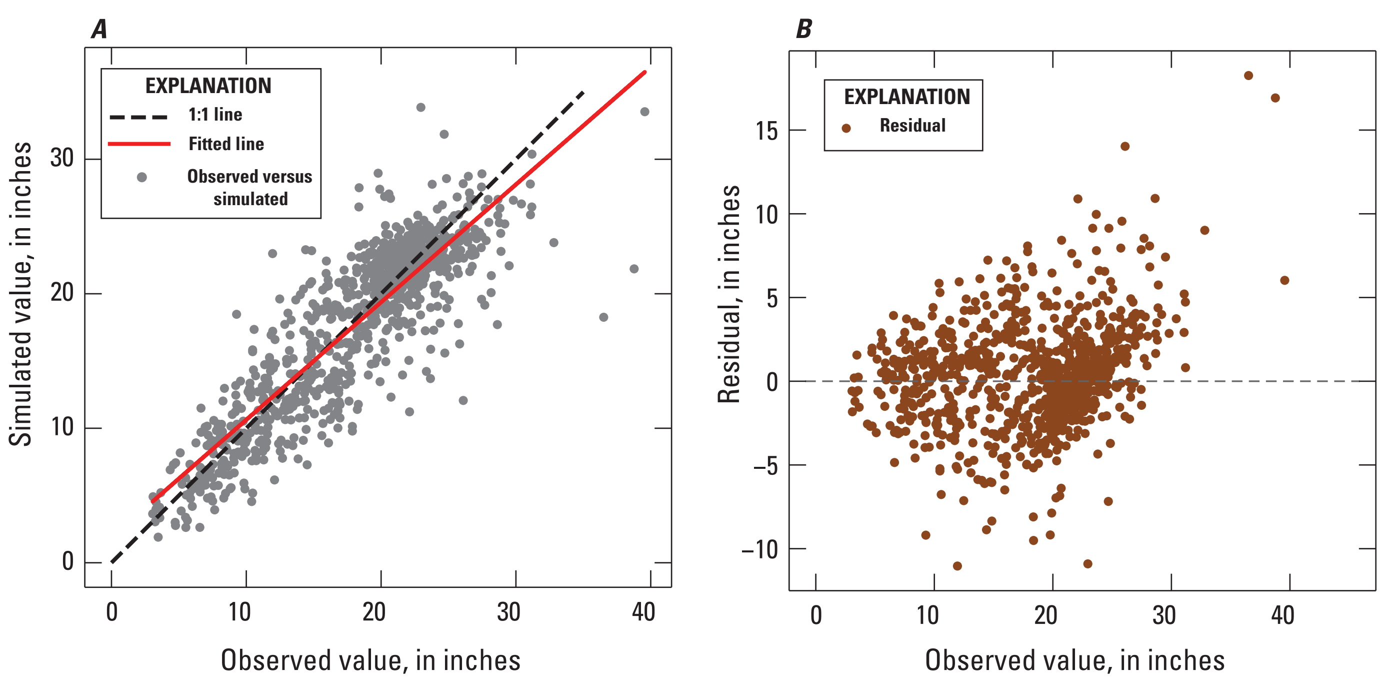


Figure 10. Overall model calibration results. *A*, observed and simulated values for all observations. *B*, model residuals.

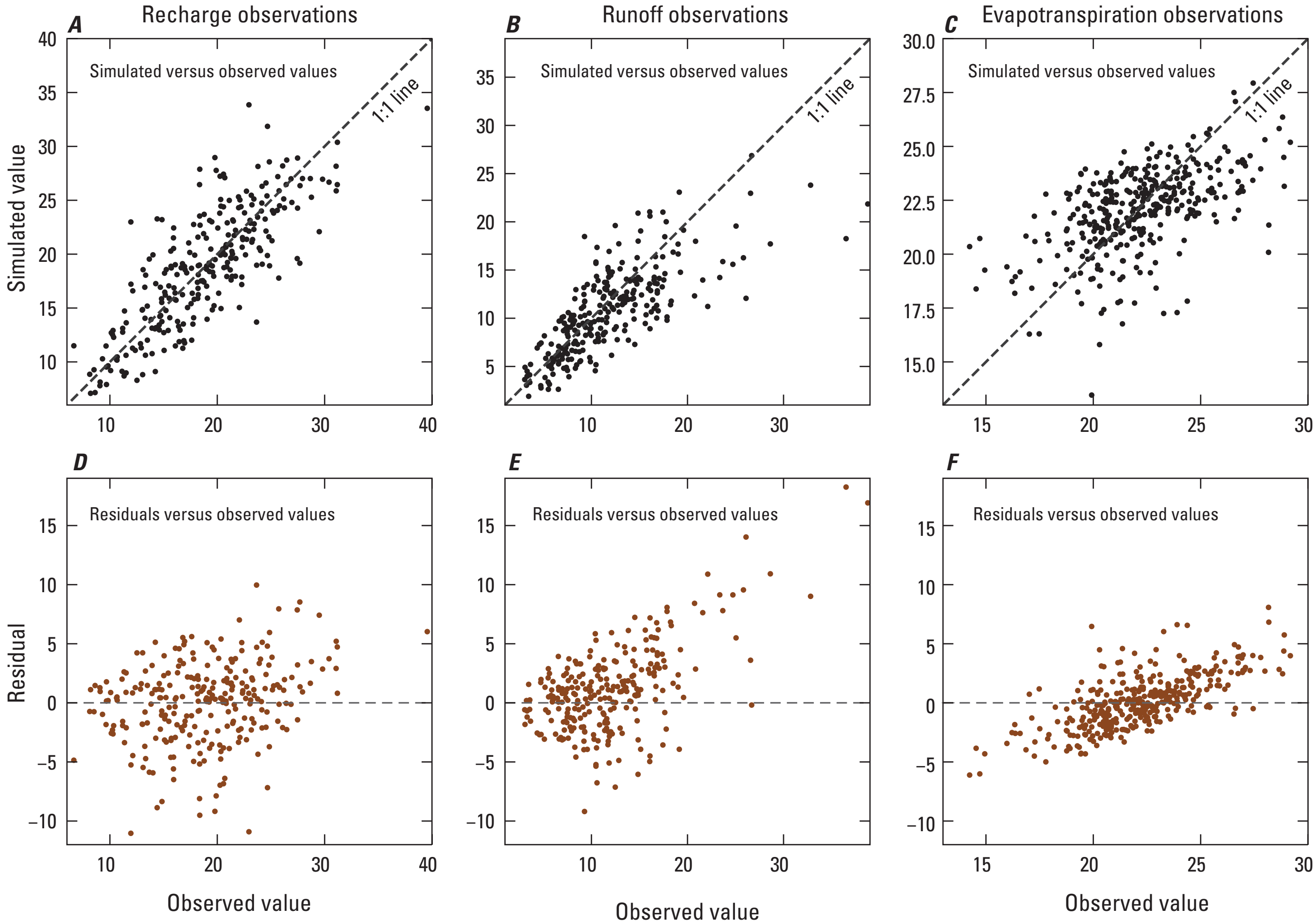


Figure 11. Relations between observed and simulated values for watershed recharge, runoff, and evapotranspiration for 32 calibration watersheds during 2000–12, and plots of residuals compared to observed values. Simulated versus observed values of *A*, recharge observations; *B*, runoff observations; and *C*, evapotranspiration observations. Residuals versus observed values of *D*, recharge observations; *E*, runoff observations; and *F*, evapotranspiration observations.

may confuse slow surface-water outflow from lakes and wetlands with groundwater discharge). The Carrabassett River watershed has the opposite—more recharge is modeled than expected, and less runoff, especially during years of high precipitation (2005–6). This watershed has a high proportion of sandy group A soils near its mouth; it is possible that the streamgage does not capture 100 percent of the recharge, and that some may exit the watershed as underflow. Overall, each watershed has its own unique set of circumstances that may help to explain variations in the degree to which the observed values of recharge and runoff agree with the simulated values.

Assuming that the streamgage for each of these calibration watersheds captures all the direct runoff and recharge in the basin (which is a good assumption for most of the watersheds), and that the remaining incoming precipitation becomes ET as estimated by the SSEBop dataset, the total height of the observed bars should equal the total incoming precipitation over the watershed, plus any snow storage that is held over from the previous year. The precipitation totals range from about 35 in/yr in a few watersheds in 2001–2, to about 70 in/yr in 2005 in several watersheds. Similarly, the total height of the simulated bars represents the total input water (DayMet precipitation) plus or minus any changes in soil or snow storage over the watershed. Because of the combination of storage effects and other possible model errors, the total DayMet precipitation does not always agree with the observed totals from the sum of the observations.

Parameter Sensitivity and Influence

An important measure of the sensitivity of a model to variations in model input parameters (when the true value of the parameter is not known) is a parameter sensitivity analysis. Sensitivity of the model to the parameter values is calculated by PEST as part of the calibration process. The PEST output for the calibration using SVD enables an analysis of the total sensitivity of the model observations, for all the

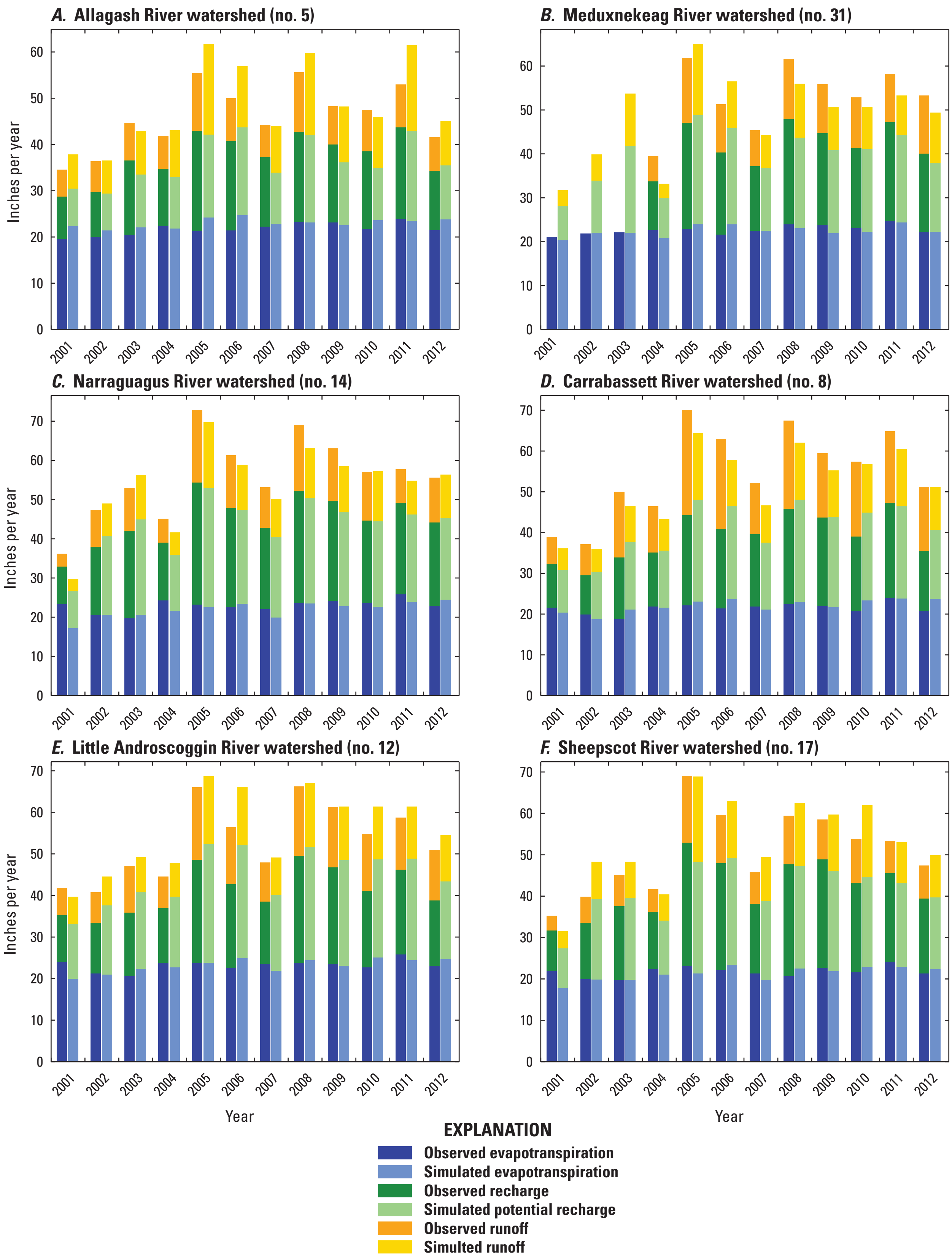


Figure 12. Annual comparisons of observed and simulated recharge, runoff, and evapotranspiration for 2001–12 in six calibration watersheds. *A*, Allagash River watershed, no. 5. *B*, Meduxnekeag River watershed, no. 31. *C*, Narraguagus River watershed, no. 14. *D*, Carrabassett River watershed, no. 8. *E*, Little Androscoggin River watershed, no. 12. *F*, Sheepscot River watershed, no. 17.

parameter types together, and for just the recharge observations by themselves. Parameter identifiability (Doherty and Hunt, 2009; Anderson and others, 2015) is a type of sensitivity analysis that analyzes the amount of information contained by the observations about each parameter. The calculation of this statistic uses SVD on the matrix expressing the sensitivity of every observation to every parameter. The result is unaffected by parameter correlation, which makes it a better statistic than weighted sensitivities (Doherty and Hunt, 2009).

Considering all the observations together, the model is most sensitive to the K_{cb} mid-season growth ET parameters (table 7; fig. 13*A*). This is understandable because these values directly control how much of the total soil moisture is moved by plants into the atmosphere during the height of the growing season and therefore how much is left in the soil to become potential recharge. The runoff curve numbers are the second most sensitive group (table 7; fig. 13*A*), and these operate at the beginning of the daily calculations to route excess water from the land surface to runoff, directly controlling what is available for plant uptake and potential infiltration.

Because the primary product of this study is the potential recharge to groundwater, a separate identifiability calculation was done for the observations of recharge. The recharge simulations are most sensitive to the runoff curve numbers (table 7; fig. 13*B*), closely followed by the mid-season K_{cb} ET parameters and maximum potential infiltration rates. The recharge calculations are more sensitive than the overall model to the maximum potential infiltration rate and rooting depth parameters. This follows from the fact that some of the observations in the overall model, the runoff calculations in particular, do not rely as heavily on these parameters.

Table 7. Identifiability of parameters and parameter groups for the Maine Soil-Water-Balance model.

[K_{cb}, transpiration crop coefficient]

Parameter group	Total identifiability of parameters in group	Number of parameters in group	Recharge identifiability of parameters in group
K_{cb} mid-season values	7.94	13	6.71
Runoff curve numbers	6.17	41	6.89
Maximum potential recharge rate	3.93	77	5.95
Rooting depths	2.64	77	3.07
Soil evaporation factors	2.55	11	1.33
K_{cb} edge season values	1.06	4	1.05

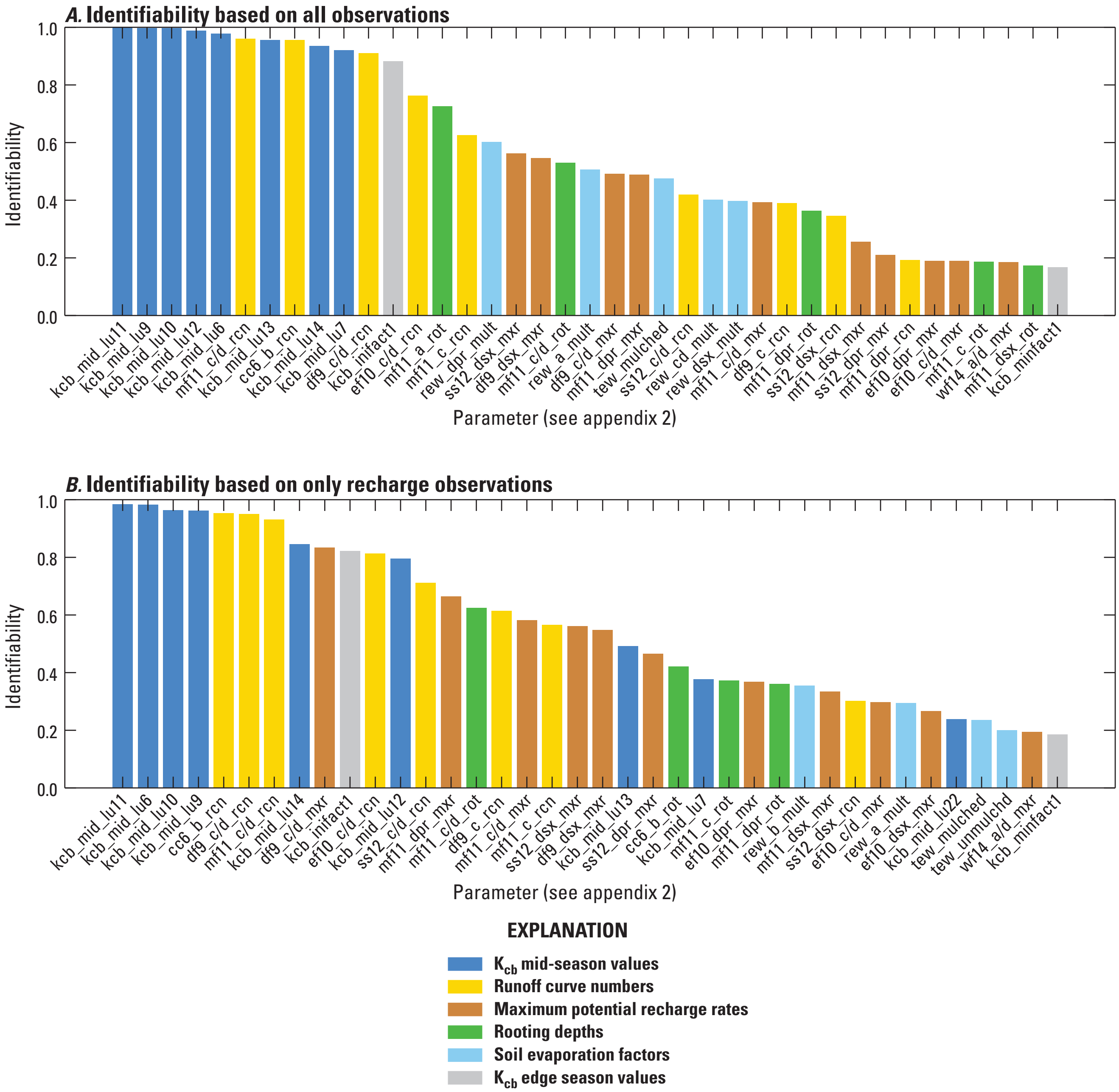


Figure 13. The identifiability of the top 40 most-sensitive parameters used in the Parameter ESTimation model calibration, by parameter group (appendix 2). *A*, Calculated using all observations (recharge, runoff, and evapotranspiration). *B*, Calculated using only recharge observations.

Groundwater Recharge Estimates for Maine, 1991–2015

Using the best-fit set of parameters from the calibration runs, the Maine SWB model was run for 25 years, from 1991 to 2015, using a 250-m grid-cell size. The 25 annual grids were used to calculate the 25-year mean annual potential recharge, median annual potential recharge, and the minimum and maximum potential recharge for the 25-year simulation. A Monte Carlo exercise (Tonkin and Doherty, 2009) was done to determine the potential uncertainty in these grids, using a distribution of alternate parameter values that fall within a reasonable range of the calibrated values for all parameters. In total, 300 alternate model realizations were run, and the standard deviation of the potential recharge value at every pixel was calculated.

Exclusion Zone

The anomalous DayMet data, discussed above in the descriptions of the model input, proved to make calibrating the model difficult. During the parameter estimation process, the two watersheds falling almost completely within this area were removed from the calibration process because their observations did not contribute to any improvements in the model fit and continually contributed a large amount to the degree of misfit of the model during early calibration runs. Based on this and the discrepancy of the DayMet data as compared to the PRISM precipitation data, an “exclusion zone” was created and used to screen out the area in northwestern Maine from the final analysis because the calculated potential recharge values in this area are not considered representative of actual conditions.

Recharge Grids—Annual Average and 25-Year Minimum, 25-Year Maximum Potential Recharge

From the 25-year simulation, the average annual potential recharge is represented by the mean and median annual potential recharge. The model grids were processed as described earlier in this report. A comparison was done to see if using the 250-m grid-cell size for the final grids gave a different result than using the 500-m grid-cell size used in the calibration, using the observation watersheds to test the annual grid outputs. At this scale, the median difference in the potential recharge was only 0.1 in., and 90 percent of the differences were within plus or minus 0.5 in., so the switch to using a 250-m grid-cell size does not introduce substantial changes in the overall results.

The statistical distributions of the values in the mean and median 25-year, 250-m grids are similar. The statewide average of the mean grid (7.7 in.) is just 0.2 in. more than the statewide average of the median grid (7.5 in.), and the statewide maximum for the mean was just 0.5 in. more than the statewide maximum for the median potential recharge. A histogram of each statewide grid (minimum, mean, median, and maximum), illustrates the overall distribution of potential recharge values across the State (fig. 14). The mean and median overall distributions are very similar, as noted above, because most values fall between 5 and about 30 in/yr across the State (fig. 14*A*, *B*). The statewide range in the minimum values is very compressed (about 2 to 20 in/yr)—almost everywhere in the State experienced a drought-year low recharge less than 10 in/yr sometime during the 25-year simulation period (fig. 14*C*). The statewide range in the maximum recharge experienced between 1991 and 2015 is much more variable, and most values are between 15 and 48 in/yr (fig. 14*D*). Very high recharge years are mostly driven by excessive precipitation, and the spatial variability in excess precipitation events would help to explain the greater range in maximum potential recharge across the State. Maps of the median, mean, minimum, and maximum estimated annual potential recharge are presented in figures 15 through 18.

A visual comparison of either of the spatial distribution of the average recharge (mean [fig. 15] or median [fig. 16]) to the average annual precipitation (fig. 8) suggests that the spatial distribution of potential recharge in Maine is driven largely by variations in precipitation patterns. Higher-than-average precipitation in the mountains in north-central Maine are mirrored by the higher-than-average potential recharge in the same areas. Other areas with higher precipitation in western Maine, central coastal areas and the furthest eastern coastal areas also have relatively high potential recharge. Conversely, the northern Maine, central Maine, and northwestern areas with lower-than-average precipitation also are mirrored by areas of lower-than-average recharge.

Keeping this in mind, there are also patterns in the potential recharge that are affected by the spatial distribution of the land-use class and hydrologic soil group categories (table 8). The land use:hydrologic soil group categories with the highest simulated median potential recharge include many land uses underlain by group A soils (sandy and well drained), particularly those land uses with low or little vegetation (blueberry barrens, developed, open space, shrub/scrub, and cropland, for example). The simulated median recharge for the categories with the 10 highest recharge values statewide range from 26.5 to 38.2 in/yr. These values are not dissimilar to previously published values for sandy, well drained soils in Maine. A detailed analysis comparing the SWB simulated potential recharge with several published study areas in Maine is presented later in the report.

The categories with the lowest potential recharge estimates across the State include impervious-surface categories (roads/runways/bare rock) and forested land uses with poorly drained, low-permeability soils (D–Poor). Rates for the impervious surface categories compare favorably to previously published values for bedrock (Gerber and Hebson, 1996). The values for the forested:D–Poor categories are on the higher end of previously published values for clay soils in Maine, which have been estimated from 2 to 12 in/yr (Gerber and Hebson, 1996), see discussion below in the section on “Comparison of Average Recharge to Previous Studies.”

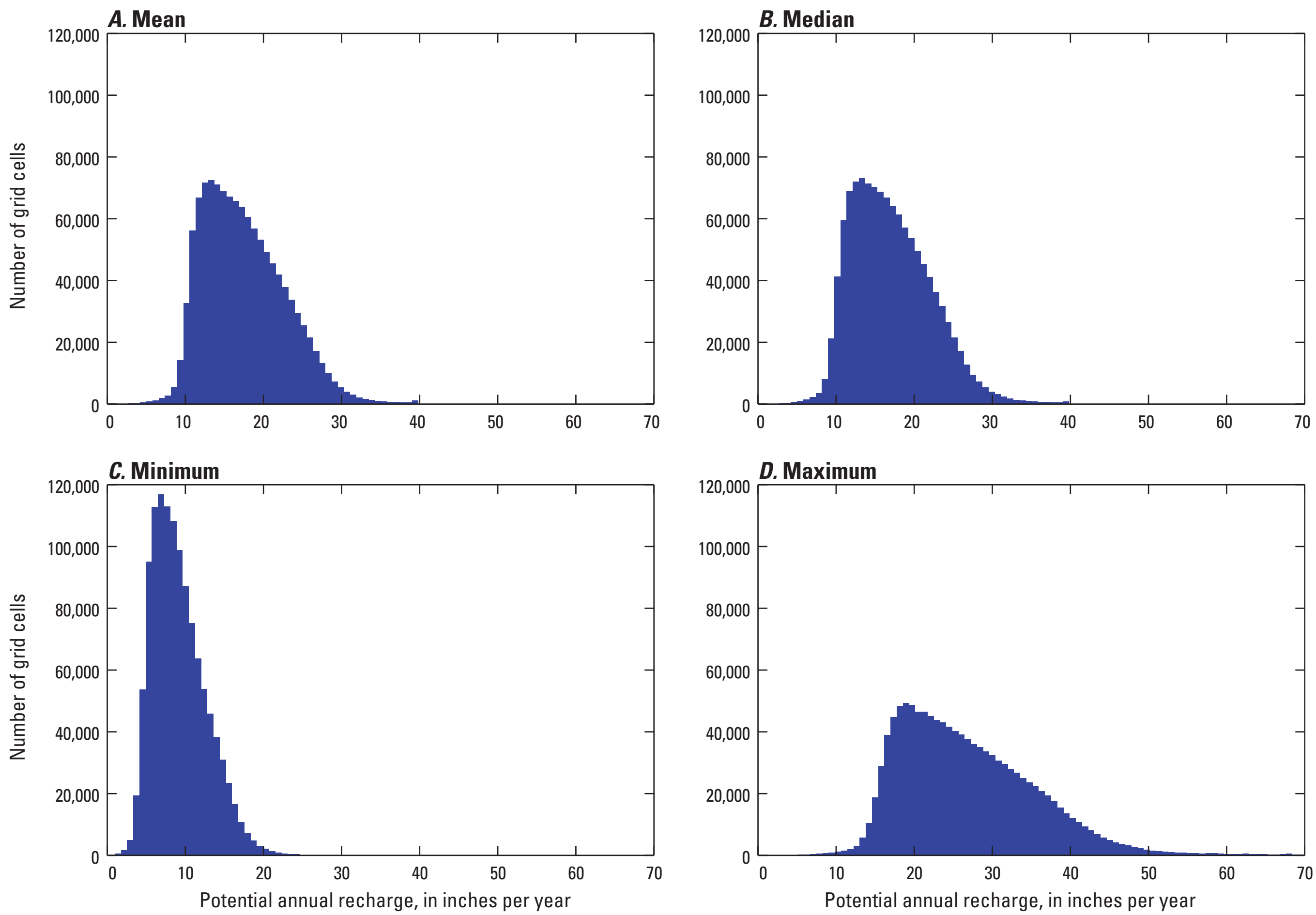


Figure 14. Range of 25-year modeled *A*, mean; *B*, median; *C*, minimum; and *D*, maximum potential annual recharge across Maine.

Uncertainty of 25-Year Recharge Grids

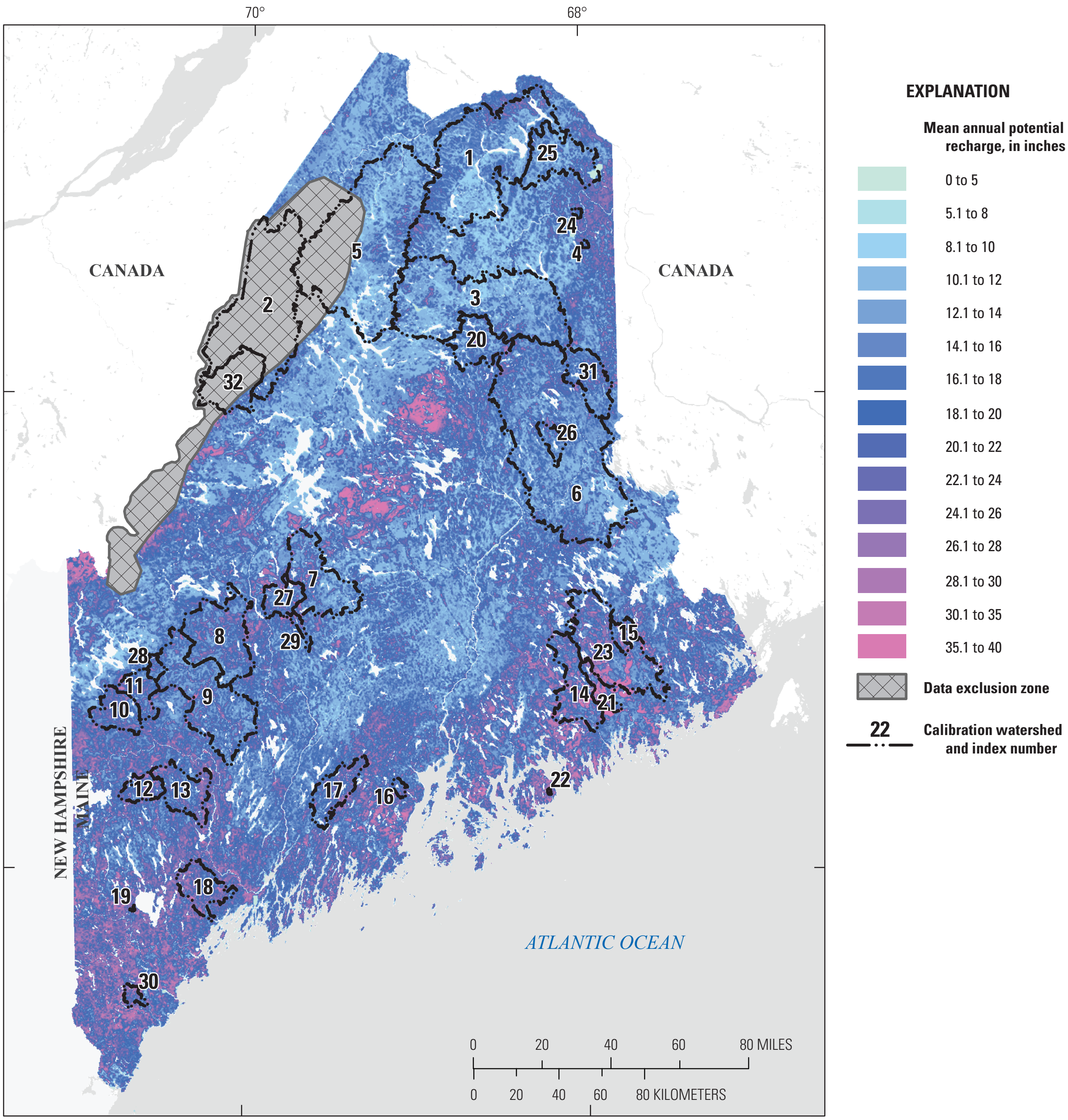
The primary reason for conducting uncertainty analysis is to improve decision-making by addressing the ability of a model to fulfill its stated purpose (Anderson and others, 2015). For this study, the purpose is to provide an estimate of potential recharge to shallow groundwater across the State, and the uncertainty analysis addresses the potential error in the estimates of the 25-year average recharge grids. This section presents the overall spatial distribution of model uncertainty, global sensitivity to the most important calibration parameters, and a discussion of intrinsic uncertainty from the uncertainty in underlying datasets and model design.

Calculated Uncertainty

As a measure of the uncertainty in the calibrated model 25-year median annual potential recharge grid, a Monte Carlo analysis was performed, using 300 potential realizations of the suite of model parameter values, using the method of Tonkin and Doherty (2009; White and others, 2016; see above section on “Modeling Uncertainty Representation”).

From each of the successful Monte Carlo runs (285 total), the 25-year median grid was calculated. The model fit of each run, as compared to the observation values used during the calibration, also was calculated. Any Monte Carlo run whose model fit fell outside a range of acceptable Φ values was discarded from the final analysis, resulting in 258 model realizations with acceptable combinations of parameter values. The range in Φ values for the “acceptable” runs was from 270 to 360 (the best-fit model from the PEST calibration had a Φ of 318). The model runs with unacceptably poor model fit included combinations of model parameter values that produced recharge estimates unlikely to represent actual conditions. Using the remaining 258 model realizations, cell-by-cell statistics were generated, and the standard deviation of all possible values for each grid cell was recorded. As in the best-fit model, each median potential recharge grid was given a screening for anomalously high values before the overall standard deviation grid was calculated.

The resulting grid of standard deviation values (fig. 19) provides a quantitative measure of the uncertainty in the Maine potential recharge grids that is a result of uncertainties in the model parameter values. The overall model uncertainty distribution is graphically shown in figure 20—the average



Base from U.S. Geological Survey digital data 1:2,000,000
Universal Transverse Mercator projection, zone 19N
Central meridian 69° W
Water bodies from Esri World Water Bodies 2018
North American Datum of 1983

Figure 15. Simulated 25-year mean annual potential recharge to groundwater for Maine, 1991 to 2015.

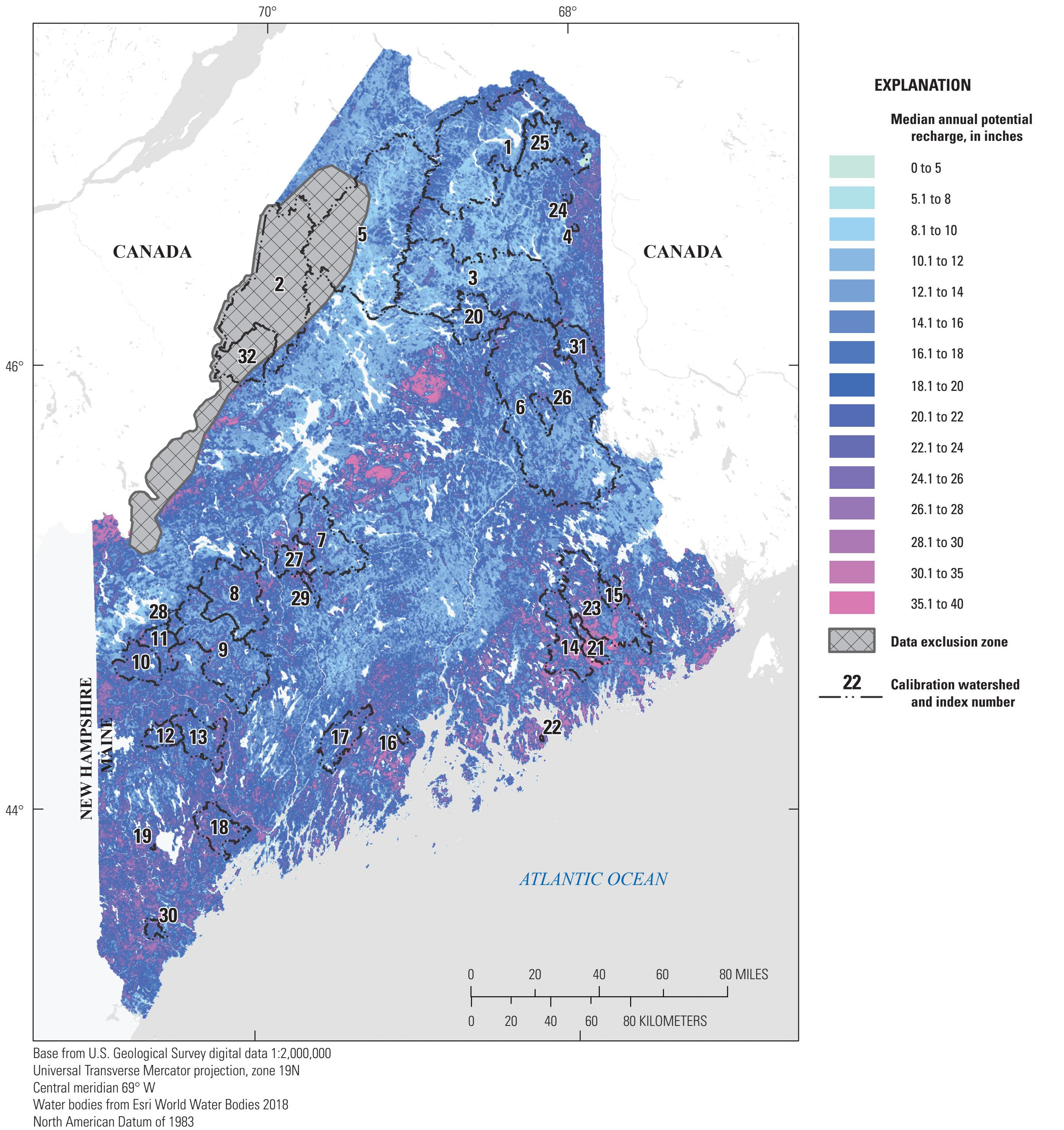
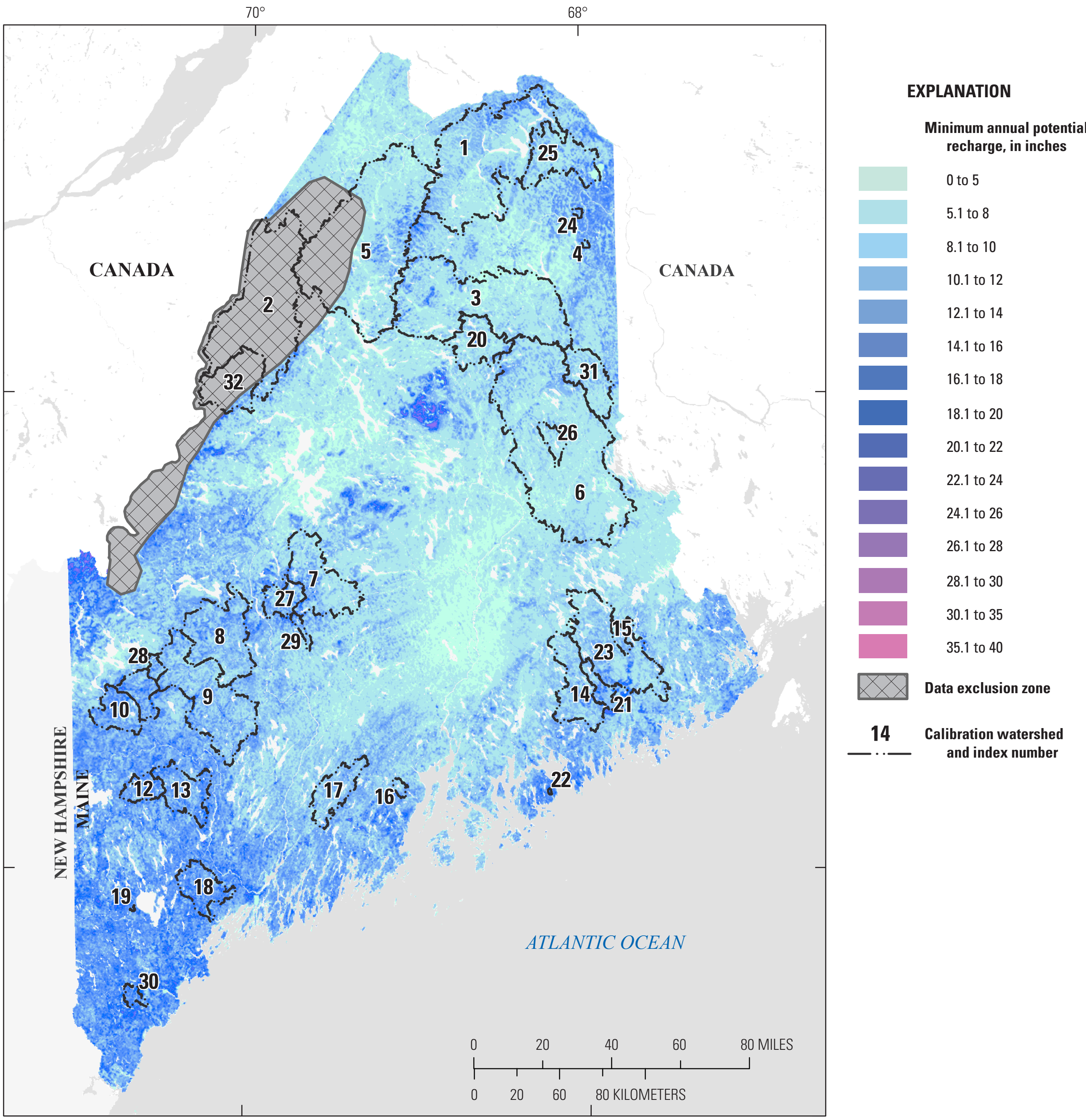


Figure 16. Simulated 25-year median annual potential recharge to groundwater for Maine, 1991 to 2015.



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Water bodies from Esri World Water Bodies 2018
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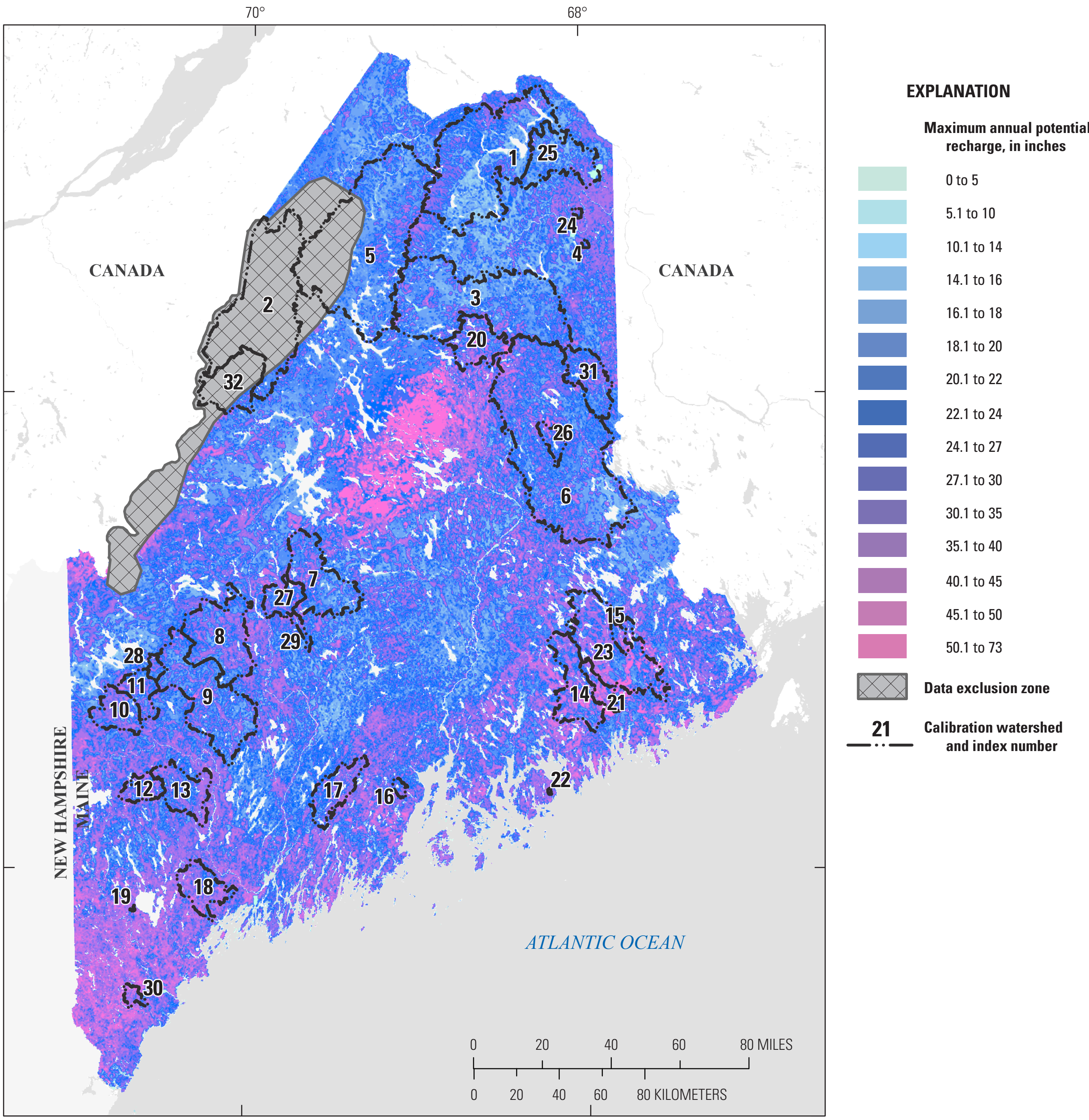
Figure 17. Simulated 25-year minimum annual potential recharge to groundwater for Maine, 1991 to 2015.



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Universal Transverse Mercator projection, zone 19N
Central meridian 69° W
Water bodies from Esri World Water Bodies 2018
North American Datum of 1983

Figure 18. Simulated 25-year maximum annual potential recharge to groundwater for Maine, 1991 to 2015.

Table 8. Median potential annual recharge rates and standard deviation for the highest and lowest 10 land-use class:hydrologic soil group categories in the Maine Soil-Water-Balance model.

[in., inch]

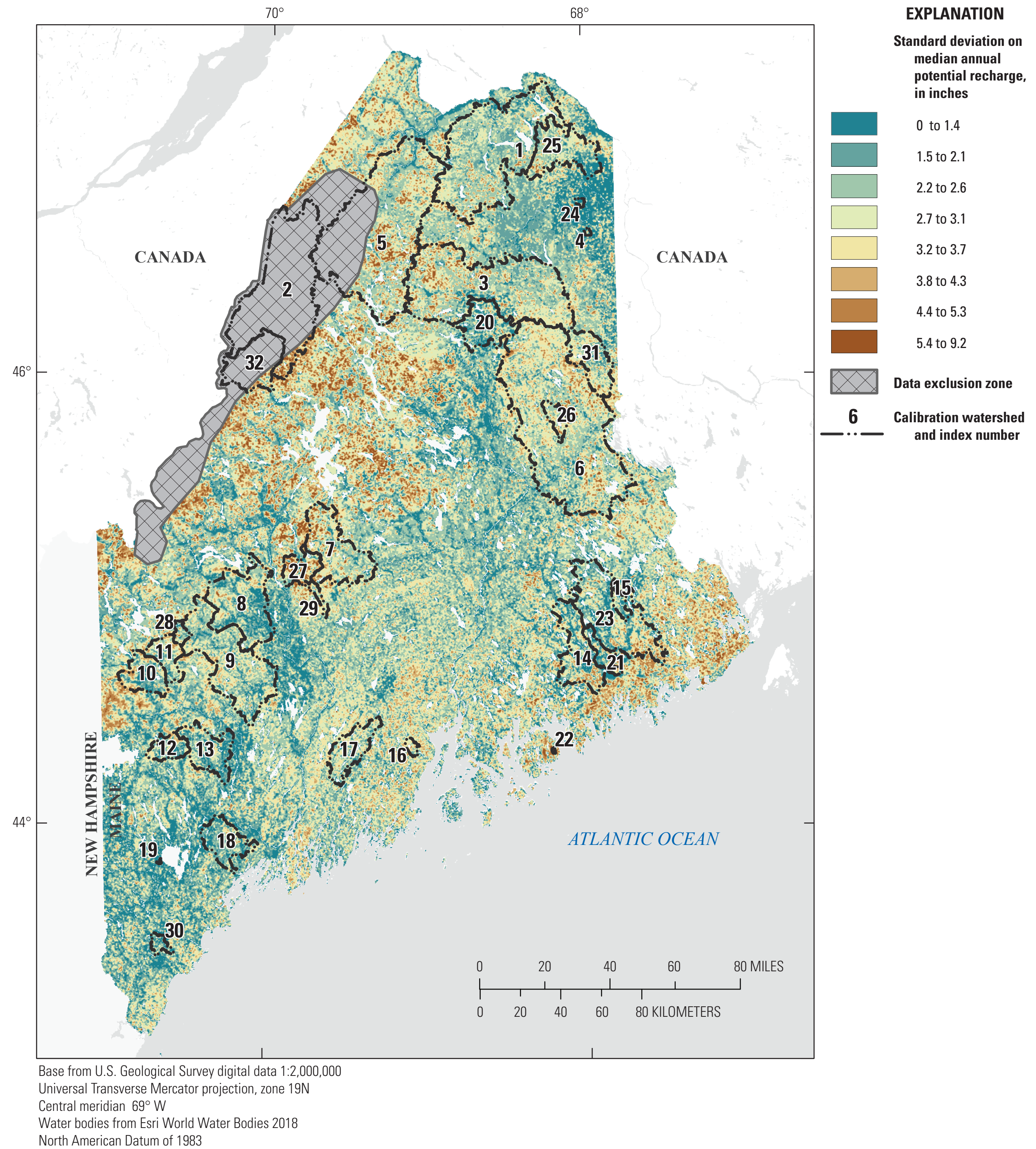
Land-use class	Land-use code	Hydrologic soil group	Median recharge (in.)	Standard deviation (in.)	Percentage of land area in model
Highest 10 categories					
Blueberry barrens	22	A	39.2	1.18	0.14
Developed–Open space	5	A	30.42	1.67	0.11
Scrub/shrub	12	A	30.37	1.65	0.52
Pasture/hay	7	A	29.47	1.35	0.24
Developed–Low intensity	4	A	29.31	1.98	0.12
Scrub/shrub	12	B	28.47	1.53	0.36
Cultivated crops	6	A	28.24	1.22	0.19
Scrub/shrub	12	A/D	27.23	2.06	0.17
Cultivated crops	6	C	27.14	1.20	0.59
Cultivated crops	6	D–SoEx	27.05	1.59	0.23
Lowest 10 categories					
Roads/runways/bare rock	16	C	3.71	1.50	0.31
Roads/runways/bare rock	16	D–Poor	3.90	2.28	0.31
Roads/runways/bare rock	16	A	3.90	1.49	0.16
Wetlands	15	B/D	6.67	2.14	0.17
Roads/runways/bare rock	16	C/D	7.03	2.70	0.26
Roads/runways/bare rock	16	D–SoEx	7.89	5.23	0.15
Evergreen forest	10	D–Poor	10.70	2.86	8.36
Mixed forest	11	D–Poor	11.34	2.81	11.76
Deciduous forest	9	D–Poor	11.99	4.21	3.07
Wetlands	15	D–Poor	12.05	3.72	0.50

(mean) value for the State is 2.62 in.; the 10th percentile is 1.49 in. and the 90th percentile is 3.78 in. To translate these into an absolute uncertainty of the average recharge, a typical method is to take plus or minus 2 times the standard deviation of a value.

Overall, most of the modeled area has a calculated uncertainty (standard deviation) between 1.5 and 4.0 in. (fig. 20). The uncertainty of the estimated recharge rates for the most abundant land-use class:hydrologic soil group categories in the State have a wide range, from 0.81 to 6.41 in. (table 9). The amount of uncertainty generally is lower for categories with group A or B soils, which are more permeable and well drained. In these areas, the standard deviation from the Monte Carlo runs reflects the fact that few of the parameters that have a high degree of identifiability (fig. 13*B*) apply to these categories. Several of the categories with more poorly drained soil groups (D–Poor in particular) have much higher standard deviation from the Monte Carlo runs than the other categories, but the values are not directly proportional to the amount of identifiability of the model parameters.

The land-use class:hydrologic soil group categories with the highest average potential recharge, most of which have group A soils and vegetation with relatively shallow root zones such as blueberry barrens, scrub/shrub, pasture/hay, and cultivated crops, also have relatively small amounts of uncertainty relative to the total recharge (fig. 21). The categories with the lowest potential recharge rates, which include land uses with relatively impervious surfaces (roads/runways/bare rock), some wetlands, and forest types with D–Poor soils, have uncertainty values that are much higher in relation to the amount of modeled potential recharge, but some of these uncertainty values are similar in absolute magnitude to the higher-recharge categories.

The standard deviation values can be used to calculate a 95-percent confidence interval around the median potential recharge value. The total 95-percent confidence range is calculated using the standard deviation (σ): minimum=median−(2×σ) and maximum=median+(2×σ). For any area of interest, the 95-percent confidence intervals can be calculated to get an estimate of the overall possible range in the modeled 25-year average potential recharge.



Base from U.S. Geological Survey digital data 1:2,000,000
Universal Transverse Mercator projection, zone 19N
Central meridian 69° W
Water bodies from Esri World Water Bodies 2018
North American Datum of 1983

Figure 19. Calculated standard deviation on the median annual potential recharge to groundwater for Maine, 1991 to 2015.

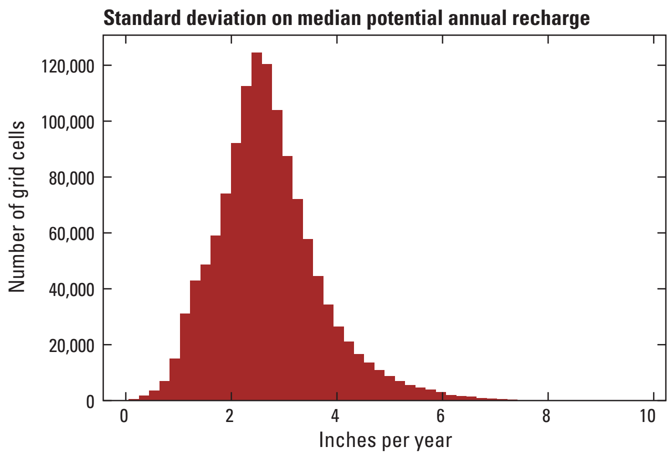


Figure 20. Distribution of the calculated standard deviation of the potential median annual recharge.

Other Sources of Uncertainty

Other factors also contribute to the overall uncertainty in the recharge estimates, but because they are nonvarying components of the model, they cannot be changed to evaluate their contribution to the total uncertainty. These include uncertainty in the DayMet climate data used in the simulation, uncertainty in the soils mapping from NRCS (including the hydrologic soil groups and AWC), and uncertainty in the land-use grid. Some of these other sources of uncertainty that are not specifically quantifiable can be discussed or evaluated in a qualitative manner.

The DayMet data (Thornton and others, 2018) are based on a model that interpolates precipitation and temperature data between climate data-collection points. Across the northwest boundary between Maine and Canada, anomalous values of annual precipitation are likely artifacts of the interpolation methods used between stations in Canada and the United States because these do not appear anywhere else in the State (fig. 8). As discussed in the "Exclusion Zone" section, an exclusion zone was set up to remove those anomalous areas from the final datasets.

Another example of underlying datasets possibly contributing to model error is that land use has changed in some areas of the State since the MELCD data were collected in 1999 and 2000. One particular land-use class, scrub/shrub, is particularly common in the northern and northwestern part of the State where logging in the 1990s produced large areas of clearcuts or patchy clearcuts, which were assigned the scrub/shrub land-use class before trees had a chance to grow back. By the end of the model simulations in 2015, these areas would have likely grown up into young forests, which would change the ET response to precipitation. Although the land use was slowly changing over the 25-year simulation period, which would be reflected in the observations of ET, base flow, and direct runoff, the model is not set up to have parameters that also change with time. Urbanization also increased a small amount during the 25-year simulation time, but this land-use class covers a relatively small percentage of the overall model area.

The other source of data for the model that could contribute uncertainty is the soils data from the NRCS. The mapping of the soil units and assignments of AWC was done originally by county soil staff, and the interpretation of surficial geology and soil classes is not uniform across the State. For example, the hydrologic soil group C/D is described in USDA, NRCS (2007) as having moderately low water transmission rates and a water table less than 60 cm from the surface, which implies that the designation would typically apply to areas with impeded drainage such as wetlands. However, some counties assigned large areas of thin glacial till soils over bedrock in mountainous areas to the C/D hydrologic soil group even if they did not have a shallow water table, whereas in other counties the thin glacial till over bedrock in mountainous areas was assigned to the D hydrologic soil group. Therefore, areas in different parts of the State may not behave very differently (in terms of the observed values of ET, runoff, and base flow), but because the soils are assigned using different criteria the model simulates them quite differently. Another source of possible uncertainty from the NRCS is the AWC data. As discussed earlier, the assignment of the AWC is not always understandable from the point of the hydrologic soil groups (see the "Model Input Data Summary" section) or underlying soil classification, so the accuracy of this dataset is unknown, and the uncertainty contribution to the overall results would be difficult to quantify (but may be important).

Comparison of Average Recharge to Previous Studies

As noted in the introduction, there are relatively few published studies that deterministically evaluated recharge in the State for a specific location. Over the last 30 years, the USGS has published only four calibrated groundwater models for the State plus a couple of other groundwater studies that evaluated recharge for a particular study area. There have been many consulting studies (some using groundwater-flow models) done for local municipalities and other organizations, but these are generally not available to the public, and many are not well calibrated to local groundwater levels and streamflows. Using available information from the USGS studies and two consulting studies, an evaluation was done to see how well the statewide SWB model represented conditions at the local scale. The studies from the USGS included a 1983 groundwater flow model of the Little Androscoggin River valley aquifer near Norway, Maine (Morrissey, 1983); a groundwater-flow model of the Saco River valley aquifer near Fryeburg, Maine (Tepper and others, 1990); a 2011 groundwater-flow model of the Freeport Aquifer area (a buried sand and gravel aquifer and surrounding watershed; Nielsen and Locke, 2012); and a 2014 groundwater flow model of the Branch Brook and Merriland River watersheds in southern Maine (Nielsen and

Table 9. Median and mean estimated annual potential recharge rates for the 20 most-abundant land-use class:hydrologic soil group categories in the Maine Soil-Water Balance model.

Land-use class	Hydrologic soil group	Median potential recharge (in.)	Mean potential recharge (in.)	Percentage of land area in model	Standard deviation on median recharge (in.)
Mixed forest	D–Poor	11.34	12.73	11.76	2.81
Evergreen forest	D–Poor	10.7	12.02	8.36	2.86
Mixed forest	C/D	13.18	15.22	7.31	2.45
Mixed forest	C	18.47	17.59	6.03	2.35
Mixed forest	D–SoEx	17.67	17.35	4.68	3.07
Scrub/shrub	D–Poor	13.61	15.75	4.61	6.41
Deciduous forest	C/D	14.21	16.92	3.83	3.43
Deciduous forest	C	20.53	19.99	3.40	1.68
Evergreen forest	C/D	13.18	13.67	3.07	2.32
Deciduous forest	D–Poor	11.99	15.39	3.07	4.21
Deciduous forest	D–SoEx	19.32	19.70	2.69	3.36
Mixed forest	A	23.55	22.42	2.56	1.10
Evergreen forest	D–SoEx	17.45	17.55	2.54	3.50
Evergreen forest	C	16.44	16.95	2.49	1.86
Wetland forest	D–Poor	12.44	13.29	1.87	3.88
Scrub/shrub	C/D	20.97	22.21	1.85	2.34
Evergreen forest	A	22.55	21.79	1.62	1.16
Wetlands from soils	A/D	16.11	18.30	1.50	3.30
Scrub/shrub	C	23.11	23.53	1.41	1.87
Mixed forest	B	20.05	19.04	1.33	0.81

Locke, 2015). The consulting reports of modeling efforts with published recharge rates include a 1986 study of the islands in Casco Bay (Robert G. Gerber, Inc., 1986), and a groundwater model prepared for the town of Bar Harbor, Maine in 2007 (Robinson and Gerber, 2007). The evaluation of each of the studies involved calculating the SWB average annual potential recharge over a zone of each modeled area with reported, calibrated annual recharge and comparing it with the published study. For each of the areas tested, the 95-percent confidence interval for the Maine SWB estimate also was calculated.

The comparisons of previous studies and the Maine SWB estimates are presented here based on the type of geology/soils in the area evaluated, or the hydrogeologic setting. The principal hydrogeologic settings evaluated include outwash sand and gravel deposits, other sandy deposits and till, silt and clay deposits, and till or other thin deposits over bedrock. Some of the studies cited above only included one hydrogeologic setting in the recharge calculations, and others have several.

Because most of the previous studies in the State have focused on groundwater availability in areas of known productive sand and gravel aquifers, there are five different areas with outwash sand and gravel deposits to compare with the SWB potential average recharge (fig. 22). The SWB potential recharge estimates compare favorably with all the outwash zones, even though some (the Little Andsroscoggin and Saco River valley aquifers) were studied in the early to mid-1980s. Two of the three sand and till deposit areas also compare very well between the SWB potential recharge and the site-specific model areas (the second of two Freeport aquifer zones, and one of three zones in the Bar Harbor model). However, as the amount of reported recharge goes down, the ability of the SWB modeled recharge to reproduce those values is decreased. None of the silt and clay zones or the till over bedrock zones is estimated very well in the SWB model, in which case it is modeling the recharge too high. The reasons for the SWB model's lack of agreement with the groundwater-flow-modeled values in these areas differs by hydrogeologic setting.

Three of the areas with previously published low modeled recharge values but higher SWB estimates are in areas with relatively thick surficial deposits of low permeability where the water table is above the underlying bedrock (a till zone in Bar Harbor and the silt and clay zones in Freeport and the Branch Brook area). The soils that are mapped over the silt and clay zones in these study areas are a mix of hydrologic soil groups A/D, B/D, and D–Poor, and wetland forest or deciduous and mixed forest land-use classes cover most of these areas. Wetlands are often represented as soil group A/D or B/D, which are peaty soils or sandy soils overlying the

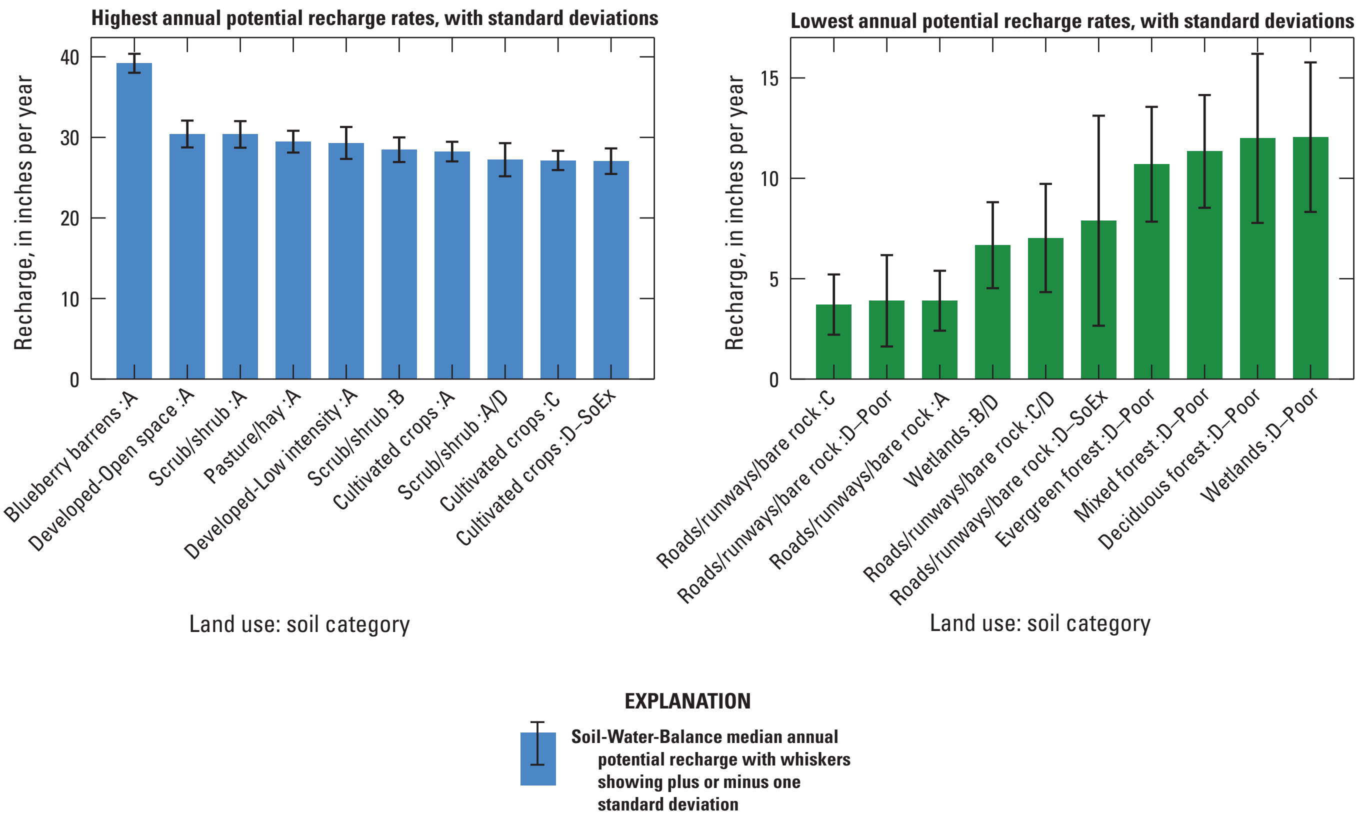


Figure 21. Highest and lowest median annual potential recharge by land-use class:hydrologic soil group category, with standard deviations.

silt and clay deposit. The SWB modeled potential recharge depends very much on what the mapped AWC is for any particular model cell. For model cells in these silt/clay areas where the available water capacity is over 3 in/ft (as would be expected for a peaty soil, or for a sandy soil that could not drain because of the underlying silt and clay), the potential recharge is closer to what would be expected (7 in/yr). However, the available water capacity is often a lower value in these model cells (less than 1 in/ft, typical of a coarse sand that is well drained), resulting in a SWB potential recharge that is much higher (often around 17 in/yr).

The remaining hydrogeologic setting to be discussed here is the fairly common situation where there is a thin soil layer (often till) over a shallow bedrock unit. Three previous studies have these settings: part of the Branch Brook model area, part of the Bar Harbor model area, and the 1980s study of islands in Casco Bay. As noted in the introduction in this report, the potential recharge modeled by SWB only takes into consideration the soil characteristics at the surface and does not have any way to simulate what may happen to infiltration below the root zone that encounters a relatively impermeable bedrock zone. In each of the studies evaluated, the recharge to bedrock is reported to be 5 in/yr or less, but the SWB potential recharge is estimated at 15 in/yr (±4 to 8 in/yr). The SWB model does predict low potential infiltration when the surface is represented as a relatively impervious surface (roads/runways/bare rock) but not where there is a mapped soil layer above the bedrock.

The conclusions to be drawn from these comparisons are that the Maine SWB model performs well in representing an accurate potential recharge under circumstances where the surficial mapped soils extend below the surface to the water-table aquifer and where the AWC data are in an appropriate range for the hydrologic soil group. The areas where the SWB model has difficulty in representing the potential recharge accurately are where there is a shallow impermeable layer in the unsaturated zone below the mapped soil unit that impeded vertical movement of potential recharge to the aquifer, such as a bedrock surface, or where the mapped AWC is not appropriate for the hydrologic soil group.

Estimated 25-Year Potential Recharge Statistics and Ranges for Calibration Watersheds

The SWB estimated median annual potential recharge for the watersheds used in the calibration of the model ranges from over 21 in/yr in several calibration watersheds (4 [Williams Brook], 14 [Narraguagus River], 18 [Royal River], 19 [Stony Brook], 21 [Pleasant River], and 22 [Otter Creek]) to less than 16.5 in/yr in the calibration watersheds 3

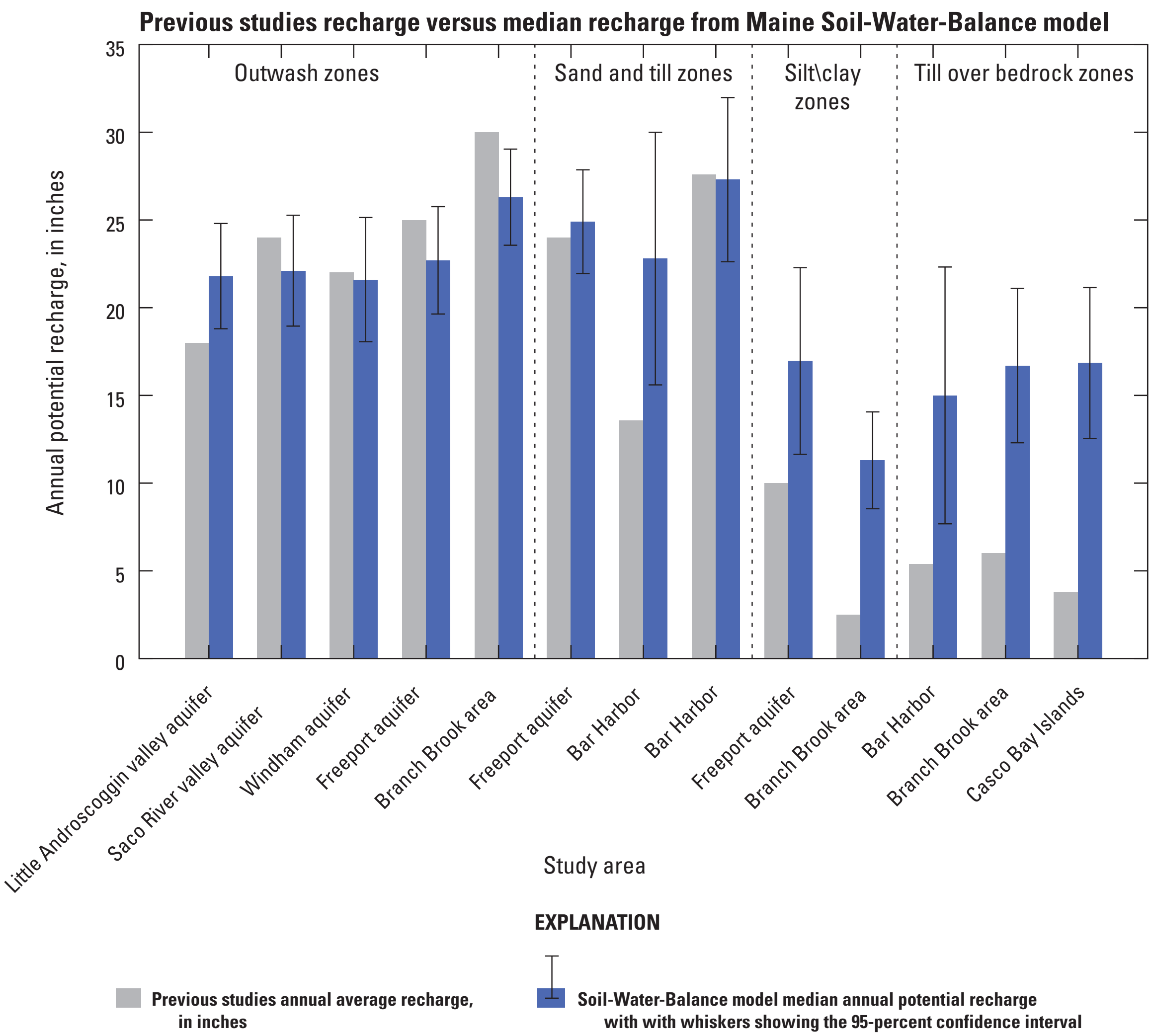


Figure 22. A comparison of previously published annual average recharge values in a selection of study areas in Maine, and corresponding median potential annual recharge from the Maine Soil-Water-Balance model, with 95-percent confidence intervals calculated from the standard deviation grid.

(Aroostook River), 5 (Allagash River), 6 (Mattawamkeag River), 7 (Piscataquis River), 20 (Seboeis River), and 25 (Little Madawaska River; table 10). Watersheds with significant amounts of sand and gravel aquifers (Dudley and Nielsen, 2011), such as 21 (Pleasant River), 14 (Narraguagus River), 18 (Royal River), and 19 (Stony Brook), have relatively high estimated total potential recharge. Several of the watersheds with lower amounts of annual potential recharge are in areas of the State receiving low amounts of total precipitation (see fig. 8).

The 95-percent confidence intervals are greatest for the calibration watersheds with highest standard deviation values (table 10): 22 (Otter Creek), 27 (Austin Stream), 16 (Ducktrap River), 29 (East Branch Wesserunsett Stream), and 7 (Piscataquis River). Some watersheds had relatively stable estimates regardless of the suite of parameters used in the Monte Carlo exercise and therefore will have narrower 95-percent confidence intervals: 24 (Hardwood Brook), 19 (Stony Brook), 4 (Williams Brook), 30 (Kennebunk River), and 13 (Nezinscot River).

The values shown in table 10 for the minimum and maximum annual recharge should be viewed as extreme values—the minimum and maximum value for each cell in the model is computed over the 25-year simulation. In larger calibration watersheds it is unlikely that the minimum or maximum values would occur for the whole watershed in a given year.

Uses and Limitations

The uses for which the grids are appropriately described and an example of such a use are included in this section. The discussion of limitations and uses of the 25-year annual potential recharge grids include geographic limitations and application limitations.

Table 10. Annual potential recharge statistics calculated for Soil-Water-Balance model calibration watersheds.

[in., inch; --, no data]

Calibration watershed index number	Calibration watershed name	Potential recharge, 1991–2015 (in.)				
		Mean annual	Median annual	Standard deviation around the median annual value	Minimum annual	Maximum annual
1	Fish River	14.76	14.49	2.55	8.51	21.93
2	St. John River	--	--	--	--	--
3	Aroostook River	13.97	13.73	2.79	7.40	22.18
4	Williams Brook	20.76	21.11	1.98	11.85	30.10
5	Allagash River	13.44	12.57	2.96	7.65	21.42
6	Mattawamkeag River	15.78	15.76	2.82	7.34	25.41
7	Piscataquis River	16.67	16.38	3.00	9.09	24.65
8	Carrabassett River	18.50	17.61	2.29	10.59	27.05
9	Sandy River—Mercer	17.38	16.76	2.54	10.42	24.94
10	Ellis River	19.92	19.44	2.52	12.41	28.57
11	Swift River	19.49	19.09	2.77	12.51	27.38
12	Little Androscoggin River	20.95	19.81	2.36	13.10	30.24
13	Nezinscot River	20.68	19.68	2.20	13.06	29.27
14	Narraguagus River	22.12	22.14	2.51	9.74	32.22
15	Old Stream	20.68	20.50	2.36	9.63	30.79
16	Ducktrap River	20.01	19.60	3.04	10.38	28.37
17	Sheepscot River	20.14	19.91	2.61	10.08	28.84
18	Royal River	22.18	21.10	2.12	13.89	32.27
19	Stony Brook	24.54	22.99	1.55	14.62	38.36
20	Seboeis River	16.43	15.89	2.15	8.07	29.75
21	Pleasant River	25.43	25.54	2.31	11.54	36.11
22	Otter Creek	28.89	28.85	5.60	18.51	38.10
23	Machias River	20.64	20.45	2.48	9.47	30.77
24	Hardwood Brook	20.82	20.30	1.57	12.18	31.87
25	Little Madawaska River	15.11	15.14	2.51	9.06	21.75
26	Wytopitlock Stream	16.29	16.21	2.92	7.61	27.20
27	Austin Stream	18.87	18.71	3.59	11.17	27.28
28	Sandy River—Madrid	18.00	17.66	2.65	10.92	25.81
29	East Branch Wesserunsett Stream	20.10	20.04	3.03	11.70	28.48
30	Kennebunk River	23.01	21.01	2.02	15.08	36.69
31	Meduxnekeag River	17.33	17.41	2.83	8.23	25.94
32	North Branch Penobscot River	--	--	--	--	--

Table 11. Example of calculations for a watershed using the annual potential recharge grids in Maine.

Calculation or result desired	How calculated	Example results
Watershed area	Calculate using StreamStats (Lombard, 2015) or geographic information system software	12.4 square miles
25-year mean potential recharge for the watershed	Calculate the areal average of the 25-year mean potential recharge grid for the watershed using geographic information system software.	16.8 inches per year
Standard deviation of potential recharge for the watershed	Calculate the areal average of the standard deviation grid using geographic information system software	2.1 inches per year
95-percent confidence interval on the mean potential recharge	Using the method provided on p. 37 and p. 44, calculate the minimum and maximum for the confidence interval.	The confidence range (or interval) would be plus or minus 4.2 inches per year, or from 12.4 to 21.0 inches per year.
25-year minimum potential recharge	Calculate the areal average of the 25-year minimum potential recharge grid for the watershed using geographic information system software.	8.1 inches per year

Appropriate Uses and Example Use Application

The grids of potential annual recharge for Maine are intended to be used to provide first-cut estimates of recharge for geographic areas no smaller than the smallest watersheds used in the calibration of the model—or about 1.5 square miles. It is recommended that the grids be used to calculate an area-wide average potential recharge for any given area of study (as compared to point-specific potential recharge), and an uncertainty around the mean should be calculated from the standard deviation grid at the same time.

One potential use of the Maine SWB potential annual recharge grids would be to create an initial estimate of recharge for an area for which one might want to calculate an overall water budget, such as for a watershed. The suggested application of the data would include the following steps. First, define the watershed boundaries for the study using GIS software or using the Maine StreamStats application (Lombard, 2015; https://streamstats.usgs.gov/ss/). A shapefile of the watershed can be downloaded from StreamStats. Using the datasets from the data release accompanying this report (Nielsen and Westenbroek, 2019), calculate the spatial average (or mean) value for the watershed for each of the potential recharge layers—mean annual, median annual, 25-year minimum, and 25-year maximum. Then, calculate the spatial mean value for the standard deviation layer. Finally, calculate the 95-percent confidence interval on the mean and median using the standard deviation grid: the 95-percent confidence range is calculated using the standard deviation (σ): minimum=median−($2\times\sigma$) and maximum=median+($2\times\sigma$).

For an example watershed located somewhere in Maine that is 12.4 square miles in area, a list of the results for calculating the mean annual potential recharge could produce the results as listed in table 11. The standard deviation grid is intended for use with the 25-year mean and median potential recharge grids but not for the 25-year minimum or maximum grids.

Limitations to the Availability and Use of the Potential Recharge Grids

Areas of no data for the State recharge grids include the White Mountain National Forest and the former Brunswick Naval Air Station, for which areas soils data were not available. In addition, the anomalous DayMet precipitation data (Thornton and others, 2018) were screened out of the final analysis with an exclusion zone in northwestern Maine along the Canadian border (figs. 15–19).

Refer to the “Model Limitations and Assumptions” section for a discussion of the potential use and interpretation limitations of the modeled output. In addition, the mapping of the AWC values does affect the ability of the Maine SWB model to accurately represent the average potential recharge. Users are encouraged to verify that the AWC is in an expected range for the hydrologic soil groups in their area of interest. The AWC and hydrologic soil groups data for this model can be found in the USGS model archive for this model at (https://doi.org/10.5066/P9GRP7DH; Nielsen, 2019).

Summary and Conclusions

To estimate average annual recharge to groundwater in Maine, the U.S. Geological Survey Soil-Water-Balance (SWB) model was used to simulate potential annual recharge across the whole State from 1991 to 2015, in cooperation with the Maine Geological Survey. The 25-year simulation results are presented as 25-year average (mean and median), minimum, and maximum potential recharge grids. Compared to previously published large-scale SWB models, the Maine SWB model presents several innovations in model calibration and uncertainty analysis. This is the first published SWB model to incorporate a rigorous parameter estimation calibration that accounts for all three of the main components of the water budged: recharge, runoff, and evapotranspiration (ET), using observations covering 32 calibration watersheds in the State. SWB's implementation of the Food and Agriculture Organization of the United Nations Drainage and Irrigation Paper 56 (FAO56) ET method was used, which provides more control over the treatment of ET in forests than the standard method. A new approach to displaying uncertainty in the SWB output was applied to the Maine SWB model, using null-space Monte Carlo analysis and several hundred alternate realizations of the model input parameters to derive a standard deviation grid of the final 25-year annual average potential recharge grid.

SWB calculates excess soil moisture (potential recharge) by dividing up input to the hydrologic system being modeled (precipitation or snowmelt) into fractions of direct runoff, plant interception, soil infiltration, actual ET, soil moisture storage, rejected recharge, and infiltration of excess soil moisture to the water table (potential recharge). The inputs required for running the Maine SWB model consists of (a) grids describing the study domain (land use, hydrologic soil groups, and soil available water capacity [AWC]); (b) grids of daily climate data; (c) lookup table values for the water balance calculations with runoff curve numbers, maximum potential infiltration rates, rooting depths, and information on how interception is handled for each combination of land-use class and hydrologic soil group; and (d) lookup table values for the implementation of the FAO56 ET calculations (plant growth settings and bare soil evaporation settings).

Land-use data for the Maine SWB model was based on the Maine Land Cover Dataset, which was compressed to 19 land-use classes for this study. The other two data inputs for SWB (hydrologic soil groups and AWC) were produced for this study using gridded soil survey data from 2016 (the Natural Resources Conservation Service [NRCS] gridded Soil Survey Geographic Database [gSSURGO] data). The hydrologic soil groups are used in SWB alongside land-use classes to classify the landscape into combinations of land use/vegetation and soil texture that should, in theory, transmit water similarly through the rooting zone and unsaturated zone to the water table under the same climatic conditions. DayMet (version 3) daily climate data from the Oak Ridge National Laboratory were the source of the daily minimum and maximum temperature and daily precipitation and have a spatial resolution of 1 kilometer .

The Parameter ESTimation (PEST) software suite was used for the calibration. The model was calibrated to optimize the output to fit 902 weighted observations of annual recharge, runoff, and ET from 32 unregulated watersheds in Maine for 2001 to 2012. The annual recharge and runoff observations were obtained using an average of nine base flow-separation techniques for the hydrograph at the streamgage for each watershed. The annual ET observations were obtained by calculating the average value of ET from national gridded ET datasets for the same watersheds. Over 500 parameters were adjusted at some point during the calibration, which were primarily values from the two SWB lookup tables: runoff curve numbers, maximum infiltration rates, rooting depths, plant ET factors, and bare soil ET factors. PEST's use of highly parameterized inversion allows for the use of hundreds of model parameters, while not introducing problems of parameter insensitivity and correlation. Tihkonov regularization was used during the PEST runs, which prevents an "overfit" model when there are many parameters. All model runs were controlled and organized using the HTCondor computer cluster at the T.C. Chamberlin computing center at the Middleton, Wisconsin USGS office.

The overall mean model error (average of all residuals) for the calibrated SWB model was 0.39 inches (in.). The mean of the absolute value of the residuals, or the mean absolute error, was 2.32 in. The root mean squared error for the calibrated model overall is 3.14 in. The r^2 value for the simulated versus observed values for the Maine SWB model is 0.76. The Nash-Sutcliffe efficiency for the Maine SWB model is 0.75. The simulated model results line up closely to the 1:1 line, indicating a relatively accurate model where the residuals do not deviate significantly from the line in one direction or another, and statistical tests show that the residuals are normally distributed.

The model was calibrated at a 500-meter (m) grid-cell size for 12 years to make the run times for the model reasonable enough to allow for thousands of model runs per calibration run. Once model parameters were calibrated, the model was run for the final time for a 25-year period using a 250-m grid size.

Using the best-fit set of parameters from the calibration runs, the Maine SWB model was run for 25 years, from 1991 to 2015, using a 250-m grid-cell size. The 25 annual grids were used to calculate the 25-year mean annual potential recharge, median annual potential recharge and the minimum and maximum potential recharge for the 25-year simulation. Based on anomalous precipitation data in northwestern Maine, an "exclusion zone" was created and used to screen out some of the area along the Canadian border from the final analysis because the calculated potential recharge values in this area are not considered representative of actual conditions. As expected, there is wide variability in the simulated 25-year median potential recharge across the State. This variability closely follows patterns of precipitation, with additional variability contributed by the patchwork nature of the intersection of land-use class and hydrologic soil groups across the State. Overall, the 25-year median potential recharge across the State is 7.98 in., ranging from a low of about 5 in. to as much as 38.7 in. The statewide range in the 25-year minimum values is very compressed—from just over 2 in. to just over 20 in.; almost everywhere in the State experienced a drought-year low of less than 10 in. of potential recharge per year sometime during the 25-year simulation period. The statewide range in the 25-year maximum potential recharge is much more variable (between 15 and 48 inches per year).

To quantify the uncertainty in the 25-year average potential recharge that results from uncertainty in the best-fit values of each of the 500 or so parameters used in the calibration, a formal uncertainty calculation was done. Portraying the uncertainty in the results of the SWB modeling exercise is difficult because the study result is not a prediction of a change in some measurable volume or measurement of interest but rather a surface across the entire State. Techniques of uncertainty analyses using linear-based first-order, second-moment methods to analyze model response to specific conditions at a particular time and place are not readily applicable to this kind of output. Therefore, the null-space Monte Carlo analysis was used, in which several hundred alternate parameter sets were generated (that could theoretically satisfy the calibration criteria) and run through the SWB model. After running hundreds of alternate models, a grid of the standard deviation of the modeled potential recharge was calculated. This is the first SWB model to use this technique for uncertainty analysis.

This standard deviation grid provides a quantitative measure of the uncertainty in the Maine potential recharge grids that is a result of uncertainties in the model parameter values. The average (mean) standard deviation for the State is 2.6 in.; the 10th percentile is 1.5 and the 90th percentile is 3.8. To translate these into a 95-percent confidence interval of the average recharge for a given area, a typical method is to take plus or minus two times the standard deviation of the average potential recharge for the same area.

Other factors also contribute to the overall uncertainty in the recharge estimates, but their values cannot be changed to evaluate their contribution to the total uncertainty. These include: uncertainty in the DayMet climate data used in the simulation, uncertainty in the soils mapping from NRCS (including the hydrologic soil groups and AWC), and uncertainty in the land-use grid.

The 25-year average potential recharge grids were compared to recharge evaluated through groundwater flow models or other methods in four hydrogeologic settings at six study areas in the State. Several zones in each study area were checked—the average potential recharge and the 95-percent confidence interval in each zone were calculated and compared to the published value. In general, the Maine SWB model reproduced the published values for outwash sand and gravel aquifers better than some other settings. A key factor in the ability of the SWB model to reproduce the earlier study results was whether the AWC data as provided in the gSSURGO data were an appropriate match for the soil hydrologic group. The Maine SWB model does a good job in representing an accurate potential recharge under circumstances where the surficial mapped soils extend below the surface to the water-table aquifer and where the AWC data are in an appropriate range for the hydrologic soil group. One setting where the SWB model has difficulty in representing the potential recharge accurately is where there is a shallow impermeable layer in the unsaturated zone below the mapped soil unit that impeded vertical movement of potential recharge to the aquifer, such as a bedrock surface. Another hydrogeologic setting that was challenging for the model was where a silt and clay layer was below a shallow soil unit that did not have AWC data that were appropriate for the hydrologic soil group. In these cases, typically the AWC data were very low, not accounting for the impedance of water flow provided by the underlying soil.

The final 25-year annual potential recharge grids for the State are released along with this report (https://doi.org/10.5066/P9052ULY). The grids of potential annual recharge for Maine are intended to be used to provide first-cut estimates of recharge for geographic areas no smaller than the smallest watersheds used in the calibration of the model—or about 1.5 square miles. It is recommended that the grids are used to calculate an areal average recharge for any given area of study, and an uncertainty around the mean should be calculated from the standard deviation grid at the same time. The user of these data also should familiarize themselves with the model limitations and assumptions are described earlier in the report. The model archive (https://doi.org/10.5066/P9GRP7DH) documents all the model construction and other model information.

Acknowledgments

Randy Hunt and Mike Fienen provided assistance in helping to guide the parameter estimation, Monte Carlo analysis and uncertainty work, and especially in making the T.C. Chamberlin computing center available for the parallel processing runs using the HTCondor computer cluster. Luke Sturtevant of the New England Water Science Center assisted in some of the initial data preparation steps. Andrew Leaf provided advice and assistance on some of the python coding tasks.

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Appendixes 1–3

Appendix 1 Details of Soil-Water-Balance Model Input for Maine

This appendix describes the data sources and data processing of the Soil-Water-Balance (SWB) model input in more detail than is presented in the main report. The climate data, land use data, and soils data are discussed. All the values of the calibrated lookup tables (land-use lookup table and irrigation lookup table) are presented in this appendix. The model input datasets and all the information needed to run this model are available in the U.S. Geological Survey (USGS) model archive for this model (https://doi.org/10.5066/P9GRP7DH; Nielsen, 2019).

Climate Data

The DayMet version 3 gridded estimates of daily climate data from the Oak Ridge National Laboratory were used in the Maine SWB model (Thornton and others, 2018; https://daac.ornl.gov/DAYMET/guides/Daymet_V3_CFMosaics.html#citation). These data have a spatial resolution of 1 kilometer. Daily minimum and maximum temperature and daily precipitation data from 1990 to 2015 were used for the model. The files were downloaded using the Network Common Data Form (netCDF) format on July 13, 2016. A python script was used to subset the national DayMet files to include only the geographic area needed to run the Maine SWB model.

Land Use

Land-use data for the Maine SWB model were based on the Maine Land Cover Dataset (MELCD), with modifications of water, wetland areas, and gravel pits using gSSURGO soil data. The MELCD data are based on Landsat Thematic Mapper 5 and 7 imagery from 1999 and 2000, and have a spatial resolution of 5 meters (Maine Office of Geographic Information Systems, 2006). Several of the original land-use classifications were condensed so that the final landcover dataset used had 19 land-use classes. Wetland and open-water areas were compared to wetland areas from the Natural Resources Conservation Service (NRCS) soils data (described below). If the NRCS soil unit indicated a wetland but the land use did not, the land use was assigned to a “wetlands from soils” category. Additional cleanup also was done to prevent inconsistencies in the treatment of open water between the soil and land use layer. The final land-use classes in the SWB model are listed in table 2 and are mapped in figure 3 of the report. The crosswalk between the original MELCD codes and the Maine SWB land-use codes are in table 1.1.

Table 1.1. Crosswalk between original Maine Land Cover Dataset and land-use codes used in the Maine Soil-Water-Balance model.

[Shaded cells highlight changes from the original. SWB, Soil-Water-Balance; NA, not applicable]

Original code	5-meter grid original classes (from melcd.tif)	Final Maine SWB land-use codes	Final Maine SWB land-use classes
2	High intensity developed	2	Developed–High intensity
3	Medium intensity developed	3	Developed–Moderate
4	Low intensity developed	4	Developed–Low intensity
5	Open space developed	5	Developed–Open space
6	Cultivated crops	6	Cultivated crops
7	Pasture/hay	7	Pasture/hay
8	Grassland/herbaceous	8	Grassland
9	Deciduous forest	9	Deciduous forest
10	Evergreen forest	10	Evergreen forest
11	Mixed forest	11	Mixed forest
12	Scrub/shrub	12	Scrub/shrub
13	Wetland forest	13	Wetland forest
NA	NA	14	Wetlands from soils
15	Wetlands	15	Wetlands
16	Roads/runways	16	Roads/runways/bare rock
19	Unconsolidated shore	21	Open water
20	Bare land	20	Bare land
21	Open water	21	Open water
22	Blueberry field	22	Blueberry barrens
23	Recent clearcut	12	Scrub/shrub
24	Light partial cut	11	Mixed forest
25	Heavy partial cut	12	Scrub/shrub
26	Regenerating forest	12	Scrub/shrub
27	Alpine	27	Alpine/tundra
NA	NA	30	Gravel pits

Soils Data from Natural Resources Conservation Service

Several groups of information for running the Maine SWB model were taken from the NRCS gridded soil survey data from 2016 (NRCS gridded Soil Survey Geographic Database [gSSURGO] data; Soil Survey Staff, 2016). The gSSURGO data are a compilation of soil survey data for all counties in the country. The gSSURGO data format is a raster of soil map unit keys at a 10-meter resolution. The map unit keys link the raster cells to many attribute tables, including (among others) soil unit names, soil unit descriptions, hydrologic soil groups, drainage classes, parent material, and available water capacity.

The soil unit names and descriptions were used in comparison with the land-use data to make sure that the input grids from the gSSURGO database were not inconsistent with the land-use data (for example, to make sure that if the land-use data indicated open water in a certain area, that the gSSURGO data were not coded for a terrestrial soil type). Cleanup of the final land-use layer and hydrologic soil group layer was done to prevent these types of inconsistencies.

Hydrologic Soil Groups

Data processing of the NRCS standard hydrologic soil groups included filling in missing data (for soils with no hydrologic soil groups code assigned) and modifying the D hydrologic group.

The gSSURGO “chorizon” table was the primary source for the hydrologic soils group (“hydgrp” field). For soils that did not have a valid value for the “hydgrp” field, values were assigned based on other soils in the same county with similar geologic material descriptions (“geomdesc” field).

As described earlier in the report, the hydrologic soil groups used for the Maine SWB model were modified from the NRCS standard hydrologic soil groups. The modification included dividing the “D” hydrologic group (high runoff potential when wet; water movement is restricted; typically clayey textures), which in Maine includes not only flat-lying clay textured soils, but also shallow bedrock “soils,” often having very high slopes. The “D” hydrologic group was divided into three subgroups based on the soil drainage class for each soil unit: “D–Ex” are the group D soils that are also excessively drained (shallow soils over bedrock, often steep slopes); “D–SoEx” are primarily soils in subdued hilly areas and often are composed of glacial till; “D–Poor” are a group of several poorly drained soil types, including glacial clay deposits, silt loam soils (farmable, but not peats), silt-loams, and silty clay loams and silt loams (no plant material or peat mentioned). Some are tidal marshes or upland areas of poor drainage (forested). The nine hydrologic soil groups used in the Maine SWB model are listed in table 3 of the report, and the distribution is mapped in figure 4 of the report.

Available Water Capacity

The available water capacity (AWC) grid was derived from the U.S. Department of Agriculture, NRCS gSSURGO for Maine, 2016 data release (Soil Survey Staff, 2016). The attribute used from the gSSURGO data for available water capacity is the “awc_r” field in the “chorizon” table, or representative available water capacity, which are given as a volume fraction. The SWB program expects AWC as inches per foot, so the values were multiplied by 12. Some soil units did not have a value for the available water capacity. In those instances, the soil description was used to find a soil unit in the same county (if possible) with a similar geologic material description (“geomdesc”) that did have a value for the available water capacity, and the value was assigned from the other soil. The available water capacity data are in units of inches of water per foot of soil (fig. 6 in the report), ranging from 0 to 7.2 inches per foot.

Soil-Water-Balance Lookup Tables

The output of the model is controlled and by many values within two lookup tables (tab-delimited text files): the land-use lookup table and the irrigation lookup table. The land-use lookup table contains values for runoff curve numbers, plant rooting depths, and maximum infiltration rates (Westenbroek and others, 2010), which are unique for every combination of land-use class and hydrologic soil group in the model. Additional lookup values for interception of rainfall on vegetation are also input and vary with vegetation type (land use). The model performs calculations to apportion water input to a cell (rainfall or snowmelt) to components of the water budget based on the input grids, daily temperature data, and the lookup table values for runoff curve, maximum infiltration rate, and plant rooting depths (fig. 2). The lookup table values for the Maine SWB model were adjusted during the calibration process; the calibrated table values for the land-use lookup table are given here in table 1.2, which is available for download at https://doi.org/10.3133/sir20195125.

The evapotranspiration calculations for the Maine SWB model were done using the optional Food and Agriculture Organization of the United Nations Drainage and Irrigation Paper 56 (FAO56) method (Allen and others, 1998; Westenbroek and others, 2018), which requires a second lookup table, the irrigation lookup table. Although this table is used to calculate crop irrigation needs, it does so by calculating crop/land use specific transpiration and soil evaporation, which are the output desired for this application of the model. The values that control the transpiration and soil evaporation calculations were modified during the model calibration process; other values were taken from example datasets (Westenbroek and others, 2018). The final (calibrated) values for the irrigation lookup table are given in table 1.3, which is available for download at https://doi.org/10.3133/sir20195125.

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Appendix 2 Details of Soil-Water-Balance Model Calibration Information

This appendix includes information on the parameters used for the land-use lookup table and the irrigation lookup table, and the recharge, runoff, and evapotranspiration observations used during the calibration. The parameter information includes whether the parameter was adjusted during the final calibration and the final calibration values used for each parameter. Also included is information on the Monte Carlo runs used to calculate the standard deviation on the median potential recharge grid.

Parameters

The model calibration used values from the land-use lookup table and the irrigation table as parameters. The individual values for the land-use lookup table entries for runoff curve numbers, maximum potential recharge, rooting depths, and interception values were treated as parameters and are included in table 2.1, which is available for download at https://doi.org/10.3133/sir20195125. The irrigation table parameters included 13 individual values for the plant-growth coefficients (K_{cb}) and 15 values that were multipliers for sections of the irrigation table. These multipliers acted on an initial set of table values. The irrigation parameters and a description of each are included in table 2.2, which is available for download at https://doi.org/10.3133/sir20195125. The land-use parameters are a one-for-one substitution of values for the land-use lookup table, but the irrigation table parameters include several multipliers that act on blocks of values in the irrigation lookup table, as well as some values that are direct substitutions for values in the irrigation lookup table.

Observations

The development of the observations for the model calibration included an extensive analysis of streamflow data for the recharge and runoff observations for each of the calibration watersheds, described below. The model calibration also used annual evapotranspiration observations for each of the calibration watersheds, which are described as well.

Analysis of Streamflow Data for Calibration Targets

The annual hydrograph for each gage location was separated into a base flow and direct runoff component using nine hydrograph separation techniques (table 2.3). Each base flow-separation technique uses different methods of identifying the base flow versus direct runoff components of flow—some assign a relatively larger portion of flow to base flow (recharge), some less. None of them can exactly represent the movement of water into and out of bank storage, which is an important process that often occurs on a shorter time scale than represented in the daily streamflow data that is used by most hydrograph separation techniques, and there is no consensus on which method most accurately achieves this division of flow, as it varies with watershed size and other factors (Risser and others, 2005). The Rorabaugh method, as implemented in the recession-curve displacement method RORA algorithm (Rorabaugh, 1964; Rutledge, 1998) incorporates more site-specific detail and event-based processes than other methods (Barlow and others, 2015; Risser and others, 2005). However, Risser and others (2005) found that the RORA method produced values greater than direct measurements using lysimeters. In a comparison of methods for this study, the RORA method yielded estimates that were often significantly higher than other methods, and less water was available for direct runoff. During initial calibration runs using only RORA as calibration targets, the Soil-Water-Balance

Table 2.3. Base flow-separation techniques used for annual recharge and runoff calculations.

Method	Reference
Base Flow Index—Standard	Wahl and Wahl, 1995; Institute of Hydrology, 1980a, b
Base Flow Index—Modified	Wahl and Wahl, 1995; Institute of Hydrology, 1980a, b
HYSEP—Fixed Interval	Sloto and Crouse, 1996; Pettyjohn and Henning, 1979
HYSEP—Sliding Interval	Sloto and Crouse, 1996; Pettyjohn and Henning, 1979
HYSEP—Local Minimum	Sloto and Crouse, 1996; Pettyjohn and Henning, 1979
PART	Rutledge, 1998
RORA and RECESS	Rorabaugh, 1964; Rutledge, 1998
SWAT Bflow (Digital Filter One Parameter)	Arnold and others, 1995; Arnold and Allen, 1999
Eckhardt Digital Filter, Two Parameter	Eckhardt, 2005; Eckhardt, 2008

(SWB) model was unable to reproduce the division of water into the two hydrograph components without using unrealistic values for many of the lookup table parameters. Therefore, the calibration targets chosen for this study are calculated as the median value of the nine methods, which is intended to average out the estimation inaccuracies inherent in each method.

Besides providing an averaged estimate of recharge and direct runoff, the use of so many different estimates enabled a mean and variance to be calculated, which was used to generate initial weights on the calibration targets (see below). The U.S. Geological Survey Groundwater Toolbox (Barlow and others, 2015) software package (version 1.3) was used to download and process the streamflow data for each streamgage location and compute the annual base flow and direct runoff values. A table of the annual mean base flow and direct runoff estimates and the variances for each year are given in table 2.4, which is available for download at https://doi.org/10.3133/sir20195125.

Evapotranspiration Observations for Model Calibration

The third set of calibration targets consisted of annual evapotranspiration (ET) across each watershed. Observations of ET were obtained from Reitz and others (2017), who have published monthly ET estimates for the conterminous United States based on remote sensing data (data downloaded from https://www.sciencebase.gov/catalog/item/59d3d13ce4b05fe04cc3d278 on October 10, 2018). The original data are gridded at a 90-meter cell size. The monthly grids were summed for each year of the calibration period (2000–12) to get an annual grid, and the average value of annual ET over each watershed was calculated to use as the annual ET observation value. The annual values of average ET for each year and each watershed are given in table 2.5, available for download at https://doi.org/ 10.3133/ sir20195125.

The model calibration used all the observations from 2000 through 2012, but because the year 2000 is a year that sets up the snow and soil moisture storage for the first calibration year (2001), it is included in the calibration data but given zero weight in the parameter estimation process. The discussion of the selection and modification of weights is given in the body of the report. The final values are listed in table 2.6, which is available for download at https://doi.org/10.3133/sir20195125.

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Appendix 3 Annual Values of Modeled Recharge, Runoff, Evapotranspiration, and Precipitation for Calibration Watersheds, 1991–2015

This appendix contains all the model-derived values of annual precipitation, recharge, runoff, and evapotranspiration for each calibration watershed, for the whole simulation period (1991–2015; table 3.1, available for download at https://doi.org/10.3133/sir20195125).

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Publishing support provided by the
Pembroke and Rolla Publishing Service Center

Nielsen and Westenbroek—**Groundwater Recharge Estimates for Maine Using a Soil-Water-Balance Model, 1991 to 2015**—SIR 2019–5125

ISSN 2328-0328 (online)
https://doi.org/10.3133/sir20195125