Methods for Computing Water-Quality Loads at Sites in the U.S. Geological Survey National Water Quality Network

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Version 1.3, August 2021

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

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By Casey J. Lee, Jennifer C. Murphy, Charles G. Crawford, and Jeffery R. Deacon

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Foreword

Sustaining the quality of the Nation's water resources and the health of our diverse ecosystems depends on the availability of sound water-resources data and information to develop effective, science-based policies. Effective management of water resources also brings more certainty and efficiency to important economic sectors. Taken together, these actions lead to immediate and long-term economic, social, and environmental benefits that make a difference to the lives of the almost 400 million people projected to live in the United States by 2050.

In 1991, Congress established the National Water-Quality Assessment (NAWQA) to address where, when, why, and how the Nation's water quality has changed, or is likely to change in the future, in response to human activities and natural factors. Since then, NAWQA has been a leading source of scientific data and knowledge used by national, regional, state, and local agencies to develop science-based policies and management strategies to improve and protect water resources used for drinking water, recreation, irrigation, energy development, and ecosystem needs (https://water.usgs.gov/nawqa/applications/). Plans for the third decade of NAWQA (2013–23) address priority water-quality issues and science needs identified by NAWQA stakeholders, such as the Advisory Committee on Water Information and the National Research Council, and are designed to meet increasing challenges related to population growth, increasing needs for clean water, and changing land-use and weather patterns.

Federal, State, and local agencies have invested billions of dollars to reduce the amount of pollution entering rivers and streams that millions of Americans rely on for drinking water, recreation, and irrigation. Long-term information on the loading of water-quality constituents is crucial for evaluating the effectiveness of pollution control efforts and protecting the Nation's water resources into the future. This report specifies methods used to compute loads at long-term NAWQA sampling sites as of 2018. All NAWQA reports are available online at https://water.usgs.gov/nawqa/bib/.

We hope this publication will provide you with insights and information to meet your water-resource needs and will foster increased citizen awareness and involvement in the protection and restoration of our Nation's waters. The information in this report is intended primarily for those interested or involved in resource management and protection, conservation, regulation, and policymaking at the regional and national levels.

Dr. Donald W. Cline
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Conversion Factors

U.S. customary units to International System of Units

Multiply	By	To obtain
	Length	
mile (mi)	1.609	kilometer (km)
	Area	
square mile (mi^2)	2.590	square kilometer (km^2)
	Mass	
ton, short (2,000 lb)	0.9072	metric ton (t)

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

°F = (1.8 × °C) + 32.

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

°C = (°F –32) / 1.8.

Supplemental Information

A water year is the period from October 1 to September 30 and is designated by the year in which it ends; for example, water year 2015 was from October 1, 2014, to September 30, 2015.

Abbreviations

NASQAN	U.S. Geological Survey National Stream Quality Accounting Network
NAWQA	U.S. Geological Survey National Water Quality Assessment Program
NWQN	U.S. Geological Survey National Water Quality Network
USGS	U.S. Geological Survey
WRTDS	Weighted Regressions on Time, Discharge, and Season
WRTDS–K	Weighted Regressions on Time, Discharge, and Season with Kalman filtering

Methods for Computing Water-Quality Loads at Sites in the U.S. Geological Survey National Water Quality Network

By Casey J. Lee, Jennifer C. Murphy, Charles G. Crawford, and Jeffery R. Deacon

Abstract

The U.S. Geological Survey currently (2020) publishes information on concentrations and loads of water-quality constituents at 110 sites across the United States as part of the U.S. Geological Survey National Water Quality Network (NWQN). This report details historical and updated methods for computing water-quality loads at NWQN sites. The primary updates to historical load estimation methods include (1) an adaptation to methods for computing loads to the Gulf of Mexico; (2) the inclusion of loads and trends computed using the Weighted Regressions on Time, Discharge, and Season (WRTDS) and Weighted Regressions on Time, Discharge, and Season with Kalman filtering (WRTDS–K) methods; and (3) the inclusion of loads computed using continuous water-quality data. Loads computed using WRTDS and WRTDS–K and continuous water-quality data are provided along with those computed using historical methods. Various aspects of method updates are evaluated in this report to help users of water-quality loading data determine which estimation methods best suit their particular application.

Introduction

Knowledge of the mass, or load, of water-quality constituents transported by streams and rivers is necessary to assess the health of receiving waters and to characterize contributions from upstream landscapes. A central objective of the U.S. Geological Survey (USGS) National Water Quality Network (NWQN) is to provide accurate water-quality loading information to stakeholders. This information is provided through consistent collection and analysis of streamflow and water-quality data at sites across the United States and through continued evaluation and improvement of procedures used to compute water-quality loads. The purpose of this report is to summarize historical methods for computing water-quality loads at NWQN sites and to describe and justify updates to load computation procedures.

The U.S. Geological Survey National Water Quality Network

The NWQN was formed in 2013 through a merger of water-quality networks managed by the National Stream Quality Accounting Network (NASQAN) (Hooper and others, 1997) and the National Water Quality Assessment Program (NAWQA) (U.S. Geological Survey, 2017b). In 2015, the NWQN was expanded to include 113 sites with the addition of reference sites previously managed by the Hydrologic Benchmark Program (Murdoch and others, 2005; Deacon and others, 2015). Three sites at the Mississippi River at Baton Rouge, Louisiana, Wax Lake at Calumet, La., and Orestimba Creek near Crows Landing, California, were eliminated from the network in early 2017 and 2018, and thus, the current (2020) NWQN consists of 110 sites. Sites within the NWQN are characterized by size, location, and upstream land use. Coastal river sites (20 sites) represent concentrations and loads being contributed to estuaries. Large inland river sites (41 sites) are at major rivers in the inland United States, whereas agricultural (9 sites) and urban indicator sites (10 sites) represent small streams with predominantly agricultural or urban upstream land use. Reference sites (30 sites) are sampled to characterize conditions at streams with minimal upstream anthropogenic effect.

Sample Collection

The scheduling and frequency of sample collection at sites in the NWQN are determined based on historically observed variability in water-quality concentrations and loads (C. Crawford, USGS, written commun., 2017). With the exception of reference sites, samples are collected through a seasonally weighted, fixed-interval sampling regime. This sampling regime was implemented to allow for consistent sampling of water quality throughout the year while improving the representation of water-quality conditions during seasons with the highest loads (C. Crawford, USGS, written commun, 2017). Typically, twelve to eighteen water-quality samples are collected per year at the coastal and inland river sites (table 1);

Table 1. U.S. Geological Survey National Water Quality Network sites in water year 2020 (October 1, 2019, to September 30, 2020).

[USGS, U.S. Geological Survey; ME, Maine; NA, not applicable; MA, Massachusetts; CT, Connecticut; NY, New York; NJ, New Jersey; PA, Pennsylvania; MD, Maryland; WV, West Virginia; DC, District of Colombia; VA, Virginia; NC, North Carolina; nr, near; SC, South Carolina; GA, Georgia; FL, Florida; Rd, Road; AL, Alabama; R, River; BL, below; L&D, Lock and Dam; IN, Indiana; TN, Tennessee; KY, Kentucky; IL, Illinois; WI, Wisconsin; MI, Michigan; OH, Ohio; St., Saint; Ont, Ontario; Cr, Creek; ab, above; Lk, Lake; MT, Montana; ND, North Dakota; MN, Minnesota; Ave, Avenue; #, number; IA, Iowa; NE, Northeast; Ne, Nebraska; CO, Colorado; Nebr., Nebraska; KS, Kansas; MO, Missouri; AR, Arkansas; L, Little; OK, Oklahoma; @, at; MS, Mississippi; bl, below; LA, Louisiana; COE, Corps of Engineers; Rk, Rock; Ck, Creek; TX, Texas; Rv, River; USIBW, United States International Boundary Water Commission; WY, Wyoming; AZ, Arizona; NIB, Northerly International Boundary; SLC, Salt Lake City; UT, Utah; C, Creek; CA, California; NV, Nevada; Rd, Road; NF, North Fork; Rpds, Rapids; WA, Washington; ID, Idaho; HWY, Highway; xing, crossing; OR, Oregon; Mt, Mount; AK, Alaska; HI, Hawaii; Co, County; S, South]

Station name	USGS station identifier	USGS station identifier or other Federal agency responsible for streamflow-data collection (if different)	Site type	Drainage area (square miles)	Typical number of samples per year
USGS National Water Quality Assessment Project, National Water Quality Network					
Wild River at Gilead, ME	01054200	NA	Reference	70	16
Green River near Colrain, MA	01170100	NA	Reference	41	18
Connecticut River at Thompsonville, CT[1]	01184000	NA	Coastal rivers	9,660	18
Norwalk River at Winnipauk, CT	01209710	NA	Urban	33	24
Canajoharie Creek near Canajoharie, NY	01349150	NA	Agriculture	60	24
Hudson River near Poughkeepsie, NY	01372043	01372058	Coastal rivers	11,700	14
Neversink River near Claryville, NY	01435000	NA	Reference	67	16
Delaware River at Trenton, NJ[1]	01463500	NA	Coastal rivers	6,780	14
McDonalds Branch in Byrne State Forest, NJ	01466500	NA	Reference	2	18
Young Womans Creek near Renovo, PA	01545600	NA	Reference	46	17
Susquehanna River at Conowingo, MD[2]	01578310	NA	Coastal rivers	27,100	14
Waites Run near Wardensville, WV	01610400	NA	Reference	13	18
Potomac River at Chain Bridge at Washington DC[1]	01646580	01646500	Coastal rivers	11,570	18
Accotink Creek near Annandale, VA[2]	01654000	NA	Urban	24	24
Swift Creek near Apex, NC	02087580	NA	Urban	21	24
Neuse River at Kinston, NC	02089500	NA	Large inland rivers	2,692	18
Contentnea Creek at Hookerton, NC	02091500	NA	Agriculture	733	24
Edisto River near Givhans, SC	02175000	NA	Coastal rivers	2,730	18
Altamaha River at Everett City, GA	02226160	02226000	Coastal rivers	14,000	14
Sopchoppy River nr Sopchoppy, FL	02327100	NA	Reference	102	18
Sope Creek near Marietta, GA	02335870	NA	Urban	31	24
Chattahoochee River near Whitesburg, GA	02338000	NA	Large inland rivers	2,430	18
Hillibahatchee Creek at Thaxton Rd, near Franklin, GA	02338523	NA	Reference	17	14
Apalachicola River near Sumatra, FL	02359170	NA	Coastal rivers	19,200	14
Alabama River at Claiborne, AL	02429500	02428400	Large inland rivers	22,000	14
Tombigbee R BL Coffeeville, L&D near Coffeeville, AL	02469762	NA	Large inland rivers	18,417	18
Ohio River at Cannelton Dam at Cannelton, IN[3]	03303280	NA	Large inland rivers	97,000	14
White River at Hazleton, IN[1]	03374100	NA	Large inland rivers	11,305	18
Wabash River at New Harmony, IN[3]	03378500	NA	Large inland rivers	29,234	14
Little River above Townsend, TN	03497300	NA	Reference	106	18
Tennessee River at Highway 60 near Paducah, KY[2,3]	03609750	Kentucky Dam outflow (Tennessee Valley Authority)	Large inland rivers	40,330	14
Ohio River at Olmsted, IL[1,3]	03612600	NA	Large inland rivers	203,100	14
Popple River near Fence, WI	04063700	NA	Reference	139	18
Clinton River at Sterling Heights, MI	04161820	NA	Urban	309	24
Maumee River at Waterville, OH	04193500	NA	Large inland rivers	6,330	18
St. Lawrence River at Cornwall, Ont, nr Massena, NY	04264331	NA	Large inland rivers	298,800	14
Swiftcurrent Cr ab Swiftcurrent Lk at Many Glacier, MT	05014300	NA	Reference	16	12
Red River of the North at Grand Forks, ND	05082500	NA	Large inland rivers	30,100	14
Kawishiwi River near Ely, MN	05124480	NA	Reference	254	16
Shingle Creek at Queen Ave in Minneapolis, MN	05288705	NA	Urban	28	24
Mississippi River below L&D #2 at Hastings, MN[3]	05331580	NA	Large inland rivers	37,100	14
Mississippi River at Clinton, IA[1,3]	05420500	NA	Large inland rivers	85,600	14
South Fork Iowa River NE of New Providence, IA	05451210	NA	Agriculture	224	24
Iowa River at Wapello, IA[1,3]	05465500	NA	Large inland rivers	12,500	15
Des Moines River at Keosauqua, IA	05490500	NA	Large inland rivers	14,038	14

Table 1. U.S. Geological Survey National Water Quality Network sites in water year 2020 (October 1, 2019, to September 30, 2020).—Continued

[USGS, U.S. Geological Survey; ME, Maine; NA, not applicable; MA, Massachusetts; CT, Connecticut; NY, New York; NJ, New Jersey; PA, Pennsylvania; MD, Maryland; WV, West Virginia; DC, District of Colombia; VA, Virginia; NC, North Carolina; nr, near; SC, South Carolina; GA, Georgia; FL, Florida; Rd, Road; AL, Alabama; R, River; BL, below; L&D, Lock and Dam; IN, Indiana; TN, Tennessee; KY, Kentucky; IL, Illinois; WI, Wisconsin; MI, Michigan; OH, Ohio; St., Saint; Ont, Ontario; Cr, Creek; ab, above; Lk, Lake; MT, Montana; ND, North Dakota; MN, Minnesota; Ave, Avenue; #, number; IA, Iowa; NE, Northeast; Ne, Nebraska; CO, Colorado; Nebr., Nebraska; KS, Kansas; MO, Missouri; AR, Arkansas; L, Little; OK, Oklahoma; @, at; MS, Mississippi; bl, below; LA, Louisiana; COE, Corps of Engineers; Rk, Rock; Ck, Creek; TX, Texas; Rv, River; USIBW, United States International Boundary Water Commission; WY, Wyoming; AZ, Arizona; NIB, Northerly International Boundary; SLC, Salt Lake City; UT, Utah; C, Creek; CA, California; NV, Nevada; Rd, Road; NF, North Fork; Rpds, Rapids; WA, Washington; ID, Idaho; HWY, Highway; xing, crossing; OR, Oregon; Mt, Mount; AK, Alaska; HI, Hawaii; Co, County; S, South]

Station name	USGS station identifier	USGS station identifier or other Federal agency responsible for streamflow-data collection (if different)	Site type	Drainage area (square miles)	Typical number of samples per year
USGS National Water Quality Assessment Project, National Water Quality Network—Continued					
Illinois River at Valley City, IL[1,3]	05586100	NA	Large inland rivers	26,743	14
Mississippi River Below Grafton, IL[3]	05587455	05587450	Large inland rivers	171,300	14
Yellowstone River near Sidney, MT[3]	06329500	NA	Large inland rivers	69,083	14
Missouri River at Omaha, NE[2,3]	06610000	NA	Large inland rivers	322,800	14
Cherry Creek at Denver, CO	06713500	NA	Urban	410	24
South Platte River near Kersey, CO[4]	06754000	NA	Large inland rivers	9,661	18
Dismal River near Thedford, NE	06775900	NA	Reference	966	12
Maple Creek near Nickerson, NE	06800000	NA	Agriculture	368	24
Elkhorn River at Waterloo, NE[1,3]	06800500	NA	Large inland rivers	6,900	18
Platte River at Louisville, NE[1,3]	06805500	NA	Large inland rivers	85,370	14
Kansas River at DeSoto, KS[1,3]	06892350	NA	Large inland rivers	59,756	14
Missouri River at Hermann, MO[1,3]	06934500	NA	Large inland rivers	522,500	14
Mississippi River at Thebes, IL[1,3]	07022000	NA	Large inland rivers	713,200	14
North Sylamore Creek near Fifty Six, AR	07060710	NA	Reference	58	16
L Arkansas River near Sedgwick, KS[1]	07144100	NA	Large inland rivers	1,239	18
North Canadian River near Harrah, OK	07241550	NA	Large inland rivers	13,775	18
AR River @ David D Terry L&D below Little Rock, AR[3]	07263620	07263450	Large inland rivers	158,429	14
Bogue Phalia nr Leland, MS[1]	07288650	NA	Agriculture	484	24
Yazoo River bl Steele Bayou nr Long Lake, MS	07288955	NA	Large inland rivers	13,355	18
Mississippi River nr St. Francisville, LA[1,3]	07373420	01100 (U.S. Army Corps of Engineers)	Coastal rivers	--[5]	16
Mississippi River at Belle Chasse, LA	07374525	NA	Coastal rivers	--[5]	14
(COE) Atchafalaya River at Melville, LA[3]	07381495	03045 (U.S. Army Corps of Engineers)	Coastal rivers	--[5]	16
Lower Atchafalaya River at Morgan City, LA[1]	07381600	NA	Coastal rivers	--[5]	14
Ouiska Chitto Creek near Oberlin, LA	08014500	NA	Reference	510	12
White Rk Ck at Greenville Ave, Dallas, TX	08057200	NA	Urban	66	24
Trinity Rv bl Dallas, TX	08057410	NA	Large inland rivers	6,278	18
Brazos Rv nr Rosharon, TX	08116650	NA	Coastal rivers	45,339	14
Frio Rv at Concan, TX	08195000	NA	Reference	389	18
USIBW Rio Grande at El Paso, TX	08364000	08-3640.00 (International Boundary and Water Commission)	Large inland rivers	32,210	14
Rio Grande nr Brownsville, TX	08475000	08-4750.00 (International Boundary and Water Commission)	Coastal rivers	176,333	12
Colorado River near Colorado-Utah State Line	09163500	NA	Large inland rivers	17,849	18
Pine Creek above Freemont Lake, WY	09196500	NA	Reference	76	12
Vallecito Creek near Bayfield, CO	09352900	NA	Reference	73	14
Colorado River at Lees Ferry, AZ	09380000	NA	Large inland rivers	111,800	14
West Clear Creek near Camp Verde, AZ	09505800	NA	Reference	241	17
Colorado River at NIB, above Morelos Dam, AZ	09522000	NA	Coastal rivers	246,700	12
Little Cottonwood Creek @ Jodan River nr SLC, UT	10168000	NA	Urban	46	24
Jordan River @ 1700 South @ Salt Lake City, UT	10171000	NA	Large inland rivers	3,438	18
Red Butte Creek at Fort Douglas near Salt Lake City, UT	10172200	NA	Reference	7	16
Sagehen C nr Truckee, CA	10343500	NA	Reference	11	16
Truckee Rv nr Tracy, NV	10350340	NA	Large inland rivers	1,580	18
Santa Ana R bl Prado Dam, CA	11074000	NA	Coastal rivers	2,258	18
Marble Fork Kaweah R ab Horse C nr Lodgepole, CA	11206800	11206820	Reference	8	16
Merced R at Happy Isles Bridge nr Yosemite, CA	11264500	NA	Reference	181	18

Table 1. U.S. Geological Survey National Water Quality Network sites in water year 2020 (October 1, 2019, to September 30, 2020).—Continued

[USGS, U.S. Geological Survey; ME, Maine; NA, not applicable; MA, Massachusetts; CT, Connecticut; NY, New York; NJ, New Jersey; PA, Pennsylvania; MD, Maryland; WV, West Virginia; DC, District of Colombia; VA, Virginia; NC, North Carolina; nr, near; SC, South Carolina; GA, Georgia; FL, Florida; Rd, Road; AL, Alabama; R, River; BL, below; L&D, Lock and Dam; IN, Indiana; TN, Tennessee; KY, Kentucky; IL, Illinois; WI, Wisconsin; MI, Michigan; OH, Ohio; St., Saint; Ont, Ontario; Cr, Creek; ab, above; Lk, Lake; MT, Montana; ND, North Dakota; MN, Minnesota; Ave, Avenue; #, number; IA, Iowa; NE, Northeast; Ne, Nebraska; CO, Colorado; Nebr., Nebraska; KS, Kansas; MO, Missouri; AR, Arkansas; L, Little; OK, Oklahoma; @, at; MS, Mississippi; bl, below; LA, Louisiana; COE, Corps of Engineers; Rk, Rock; Ck, Creek; TX, Texas; Rv, River; USIBW, United States International Boundary Water Commission; WY, Wyoming; AZ, Arizona; NIB, Northerly International Boundary; SLC, Salt Lake City; UT, Utah; C, Creek; CA, California; NV, Nevada; Rd, Road; NF, North Fork; Rpds, Rapids; WA, Washington; ID, Idaho; HWY, Highway; xing, crossing; OR, Oregon; Mt, Mount; AK, Alaska; HI, Hawaii; Co, County; S, South]

Station name	USGS station identifier	USGS station identifier or other Federal agency responsible for streamflow-data collection (if different)	Site type	Drainage area (square miles)	Typical number of samples per year
USGS National Water Quality Assessment Project, National Water Quality Network—Continued					
San Joaquin R near Vernalis, CA[1]	11303500	NA	Coastal rivers	13,539	18
Sacramento R at Freeport, CA[1]	11447650	NA	Coastal rivers	NA	14
NF Skokomish R bl Staircase Rpds nr Hoodsport, WA	12056500	NA	Reference	57	16
Andrews Creek near Mazama, WA	12447390	NA	Reference	22	7
Granger Drain at Granger, WA	12505450	NA	Agriculture	62	24
Yakima River at Kiona, WA	12510500	NA	Large inland rivers	5,615	18
Henry's Fork nr Rexburg, ID	13056500	NA	Large inland rivers	2,920	18
Rock Creek ab HWY 30/93 xing at Twin Falls, ID	13092747	NA	Agriculture	259	24
Snake River at King Hill, ID	13154500	NA	Large inland rivers	35,800	14
Lookout Creek near Blue River, OR	14161500	NA	Reference	24	15
Zollner Creek near Mt. Angel, OR	14201300	NA	Agriculture	15	24
East Fork Dairy Creek near Meachan Corner, OR	14205400	NA	Reference	34	12
Fanno Creek at Durham, OR[2]	14206950	NA	Urban	32	24
Willamette River at Portland, OR[1]	14211720	NA	Large inland rivers	11,200	18
Columbia River at Port Westward, near Quincy, OR[2]	14246900	NA	Coastal rivers	256,900	12
Talkeetna R nr Talkeetna, AK	15292700	NA	Reference	2,010	8
Yukon R at Pilot Station, AK	15565447	NA	Coastal rivers	321,000	7
Kahakuloa Stream near Honokohau, Maui, HI	16618000	NA	Reference	3	12
Mississippi River above Vicksburg at Mile 438, MS[1,6]	322023090544500	Computed	Large inland rivers	1,131,100	14
Sugar Creek at Co Rd 400 S at New Palestine, IN	394340085524601	03361650	Agriculture	93	24
Big Thompson bl Moraine Park nr Estes Park, CO	402114105350101	NA	Reference	40	16
USGS Cooperative Water Program Sites					
Grand River near Sumner, MO[3]	06902000	NA	Large inland rivers	6,880	12
Osage River below St. Thomas, MO[3]	06926510	NA	Large inland rivers	14,584	6

[1]Real-time nitrate data are currently (2020) collected at or near this site.

[2]Sites used to evaluate procedures for aggregating uncertainty among multiple models (see the section entitled "Evaluation of Confidence Interval Summing Procedure" herein).

[3]Indicates sites (or sites near sites) in which loads have historically been computed as part of the National Stream Quality Accounting Network, Mississippi-Atchafalaya River Basin Subnetwork; Loads are published at these sites starting as early as 1968, loads at other sites are first published in 1993.

[4]Streamflow data after water year 2007 are collected by the Colorado Division of Water Resources.

[5]Drainage area is not displayed for sites downstream from diversion of Mississippi River at the Old River Outflow Channel (fig. 3).

[6]Streamflow is computed by subtracting daily streamflow from USGS station identification number 07288955 from daily flows from USGS station identification number 07289000.

the number of samples at a particular site was determined based on site-by-site reviews of the variability in water-quality concentration and loads (C. Crawford, USGS, written commun, 2017). Six of these samples are collected at bimonthly fixed intervals, and the remaining 6–12 are collected during months of the year historically characterized to have increased water-quality loading (C. Crawford, written commun., 2017). Only seven samples are collected at the coastal site at Yukon River at Pilot Station, Alaska, because of seasonal access limitations. Eighteen samples are collected per year at other large inland river sites (6 at fixed, bimonthly intervals and 12 during months characterized to have high loading conditions), and 24 samples are collected per year at agricultural and urban indicator sites (12 fixed monthly samples and 12 during months observed to have high loading conditions). Reference sites are sampled using a monthly, fixed-interval sampling regime because they typically have less variability in water-quality constituent concentrations (C. Crawford, USGS, written commun., 2017). Samples at Andrews Creek near Mazama, Wash., and Talkeetna River near Talkeetna, Alaska, sites have reduced sampling (about seven and eight samples collected per year, respectively) because of difficulty accessing these sites during the cold season. Water-quality loads are also currently (2020) computed at two sites operated by the USGS cooperative water program in which loads have historically been computed as part of the NASQAN Mississippi River Basin Program (Aulenbach and others, 2007; table 1). Streamflow and water-quality data may be collected at different, but nearby, locations because of difficulties related to accessing a site for either purpose or because an agency other than USGS collects streamflow data (table 1).

Sample Analysis

Samples collected at NWQN sites are analyzed for concentrations of suspended sediment, inorganic and organic carbon, and selected nutrients, pesticides, major ions, trace elements, and physical properties. Total and particulate constituents (such as total Kjeldahl nitrogen, total phosphorus, and suspended sediment) are not currently (2020) analyzed from samples collected at reference sites. Water-quality loads in water year 2017 will be reported for dissolved ammonia, dissolved nitrate plus nitrite, total nitrogen, orthophosphate, total phosphorus, dissolved silica, dissolved organic carbon, and suspended sediment at sites with adequate data (a water year is the 12-month period from October 1 through September 30 designated by the calendar year in which it ends). See Deacon and others (2015) for more detailed information on analytical and data preparation procedures at NWQN sites.

History of Load Computation at National Water Quality Network Sites

Water-quality loads were first published on a national scale by the NASQAN program in the Mississippi-Atchafalaya River Basin from 1980 to 1996 as part of the National Oceanic and Atmospheric Administration's integrated assessment on hypoxia in the Gulf of Mexico (Goolsby and others, 1999). Loads in that study were computed using a multiple regression approach that used the logarithm of streamflow, the logarithm of streamflow squared, and seasonal and time terms as explanatory variables. A follow up report used the Load Estimator 2 (LOADEST2) program (Crawford, 1996), a precursor to the USGS Load Estimator (LOADEST) program (Runkel and others, 2004) that used similar variables to publish loads for major ions, nutrients, and sediment in the Mississippi, Rio Grande, Colorado, and Columbia River Basins from 1996 to 2000 (Kelly and others, 2001). The NASQAN program later published nutrient loads for the Susquehanna, St. Lawrence, Mississippi-Atchafalaya, Columbia, and Willamette River Basins from 1968 to 2004 using the same explanatory variables as Goolsby and others (1999) but implemented with the USGS LOADEST program (Aulenbach, 2006). That study used a 10-year moving window approach (previous studies used all available data) for sites in the Mississippi River basin such that regression relations were developed using water-quality and streamflow data for the target water year and the previous 9 years. This moving window approach was used to allow models to adapt to potential changes in relations between streamflow and water-quality conditions through time, while still using enough data to adequately characterize the form and uncertainty of regression relations.

The NASQAN load computation process was formalized for Mississippi/Atchafalaya River basin sites in 2007 (Aulenbach and others, 2007). This process used a 5-year moving window and the "best model selection" routine within the USGS LOADEST program (Runkel and others, 2004) to define unique regression relations for a given water-quality constituent and water year. Loads were published using this methodology until 2013, when networks managed by the NASQAN and NAWQA programs were merged to form the USGS National Water Quality Network (NWQN). At this time, load estimation methods were updated to include additional explanatory variables, including the logarithm of cubic streamflow and variables indicative of short, medium, and long-term history of streamflow conditions (Ryberg and Vecchia, 2012; table 2). The method was updated to allow an analyst to inspect the fit of candidate models through a series of graphs before publication (Deacon and others, 2015).

Table 2. Explanatory variables considered in load estimation models.

[*ln*; natural log; *Q*, streamflow; *T*, decimal time]

Explanatory variable abbreviation	Description
$\ln(Q)$	Natural log of daily streamflow (centered).
$\ln(Q)^2$	Natural log of squared daily streamflow (centered).
$\ln(Q)^3$	Natural log of cubed daily streamflow (centered).
T	Decimal time.
T^2	Decimal time squared.
$\sin(2\pi T)$; $\cos(2\pi T)$	Fourier representations of season.
FA_1_10day	Subtraction of the average daily streamflow (log transformed) during the past 10 days from the log of streamflow on the day of sampling.
FA_1_30day	Subtraction of the average daily streamflow (log transformed) during the past 30 days from the log of streamflow on the day of sampling.
FA_30_365day	Subtraction of the average daily streamflow (log transformed) during the past 365 days from the average daily streamflow (log transformed) during the past 30 days.
FA_100dayall_minus_365dayall	The average daily streamflow (log transformed) during the past 100 days is subtracted from the average daily streamflow (log transformed) during the period of record, this quantity is then subtracted from the average daily streamflow (log transformed) during the past 365 days, which is subtracted from the average daily streamflow (log transformed) during the period of record.

This report describes current (2020) load estimation procedures published by Deacon and others (2015) and updates designed to improve the accuracy and interpretability of load estimates. These updates include (1) a simplification of procedures used to compute water-quality loads at the Mississippi River at St. Francisville, which is a site used to estimate water-quality loads to the Gulf of Mexico; (2) a description of methods for computing loads using the Weighted Regressions on Time, Discharge, and Season (WRTDS) and Weighted Regressions on Time, Discharge, and Season with Kalman filtering (WRTDS–K) methods (Lee and others, 2019); and (3) a description of methods that use continuous water-quality data for load computation. This report also evaluates specific aspects of updated methods to help users of water-quality loading data determine how to best use data from the various methods.

National Water Quality Network Load Estimation Methods

Effective for water year 2019, two primary methods are used to compute loads at NWQN sites. These methods include the adapted LOADEST method (Deacon and others, 2015), which has been used at NWQN sites since 2013, and the WRTDS and WRTDS–K methods (Lee and others, 2019; Zhang and Hirsch, 2019). Because LOADEST procedures have not changed substantially since their initial publication, loads published through 2013 using methods described by Aulenbach and others (2007) will remain unchanged; however, because all WRTDS and WRTDS–K estimates have the potential to change as new data are added, all loads for these methods will be updated annually. The following sections describe the adapted LOADEST and WRTDS/WRTDS–K methods used for estimating loads in the NWQN.

Adapted LOADEST Method

The adapted LOADEST method establishes regression relations among constituent concentrations and continuous information on streamflow and time within a 5-year moving window (that is, sample results are used for the year in which loads are being computed and the four previous water years; Deacon and others, 2015). The 5-year window was first used to compute loads in the Mississippi River Basin (Aulenbach and others, 2007) to use enough data to adequately characterize recent (past 5 year) relations between water-quality analyses and explanatory variables (Aulenbach, 2007). The LOADEST method and the 5-year moving window continue to be used to maintain consistency with historical loads published by Aulenbach and others (2007).

Loads are computed for a particular site, water-quality constituent, and water year using the adapted LOADEST method only if sampling was done for the year in which loads are being computed and if at least 20 samples are present during a 5-year sampling window. With less than 30 (but at least 20) samples present within the sampling window, the natural log of streamflow is the only explanatory variable considered; additional explanatory variables are considered when at least 30 samples are present (although typically many more samples are collected).

Explanatory variables considered in regression relations include the natural logarithm of daily streamflow, the natural logarithm of daily streamflow squared, and the natural logarithm of daily streamflow cubed on the day of sampling. Although cubic streamflow terms were identified as producing extreme errors in decadal water-quality loads in a few instances (Lee and others, 2016), the inclusion of this term improved the accuracy of load estimates on the whole, and the visual inspection of model results (described in the Use of Unit-Value Streamflows at Small Stream Sites" section) is used in part to prevent extremely biased load estimates. Streamflow variables are centered (as in Cohn and others, 1992) to reduce multicollinearity among explanatory variables. Fourier sine and cosine series are also used to represent variability associated with season, and decimal time and decimal time-squared are included to simulate variability in time (table 2). Four additional variables are also included to represent short to long term historical streamflow conditions (table 2; Ryberg and Vecchia, 2012; Deacon and others, 2015).

A combined automated and manual process is used to evaluate if assumptions of selected regression models are met. These assumptions are (1) that a relation exists between the natural log of observed water-quality loads and explanatory variables, (2) that model errors are normally distributed, and (3) that model errors are independent of variables used in the regression model. The automated process develops regression models for all possible combinations of potential explanatory variables. Any model that has an explanatory variable with a variance inflation factor greater than 10 is removed from consideration to reduce the potential for multicollinearity among explanatory variables. One to three models computed through this automated process are selected for further inspection to determine which model will be used to compute loads. Candidate models include the model with the smallest Akaike information criteria (a measure of model error that includes penalties for additional explanatory variables; Helsel and Hirsch, 2002) and the model with the smallest *p*-value (a measure of the significance of the overall regression). In addition, the regression relation from the previous water year (if loads were estimated) is selected for inspection. Plots are then made to confirm that water-quality observations look reasonable and to select the candidate model for load computation that best conforms to regression assumptions. Model residuals are visually inspected to select the model used to compute loads because single (or even multiple) model diagnostics have not been proven to identify models that produced unbiased loads (Helsel and Hirsch, 2002; Hirsch, 2014; Deacon and others, 2015; Lee and others, 2016). Water-quality loads may not be computed for a particular site, constituent, or water year if samples are not collected among a range of hydrologic conditions or if a candidate model could not be identified to meet regression assumptions.

Use of Unit-Value Streamflows at Small Stream Sites

Runoff flows through headwater stream reaches more quickly than through larger rivers, and thus, agricultural, urban, and reference NWQN fixed sites, which have smaller drainages than larger river sites, experience more subdaily variability in streamflow conditions compared to large-inland river or coastal river sites. It is important to accurately represent streamflow conditions at the time of water-quality sampling to develop unbiased load regression relations. Because of this, hourly streamflow is used to compute water-quality loads at agricultural, urban, and reference stream sites in the NWQN (Deacon and others, 2015). Because differences in load estimates using hourly and daily streamflow values have not previously been quantified, these differences are evaluated herein. Annual loads computed with hourly and daily streamflow are compared among all agricultural, reference, and urban NWQN sites on days when complete hourly records are present (fig. 1).

Loads computed using hourly and daily streamflow are within plus or minus (±)20 percent of each other for the majority of cases for all constituents evaluated (94 percent of nitrate plus nitrite loads, 90 percent of total nitrogen loads, 81 percent of total phosphorus (TP) loads, and 72 percent of suspended-sediment (SSC) loads were within ±20 percent of each other using hourly and daily streamflow); however, more extreme differences were observed for total phosphorus and suspended-sediment constituents, which are transported almost exclusively during high flow conditions (Lee and others, 2016). The 90th percentile of differences among hourly and daily loads were 30 and 60 percent for TP and SSC, respectively, and maximum differences were 1,280 and 2,680 percent, respectively.

Instantaneous streamflow values recorded by USGS personnel at the time of water-quality sampling are used to develop regression relations at agricultural, urban, and reference sites in the NWQN. These relations are applied to hourly streamflow obtained from the USGS Instantaneous Data Archive, which is now (2017) served on the USGS NWIS interface (U.S. Geological Survey, 2017a). Hourly streamflows are used because some sites do not record streamflow at finer time scales and because hourly data are the finest time step allowed within LOADEST. In cases in which instantaneous streamflow values are not recorded at the time of sample collection, hourly data from the streamflow record nearest the time of sample collection are used to develop regression relations.

Two additional steps are necessary to use hourly streamflow to compute water-quality loads. First, subdaily streamflow values not recorded on the hour are rounded to the nearest hour. Second, gaps in time-series streamflow data are addressed. Subdaily streamflow time series often have extended gaps because these data are not typically estimated during periods in which gages were inoperable (because of equipment malfunction, ice, or other reasons). On days in

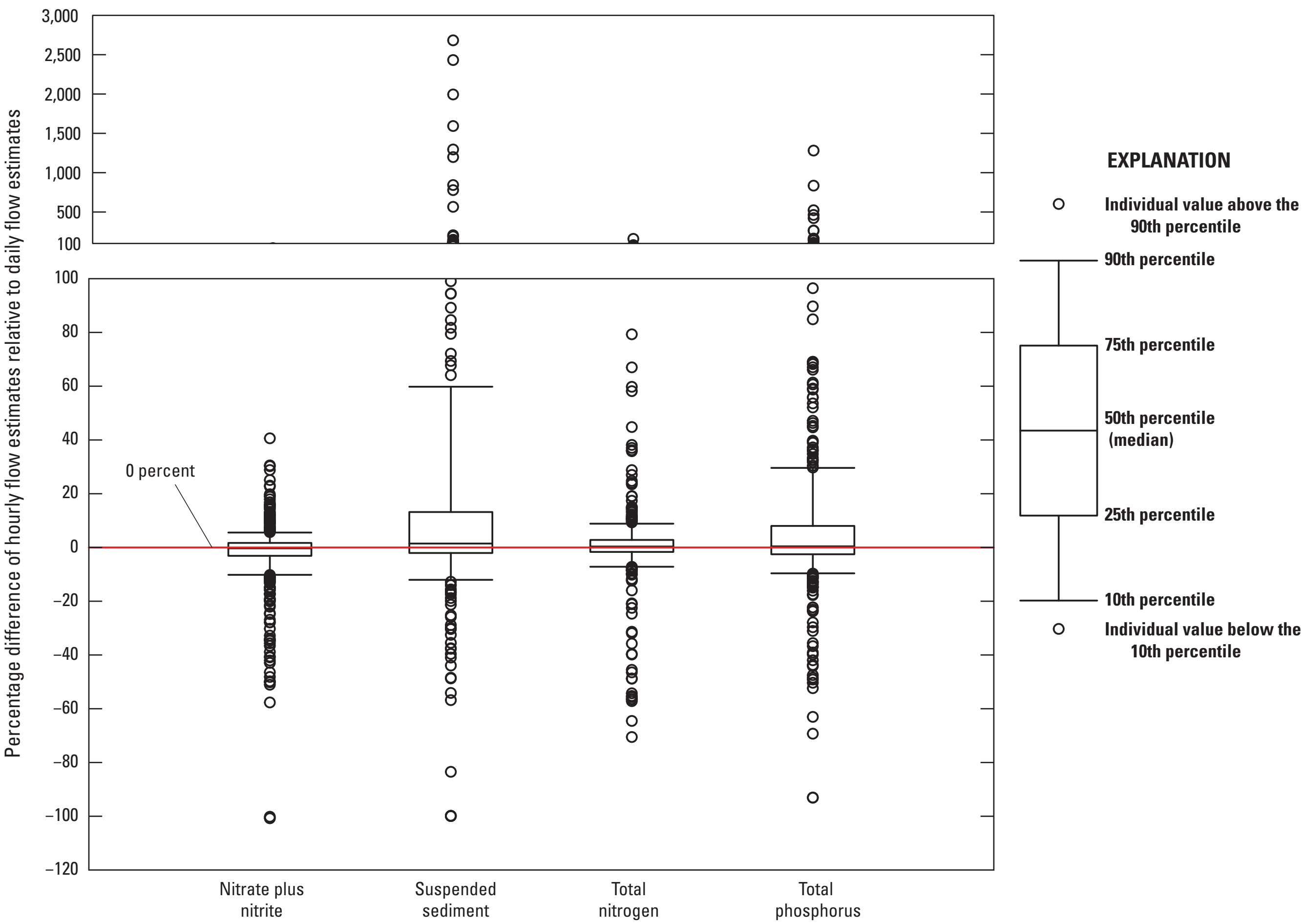


Figure 1. Relative percentage differences among loads computed using hourly and daily time steps at agricultural, urban, and reference sites in the National Water Quality Network from 1993 to 2016.

which a complete hourly streamflow record is not available, daily streamflows (published on the USGS NWIS; U.S. Geological Survey, 2017a) are used to compute loads (using the same regression relation developed using hourly streamflows). If hourly streamflows are not complete for at least half of the water year, daily streamflows are used to compute loads for the entire water year, otherwise water-year loads are computed by adding loads computed from days with daily and days with hourly streamflows.

Evaluation of Confidence Interval Summing Procedure

The USGS LOADEST program does not have procedures for computing the uncertainty of water-year loads using regression models with two different time steps. Previous studies have estimated the uncertainty of water-year loads from different models by adding the standard error (or the size of the confidence interval above or below the load estimate—procedures are mathematically the same) of the two fluxes in quadrature, meaning that errors are squared, added, and then square rooted (Aulenbach, 2007). This approach is currently (2019) being used to estimate the uncertainty of monthly loads to the Great Lakes using models with different time steps and explanatory variables (Robertson and others, 2018). Aulenbach (2007) also used this procedure to estimate the uncertainty of loads to the Gulf of Mexico from the Mississippi and Atchafalaya Rivers; however, this method assumes that the errors among the regression models used are independent, which may not be the case in practice. Because this procedure is not known to have been evaluated previously, it is evaluated herein to characterize potential differences in the uncertainty of annual load estimates derived from two models as compared to the results from a single regression model.

The procedure for aggregating errors was evaluated by comparing 95-percent confidence intervals summed in quadrature from subsets of whole records to whole-record 95-percent confidence intervals. Nitrate, total nitrogen, total phosphorus, and suspended-sediment records at 6 NWQN sites across the United States with varying upstream drainages and at least 15 years of annual load data for each constituent (table 1) were subset by randomly parsing the number of days in the period of record into two records of various lengths. Record lengths considered include dividing the number of days into 50 percent of days in each subset, 40/60 percent of days in each, 30/70 percent of days in each, 20/80 percent of days in each, and 10/90 percent of days in each. Confidence intervals were summed in quadrature 10 times (randomly selecting days for each case) for each subset type and water year in which a water-quality model had been developed. Percentage differences among the size of 95-percent confidence intervals summed in quadrature compared to the confidence interval for entire records are displayed in figure 2.

The summation of 95-percent confidence intervals in quadrature resulted in less uncertainty as compared to whole-record LOADEST estimates (fig. 2). Median percentage differences of 95-percent confidence interval bands computed by summing in quadrature were 14, 13, 13, and 10 percent smaller than those computed for whole records of nitrate plus nitrite, suspended sediment, total phosphorus, and total nitrogen loads, respectively. Ninety percent of confidence interval estimates among all sites and constituents summed in quadrature underestimated whole-record estimates by less than 25 percent. Differences among methods were primarily related to the percentage of record being subset and the sampling site. Subsets that were nearly equal in record length (50/50 or 40/60) constituted 75 percent of the cases in which confidence-interval bands summed in quadrature deviated from whole-record estimates by more than 20 percent. At two sites with small drainage areas (where this procedure is being used to sum daily and hourly load estimates), summing in quadrature more closely mimicked whole-record 95-percent confidence-interval bands. Of the 95-percent confidence-interval bands summed in quadrature at these two sites, 90 percent were within 3 and 0.2 percent of whole-record 95-percent confidence-interval bands at the Accotink Creek near Annandale, Va., and Fanno Creek at Durham, Oreg., sites, respectively; however, the most extreme differences for suspended sediment that ranged from 30 to 60 percent below whole-record estimates (fig. 2) existed for suspended sediment at the Accotink Creek site. Based on this analysis, NWQN load data at agricultural, reference, and urban-indicator sites with missing hourly records may underestimate uncertainty by as much as 25 percent as compared to whole-record estimates, although the procedure more closely mimicked whole-record uncertainty at the two sites with small drainage areas for which this procedure is used. The degree of this underestimation is likely to be larger in cases where a large amount (that is, 40 to 50 percent) of the hourly streamflow record is missing.

Types of Loads Computed

The processes above are used to compute water-year loads at NWQN sites with sufficient water-quality and streamflow data. Four additional types of loads are computed at NWQN sites as described below:

1. Monthly water-quality loads have previously been published at NASQAN sites in Mississippi-Atchafalaya River Basin Subnetwork (table 1; Aulenbach and others, 2007). Monthly loads will be updated annually at these sites.

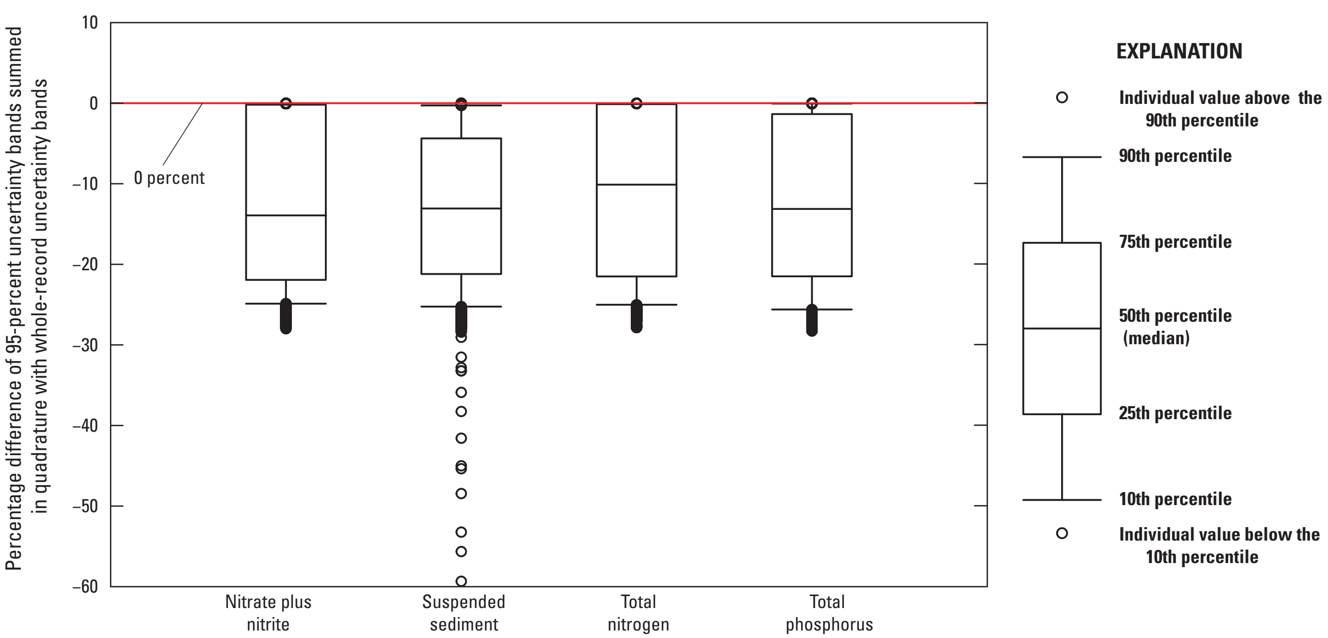


Figure 2. Percentage difference among 95-percent confidence interval bands summed in quadrature relative to whole-record 95-percent confidence intervals at selected National Water Quality Network sites from 1993 to 2016.

2. The composite method, which adjusts daily load computations based on local departures from measured values (Aulenbach and Hooper, 2006), has been used historically to compute loads at the Mississippi River at St. Francisville and at the Atchaflaya River at Melville (Aulenbach and others, 2007) for potential improvements in accuracy this method may offer for loads to the Gulf of Mexico (fig. 3). This method will continue to be used to compute loads at these sites moving forward.

3. Continuous nitrate sensors are operated at locations throughout the United States and at selected NWQN sites (table 1), in part, to improve the accuracy of computed nitrate loads. Nitrate loads are computed using continuous nitrate data in addition to streamflow-based estimates at NWQN sites when adequate data are available. Annual loads (in English tons) are computed by summing the product of daily sensor values (in milligrams per liter), streamflow values (in cubic feet per second), and a unit conversion factor (0.026969). Methods used to compute 95-percent uncertainty estimates surrounding nitrate loads using continuous nitrate data are similar to streamflow based loads described previously. Regression relations are established between the natural log of discrete nitrate loads and mean-daily streamflow and sensor-based nitrate concentrations through the LOADEST program. Residual plots (as shown in fig. 10 in Deacon and others, 2015) are evaluated to verify that regression assumptions are being met before computing loads. Two main differences exist in the load estimation process when using continuous nitrate data compared to streamflow-based estimates. First, in contrast to streamflow data, sensor malfunctions, environmental fouling, and other factors can make it difficult to obtain a complete record of daily nitrate concentrations necessary to compute loads for an entire water year; thus, in cases where 1–7 days of sensor data are missing during relatively stable streamflow conditions, daily nitrate concentrations obtained from sensors may be linearly interpolated among measured values to obtain a complete record for the water year. At sites with longer periods of missing record or in which there is missing record during rapidly changing or extreme conditions, daily loads during periods without daily sensor data are estimated using LOADEST-based procedures described above. Second, because laboratory analyses of discrete nitrate samples and nitrate sensor values have been observed to have near 1:1 relations with little variability (Pellerin and others, 2014), only 10 samples are required to compute loads (as opposed to 20 sample for streamflow-based estimates); thus, nitrate loads may be computed at continuously monitored sites for the first water-year in which data are available (provided 10 samples have been collected). As with streamflow-based estimates, data collected in subsequent years are added to the regression relations for estimates produced for the following water years until 5 years of data have been collected. At that point, loads will be computed using a 5-year moving window as is done with streamflow-based estimates.

4. Preliminary monthly loads have historically been published for October to May of the most current water year (currently 2017) for the Mississippi River at St. Francisville (table 1) and the Atchafalaya River at Melville (table 1) for purposes of estimating the size of the summer Gulf hypoxic zone (Scavia and others, 2003; Scavia and others, 2004; Turner and others, 2006; Turner and others, 2008). These loads use water-quality data collected from October through May of the current water year and the previous 4 water years. These preliminary loads will continue to be published in the beginning of June each year on the USGS Mississippi River Basin website (Lee and others, 2017). Preliminary load data are superseded by monthly load estimates later published for the entire water year through the annual data releases (see the "Data Publication" section for more information).

Updates to Procedures for Computing Loads to the Gulf of Mexico

The sum of water-quality loads computed from flow and water-quality data collected at the Mississippi River near St. Francisville and at Tarbert Landing, respectively, (labeled as observed near the St. Francisville site; table 1) and water-quality and flow data collected at the Atchafalaya River at Melville and at Simmesport, respectively, (labeled as observed at the Melville site; table 1) have historically been used to estimate loads to the Gulf of Mexico (Aulenbach, 2007; fig. 3). Additional downstream sites on the Mississippi River at Belle Chasse, La., the Lower Atchafalaya at Morgan City, La., and Wax Lake at Calumet, La., (table 1; fig. 3) are monitored to evaluate potential differences in concentrations and loads between upstream and downstream sites, and between sites with and without continuous nitrate sensors. Aulenbach and others (2007) used streamflow upstream from the diversion of the Mississippi River to the Atchafalaya River (through the Old River Outflow Channel) to estimate loads at the Mississippi River at St. Francisville site (table 1) using the rationale that upstream flows represented natural variations in nutrient concentrations (Aulenbach and others, 2007; fig. 3). The resulting loads were then multiplied by the fraction of streamflows that continued to the Mississippi main stem after the diversion at the Old River Outflow Channel to obtain loads at the Mississippi River at St. Francisville site (which is downstream from the Old River diversion); however, because the percentage of streamflow diverted to the Atchafalaya River remains relatively constant through time, an evaluation is done herein to test whether simplifying this procedure by using streamflow downstream from the Old River diversion (at Tarbert Landing) results in substantial changes to monthly

[MO, Missouri; USGS, U.S. Geological Survey; RT, real-time water-quality data was collected; IL, Illinois; QW, discrete water-quality data was collected; Flow, streamflow data was collected; MS, Mississippi; LA, Louisiana; USACE, U.S. Army Corps of Engineers; St., Saint]

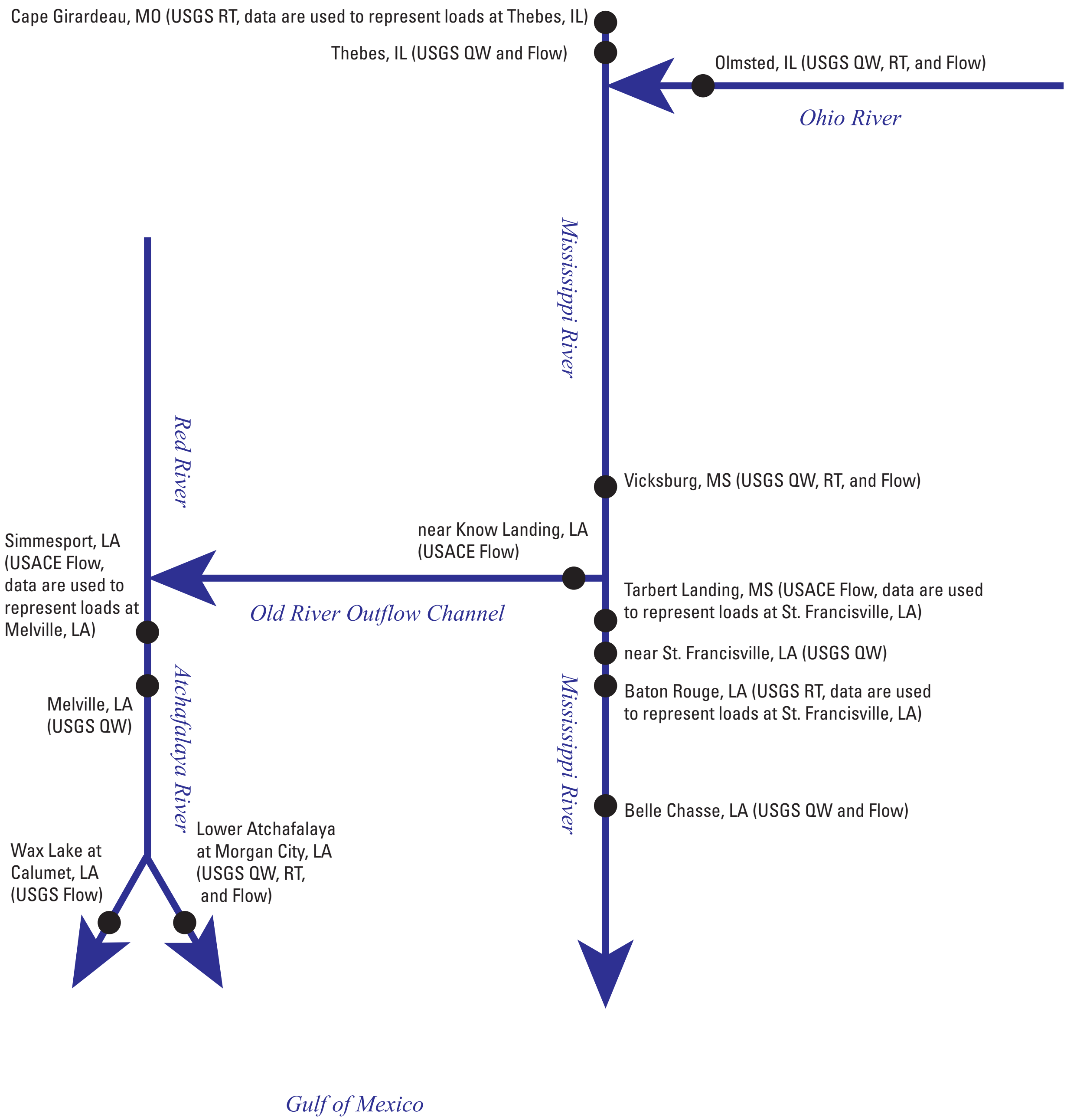


Figure 3. Schematic of streamflow and water-quality monitoring sites in the Lower Mississippi River Basin as of 2017 (not drawn to scale).

or annual water-quality loads. Simplifying this procedure by using streamflow downstream from the diversion would make load computations more reproducible and would improve the ability to use WRTDS (see the following section) for load computation at the Mississippi River at St. Francisville site.

Water year and May loads of nitrate plus nitrite and total phosphorus at the Mississippi River at St. Francisville (using flow from Tarbert Landing; fig. 3) are compared to published loads using the Aulenbach and others (2007) method to evaluate if simplified procedures for computing loads to the Gulf of Mexico differ from historically computed loads (fig. 4). Nitrate plus nitrite and total phosphorus were selected for comparisons because they represent constituents transported primarily in dissolved (nitrate plus nitrite) and solid (total phosphorus) phases. May loads are used to represent monthly loads because they are used in estimating the size of the hypoxic zone in the Gulf of Mexico (Turner and others, 2006; Turner and others, 2008).

Water year nitrate plus nitrite and total phosphorus loads were within 2 percent of each other between the 2 methods for 30 of 31 years, with a maximum difference of 3.2 percent for total phosphorus and 2.1 percent for nitrate plus nitrite. May loads were within 2 percent between the 2 methods for 29 of 31 years for nitrate plus nitrite (maximum difference was 10 percent in 1994) and 27 of 31 years for total phosphorus (maximum difference was –8.9 percent in 1998). These relatively small differences justify using streamflow values downstream from the Old River diversion to compute loads at the Mississippi River at St. Francisville starting in 2017. Historical results before water year 2017 will remain unchanged at Deacon and others (2015) and in future data releases.

Load and Trend Computations using Weighted Regressions on Time, Discharge, and Season

The WRTDS and WRTDS–K methods are used in addition to the adapted LOADEST method to compute loads at NWQN sites starting for loads computed in water year 2019. A central benefit of this method is the ability to compute flow-normalized loads, a measure which provides stakeholders an understanding of water-quality loading outside the context of year-to-year variation in hydrologic conditions (Hirsch and others, 2010). The WRTDS method also has a variety of tools to evaluate potential trends in water-quality concentrations and loads. WRTDS–K proved to be the most accurate method for computing annual loads among methods studied by Lee and others (2019) and thus is used in addition to previously described methods for computing annual loads at all NWQN sites. Because the Kalman filtering process in WRTDS–K does not affect the process of computing flow-normalized concentrations and loads, these metrics are computed using the typical WRTDS method. Flow-normalized concentration and loads are provided for the purpose of assessing the magnitude of potential changes in water-quality concentration and load over time.

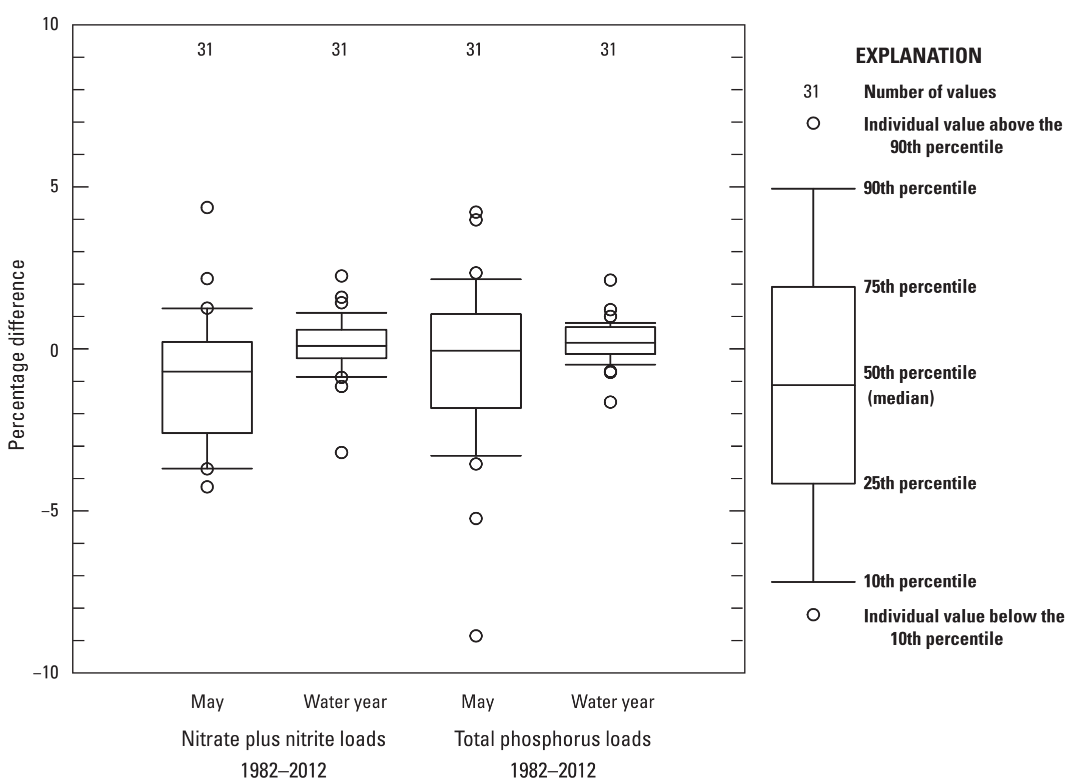


Figure 4. Relative percentage differences among May and water year loads at the Mississippi River at St. Francisville from 1982–2012 computed using streamflow upstream and downstream from the Old Flow control structure.

WRTDS–K is implemented using methods described in Lee and others (2019) and WRTDS is implemented through the EGRET package (Hirsch and others, 2015), with uncertainty analyses through the EGRETci package, both of which are open-source R packages available from the Comprehensive R Archive Network at http://cran.r-project.org/web/packages/. Water-quality data used in the formation of WRTDS–K and WRTDS models are identical to data used in historical and adapted LOADEST methods. Daily streamflow data are used in all WRTDS–K and WRTDS models because these methods are not currently (2020) equipped to use unit-value streamflow data. The WRTDS and WRTDS–K models are computed with 7-year half-window widths and a minimum of 50 total observations with at least 25 uncensored observations. WRTDS and WRTDS–K load and flow-normalized load concentration estimates are computed for years with at least four observations in the respective year and for years with less than four observations that are bounded by years with at least four observations within 2 years before and after the respective year. Ninety-percent confidence intervals are computed using a bootstrap block of 200 days (Hirsch and others, 2015) with 100 replicates. Models are visually inspected for fit before publishing loads using the same graphics used with the adapted LOADEST method. The use of 7-year half-window widths in WRTDS means that as a new year of water-quality data is added, the past 7 years of load estimates are subject to change; however, because flow-normalized estimates from all years at a given site use data from the newest water year, flow-normalized estimates from the entire period of record are subject to change as additional years of water-quality data are considered. Flow-normalized estimates are computed using both stationary and generalized processes (Hirsch and DeCicco, 2018).

As noted on the "Tracking Water Quality in U.S. Streams and Rivers" website (U.S. Geological Survey, 2020), estimates of trends in flow-normalized, water-quality concentrations and loads are provided among the most recent water year with available data (2020 for example), and consecutive decades before the most recent water year (that is, 1980, 1990, 2000, and 2010) are provided as a table underneath graphs when adequate data are available. Tables indicate the percentage change in flow-normalized concentrations and loads for the selected water-quality constituent among the water years selected. Tables also indicate a 90-percent confidence interval about the trend, the part of the total trend attributed to trends in streamflow conditions, and the part of the total trend attributed to other changes in the upstream drainage basin. The magnitude of the trend attributed to other changes in the upstream watershed sources is the stationary flow-normalized estimate (Choquette and others, 2019; Murphy and Sprague, 2019), which assumes that the distribution of streamflow is constant over a given trend period (a windowSide argument of 0; Hirsch and DeCicco, 2018). The magnitude of the trend attributed to trends in streamflow conditions is computed by subtracting the generalized flow-normalized estimate, which incorporates both trends in streamflow and upstream constituent sources (Murphy and Sprague, 2019), from the stationary flow-normalized estimate.

Water-quality constituents and (or) trend-related information are only provided when the underlying sample data met completeness thresholds for WRTDS nutrient trends based on procedures defined by Oelsner and others (2017). WRTDS trends are only published among years in which (1) quarterly data were available during the first 2 years and last 2 years of the trend period, (2) where at least 70 percent of years during the trend period had quarterly samples, and when (3) at least 14 percent of samples were categorized as high-flow samples for at least half the decades during the trend period, and at least 10 percent of samples were categorized as high-flow samples during the remaining half of decades in the trend period. However, unlike the criteria defined in Oelsner and others (2017), high-flow samples are defined as any sample in the 80th percentile (Oelsner and others [2017] used the 85th percentile) of flows for a given month and trend period for large coastal and inland river sites. This slightly reduced threshold for high-flow samples is consistent with findings in Oelsner and others (2017) that indicated lower high-flow thresholds were suitable for larger streams (page 72). See pages 38–39 in Oelsner and others (2017) for more details on data adequacy thresholds.

Because recent load estimates are more likely to change as additional years of water-quality and streamflow data are considered, the degree to which recent water-quality loads (actual and flow-normalized) change with the addition of new water-quality data was analyzed. This analysis can help users of these data better understand the certainty of recent water-quality load estimates. Twelve NWQN sites (table 3) at major subbasins in the Mississippi River Basin were selected to evaluate the certainty of recent WRTDS load estimates for as many as five constituents per site (depending on data availability), including total nitrogen, nitrate plus nitrite, total phosphorus, orthophosphate, and suspended-sediment concentration. The datasets used for this analysis began between 1980 and 1993 and extended through 2015 or 2016, depending on the site and constituent (U.S. Geological Survey, 2017a).

Each site and constituent were compared to evaluate how WRTDS load and flow-normalized load estimates change as additional years of calibration data (that is, water-quality and streamflow data) are considered. The WRTDS loads were computed using an initial calibration period that included the first 10 years of calibration data; successive WRTDS loads were then computed using each additional year of calibration data through the end of the record; for example, at the Mississippi River below Grafton, Illinois, (table 1; GRAF) a total of 25 WRTDS runs of total nitrogen were completed beginning with the 1981–91 initial calibration and ending with the 1981–2015 calibration (fig. 5). All annual and flow-normalized load estimates were retained from each WRTDS run, allowing an "age" to be assigned for annual load estimate based on how far a given year is from the last year of the water-quality calibration record used; for example, at GRAF,

Table 3. National Water Quality Network sites used to explore the variability of recent load estimates as new data are added to the calibration record.

[NO23, nitrate plus nitrite; OP, orthophosphate; SSC, suspended-sediment concentration; TN, total nitrogen; TP, total phosphorus; ALEX, Alexandria; R, river; @, at; LA, Louisiana; *n*, number of samples; --, not considered; CLIN, Clinton; IA, Iowa; GRAF, Grafton; IL, Illinois; GRAN, Grand Chain; HAZL, Hazleton; IN, Indiana; HERM, Hermann; MO, Missouri; LITT, Little Rock; L&D, Lock and Dam; AR, Arkansas; MELV, Melville; COE, Corps of Engineers; STRF, Saint Francisville; St., Saint; THEB, Thebes; VALL, Valley City; WAPE, Wapello; IA, Iowa]

Site abbreviation	Site name	NO23	OP	SSC	TN	TP
ALEX	Red R @ Alexandria, LA	1980–2015 (*n*=621)	--	--	1980–2015 (*n*=621)	1980–2015 (*n*=621)
CLIN	Mississippi River at Clinton, IA	1980–2015 (*n*=621)	1982–2015 (*n*=550)	1980–2015 (*n*=621)	1980–2015 (*n*=621)	1980–2015 (*n*=621)
GRAF	Mississippi River below Grafton, IL	1983–2015 (*n*=525)	1983–2015 (*n*=525)	--	1983–2015 (*n*=525)	1983–2015 (*n*=525)
GRAN	Ohio River at Olmsted, IL	1980–2015 (*n*=621)	1982–2015 (*n*=550)	1980–2015 (*n*=621)	1980–2015 (*n*=621)	1980–2015 (*n*=621)
HAZL	White River at Hazleton, IN	1993–2015 (*n*=231)	1993–2015 (*n*=231)	1993–2015 (*n*=231)	1993–2015 (*n*=231)	1993–2015 (*n*=231)
HERM	Missouri River at Hermann, MO	1980–2015 (*n*=621)	1981–2015 (*n*=585)	1980–2015 (*n*=621)	1980–2015 (*n*=621)	1980–2015 (*n*=621)
LITT	AR River @ David D Terry L&D below Little Rock, AR	1980–2015 (*n*=621)	1981–2015 (*n*=585)	1980–2015 (*n*=621)	1980–2015 (*n*=621)	1980–2015 (*n*=621)
MELV	(COE) Atchafalaya River at Melville, LA	1980–2015 (*n*=621)	1981–2015 (*n*=585)	1980–2015 (*n*=621)	1980–2015 (*n*=621)	1980–2015 (*n*=621)
STFR	Mississippi River nr St. Francisville, LA	1980–2015 (*n*=657)	1982–2015 (*n*=584)	1993–2015 (*n*=254)	1980–2015 (*n*=657)	1980–2015 (*n*=657)
THEB	Mississippi River at Thebes, IL	1980–2015 (*n*=621)	1981–2015 (*n*=585)	--	1980–2015 (*n*=621)	1980–2015 (*n*=621)
VALL	Illinois River at Valley City, IL	1980–2015 (*n*=621)	1982–2015 (*n*=550)	--	1980–2015 (*n*=621)	1980–2015 (*n*=621)
WAPE	Iowa River at Wapello, IA	1980–2015 (*n*=621)	1982–2015 (*n*=550)	1993–2015 (*n*=231)	1980–2015 (*n*=621)	1980–2015 (*n*=621)

there are 21 estimates of total nitrogen load (actual and flow-normalized) for 1995, which includes an estimate from each of the calibration datasets ending in 1995 through 2015 (fig. 5). The 1995 estimate determined using the 1981–95 calibration is assigned an age of “0” since the estimate year is at the very end of the calibration record. The 1995 estimate determined using calibration data from 1981 to 1996 has an age of 1 year because the 1995 estimate is now 1 year from the end of the calibration record. Similarly, the whole-record calibration has an age of 20 years because an additional 20 years of calibration data are considered between the year of the estimate (1995) and the end of the calibration record (2015).

To assess the potential variability of WRTDS estimates as new data are added, estimates from successive calibrations were compared to estimates using data from the entire calibration record. Models of WRTDS that use the entire calibration record were presumed to give the most accurate load estimates for any given year in the period of record. The percentage difference of estimates obtained using various calibration record lengths from the estimate obtained using the entire calibration dataset were used to illustrate the degree to which WRTDS estimates are likely to change as additional water-quality data are considered; for example, a flow-normalized, total nitrogen load of 506,000 tons per year was estimated for 1995 using the initial calibration dataset for GRAF from 1981 to 1995. With one additional year of calibration data (that is, a calibration record from 1981 to 1996), the 1995 estimate was reduced to 497,000 tons per year. The 1995 estimate obtained using the entire record (1981–2015) is 533,000 tons per year; thus, flow-normalized loads using the initial (1981–95) calibration and 1981–96 calibration were –5 percent different and –6.7 percent different from the whole-record calibration respectively. An example in which the percentage difference of estimates from successive-year calibrations of total nitrogen at GRAF are compared to whole-record estimates (estimates for year 1995 are highlighted in blue) is shown in figure 6. The outermost points on this plot illustrate the maximum percentage difference for a given age of load estimates and indicate how many additional years of calibration data were needed for load estimates to stabilize (for example, not fluctuate as more data are added to the calibration record).

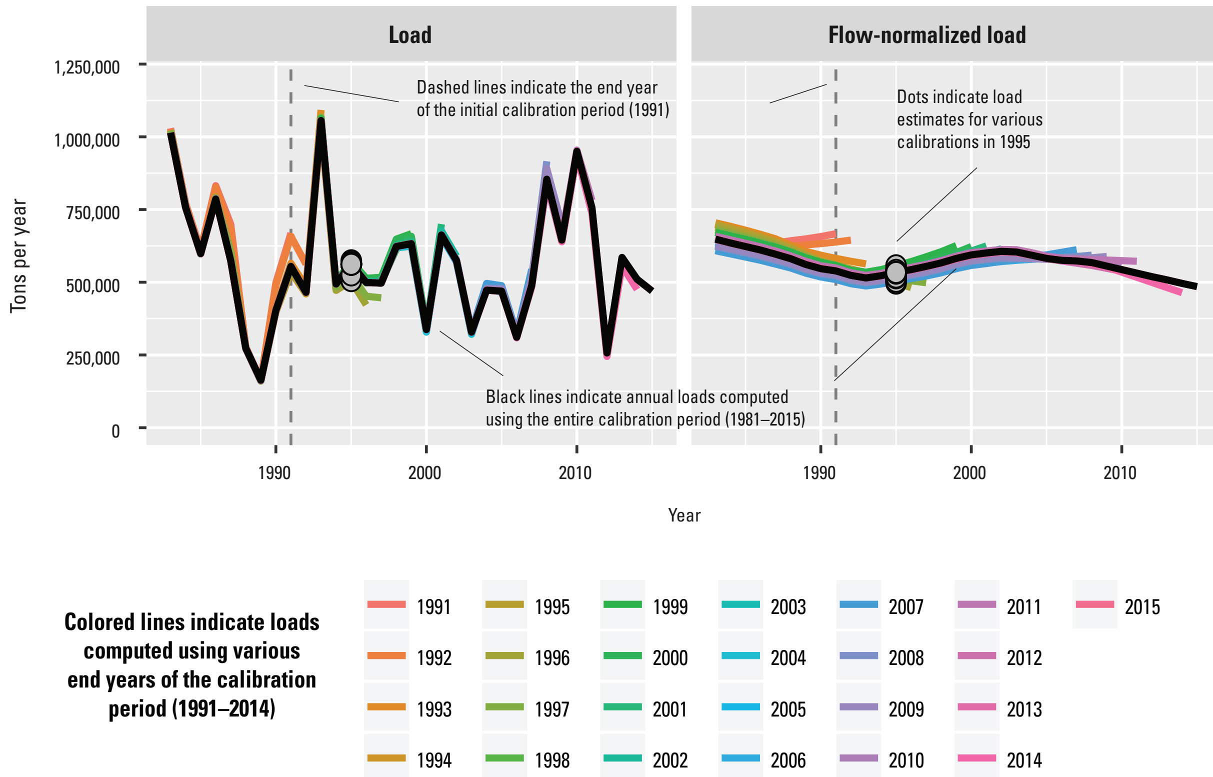


Figure 5. Results from successive calibrations of Weighted Regressions on Time, Discharge, and Season at the Mississippi River below Grafton, Illinois, for total nitrogen.

[WRTDS, Weighted Regressions on Time, Discharge, and Season]

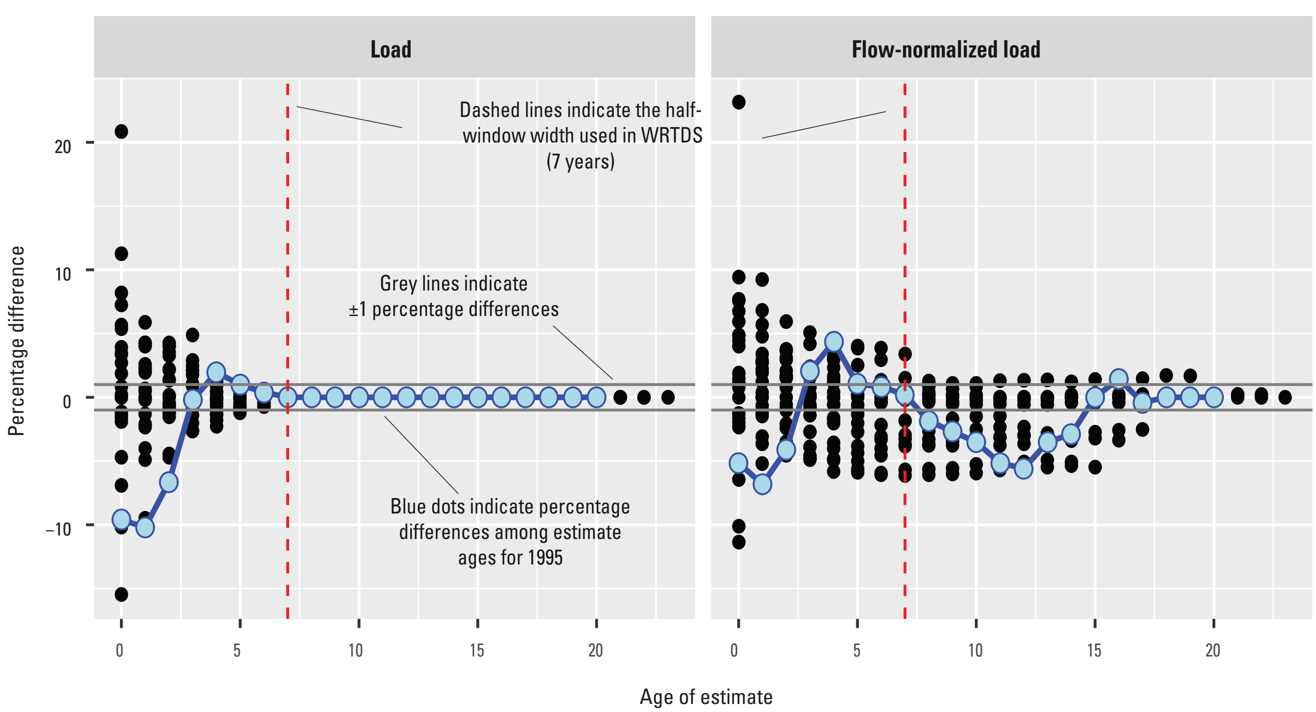


Figure 6. Percentage difference in total nitrogen load estimates of various ages compared to the whole-record estimate at the Mississippi River below Grafton, Illinois (U.S. Geological Survey station number 05587455).

Among all sites and constituents, the largest percent differences with whole-record estimates existed when the year of the estimate is the last year in the calibration period (age 0). Using total nitrogen at GRAF as an example, estimates for the last year of a calibration period can be 20 to 23 percent (for load and flow-normalized load, respectively) different from estimates for the same year using the whole-record calibration. As the age of the estimate increases (that is, more years of data between the estimate year and the end of the calibration record are added) the percentage difference compared to the whole-record estimate decreased. Load estimates were within ±1 percent of the whole-record estimate after about 6 years, which is not surprising given that the half-window width used for WRTDS is 7 years. The only time the actual load estimates could vary beyond 7 years is if window widths were automatically expanded during the model calibration process because there were too few samples (or relatively too many censored values); however, 20 additional years of calibration data were needed to obtain flow-normalized load estimates within ±1 percent different from the whole-record calibration at GRAF. Flow-normalized loads require more years primarily because the probability distribution of flows, which is used to compute flow-normalized loads, changes as each additional year of streamflow data are considered.

Among sites and constituents, loads computed without calibration data beyond the target year (i.e. an age of 0) were as much as 118 percent different from loads using the entire calibration period. Flow-normalized loads for estimates with an age of 0 were as much as 130 percent different from whole-record loads (fig. 7); however, load estimates generally converged rapidly to 0 as additional years were added to the calibration record, while flow-normalized load estimates were still relatively variable, even when calibration records extended 7 years beyond the estimate year.

Annual load computations for some constituents were more sensitive to additional calibration data than others. Flow-normalized suspended-sediment loads exhibited much more variability than other constituents near the end of calibration records (fig. 8). These loads were as much as 130 percent different from estimates that used the entire calibration period, whereas most of the other constituents were less than ±50 percent different. Flow-normalized total nitrogen and total phosphorus load estimates varied within ±10 percent of the whole-record estimate with 10 additional years of calibration data beyond the target year, whereas suspended sediment, orthophosphate, and nitrate plus nitrite took 12 to 14 years of additional data before flow-normalized load estimates were within ±10 percent (fig. 8). As with total nitrogen at the GRAF site, flow-normalized loads stabilized more slowly because additional years of streamflow data altered the probability distribution of streamflows used to estimate flow-normalized loads.

The number of additional years of calibration data (by site and constituent) beyond which both load and flow-normalized load estimates converged within ±10 percent of the whole-record calibration is shown in figure 9. For most sites

[WRTDS, Weighted Regressions on Time, Discharge, and Season]

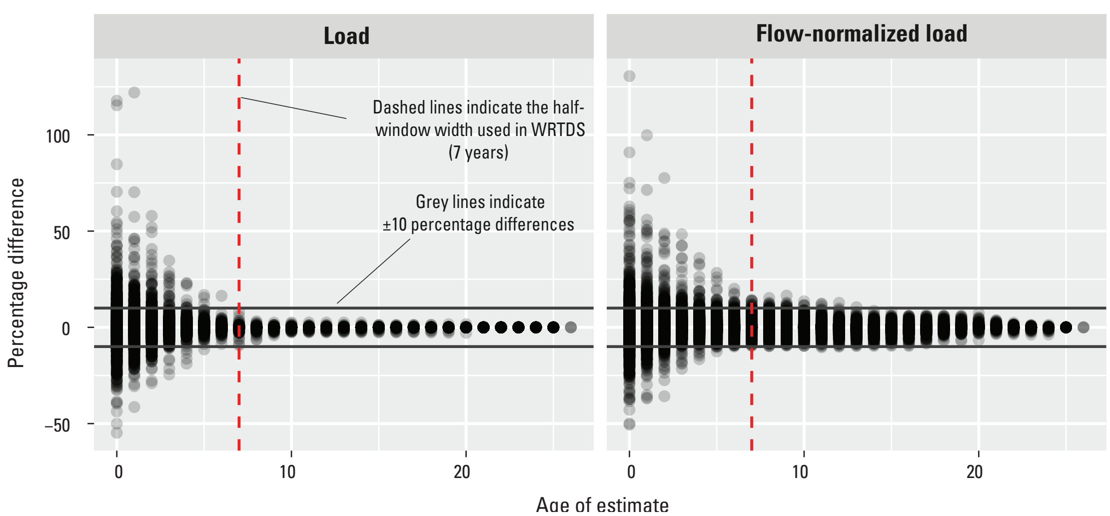


Figure 7. Percentage difference of annual loads using partial calibration periods from whole-record estimates for all constituents at the 12 selected sampling sites.

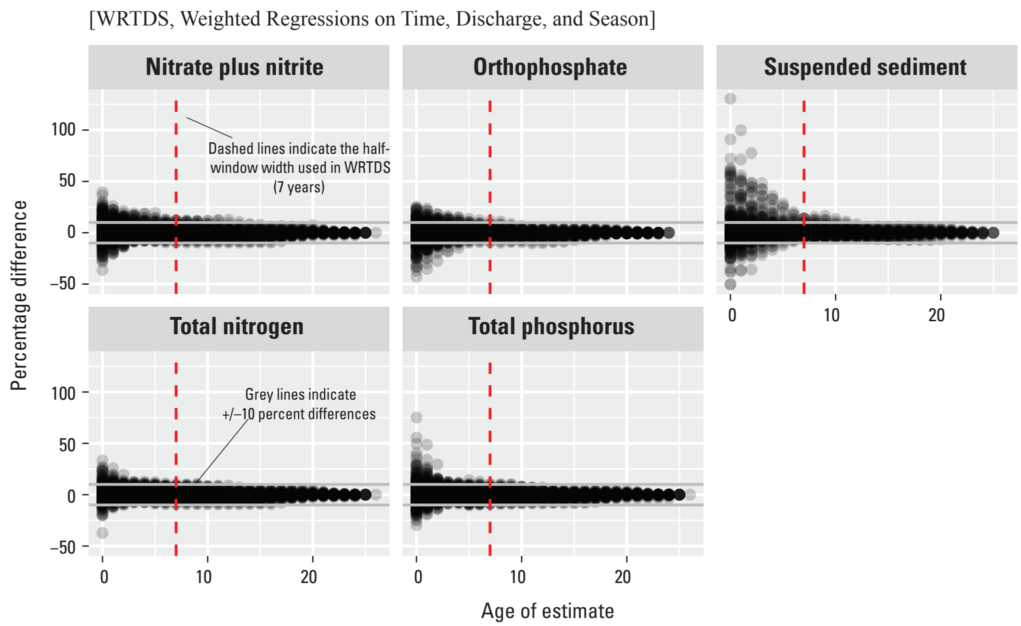


Figure 8. Percentage difference in flow-normalized annual loads for partial calibration periods compared to whole-record estimates at the 12 selected sampling sites.

and constituents, load estimates converged within ±10 percent of the whole-record estimate in less than 6 years (fig. 9); however, suspended-sediment load computations generally needed additional years of calibration to reach this criteria, whereas orthophosphate required additional years to reach ±10 percent at the Mississippi River at Clinton and the Iowa River at Wapello (fig. 9). At a few sites, the Red River @ Alexandria, the Missouri River at Hermann, and the Arkansas River at David D Terry Lock and Dam below Little Rock (table 3), flow-normalized loads required more than 5 years of calibration data for all constituents to converge within ±10 percent of the whole-record estimates (fig. 9).

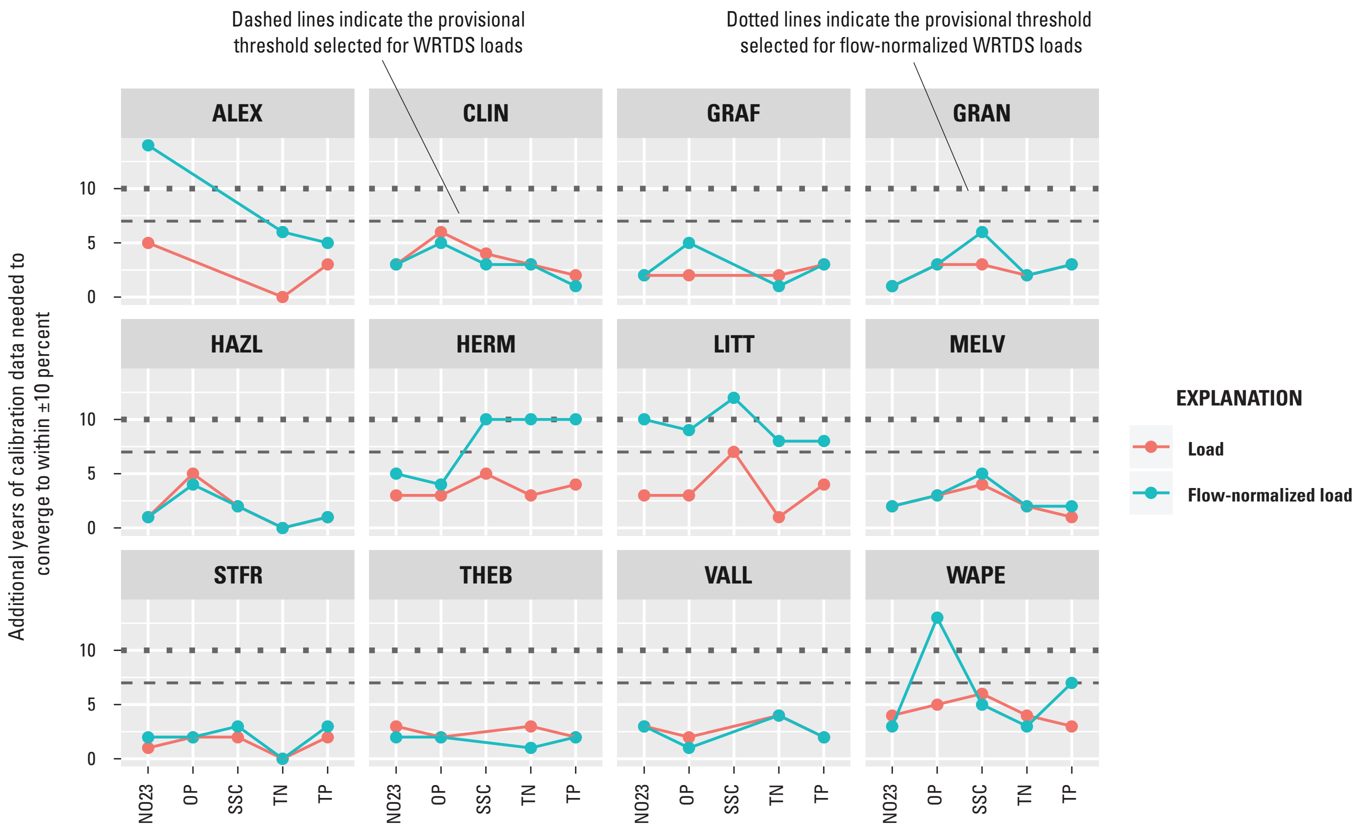
The sensitivity of load and flow-normalized load estimates computed at, or near, the end of the calibration record requires that these estimates be designated as “provisional.” To be consistent among sites and constituents, all load estimates less than 7 years from the end of the calibration record are considered provisional. Because of increased sensitivity, estimates 10 years or less from the end of the calibration record for flow-normalized loads are considered provisional.

Load Computations using Continuous Water-Quality Data

Before water year 2017, water-quality sensor data, such as water temperature, specific conductance, pH, dissolved oxygen, turbidity, and fluorescent dissolved organic matter (FDOM), were not used to compute loads at NWQN sites. Previous studies (Christensen and others, 2000; Rasmussen and others, 2005; Lee and others, 2008) have illustrated the potential for water-quality sensor data to improve estimates of concentrations and loads for some water-quality constituents, particularly during relatively short time intervals, such as for monthly loads. However, a major limitation to the use of water-quality sensor data in load computation is that these data are typically incomplete for a given water year because of sensor malfunctions, environmental fouling, ice, or other reasons.

Beginning in water year 2017, the natural log of continuous water-quality sensor data are considered as potential explanatory variables in the load computation process at NWQN sites (when available). As with estimates using continuous nitrate sensor data, in cases where sensor data are thought to improve the accuracy of load estimates but have less than 7 days of missing record during relatively stable streamflow conditions, missing data are linearly interpolated among measured values to obtain a complete record for the water year. Water-quality loads computed using continuous water-quality data are published in addition to streamflow-based load estimates.

When continuous water-quality data are thought to improve the accuracy of load estimates but these records have extended periods of missing data (or have missing record during changing streamflow conditions), an alternate method is required to estimate loads during these missing periods (including for nitrate sensor data). As described previously in the “Evaluation of Confidence Interval Summing Procedure” section, loads and confidence intervals are estimated by summing data from streamflow and continuous water-quality-based methods in quadrature.



[WRTDS, Weighted Regressions on Time, Discharge, and Season; ALEX, Red River near Alexandria, Louisiana; CLIN, Mississippi River at Clinton, Iowa; GRAF, Mississippi River below Grafton, Illinois; GRAN, Ohio River at Olmsted, Illinois; HAZL, White River at Hazleton, Indiana; HERM, Missouri River at Hermann, Missouri; LITT, Arkansas River at David D. Terry Lock and Dam below Little Rock, Arkansas; MELV, Atchafalaya River at Melville, Louisiana; STFR, Mississippi River at St. Francisville, Louisiana; THEB, Mississippi River at Thebes, Illinois; VALL, Illinois River at Valley City, Illinois; WAPE, Iowa River at Wapello, Iowa]

Figure 9. The number of additional years of calibration data (beyond a given estimate year) needed before load and flow-normalized load estimates converge within ±10 percent of corresponding whole-record estimate, by site, parameter, and estimate type.

Data Publication

Through successive annual data releases, NWQN discrete water-quality concentration, streamflow, and water-quality load data are published on the USGS ScienceBase platform (https://www.sciencebase.gov). Although the release of data from the most recent water year is the primary rationale for annual data releases, all historical data are republished in each new release to update historical loading data from sites that now have enough samples to publish loads from past years and to correct for any errors in the past release. The USGS Water Quality Tracking website (https://nrtwq.usgs.gov/nwqn; Lee and Henderson, 2020) provides maps and graphics to aid in the interpretation of concentrations, loads, and trends at NWQN sites, as well as links to the most recent ScienceBase release.

Summary

The U.S. Geological Survey publishes information on concentrations and loads of water-quality constituents at 110 sites across the United States as part of the U.S. Geological Survey National Water Quality Network (NWQN). This report describes historical and updated methods for computing loads at NWQN sites. Updates to load computation methods include (1) an adaptation to methods for computing loads to the Gulf of Mexico, (2) the inclusion of loads computed using the Weighted Regressions on Time, Discharge, and Season method, and (3) the inclusion of loads computed using continuous water-quality data. Beginning in water year 2019, loads computed using the Weighted Regressions on Time, Discharge, and Season with Kalman filtering method and continuous water-quality data will be published along with loads computed using historical methods. This report details and evaluates changes to load computation methods to aid users of water-quality loading information in determining which data best fit their particular application.

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