U.S. Geological Survey National Produced Waters Geochemical Database v2.0 (PROVISIONAL)

Documentation
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intervals, and workovers. Water samples are commonly collected when a well has production problems or during the initial development of a well. Although criteria were applied to remove the obviously contaminated samples, the culling of unrepresentative data is considered incomplete. Most obvious redundant entries were removed from the database, many of the records represent multiple samples of the same well. Therefore aggregate statistics may be weighted by relatively few wells.

Introduction

During hydrocarbon exploration and extraction, water is typically co-produced from the same subsurface geologic formations. Understanding the composition of these produced waters is important to help investigate the regional hydrogeology, the source of the water and hydrocarbons, the necessary water treatment and disposal plans, potential economic benefits of commodities in the fluids, and the safety of potential sources of drinking or agricultural water. Additionally, during geothermal development or exploration, other deep formation waters are brought to the surface and may be sampled. This U.S. Geological Survey (USGS) Produced Waters Geochemical Database, which contains geochemical and other information for produced waters and other deep formation waters of the United States, is a provisional, updated version of the 2002 USGS Produced Waters Database (Breit and others, 2002). In addition to the major element data presented in the original, the new database contains trace elements, isotopes, and time-series data, as well as nearly 100,000 new samples with greater spatial coverage and from both conventional and unconventional well types, including geothermal. The database is a compilation of 25 individual databases, publications, or reports. The database was created in a manner to facilitate addition of new data and fix any compilation errors, and is expected to be updated with new data as provided and needed. Table 1 shows the abbreviated names (IDDB) of each input database, the number of samples from each, and its reference. Table 2 defines the 241 variables contained in the database and their descriptions. The database variables are organized first with identification and location information, followed by well descriptions, dates, rock properties, physical properties of the water, and then chemistry. The chemistry is organized alphabetically by elemental symbol, each element is followed by any associated compounds (e.g. H_2S is found after S). After Zr, molecules containing carbon follow, including measures of alkalinity, dissolved organic carbon (DOC), and hydrocarbons. Isotopic data are found at the end of the dataset.

Database Compilation Procedure

Modification of the data or variable names is necessary to create a database with consistent headers, compositional units, and numeric data that can be plotted or analyzed as a whole. One of the main goals of this updated database is to create a compiled dataset where every change to the original datasets is reversible and recorded. Thus if errors are found, there is a coded record that can be adjusted as needed, and the compiled dataset can be easily recreated from scratch. To meet this goal, the USGS National Produced Waters Geochemical Database v2.0 is compiled using the statistical and data analysis program, Stata (StataCorp, 2014)[1]. A Stata routine is written for each input database that imports the original data,

[1] Disclaimer: Use of brand or trade names are for descriptive purpose and do not imply endorsement by the U.S. Government.

renames the variables to match the template (table 2), and then appends the existing columns to a template header. Non-numeric characters within numeric variables (for example, chemistry and pH) are fixed, deleted, or replaced with the following numeric codes:

-1 = Trace, minor, present, or a qualitative description of some amount.
-2 = None detected, absent, null, or negative
-3 = NA, not analyzed, unknown
-4 = Transcription error or otherwise nonsensical entry

Negative values are used for concentration data codes because all true concentrations are positive and therefore will not overlap with the codes. Negative values can easily be removed by the user when manipulating data. Furthermore, dates are formatted into a consistent date form and extra variables are removed. Units for all variables other than the major and minor ions are defined in table 2. The major and minor ions are generally reported in units of milligrams per liter (mg/L) or parts per million (ppm) on a mass basis, also defined as milligrams per kilogram (mg/kg). If the ion concentrations were originally reported in mg/L, a "1" is added to the MGL variable column of the database. If the ion concentrations were originally reported in ppm, a "1" is added to the PPM variable column of the database. The user of this database must be careful to examine these units when using the data, and can convert between the two using measurements or estimates of brine density.

Each individual input database is then appended to the template using a global Stata routine. The database is further standardized here with internally consistent 14-digit American Petroleum Institute well identification numbers (API), state names (STATE), and one of seven well type (WELLTYPE) designations (Conventional Hydrocarbon, Shale Gas, Tight Oil, Tight Gas, Coal Bed Methane, Geothermal, and Groundwater). Future standardization will be performed on other important variables such as FORMATION.

Removing duplicates

Duplicates were found within single datasets and between them. Duplicate culling is done using API well numbers and the concentrations of variables with large numbers of significant figures because it is highly unlikely that even samples taken from the same well at the same time will have the exact same values for three or more elements. API, Calcium (Ca), Chloride (Cl), and bicarbonate (HCO_3) concentrations are used to search for duplicates. Care was taken to avoid false duplicates (for example, where all three ions had the code of "-4" or all three ions had null data). There were 91,007 unique observations according to these duplicate search criteria, 8,352 groups of 2 observations (duplicates), 1,173 groups of 3 observations (triplicates), 156 groups of 4 observations, 13 groups of 5 observations, 5 groups of 6 observations, and 2 groups of 7 observations (table 3). After locating these duplicates, a second check was often performed using Mg, Na, or sample collection date to determine if they were true duplicates. The duplicate observation retained was generally the one in the database that contained more information. The order of which database had primacy follows the order of table 1.

Culling data based on chemistry

Quality control of the dataset can be performed by culling based on geochemical criteria. In this version 2.0 of the provisional database, the data that fall outside of the bounds of the following criteria are flagged, rather than culled. There are six temporary columns in the database that represent the failure of specific culling criteria, based on those published in Hitchon and Brulotte (1994). An "X" is placed in the columns shown in table 4 where the sample falls outside of the pH range of 4.5 – 10.5, where Mg > Ca, K > Cl, K > 5xNa, and the charge balance is greater than 5%.

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Tables

Table 1. Short names of input databases, number of samples after removal of duplicates, and references on input databases.

ID of database	Samples	Reference
USGSMAIN	62,792	Breit and others (2002)
USGSOK	9,304	Breit and others (2002)
USGSARK	1,125	Breit and others (2002)
ROCKIES	3,190	Department of Energy, National Energy Technology Laboratory (2005)
MICHIGAN	429	Vugrinovich (2013, written communication)
WYOGCC	9,263	Wyoming Oil and Gas Conservation Commission (2013)
BAKKEN	12	Thamke (2013, written communication)
PARADOX	89	Hanshaw and Hill (1969)
POWDERRIVERCBM	48	Rice and others (2000)
APPALACHIAN	1,644	multiple – see references
INDIANA	470	Keller (1983)
CBM	3,220	Dahm (2013, writen communication)
OHBRINE	579	Ohio DNR, Division of Geologic Survey (2013, written communication
PASHIN	126	Alabama Geological Survey (2013, written communication)
ARKMOLDOVANY	41	Moldovanyi and Walter (1992)
CIMAREX	2,891	Cimarex Energy Company (2013, written communication)
FERRON	49	Rice (2003)
ILLINOIS	347	Meents and others (1952)
MISSISSIPPI	82	Carpenter and others (1974)
MONTANACBM	21	Meredith and others (2010)
PALODURO	16	Bassett and Bentley (1983)
EASTPOPLAR	22	Thamke (2013, written communication)
NORTHDAKOTA	7,334	North Dakota Oil and Gas Division (2013)
ANTRIM	53	Walter and others (1997)
NATCARB	57,208	Department of Energy, National Energy Technology Laboratory (2013)
Total	**160,355**	

Table 2. Variable names and descriptions.

Variable Name	Description
IDORIG	ID in original database
IDDB	ID of database
SOURCE	Source of data
REFERENCE	Publication
LAT	Latitude
LONG	Longitude
FLAT	Field Latitude (estimate)
FLONG	Field Longitude (estimate)
API	API well number
USGSPROV	USGS Province
USGSREGION	USGS Region
BASIN	Basin
BASINCODE	Basin Code
STATE	State
STATECODE	State Code
COUNTY	County
COUNTYCODE	County Code
FIELD	Field
FIELDCODE	Field Code
WELL	Well name
WELLCODE	Well code
WELLTYPE	Well type
WELLCLASS	Well class
TOWNSHIP	Township
TWNDIR	Township Direction
RANGE	Range
RNGDIR	Range Direction
SECTION	Section
QUARTER	Quarter
REGDIST	Regional District
LOC	Location
QUAD	Quad
DATESAMPLE	Date of sample
DATEANALYS	Date of analysis
DATECOMP	Date of well completion
METHOD	Sample Method
OPERATOR	Well operator
DRILLER	Well driller
PERMIT	Well permit holder
FORMATION	Geologic formation name
DFORM	Geologic formation name of greatest depth
MEMBER	Geologic member name
GEOLAGE	Geologic age
AGECODE	Geologic Age code
ERA	Geologic Era name
SYSTEM	Geologic System name
SERIES	Geologic Series name
DEPTHUPPER	Upper perforation depth
DEPTHLOWER	Lower perforation depth
DEPTHSAMP	Depth of sample, may be average

Variable Name	Description
DEPTHTOTAL	Total depth of well
ELEVATION	Elevation of well
SUBSEA	Depth below seafloor
LAB	Laboratory
REMARKS	Remarks or comments
LITHOLOGY	Lithology
SILT	Silt 1 = sample is this rock type
SHALE	Shale 1 = sample is this rock type
SAND	Sand 1 = sample is this rock type
CHERT	Chert 1 = sample is this rock type
CARBONATE	Carbonate 1 = sample is this rock type
DOLOMITE	Dolomite 1 = sample is this rock type
LIMESTONE	Limestone 1 = sample is this rock type
ANHYDRITE	Anhydrite 1 = sample is this rock type
OTHERLITH	Other Lithology 1 = sample is this rock type
POROSITY	Porosity
PERM	Permeability
TEMP	Temperature, deg F
PRESSURE	Pressure, psi
SPGRAV	Specific Gravity
SPGRAVT	Temperature of Specific Gravity measurement, deg F
RESIS	Resistivity, Ohm m
RESIST	Temperature of Resistivity measurement, deg F
PH	pH
PHT	Temperature of pH measurement, deg F
EHORP	Eh / Oxidation Reduction Potential (mV)
COND	Conductivity, uS/cm
CONDT	Temperature of Conductivity measurement, deg F
TURBIDITY	Turbidity
SEDIMENT	Sediment
HEM	Oil and Grease
MBAS	Surfactants and Detergents
MGL	Units, mg/L; 1 = data are in these units
PPM	Units, mg/kg; 1 = data are in these units
TDS	Total Dissolved Solids, measured
TDSCALC	Total Dissoved Solids, calculated
TSS	Total Suspended Solids
CHARGEBAL	Charge Balance (%)
MASSBAL	Mass Balance (%)
Ag	Silver
Al	Aluminum
As	Arsenic
Au	Gold
B	Boron
BO3	Borate
Ba	Barium
Be	Beryllium
Bi	Bismuth
Br	Bromide
BrO3	Bromate
CO2	Carbon dioxide
CO3	Carbonate

Variable Name	Description
HCO3	Bicarbonate
Ca	Calcium
Cd	Cadmium
Ce	Cerium
ClO3	Chlorate
ClO4	Perchlorate
Cl	Chloride
ClO2	Chlorite
ClO	Hypochlorite
Co	Cobalt
Cr	Chromium
Cs	Cesium
Cu	Copper
F	Fluoride
FeTot	Iron, total
FeIII	Iron, 3+
FeII	Iron, 2+
FeS	Iron sulfide
FeAl	Iron plus Aluminum, reported as elements
FeAl2O3	Iron plus Aluminum, reported as oxides
Ga	Gallium
Ge	Germanium
Hg	Mercury
Hf	Hafnium
I	Iodine
In	Indium
Ir	Iridium
K	Potassium
KNa	Potassium plus Sodium
La	Lanthanum
Li	Lithium
Mg	Magnesium
Mn	Mangansese
Mo	Molybdenum
N	Nitrogen, total
NO2	Nitrite
NO3	Nitrate
NO3NO2	Nitrate plus Nitrite
NH3	Ammonia
NH4	Ammonium
TKN	Kjeldahl Nitrogen
Na	Sodium
Nb	Niobium
Ni	Nickel
O	Oxygen
DO	Dissolved Oxygen
OH	Hydroxide
Os	Osmium
P	Phosphorus
PO4	Phosphate
Pb	Lead
Pd	Palladium

Variable Name	Description
Re	Rhenium
Rh	Rhodium
Rb	Rubidium
Ru	Ruthenium
S	Sulfide
SO3	Sulfite
SO4	Sulfate
HS	Bisulfide
H2S	Hydrogen Sulfide
HSO4	Bisulfate
Sb	Antimony
Sc	Scandium
Se	Selenium
Si	Silica
Sn	Tin
Sr	Strontium
Ta	Tantalum
Te	Tellurium
Th	Thorium
Ti	Titanium
Tl	Thallium
U	Uranium
V	Vanadium
W	Tungsten
Y	Yttrium
Zn	Zinc
Zr	Zirconium
ALKTOTAL	Alkalinity, total
ALKCACO3	Alkalinity as CaCO3
ALKHCO3	Alkalinity as HCO3
ALKCO3	Alkalinity as CO3
ACIDITY	Acidity as CaCO3
DIC	Dissolved Inorganic Carbon
DOC	Dissolved Organic Carbon
TOC	Total Organic Carbon
CN	Cyanide
BOD	Biochemical Oxygen Demand
COD	Chemical Oxygen Demand
CH4	Methane
C2H3O2	Acetate
C2H4O2	Acetic Acid
C2H6O2	Ethylene Glycol
C3H6O	Acetone
C6H6	Benzene
C6H6O	Phenols
C7H8	Toluene
C8H10_XY	Xylene
C8H10_ETH	Ethybenzene
ALPHA	Alpha particle (4He), pCi/L
BETA	Beta particle, pCi/L
dD	delta 2H, per mil
H3	Tritium, 3H, tritium units

Variable Name	Description
d11B	delta 11B, per mil
B11_10	11B / 10B
d13C	delta 13C, per mil
C14	14C, pCi/L
d18O	delta 18O, per mil
d34S	delta 34S, per mil
d37Cl	delta 37Cl, per mil
K40	40K, pCi/L
Sr87_86	87Sr / 86Sr
Cs127	127Cs, pCi/L
I129	129I, pCi/L
Tl206	206Tl, pCi/L
Pb210	210Pb, pCi/L
Pb212	212Pb, pCi/L
Ra223	223Ra, pCi/L
Ra226	226Ra, pCi/L
Bi211	211Bi, pCi/L
Bi212	212Bi, pCi/L
Bi214	214Bi, pCi/L
Pb214	214Pb, pCi/L
Rn222	222Rn, pCi/L
Th227	227Th, pCi/L
Ac227	227Ac, pCi/L
Ac228	228Ac, pCi/L
Ra228	228Ra, pCi/L
Th228	228Th, pCi/L
Th230	230Th, pCi/L
Pa231	231Pa, pCi/L
Th232	232Th, pCi/L
Th234	234Th, pCi/L
Pa234	234Pa, pCi/L
U234	234U, pCi/L
U235	235U, pCi/L
Np237	237Np, pCi/L
U238	238U, pCi/L

Table 3. Observed duplicates in combined database based on exact same Ca, Cl, HCO3, and API.

Copies	Observations	Surplus
1	91007	0
2	16704	8352
3	3519	2346
4	624	468
5	65	52
6	30	25
7	14	12

Table 4. Chemical culling criteria for water data quality control.

Criteria	Column Name
pH < 4.5 or pH > 10.5	cull_PH
Mg > Ca	cull_MgCa
K > Cl	cull_KCl
K > 5xNa	cull_K5Na
charge balance > 5%	cull_CHARGEB and chargebalance