THESIS

DEVELOPMENT OF A GIS BASED TOOL TO ANALYZE PRODUCED WATER FROM

OIL AND GAS WELLS AND PREDICTION OF EQUILIBRIUM CONCENTRATIONS

USING CALCAQ

Submitted by

Ashwin Dhanasekar

Department of Civil and Environmental Engineering

In partial fulfillment of the requirements

For the Degree of Master of Science

Colorado State University

Fort Collins, Colorado

Fall 2013

Master's Committee:

    Advisor: Kenneth H Carlson

    Mazdak Arabi
    Sally Sutton

ABSTRACT

DEVELOPMENT OF A GIS BASED TOOL TO ANALYZE PRODUCED WATER FROM

OIL AND GAS WELLS AND PREDICTION OF EQUILIBRIUM CONCENTRATIONS

USING CALCAQ

New extraction techniques based on hydraulic fracturing and horizontal drilling have significantly increased the available oil and gas in the United States. Producing oil and gas from shale formations is the main source of these unconventional resources. When shale formations are hydraulically fractured to increase the permeability, up to 5 million gallons of water can be used for each well. The significant use of water has caused concerns by several stakeholders, particularly in regions that are constantly facing water shortages such as Texas or Colorado. After the well is fractured, large amounts of water return as frac flowback and then after the well is put into production, water that is coproduced with oil and gas must be collected for the life of the well. The produced water has hazardous characteristics since it has been in contact with oil and gas for millions of years and disposal or reuse is an important part of an oil and gas operation. Current water management for produced water includes underground injection and surface disposal or reuse. Owing to a large amount of total dissolved solids (TDS), metals and hydrocarbons (e.g. BTEX) in the produced water, the brine needs to be treated to achieve acceptable water quality for subsequent disposal or reuse. Reusing and recycling of produced water for drilling and fracturing after appropriate treatment has multiple advantages including less truck traffic and lower fresh water demands. The objective of the research in this thesis was to integrate the OLI chemical equilibrium model into the OWM (Optimized Water Management) tool framework to allow chemical equilibrium calculations to be made for each well and in the aggregate throughout the Wattenberg oil and gas field of northern Colorado. The calculations

from this model can then be used as design criteria for treatment train definition based on the desired water disposal outcome. OLI Systems software was developed for the chemical and oil and gas industry and is well suited as a module for calculating chemical equilibrium values for produced water and frac flowback water. The research described in this thesis includes predictions of equilibrium chemistry, solids precipitation and scale forming index, based on water quality data collected in the field. The model can also predict requirements for combining and treating produced water streams to achieve process objectives. At the same time, water quality will be analyzed after detailed sampling from various parts of the field. Finally, water quality after precipitation, settling and filtration has been used to estimate the osmotic pressure and design reverse osmosis processes for different levels of TDS rejection. This will be integrated with a customized ArcGIS tool that will help in predicting treatment specifics on a spatial scale.

ACKNOWLEDGMENTS

I would like to express my deepest appreciation to my advisor Dr. Ken Carlson for having the faith in me all along my time here at Colorado State University. Without his guidance and persistent help, this thesis would not have been possible. He has been the greatest mentor throughout my time here helping me out consistently in all aspects. In fact, it was under his tutelage that I developed a focus and became interested in the real world industrial applications of GIS. If not for him, I would not be where I am. I doubt that I will ever be able to convey my appreciation fully, but I owe him my eternal gratitude.

I would like to express my sincere thanks to Dr. Mazdak Arabi, for introducing me to the world of Geographic Information Systems, and changing my life forever. I would also like to thank Dr. Sally Sutton for being the nicest and always having the patience to listen and guide me with an ever-smiling face. I am truly grateful to Dr. James Hardy for bringing OLI into the picture.

I cannot find words to express my deepest gratitude to my team members Stephen Goodwin, Huishu Li, Bing Bai, Ildus Mingazetdinov, Amol Kitwadkar for their support and positive input. They each helped me make my time here more fun and enthralling. Special thanks to Mary Kay Wedum for her academic writing assistance. I am indebted to my best friend Asma Hanif who supported me throughout my time here with her care and support.

I would also like thank my uncle Dr.P.M.Gopinath for his unconditional love and financial support throughout my educational career. Last but not least, I would like to thank my parents Chitra and Dhanasekar for their patience and belief in me to pursue a Master's degree.

TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

Legend

● Oil & Gas Wells

— Highways

▢ Wattenberg Field

Data Source: COGCC Database, Colorado State University

A Map of the Wattenberg Field with its numerous Oil and Gas Wells

1

1. INTRODUCTION

1.1 Current Scenario and Limitations:

The state of Colorado is known for its semi-arid environment. This is one of the main reasons water resources are constrained here. The other important cause of concern is the historical agricultural needs. The oil and gas industry is experiencing new development in the country and therefore the pressure on water and other natural resources is bound to intensify. Hydraulic fracturing is one of the common methods used that is important to the new development. Its effects are causes of concern to water supply, air quality, water quality, ecosystem impacts and community impacts such as noise, truck traffic and road damage. Formation water is the water residing in formations where there are accumulations of oil and gas. Hydraulic fracturing is the process of pumping in water along with chemicals and sand to create fissures in rocks to extract oil and gas. The water which comes out during the initial drilling process is called flowback. The water which comes out after production starts is defined as produced water. This produced water is highly contaminated and requires different levels of treatment. Usually, in most cases, the produced water is injected into disposal pits, or deposited in evaporation ponds. The recycling of produced water is desirable since it is a valuable water resource even though it's contaminated. In some cases, it can be treated to be used as fracking fluid reducing the amount of freshwater used for the process of hydraulic fracturing. In order to do this, the produced water quality data should be collected for each specific area, since the produced water quality is relative to the formation water, thereby the characterization becomes really important. There is no real produced water quality data available for the public, this serves as a main limitation in most cases of treatment plans.

1.2 Framework of Thesis:

The main objective of the research was to utilize a chemical equilibrium model and link it with a GIS database that is primarily used to display the data to the end user. This tool was developed using ESRI's ArcGIS Online program, in such a way that it could be hosted on a single server or computer and people could view the end product without buying or installing additional software. An additional objective was to develop a link between the Excel file with CalcAQ programming to the GIS map hosted on ArcGIS online. This was done using re-programming on one of ESRI's commercially available tools. The structure of the thesis will be in three parts:

GIS Tool Development:

This part involves collecting data, creating databases, processing them and implementing them in an ArcGIS Map in order to analyze them spatially.

Chemistry Analyzer Modeling:

This part involves collecting water quality data, processing and modeling an analyzer tool based on the current water quality.

Integrating the GIS tool and the Chemistry Tool:

This part involves integrating the GIS tool and the Chemistry Model to develop a user-friendly application.

The tool as presented here is Phase I of the upcoming two-year, DOE-funded project "Development of GIS Tools for Optimization of Fluids Management for Shale Gas Operations".

2. LITERATURE REVIEW

2.1 Recent developments in the Shale Gas industry

Since the first natural gas production started in 1821 from an organic rich shale, it has come a long way to where it is now (Curtis 2002). North America, along with Europe is on the higher end of consumption of natural gas for electricity and heat production (Siemek, Nagy et al. 2013). Horizontal drilling and hydraulic fracturing, being some of the popular shale gas production techniques, are being used in a constantly increasing natural gas industry in huge reserve areas like the Marcellus Shale (Weltman-Fahs and Taylor 2013). Hydraulic fracturing is one of the most popular, and commonly used methods for maximizing well performance (Dmour 2013). Hydraulic fracturing is now a common process engaged by the industry for extracting oil and gas from underground resources inaccessible by regular drilling. This has clearly led the path for making new commercial sources available (Hatzenbuhler and Centner 2012). Some of the shale plays actively involved in the industry today is depicted in Figure 1.

The early 21st century saw a steady decline of the US gas production despite increased drilling activity, but the shale gas phenomenon picked up from 2004 and brought back the momentum (Rogers 2011). Many gas companies are changing their attention from the relatively easy to access conventional reservoirs in order to gain entry to the large volumes available in the shale formations even though they are complex to develop (Warlick 2006).
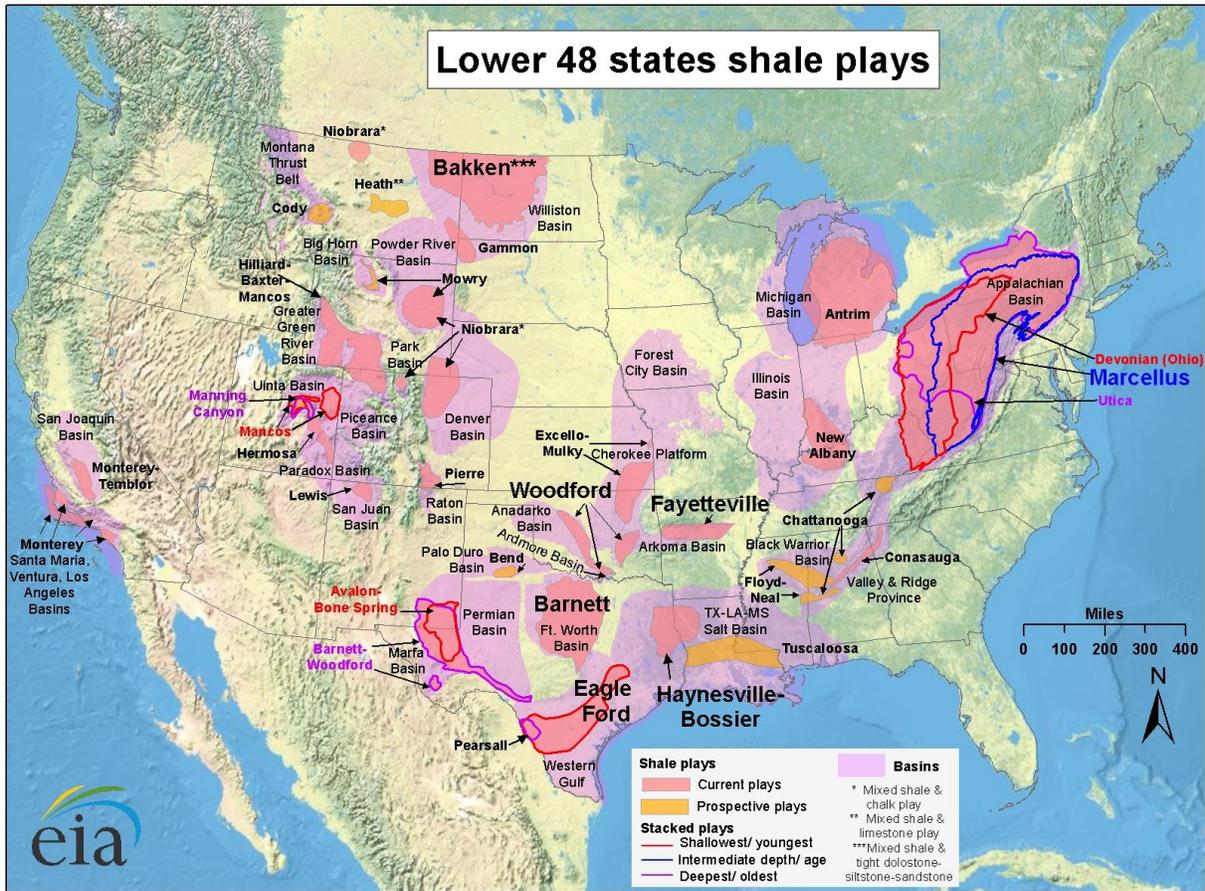
Figure 1.   An illustration of the shale plays in the US (Source: EIA Website)

Additions to the natural gas production associated with shale gas activity have been instrumental in increasing overall wet gas proved reserves. Shale gas has accounted for more than 90 percent of total additions. Key shale states in 2009 included Arkansas (the Fayetteville Shale), Louisiana (the Haynesville), Oklahoma (the Woodford), Pennsylvania (the Marcellus), and Texas (the Barnett and Haynesville/Bossier) (EIA Website 2009).

North America has a vast amount of shale gas, cumulative about 5,146 Tcf (146 trillion cubic meters). In the five leading shale gas basins, Barnett basin, Fayetteville basin, Woodford basin, Haynesville basin and Marcellus basin, up to 3,760 trillion cubic feet of shale gas is stored underground and over 12% of the total shale gas is a recoverable resource (CSM Website 2009).

Hydraulic fracturing has proven to be the key technology to facilitating economic recovery of natural gas from shale. While methods of hydraulic fracturing continually change (mostly changes in the design process and updates to additives and propping agents), this technology is utilized by the natural gas industry to increase production and to support an ever increasing demand for energy (Arthur, Bohm et al. 2009).

Water required for drilling and fracturing depends largely upon the type of wells being drilled. Usually, horizontal wells need much more water than vertical and directional wells due to the long distance. For each stage of a hydraulic fracture, an average of 5,000 gallons (119 bbl. diluted acid stage) up to 50,000 gallons (1190 bbl. prop stages) of fracturing fluid is needed, which means that the entire fracture operation would require approximately 2-4 million gallons of water, 3 million gallons (71,428 bbl.) being most common (Satterfield, Mantell et al. 2008).

A regular horizontal well needs approximately 600,000 gallons (14,000 bbl.) for drilling and 2-4 million gallons of water for hydraulic fracturing. For vertical and directional wells, water needed for fracturing is between 100,000 and 1,000,000 gallons (2,300 – 23,000 bbl.). Also, substantial amounts of water are needed for hydraulic fracturing, usually several times more than for drilling (DOE 2009).

One of the challenges of the hydraulic fracturing process is the fact that it relies on the use of chemical additives to ensure that the fracturing functions well. Water consumed by hydraulic fracturing contains more than 99% water and sand, with low probability of fracture fluid migration from the shale up to fresh water zones. Although the percentage of chemical additives in typical hydraulic fracture fluid is usually less than 0.5 percent by volume, the quantity of fluid used in these hydro-fractures is so large that the additives in a three million gallon hydro-fracture operation will be considerable (Halliburton 2008).

2.2 Current Environmental Practices

One important concern about the production of shale gas is the consideration of the possibility that hydraulic fracture fluid leaking upward along an interconnected network of fractures may contaminate groundwater. Though it's been an advantage to have shale gas as a potentially high domestic source of energy, the concerns for its impacts on the environment are growing. Earthquakes have an increased possibility because of horizontal drilling. Groundwater contamination is always a big concern, when the drilling is really deep. Land destruction and air pollution are also considered equally big concerns with these production activities (Hatzenbuhler and Centner 2012).

Oil and gas production is bound to have defective well completions and surface spills as a possibility in some cases. There are also abandoned wells and faults, other potential environmental risks (Nicot and Duncan 2012).

Produced water contains a lot of toxins, which are released to the atmosphere, when it's stored in evaporation ponds or fracking ponds waiting for recycling. These mix with the water table with

rain. These toxins may enter the human body with ingestion of contaminated water, or through the air we breathe or it might penetrate through the skin (Lauver 2012).

Some of these environmental threats were cited by the EPA when it estimated 35,000 wells were fractured every year. When each well requires around 2-4 million gallons of water, the 35,000 wells represent water consumption by 5 million people for a year. Since this water is mostly transported by trucks, road systems are disintegrated, and accidents happen with an increased risk (Schmidt 2011). Also, chemicals make up 0.5-20% of what's found in fracing fluids. Earlier studies done at Colorado State University about the life cycle analysis of water use and the intensity of oil and gas recovery in Wattenberg field have been used as a base. The water intensity was assessed by a detailed material balance as shown in Figure 3 below (Goodwin, Carlson et al. 2012).
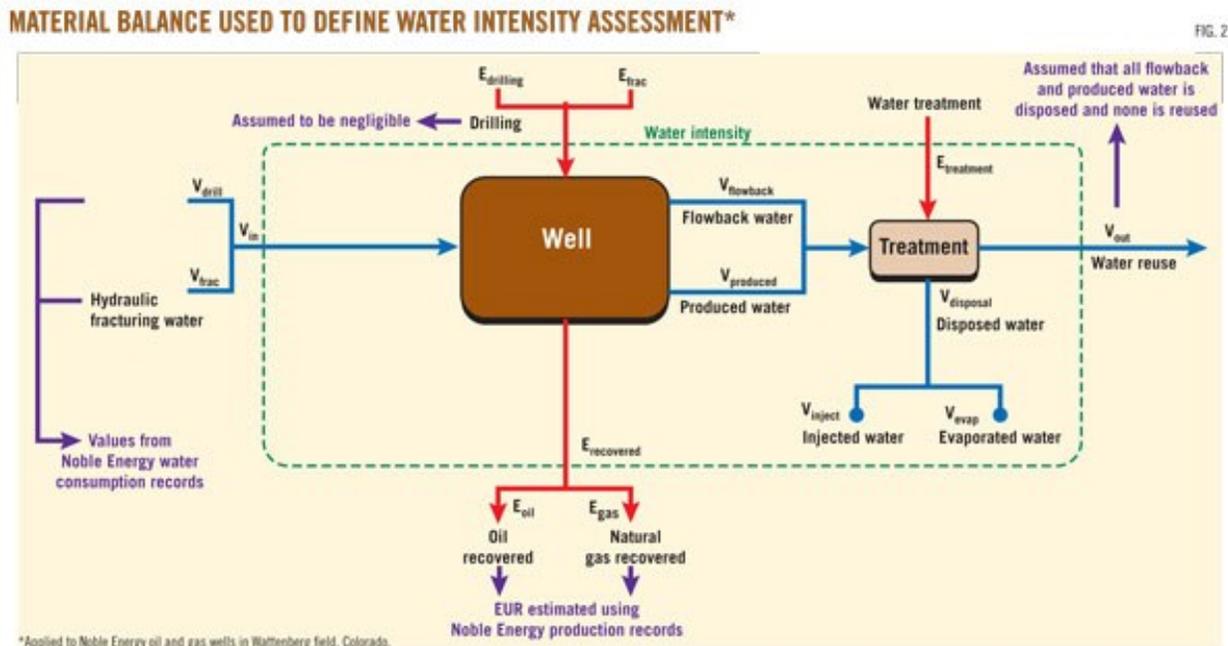
Figure 2.   Material balance used to define water intensity assessment (Goodwin, Carlson et al. 2012)

The natural gas industry believes fracing has never contaminated groundwater. Groundwater resources are protected by thousands of feet of intervening rock between aquifers and shale gas deposits located deeper underground (as shown in Figure 4).
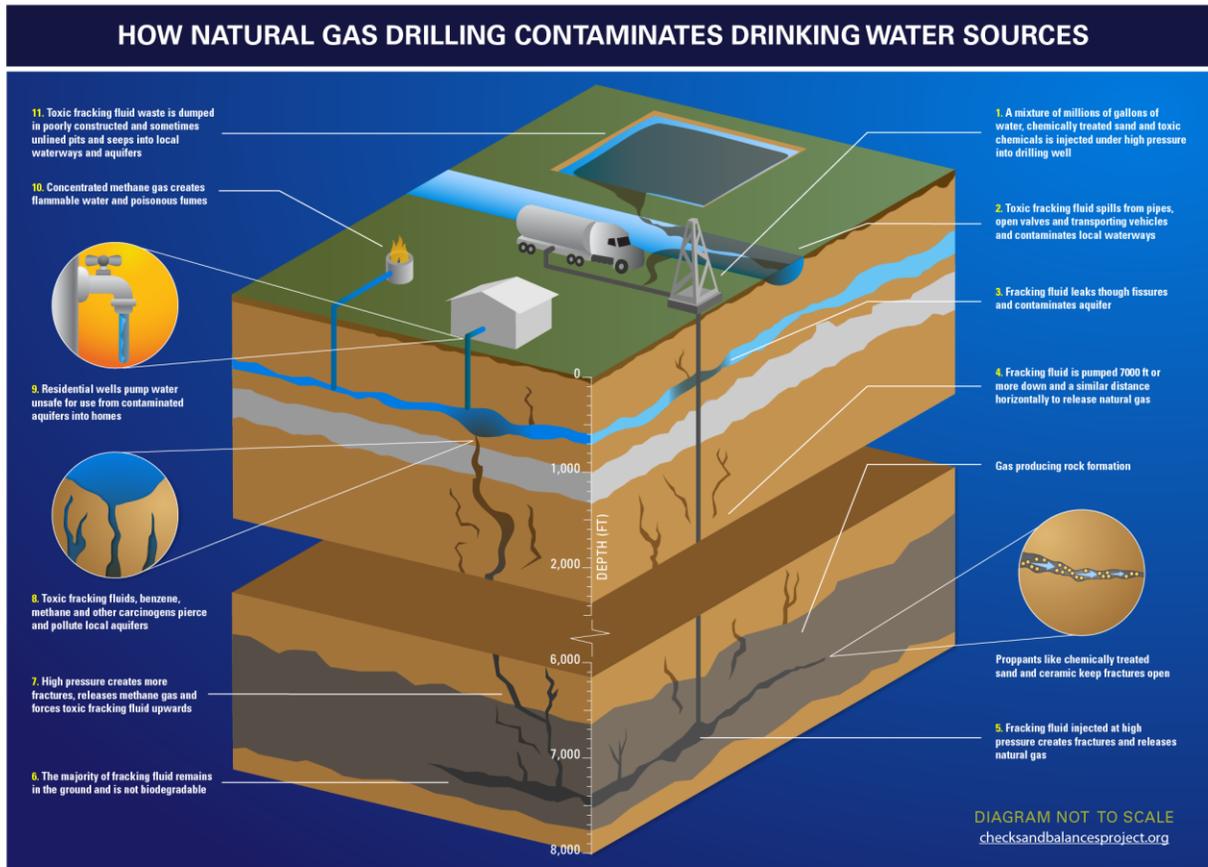
Figure 3.   Natural gas drilling's contamination effects (Source: Texas Green Report (checksandbalanceproject.org))

2.3 Produced Water Volumes:

Produced water is essentially water from underground formations that is brought to the surface during oil or gas production. Produced water is probably the largest volume by-product or waste stream associated with oil and gas exploration and production (Veil, Puder et al. 2004). Hence, it

is key to manage such a huge volume of water for any oil and gas producer. Early estimates of national produced water volume are in the range of 15 to 20 billion barrels (bbl.; 1 bbl. = 42 U.S. gallons) equivalent to a volume of 1.7 to 2.3 billion gallons per day. For example, a backyard swimming pool that is 20 ft wide by 50 ft long and 5 ft deep can be considered in comparison. The volume of water needed to fill such a pool is about 37,000 gal or about 900 bbl.

Geological characteristics differ from shale to shale and they occur in areas with different water resources and demand. For instance, Eagle Ford Shale located in Texas has nearly no flowback water after hydraulic fracturing, while in the Marcellus shale play, 20-40% of the injected water volume has flowed back (Jarvie, Hill et al. 2007).

It is estimated that more than 2 million gallons of water per well is being used in fracturing operations, and most of that water is then re-injected for disposal. More than 50% of this produced brine can be reused in subsequent well fractures, and 24% can be recovered as fresh water for beneficial use (Kurihara, Yamamura et al. 1999). The recovery volume is between 20 to 40% of the volume that was initially injected into the well. The rest of the fluid gets absorbed into the shale gas formation. A standard flowback of drilling fluids might be up to 40,000 bbl. After the first 3-4 week recovery of drilling fluids, after fracturing, an additional 12,000 to 32,000 bbl of produced water might flow for up to two years (Rey, Rey et al. 2010). Typically, 500,000 to 600,000 gallons per well will be generated in the first 10 days in the Barnett, Fayetteville and Marcellus shale plays, representing 10% to 15% of the total water used in fracturing and drilling. In contrast, 250,000 gallons per well is generally produced in the first 10 days in the Haynesville shale play, which is actually just 5% of the total water injected.

The volume of produced water from conventional oil and gas wells does not remain constant, and it increases progressively with the age of the crude oil and natural gas well. API calculated a water-to-oil ratio of approximately 7.5 barrels of water for each barrel of oil produced for the conventional hydrocarbon productions. For the survey of 2002 production prepared for this white paper, the water-to-oil ratio was calculated to have increased to approximately 9.5. For crude oil wells reaching the end of their lives, it has been reported that water can comprise 98% of the material brought to the surface. These stripper wells can produce 10 to 20 bbl (barrel) of water for each barrel of conventional crude oil produced (Wiedeman 1996).

2.4 Produced Water Quality:

Produced water, derived from seawater or formation water, has a high concentration of dissolved solids and other chemical ions due to multiple reactions with formation rocks. It is a combination of formation water and fracture fluids. The composition of fracturing fluids is described in Table 1.

The produced fluid composition is dependent on factors such as whether crude oil or natural gas is being produced, and also its constituents such as hydrocarbons, produced water, dissolved or suspended solids, sand, silt, injected fluids, additives, and all other constituents in the formation when early exploratory research was conducted before actual drilling began. Geographic location also has a diverse effect on the chemical and physical properties of produced water (McFarlane, Bostick et al. 2002) as does the geological formation which has been in contact with the produced water and the hydrocarbon. Understanding the produced water is essential for regulatory compliance and also for the selection of treatment or disposal options.

11

Table 1. Fracturing Fluid Additives, Main Compounds and Common Uses.

(Source: http://geology.com/energy/hydraulic-fracturing-fluids/)

Additive Type	Main Compound(s)	Purpose	Common Use of Main Compound
Diluted Acid (15%)	Hydrochloric acid or muriatic acid	Help dissolve minerals and initiate cracks in the rock	Swimming pool chemical and cleaner
Biocide	Glutaraldehyde	Eliminates bacteria in the water that produce corrosive byproducts	Disinfectant; sterilize medical and dental equipment
Breaker	Ammonium persulfate	Allows a delayed break down of the gel polymer chains	Bleaching agent in detergent and hair cosmetics, manufacture of household plastics
Corrosion Inhibitor	N,n-dimethyl formamide	Prevents the corrosion of the pipe	Used in pharmaceuticals, acrylic fibers, plastics
Crosslinker	Borate salts	Maintains fluid viscosity as temperature increases	Laundry detergents, hand soaps, and cosmetics
Friction Reducer	Polyacrylamide	Minimizes friction between the fluid and the pipe	Water treatment, soil conditioner
	Mineral oil		Make-up remover, laxatives, and candy
Gel	Guar gum or hydroxyethyl cellulose	Thickens the water in order to suspend the sand	Cosmetics, toothpaste, sauces, baked goods, ice cream
Iron Control	Citric acid	Prevents precipitation of metal oxides	Food additive, flavoring in food and beverages; Lemon Juice ~7% Citric Acid
KCl	Potassium chloride	Creates a brine carrier fluid	Low sodium table salt substitute
Oxygen Scavenger	Ammonium bisulfite	Removes oxygen from the water to protect the pipe from corrosion	Cosmetics, food and beverage processing, water treatment
pH Adjusting Agent	Sodium or potassium carbonate	Maintains the effectiveness of other components, such as crosslinkers	Washing soda, detergents, soap, water softener, glass and ceramics
Proppant	Silica, quartz sand	Allows the fractures to remain open so the gas can escape	Drinking water filtration, play sand, concrete, brick mortar
Scale Inhibitor	Ethylene glycol	Prevents scale deposits in the pipe	Automotive antifreeze, household cleansers, and de-icing agent
Surfactant	Isopropanol	Used to increase the viscosity of the fracture fluid	Glass cleaner, antiperspirant, and hair color

Note: The specific compounds used in a given fracturing operation will vary depending on company preference, source water quality and site-specific characteristics of the target formation. The compounds shown above are representative of the major compounds used in hydraulic fracturing of gas shales.

Oil and grease are also constituents of produced water which might receive a lot of attention in both onshore and offshore operations, while salt content (expressed as salinity, conductivity, or TDS) is a primary constituent of concern in onshore operations. Produced water contains many organic and inorganic compounds. These vary greatly according to the location and even temporally in the same well (Zangaeva 2010). The physiochemical properties of fresh and formation water samples in various compositions, tested in earlier research are presented in Table 2.

Table 2. Physiochemical properties of fresh and formation water samples (Stevenson 1997):

S/N	PARAMETERS	A	B	C	D	E	F	G	H
1.	pH	4.43	5.03	6.10	9.34	4.80	6.35	5.26	7.94
2.	Temperature ($^{\circ}$F)	79	185	73	185	76	185	77	185
3.	TDS (mg/l)	51	78	120	430	57	77	73	108
4.	EC (μScm^{-1})	105	155	241	850	115	155	147	218
5.	Colour (PtCo)	0.0	0.0	10.0	3.0	3.0	0.0	5.0	0.0
6.	Oil & Grease (mg/l)	0.0	0.0	4.35	1.40	0.32	0.2	2.70	0.6
7.	PO_4^{3-} (mg/l)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
8.	SO_4^{2-} (mg/l)	0.0	0.0	9.02	6.74	<0.001	0.0	<0.001	0.0
9.	Cl^- (mg/l)	<0.001	<0.001	0.10	0.10	<0.001	<0.001	<0.001	<0.001

A = 100% Lab Water (82₀F), B = 100% Lab water (185₀F), C = 100% Formation Water (82₀F), D = 100% Formation water (185₀F), 90% Lab water +10% Formation water (82₀F), F = 90% Lab water + 10% Formation water (185₀F), G = 50% Lab water + 50% Formation water (82₀F), H = 50% Lab water + 50% Formation water (185₀F)

The inorganic constituents of produced water are determined by the geology of the basin. The quantity and characteristics of organic contaminants in produced water is impacted by a number of factors like the type of hydrocarbon product the water is in contact with, the volume of water produced, the lift technique used and the age of production (Benko and Drewes 2008). The organic data presented in Table 3 was derived from sources that reported on the organic content of produced water. The data presented in Table 3 does not differentiate between water from oil operations and water from gas operations, still, water from gas production tends to have higher

concentrations of low molecular-weight aromatic hydrocarbons, such as benzene, toluene, ethyl benzene, and xylene, than water from oil production (Benko and Drewes 2008). Small concentrations of volatile organics are found in 75 to 80% of all gas produced water samples. Semi volatile organics are rarely found in gas produced water and are much more prevalent in oil produced water (Benko and Drewes 2008).

Table 3. Concentration ranges of organic material in produced water from conventional oil and gas (Benko and Drewes 2008)

Constituent	Low	High	Median	Technique (method)	Reference
TOC (mg/L)	ND	1,700	Unknown	UV Oxidation/IR (EPA 415.1)	Tibbetts et al. 1992
TSS (mg/L)	1.2	1,000	Unknown	Gravimetric (EPA 160.2)	Tibbetts et al. 1992
Total volatile organics (mg/L)	0.39	35	Unknown	GC/MS (EPA 1624 Rev B and EPA 24 & CLP)	Tibbetts et al. 1992
Total polar compounds (mg/L)	9.7	600	Unknown	Florisil column/IR	Tibbetts et al. 1992
Volatile fatty acids (mg/L)	2	4,900	Unknown	Direct GC/FID of water	Tibbetts et al. 1992
Total recoverable oil and grease (mg/L)	6.90	210.0	39.8	Unknown	Science Applications, 1994
2-Butanone (mg/L)	ND	0.37	Unknown	Unknown	Wesolowski et al., 1986
Benzene (mg/L)	ND	27	10	EPA Method 1624 and 624	Fillo et al., 1992
Benzoic acid (mg/L)	ND	13.5	3.80	Unknown	Science Applications, 1994
Bis (2-chlorethyl) ether (mg/L)	ND	0.03	Unknown	Unknown	Wesolowski et al., 1989
Ethyl benzene (mg/L)	ND	19	1.8	EPA Method 1624 and 624	Wesolowski et al., 1989
Hexanoic acid (mg/L)	ND	3.43	0.815	Unknown	Science Applications, 1994
Methylene Chloride (mg/L)	1.41	1.71	0.179	Unknown	Science Applications, 1994
m-xylene (mg/L)	0.015	0.611	0.137	Unknown	Science Applications, 1994
Naphthalene (mg/L)	ND	0.556	0.119	Unknown	Science Applications, 1994
N-decane (mg/L)	ND	0.797	0.116	Unknown	Science Applications, 1994
N-dodecane (mg/L)	ND	2.89	0.245	Unknown	Science Applications, 1994
N-hexadecane (mg/L)	ND	1.11	0.298	Unknown	Science Applications, 1994
N-octadecane (mg/L)	ND	0.246	0.106	Unknown	Science Applications, 1994
N-tetradecane (mg/L)	ND	0.404	0.138	Unknown	Science Applications, 1994
p-cresol (mg/L)	ND	0.541	0.123	Unknown	Science Applications, 1994
Phenol (mg/L)	0.009	23	NA	Silylation GC/MS	Tibbetts et al., 1992
Toluene (mg/L)	ND	37	9.7	EPA Method 1624 and 624	Fillo et al., 1992

ND, below detection limit; unknown, information was not provided by reference.

The composition of produced water is capable of varying with a dependence of various factors such as location, extraction type, chemicals used, and the well age. These qualities are spatially varying and need to be analyzed independently according to their location. The characteristics include salinity, TDS, pH, DO and conductivity. The treatment of these varying characteristics may potentially increase the reuse of water for irrigation purposes (Murray-Gulde, Heatley et al. 2003).

When produced water is treated or distilled, the salt content which is filtered out must still be transported and disposed of properly. Common constituents in produced water are described in Table 4.

Table 4.   Common components in produced water (McFarlane, Bostick et al. 2002)

Organic compounds	Inorganic components	Production chemicals
Aliphatic, aromatic, polar compounds, e.g., fatty acids, oil, grease, benzene, phenol	Na^+, K^+, Ca^{2+}, Mg^{2+}, Cl^-, SO_4^{2-}, CO_3^{2-}, silicates (H_4SiO_2), borates (H_3BO_3)	Emulsion breakers to improve separation of oil and water, corrosion inhibitors

2.5 Equilibrium Chemistry Software

Problems with pH calculations, solubility calculations, and redox calculations are complex issues for researchers and students in the field of chemistry or advanced chemical engineering. The easiest way to solving these problems is to write out the equilibrium expressions or the K equations and their corresponding equations such as mole balance, charge balance, while making simple assumptions along the way wherever useful and possible, and finally to combine the remaining equation to solve the resulting polynomial. These problems are very time consuming even for a simple setup such as one acid in water or a one dissolving salt. Environmental engineers and water engineers among many have to deal with such problems every day in the

field. For this purpose, they use many different software packages ranging from simple to very detailed.

Most equilibrium software is thought of as having two critical parts: the algorithm to solve any distinct industrial problem, and the complete datasets that contains the thermodynamic constants or K values for all these problems. Additional constituents such as ionic strength corrections, adsorption equations, and titration simulations, however, vary from program to program.

A dependable aqueous equilibrium chemistry calculator must have an interactive and self-instructive interface for clarifying reactions, the ability to work with all kinds of common equilibrium reactions, a strong solution algorithm, expressive and easily understandable displays for results, and the ability to produce results in multiple formats according to different use requirements. Depending on the application it's being used for, it may be more sensible to include a database of reactions relevant to this specific purpose, specific models of complex systems or the ability to vary temperature, pressure and ionic strength. For example, the OLI Systems Analyzer can do all this with the additional option of customizing every feature according to requirements and simulating them using the OLI ESP Program (OLI Website 2005).

The Stream Analyzer is OLI's simplest and clearest answer to the electrolyte thermodynamic water problems of the oil and gas industry. This software features single point equilibrium calculations, multiple point survey calculations for calculating a complete trend analysis for characteristics like temperature, pressure, pH and composition effects, and simple mix and separate capability. The calculations provide vapor, liquid, solid, and 2nd liquid phase separations for a fully specialized model. Properties such as pH, ORP, viscosity, density, enthalpy as well as compositions are reported (OLI Website 2005).

The program computes the gas-liquid-oil-solid chemistry part of produced fluids, and provides operators and engineers with clear chemical analysis about their wells, surface facilities, and water injection and disposal operations, thereby helping them understand processes better. ScaleChem is software from OLI which works with specialties like brines, gases, and hydrocarbons, collected as samples and input into the program (Amiri and Moghadasi 2010). Calculation types include a scale scenario that is general for well profiles, mixing waters to find non-scaling ratios, reservoir equilibrium to simulate downhole conditions, and facilities with simple mix and separate abilities to simulate collection and disposal" (Amiri, Moghadasi et al. 2013). Output includes the (thermodynamic) scale tendencies for all solids in the model, as well as scale amount produced, if any (Amiri and Moghadasi 2012). ScaleChem was written originally by Shell Oil Company using the OLI thermodynamic model. OLI has maintained, extended and supported ScaleChem and ScaleChem clients since then (OLI Website 2005). In addition, ScaleChem simultaneously has the ability to compute scale tendency and deposition at key process points (OLI Website 2005).

CalcAQ which is an add-on to OLI, provides access to advanced thermodynamic calculations through the Excel spreadsheet interface. It integrates the OLI aqueous simulation engine and database with an Excel spreadsheet that is easier to use. Many types of applications can be created for needs ranging from simple calculators of stream parameters to titration curves or surveys (Turner 2012).

There are other comparatively competent programs like Aspen Plus and Corrosion Module from COMSOL. Since the compatibility for the current issues in this project were more related to customization based on different modules, we chose to use OLI to continue our work. Although the other programs have relatively large databases and various options to use in terms of

equilibrium calculations, they were not compatible with the GIS application that was simultaneously developed for our current purpose.

2.6 Common Treatment Methods:

Softening:

Softening is the process of essentially removing hardness from water streams. Its cause is mainly calcium and magnesium salts. The water percolates, and these substances dissolve from the deposits formed. The contact time between the water and the hardening material is an important hardness determining factor. To soften water by the lime or soda-ash method, its degree of alkalinity has to be considered (Al-Deffeeri 2008).
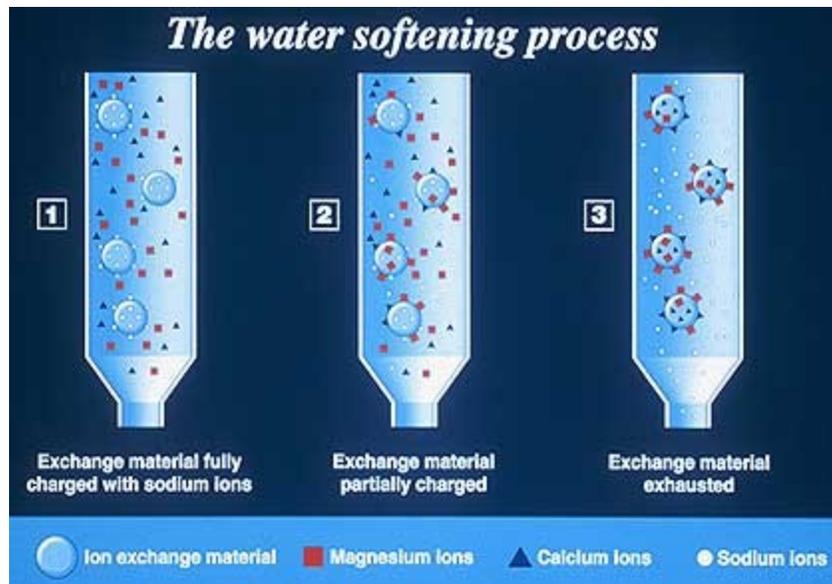
Figure 4.   An illustration of the softening process

The acid neutralizing capacity of the water sample is measured by its alkalinity. This mostly is the result of the presence of hydroxides of calcium, magnesium, and sodium, bicarbonates and carbonates, in natural and treated waters. Most of the chemicals used in treatment of such water samples, like alum, chlorine, or lime, cause changes in alkalinity. Estimating alkalinity is useful during calculating chemical doses for the water-softening processes and coagulation. The alkalinity must also be known when calculating corrosivity of the water and estimating its carbonate hardness (Al-Deffeeri 2008). Alkalinity is usually expressed in terms of calcium carbonate:

Alkalinity = hydroxyl ion concentration [OH], expressed as calcium carbonate $CaCO_3$ + bicarbonate ion concentration [HCO_3] + carbonate ion concentration [CO_3]

The hardness in water is formed by it constantly being in contact with soluble, divalent, metallic cations. Calcium dissolves in water as the water passes over and through limestone ($CaCO_3$) deposits. Magnesium dissolves along the way with magnesium bearing formations like dolomite. Because groundwater is in contact with these geologic formations for a longer period of time than surface water, groundwater is usually harder than surface water (Boulding and Ginn 2003).

Other chemicals like strontium, aluminium, barium, iron, manganese, and zinc also have the tendency to cause hardness in water, however the concentrations that they are present in doesn't help contribute (Crittenden, Trussell et al. 2012).

The following table shows a classification of water hardness:

Table 5.   Hardness classification:

Hardness mg/L as CaCO3	Soft	0 to 75
Moderate		75 to 150
Hard		150 to 300
Very Hard		Above 300

The degree of hardness acceptable for finished water varies with the consumer or industry served. In 1968, the American Water Works Association (AWWA) established a water quality goal for total hardness of 80 to 100 mg/l as calcium carbonate.

Reverse Osmosis:

Produced water is generally treated through a set of different physical, chemical, and biological methods. In offshore platforms due to limited space, compact physical and chemical systems are utilized. However, current technologies are not considered powerful enough to remove minute-suspended oil particles and dissolved elements. Also, many chemical treatments, whose initial and/or running costs are high, produce hazardous sludge. In onshore facilities, biological pretreatment of oily wastewater can be a cost-effective and environmental friendly method. As high salt concentration and variations of influent characteristics have direct influence on the turbidity of the effluent, it is appropriate to incorporate a physical treatment, e.g., membrane based filtration to refine the final effluent. Hence, reverse osmosis as a means to the use of

combined physico-chemical and/or biological treatment of produced water in order to comply with reuse and discharge limits is a good alternative (Ayatollahi and Zerafat 2012).

Earlier in California, a state of the art process was used to convert produced water to freshwater. This process included chemical clarification, softening, filtration, and reverse osmosis. The plant could successfully handle water with about 7,000 mg/l. of total dissolved solids, 250 mg/l. silica, and 170 mg/l. soluble oil, complying with the California drinking standard (Tao, Curtice et al. 1993).

Diffusion is defined as the transportation of molecules from regions of higher concentration to a lower concentration. Osmosis is the process in which the molecules are water and the change in concentration occurs through a semi-permeable membrane. Barring the exception of water, ions or bigger molecules are not allowed to pass. These processes continue till equilibrium. When pressure is applied in a suggested amount to the high concentration side of the membrane, the process can be abruptly stopped, reduced or even reversed (Sourirajan 1970).

Reverse osmosis occurs when the water is passed through a membrane from lower concentration to higher concentration (Toray Industries Website 2013). Here the pressure is applied to the high concentration side, to pass the molecules through the semipermeable membrane, to obtain pure water as shown in Figure 6.
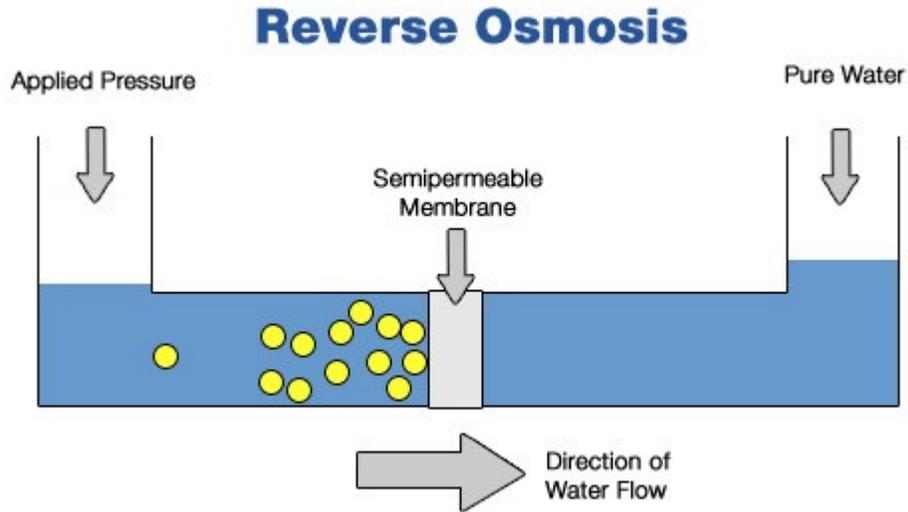
Figure 5. Reverse Osmosis (HCTI Website 2008)

Reverse osmosis is commonly used in the filtration processes of commercial and residential water. It is also one of the most commonly used methods to desalinate seawater. Sometimes it is also used to remove or filter out water from other solvents like ethanol (Helmenstine).

Dissolved Air Flotation:

Dissolved air flotation is a simple process where the suspended solids, oils and greases and other impurities are removed from water slurries by dissolving air into water. The micro-bubbles act on the particles causing them to float to the top of a vessel where they are skimmed and removed (Yeh 1995). Superior effluent quality, reduced footprint, and maximum recovery of solids are some of the benefits that this process could support. It does not have to be operational for a long time, and there is a considerable reduction in capital cost when compared to other processes.
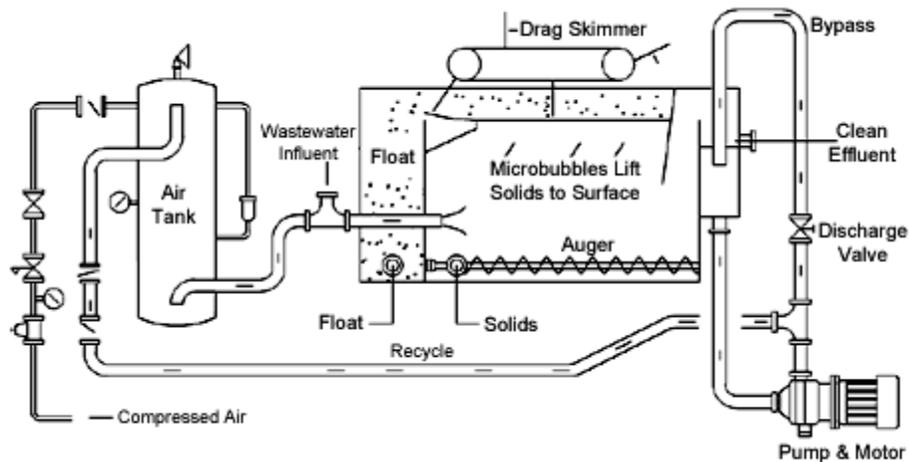
Figure 6.   Dissolved Air Flotation Process (Pan America Website 2007)

Dissolved air flotation is basically a common treatment process where wastewater is clarified by removing suspended matter like oil or solids (Mollah, Schennach et al. 2001). Air is dissolved in the water or wastewater under pressure and then releasing the air at atmospheric pressure in a flotation tank or basin, hence making it more effective. The released air forms tiny bubbles which stick to the freely suspended matter making it float to the surface of the water where it may then be removed by a skimmer or a similar device. However in the petroleum industry, natural gas replaces air as the primary flotation medium, because of the former's explosive nature. The feed water is concentrated with a coagulant like $FeCl_3$ or Al_2SO_4 to flocculate the suspended matter. Typical bubble sizes range from 50 to 70 μm for this process (Stevenson 1997). The advantages of DAF is that it can be started up easily, it can operate from high surface loading and it can achieve a steady water quality in less than 45 minutes (Zabel 1985).

2.7 Geographic Information Systems

Geographic information systems (GIS) have gained much attention in many research fields, because the output for spatially dispersed data be viewed easily (Singh and Yadava 2003). GIS is an all-purpose module of technology for handling large datasets of geographical data in digital form. It can also preprocess data into a form suitable for analysis, for spatial analysis and modeling directly, and posting processed results in an illustrative format (Steyaert and Goodchild 1994). GIS depict a spatial representation of a lot of systems including water resources systems. A GIS can illustrate spatial aspects for a traditional water resource data base, simultaneously presenting an integrated view by combining various factors like social, economic and environmental (McKinney and Cai 2002). In particular, the visual depiction capacity of GIS compliments the user interface of water resources models, allowing the user to control completely the data input and manipulation. Complicated graphical user interfaces can provide user-dictated applications, so that the user can decide how features will respond to changes to the environment, and to create rules to supervise the modeling process (McKinney and Cai 2002).

For water resource problem solving, both a spatial look of the system and a general idea about water resource problems are necessary (McKinney and Cai 2002). GIS can represent the geo-referenced characteristics and spatial relationships of systems however the predictive and related analytical capacities are more useful for problem solving (Boulos 2004).

Spatial interpolation methods are frequently used to estimate values of physical or chemical constituents in locations where they are not measured. To date, the research conducted to see the different capacities of interpolation methods in effective water management, has been trivial (Aspinall and Pearson 2000). GIS is more of a tool which is used for storing, analyzing and

displaying spatial data, as well as it can be used for investigating ground water quality information. GIS has been used in the map classification of groundwater quality, based on correlating total dissolved solids (TDS) values with some aquifer characteristics or land use and land cover. Other similar studies have used GIS as a complex database management system for preparing maps of water quality according to their corresponding concentration values of various chemical constituents (Kouli, Lydakis-Simantiris et al. 2008). In such studies, GIS is utilized to locate groundwater quality areas suitable for different purposes like irrigation and domestic use.

Geographic Information Systems (GIS) have been used frequently in monitoring utilities for cities and states in an organized way viewable in a map format. They have been used in the monitoring of pipelines, utilities like water, electricity, and gas on a spatial basis. There has been a lot of development in GIS since it was originally framed years back (Abbott and Argentati 1995). It has been applied to almost every industry in the world since it is an excellent way to view work. GIS has been influential in the oil and gas industry as it has been used to map the well locations and drilling pads for accurate plans. It has also been a modern media for recording data for the particular industry in a spatial format. However there has not been much progress in its use for water based applications in the oil and gas industry.

GIS was used in this study to prepare layers of maps to locate promising well sites based on water quality and availability. A GIS-based groundwater quality index method was proposed earlier which takes in various available water quality data and indexes them numerically relative to the WHO standards (Clark 1998). For spatial interpolation Inverse Distance Weighted (IDW) approach in GIS had been used in that study to characterize the locational distribution of groundwater pollutants.

25

Other spatial interpolation techniques include Kriging, Cokriging, Spline. Kriging is when spatial structures and observations close to each other are assumed to be more alike than those that are far apart (spatial autocorrelation) (Ali, Younes et al. 2011). Usually, when Kriging is used, the experimental variogram calculates the average degree of dissimilarity between none data values points and a nearby data value point thereby depicting autocorrelation at various distances (Sahebjalal 2012). After analyzing the experimental variogram, a suitable model is deduced by using the parameters and their weighted least squares (Robinson and Metternicht 2006). The combination of affiliation and the applicable error surface output are some benefits of using these methods (Anderson 2002).

A disadvantage is that it requires substantially more computing and modeling time and Kriging requires more input from the user. In co-kriging, the correlation between two variables, groundwater quality in this case and another easily accessible variable, can be exploited for our estimation purposes (Nourani and Ejlali).

To date, GIS has not been used to manage produced water in an oil and gas field. It, however, can be developed to be a really effective tool in field management. It can be used effectively to interpolate water quality in a specific area, or to optimize truck routes and optimized pick-ups, routing for a pipeline system and also for determining an optimum location for a centralized treatment facility.

2.8 Summary and Research Objectives

The oil and gas industry is an economically important industry, with direct and indirect effects on the current job market and increased energy security for the country. In spite of these benefits, it still has its environmental and social concerns. Most importantly the issues relating to the water use is critical. A key management strategy is the reuse of produced water, as it addresses both water availability and disposal along with some environmental issues.

Produced water quality is one of the key aspects in optimizing water management in this industry. The oil and gas industry is over one hundred years old, and there has been a lot of research done in this field. However, there is a deficiency in the part of predicting water quality in different stages of treatment for optimization of reuse. Since produced water recycling is a highly spatially diverse problem, it is important to utilize GIS when evaluating options.

Work will be done to collect sample water quality data in the research area. A model will be designed based on this sample quality. Using this model, predictions will be made for different stages of treatment. Specific research objectives include:

1. Create GIS application for display of water quantity and water quality data.
2. Using OLI Systems Stream Analyzer, model equilibrium conditions for water quality and develop case study for solution mixing and optimizing a treatment scheme.
3. Develop framework for integrating OLI model and GIS application that will allow the user to make chemical treatment predictions with a spatially diverse data set.

3. DEVELOPMENT OF A GIS BASED CHEMISTRY TOOL TO OPTIMIZE PRODUCED WATER TREATMENT

3.1 Area of Research:

The research was focused on the Wattenberg Field in Northern Colorado. It is an important part of Colorado's shale oil and gas industry and is part of the Denver-Julesburg basin. This field has produced more than 4.0 trillion cubic feet (TCF) of natural gas from its diverse geological formations such as Niobrara, J Sandstone, Codell Sandstone, and T Sandstone and currently is producing significant quantities of shale oil. Water sampling was done in this field since the project involved collaboration with Noble Energy Inc. and many of their wells are located in this area.

Figure 7.   An image of a drilling rig in the Wattenberg Field

The water quantity values from the wells located in this field were obtained from the Colorado Oil and Gas Conservation Commission and also through Noble Energy Inc. The data included dates of production, dates of drilling, water used for fracturing, water used for completion, dates

of recompletion, period of production, and flow back data. A lot of other producers operate their wells in this field as well.

This has multiple formations as illustrated in the image below and is a source for shale gas. Some of the formations depicted below are the Dakota, J Sandstone, Codell, Niobrara, Shannon, and Sussex. Most of the wells we have studied are in the Niobrara formation.
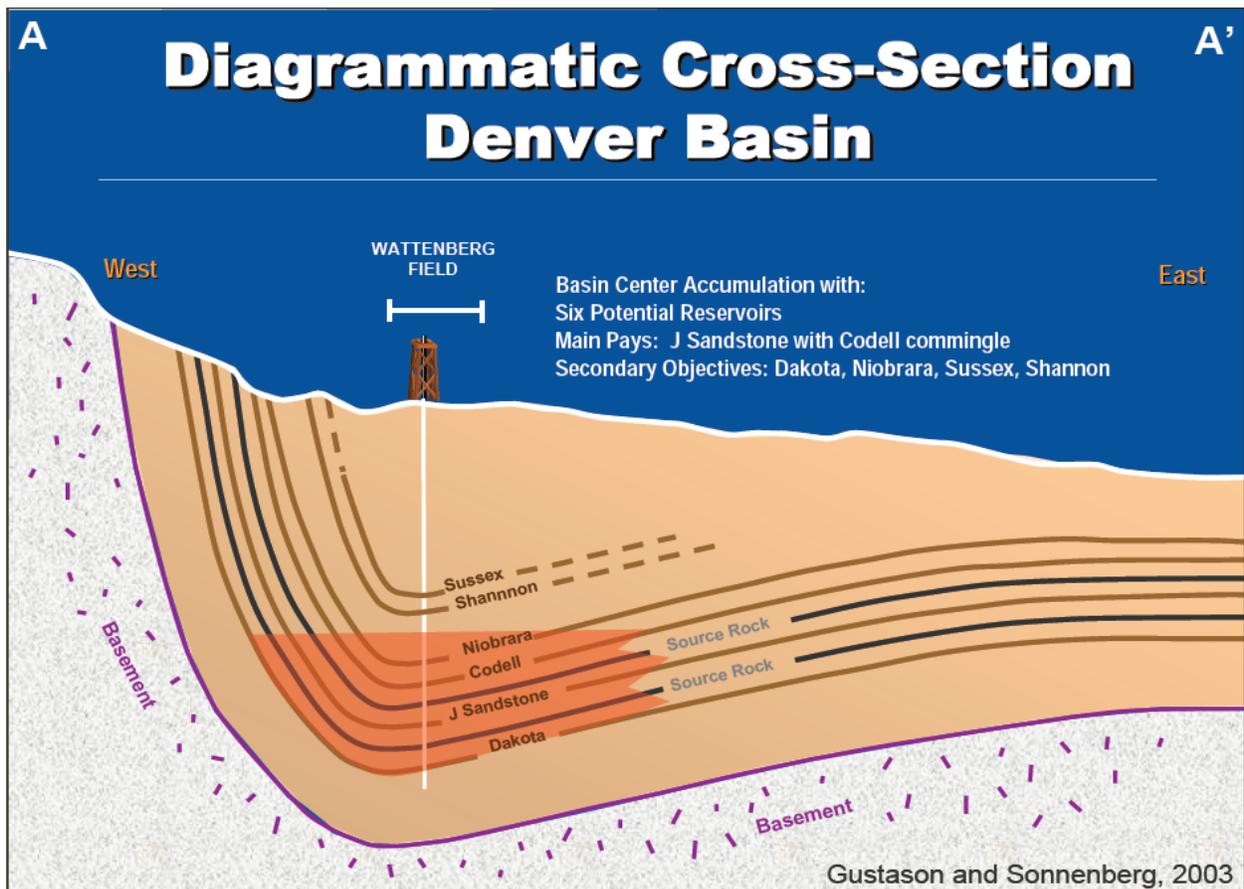
Figure 8.   Illustration of the Cross-Section of the Denver Basin and the Wattenberg Field

The average well depth of wells in this field range from 7600 – 8400ft (Smith, Holman et al. 1978).

The Wattenberg field is known for its rich history of producing oil and gas for the past 40 years. Initially, petroleum companies started producing oil from the Denver Julesburg sandstone formation mainly in Weld County, located in the north east of Denver, but recently the number of wells being drilled has increased considerably. It has been estimated that 1.6-2.4 trillion cubic feet of natural gas could be extracted from Wattenberg field at a time when energy companies could only use conventional approaches from relatively high permeability formations. However, the developing trend of horizontal drilling and hydraulic fracturing technologies, unconventional natural gas is becoming the major form of gas production in the Wattenberg comprised of shale gas and tight sandstone among others. Nearly 5.2 trillion cubic feet of natural gas is being stored in the formations in Wattenberg field.

3.2 Water Quality Data and GIS Integration:

Data was collected from the operator of the wells, Noble Energy Inc., and the Colorado Oil and Gas Conservation Committee's public database. They were obtained in the form of Microsoft Access files for each year in the format of annual production for each well. This data was organized for the required conditions such as owned by Noble Energy Inc., and situated geographically in the Wattenberg Field using custom relative queries. They were then filtered as oil wells and gas wells respectively according to their corresponding gas/oil ratio. Once the filtration was done, their gas production, oil production and water production were compared against each other to get an idea of how the trend is and how the produced water varies according to the type of well. The annual data was summarized for each year for each type of well i.e. gas well or oil well tabulated and finalized as a report.

Sampling was done by Colorado State University research students certified by Safeland PEC Basic with secure access to Noble Energy wells in the Wattenberg. Samples were collected and tests were done partly in the Colorado State University Environmental Engineering Laboratory and ACZ Laboratories. The tests are classified in Table 6.

Table 6.   Classification of tests and the labs they were tested

	Analysis
ACZ	Na, Ca, Mg, Sr, Ba, B, Cl$^-$,SO$_4^{2-}$, PO$_4^{3-}$, TDS, HCO$_3^-$
CSU lab	pH, Electric Conductivity, TC, TN, TOC,
On site	Temperature

The pH was tested in the CSU lab by EPA 150.1 using Fisher Scientific Accumet AB15 Basic and Bio-Basic pH/mV/C meter. For determining the dissolved elements, water samples were filtered by the standard method 200.7 section 8.2. They were filtered using a 0.45 μm pore diameter membrane filter after the pH test, as filtration should be tested at the time of collection and taking into consideration the practical possibility.

For the dissolved wet chemistry methods (chloride, phosphorous, TDS, sulfate) samples were filtered using Whatman Glass Microfibre Filters 934-AH. HACH method 8146 was used for testing Dissolved Ferrous. The 1-10 phenanthroline indicator in the ferrous iron reagent reacts with ferrous iron (Fe2+) in the sample to develop an orange color proportionate to the iron concentration. Ferric iron (Fe3+) does not react. The ferric iron concentration can be obtained by finding the difference in the ferrous iron concentration from the results of a total iron test.

Test results are measured at 510 nm by a Model DR/2500 (HACH Instruments, Loveland, CO) Laboratory Spectrophotometer. The detective range of Fe2+ is 0.02 to 3.00 mg/L with 95%

confidence limits of distribution from 1.98 to 2.02 mg/L. Total carbon (TC), inorganic carbon (IC), total organic carbon (TOC) and total nitrogen (TN) were measured by SHIMADZU (Kyoto, Japan) TOC-VWS/TOC-VWP.

COD was tested using HACH method 8000 (high range plus), adapted from standard methods 5220D. The results in mg/L COD are defined as the milligrams of O_2 consumed per liter of sample under the conditions of this procedure.

As EPA suggested, inductively coupled plasma-atomic emission spectrometry (ICP-AES) was used to determine metals and some nonmetals in the solution, following *Method 200.7*. Chloride was tested by EPA *Method 300.1*. Total hardness as CaCO3 was calculated by following equation

$$Total\ Hardness\ (as\ CaCO_3) = 2.497 \times [Ca^{2+}] + 4.118 \times [Mg^{2+}]$$

TDS can be measured using EPA 160.1 or Standard Method 2540B. Titration is used to measure bicarbonate and carbonate concentration, following Standard Method 2320B.

3.3 Development of GIS Model Application:

The GIS map was developed using the ArcGIS Explorer tool (shown in Figure 9) so that it could be published as a web map and was readily available online and could also be made public if required. The chemistry tool was programmed on a single system and would be essentially hosted on the server. The input and output would be an excel file which would be hosted on the server as well. This excel file will be linked to the GIS map so that the user could do custom analysis/calculations and view it cartographically according to their exact locations. Custom analysis/ calculation options could be made available in a compact toolbox in the map.
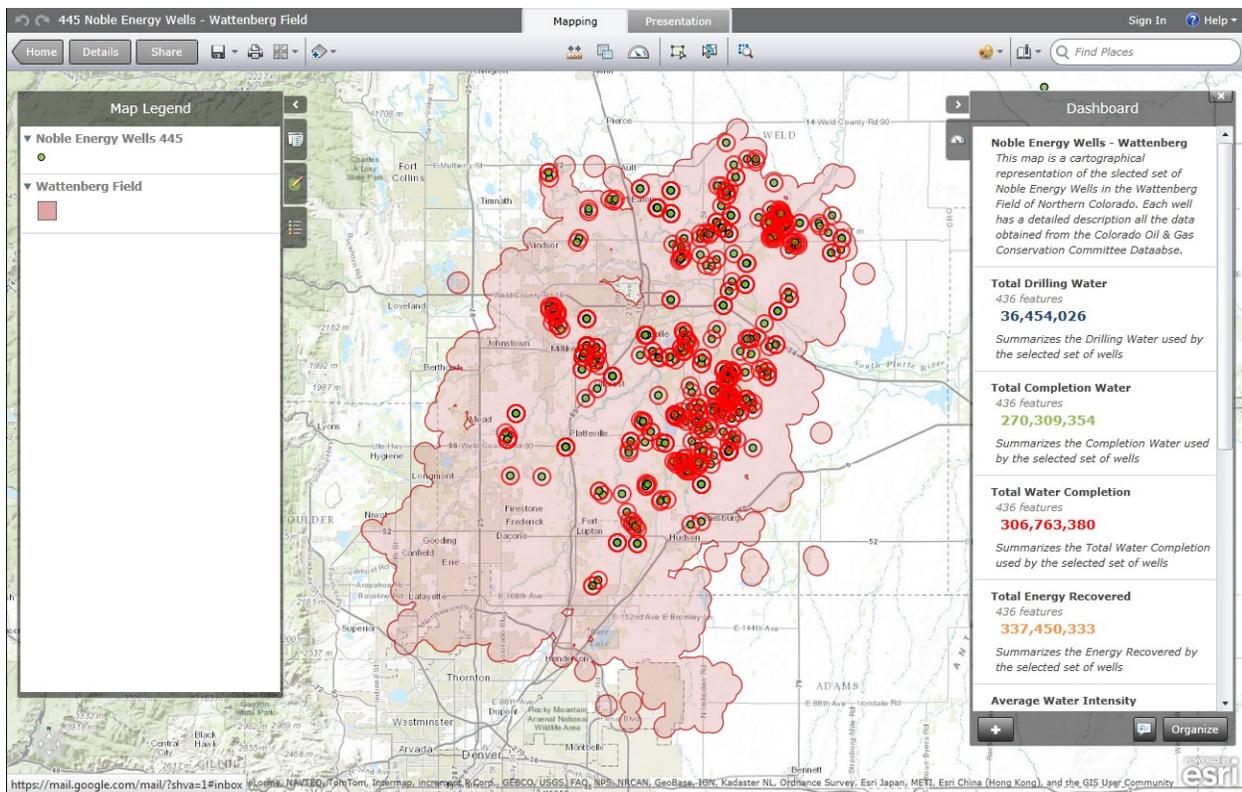
Figure 9.   Screenshot of the model GIS application

3.4 Description of Water Analyzer:

For the OLI Systems electrolyte simulation, we ran a sample simulation with assumed values of temperature, pressure, and pH. We also took the acid titrant as sulphur trioxide and the base titrant as sodium hydroxide. We ran the inputs for a sample simulation calculation trying with a sole objective of adjusting the pH to 9. We assumed the temperature to be standard room temperature of 25 °C, the pressure to be standard atmospheric pressure of 1 atm and the desired pH to be 9. Once we input the values in the OLI Systems Chem Analyzer (shown in Figure 11), we get a summarized calculation as follows. The input anions and cations were assumed on an approximation based on the area selected. The results show a complete calculation summary of

33

the simulation run. This will be used in predicting treatment in stages according to the specific characteristics.
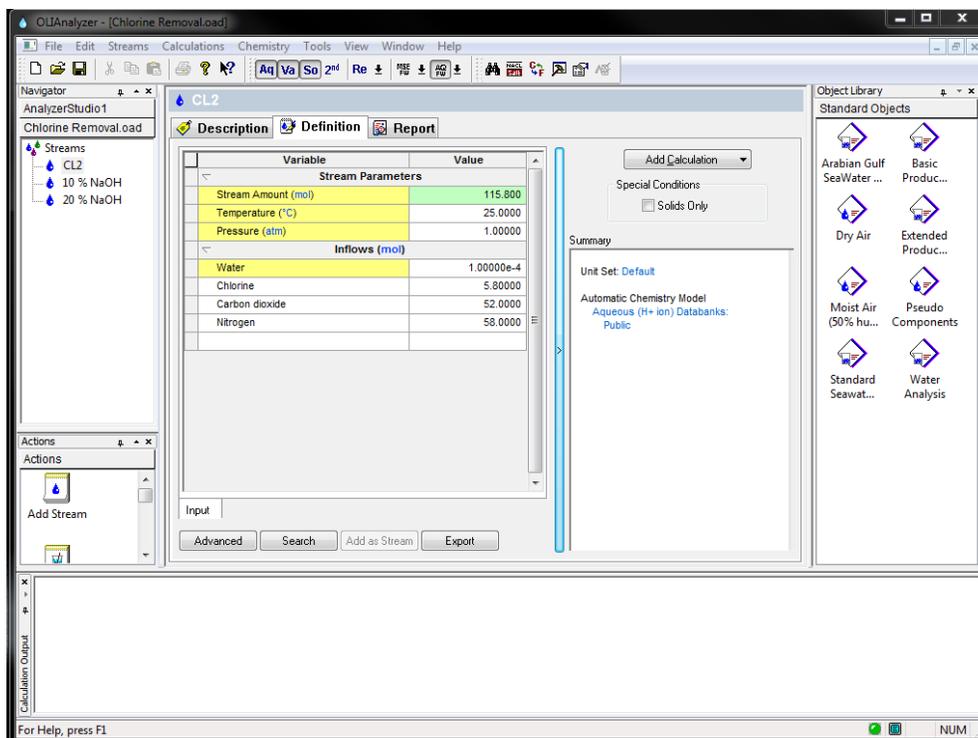
Figure 10. Screenshot of OLI Stream Analyzer Studio

3.4.1   Water Quality Input:

As mentioned earlier, water quality data for produced water in the Wattenberg Field was sparse to non-existent. There was no current data that was available for our research. Sampling plans were made after industrial collaborations helped. Sampling was done on a specific set of wells in the Wattenberg Field. The collected samples were prepped in university labs and sent to certified labs for additional tests. Once these results were obtained, the values for our base model development were ready (shown in Figure 12).
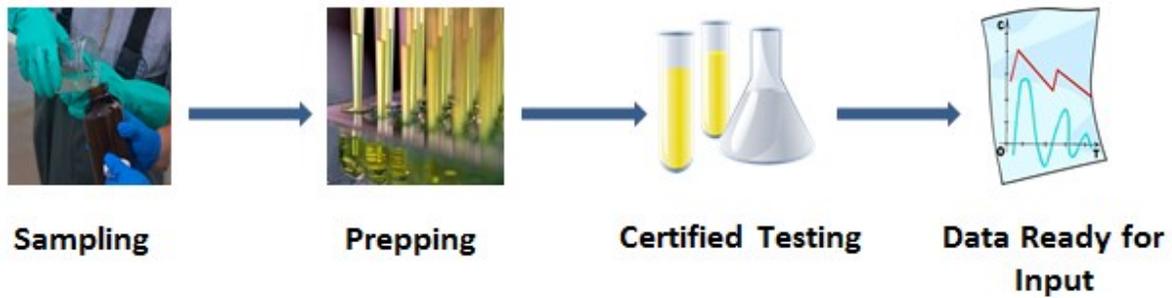
Figure 11. Process schematic for water quality data preparation

The data obtained from the certified labs are presented in the Appendix Section A1 . A selected set of these datasets were used for further processing.

3.4.2 Base Model Development:

With the obtained water quality values for the sampled wells, tests were run on the OLI Process Simulation Analyzer to simplify the equilibrium changes in different stages. Specific characteristics were monitored along the way to maintain equilibrium. Initial samples were run on OLI Analyzer Studio to get an idea of the equilibrium characteristics after reconciliation to balance charges and adjusting pH for optimum treatment specifics. One of the samples run are explained below in a case study. In this case study, we simulated mixing water samples from different wells, and getting equilibrated water quality specifics for the mixtures in different percentages to identify optimizing treatment accordingly. The steps involved in this process are explained below in the case study.

3.4.3 Case Study – OLI Analyzer:

A case study was done using the OLI Analyzer on a particular set of water qualities, to optimize an electro-coagulation process in an existing treatment train. A set of 4 scenarios were tested by CSU students. We took one of the scenarios to do a comparative case study to find the accuracy of the predictions by OLI. The scenario chosen involved a three step process starting with electro-coagulation, softening and pH reduction. The tests were conducted experimentally and compared with OLI predictions using the same water quality values.

The chosen treatment train is demonstrated in Figure.
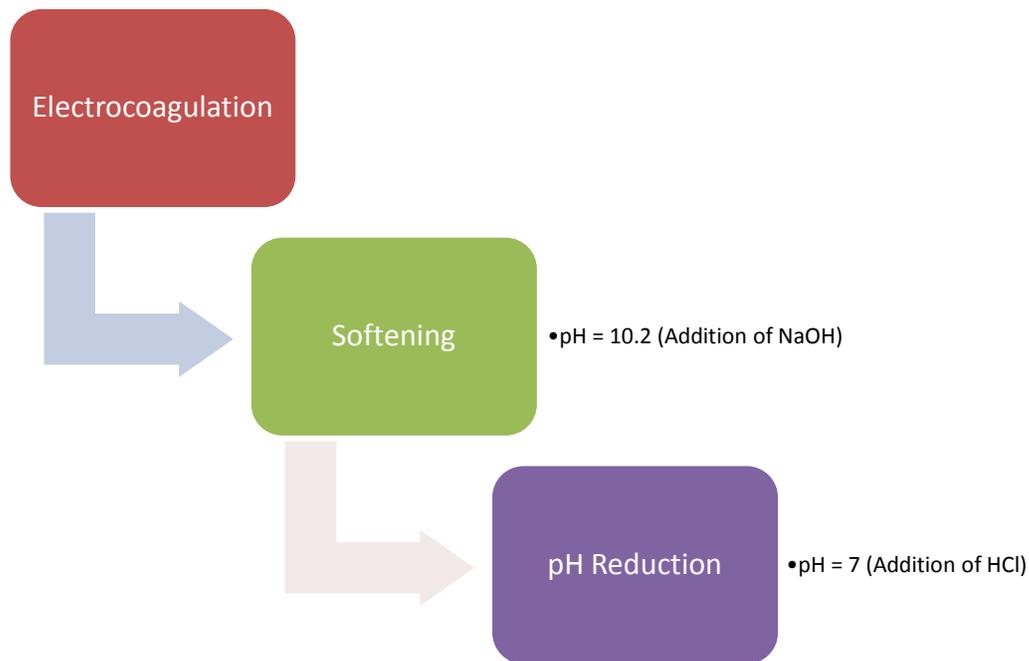
Figure 12. Schematic of chosen treatment scheme

The analysis were done experimentally in three phases, starting with the raw sample, filtered raw sample, post EC filtered sample and the pH adjusted sample. The final characteristics were compared to predictions done in OLI, to measure its accuracy in a real-field case study.

The results of the comparisons are explained below in distinct graphs and Table 7.

Table 7. Results from the Case Study – Three Stage Optimization:

Temperature	33.8 F				
Pressure	839mb				
Well No.	NO.14-66-3				

			EC+pH10.2		OLI
	Raw Sample	Raw Filtered	Post EC Filtered	Final	Final
Potassium ion(+1)	1032	1005	966	889	965.649
Sodium Ion(+1)	13895	13456	13115	12002	13370.3
Barium ion(+2)	30.6	29.2	19.3	17.2	0.393525
Calcium ion(+2)	301	290	283	256	4.47953
Copper(II) ion (+2)	0.577	0.563	0.551	0.556	0.000974863
Iron ion(+2)	189	166	131	117	1.14156
Magnesium ion(+2)	54.8	52.6	54.3	48.4	54.2803
Aluminum ion(+3)	1.6	1.09	6.94	1.6	2.47435E-05
Manganese ion(+2)	2.54	2.39	2.41	2.2	0.299665
Strontium ion(+2)	52.7	51.4	47.7	43.5	1.66198
Anions					
Chloride ion(-1)	21613	20412	20349	18489	21576
Bicarbonate ion(-1)	898	816	664	588	
Sulfate ion(-2)	89.9	106	86.5	139	
Boron tetrahydroxide ion(-1)	13.3	11.6	11	9.74	1.50771
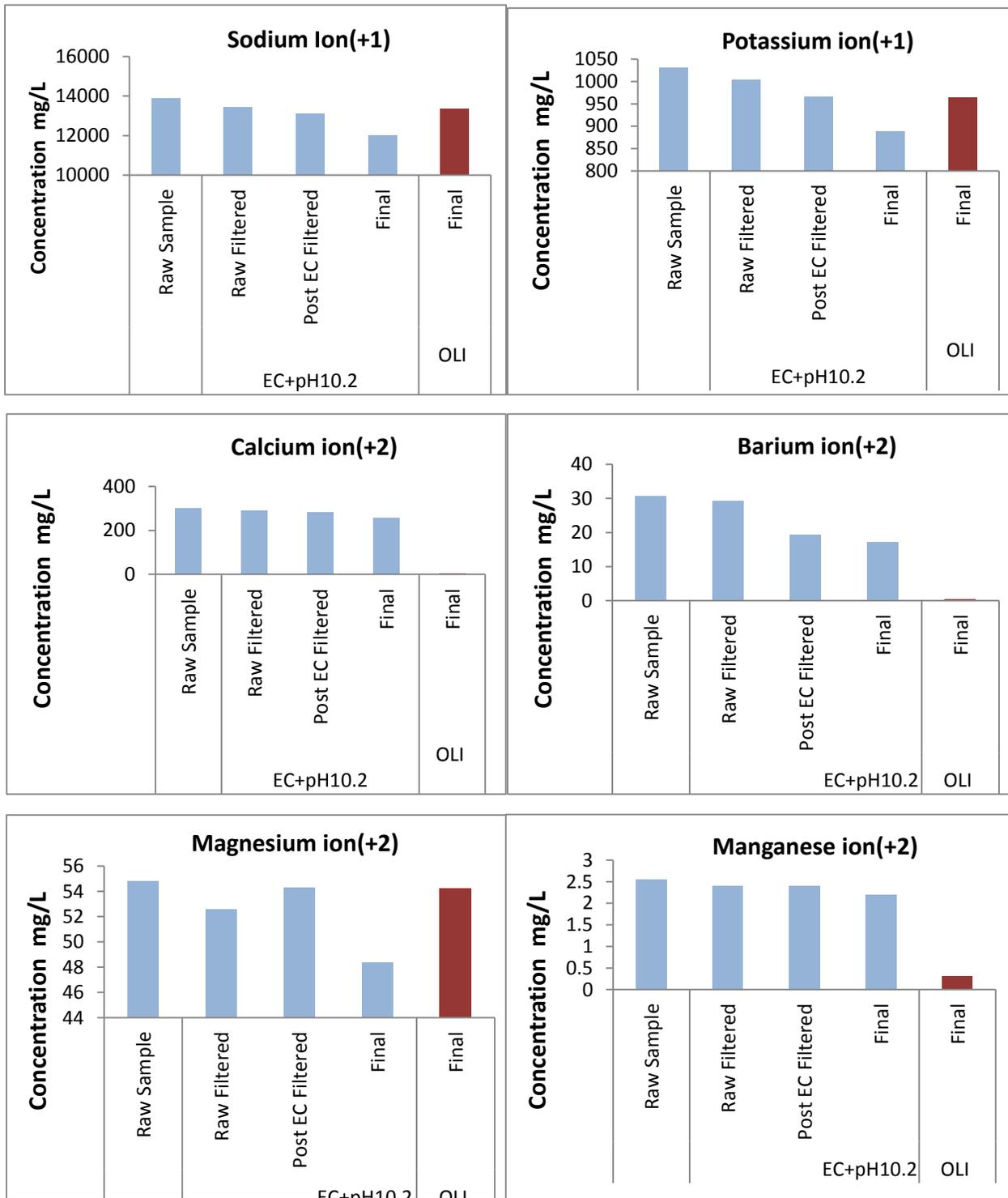
Figure 13. Experimental and predicted results – a comparison

The results turned out really close to the experimental values, except for the cases of the solids like Calcium, Barium. The huge difference in the comparisons of Calcium, Barium was due to the fact that solids were removed as a separate stream when simulating in OLI Analyzer, thus explaining the huge variations.

Instructions for running analyses and simulations in OLI are as follows:

- The OLI Analyzer Studio window was opened. A new analyzer window is started and streams are added by clicking on the "Add Stream" option as shown below in Figure 13.
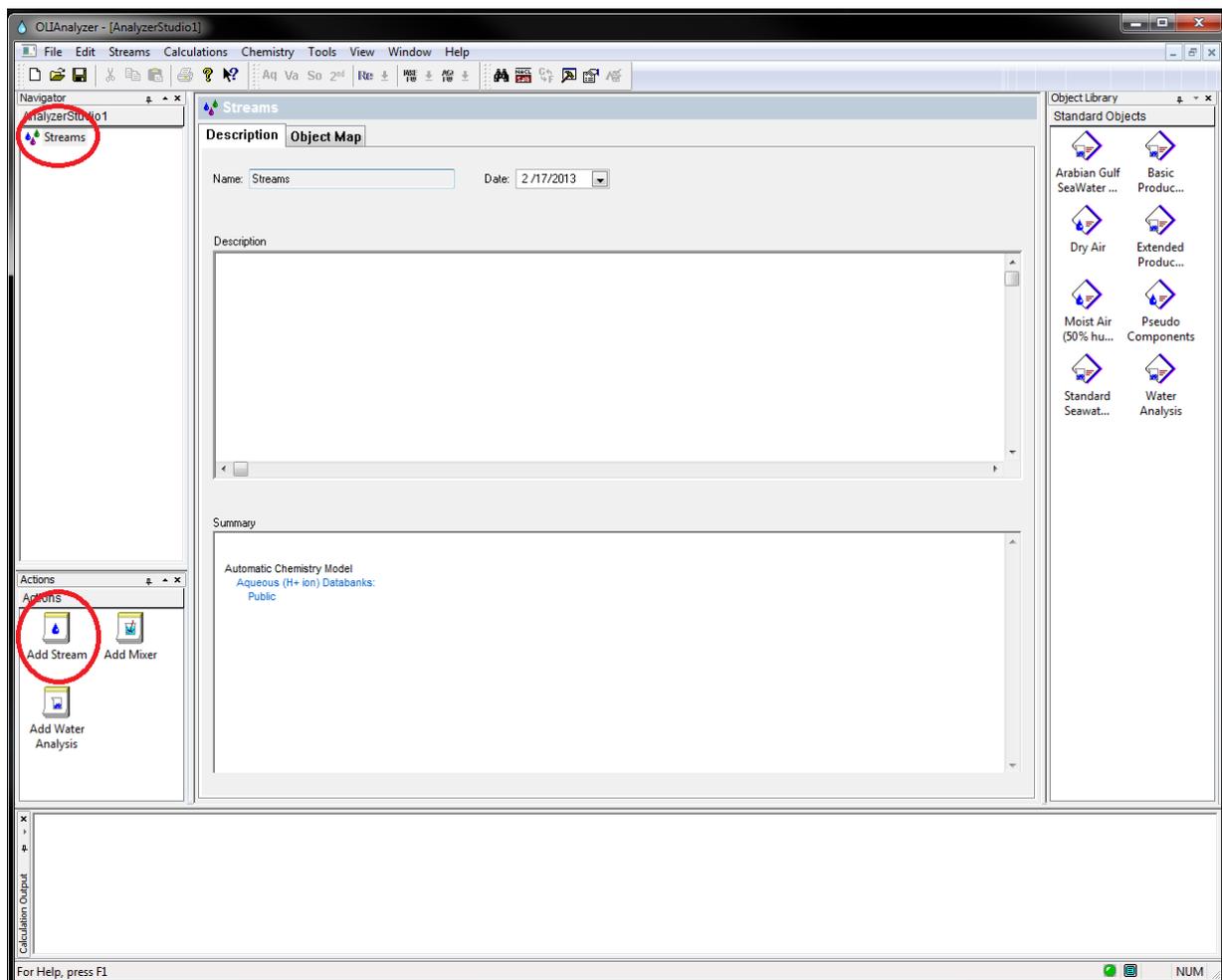
Figure 14. Screenshot of the Add Stream Step

- Once the stream is added successfully, double click on the stream and rename the stream to the corresponding well or sample name as shown in Figure below.
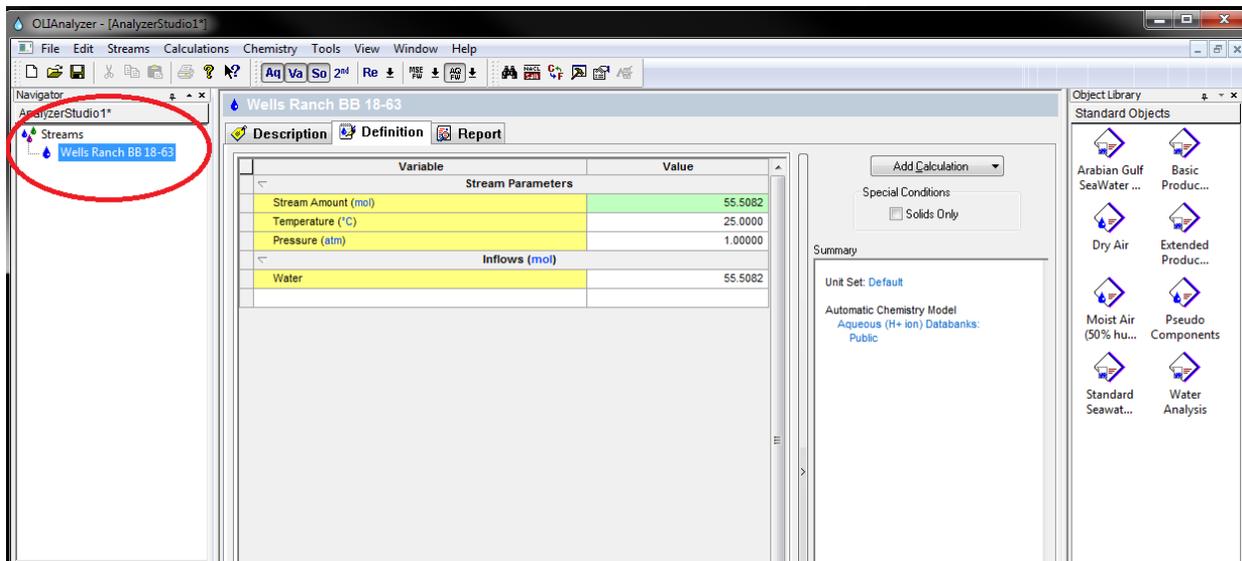
Figure 15. Screenshot of Stream naming step

- The next step would be to add the corresponding water analysis, such that you can input all your well water quality data. Since it is a long process of typing in all the constituents one by one, it would be easier to use a built-in template to get an idea of basic constituents in produced water. You can click on the Extended Produced Water Analysis object in the object library and drag it into the Analyzer Studio workspace. Now, you get a list of components where you can click on change values. If you have additional components, you can just click on empty spaces in the inflows window and enter them manually (shown in Figure 15).
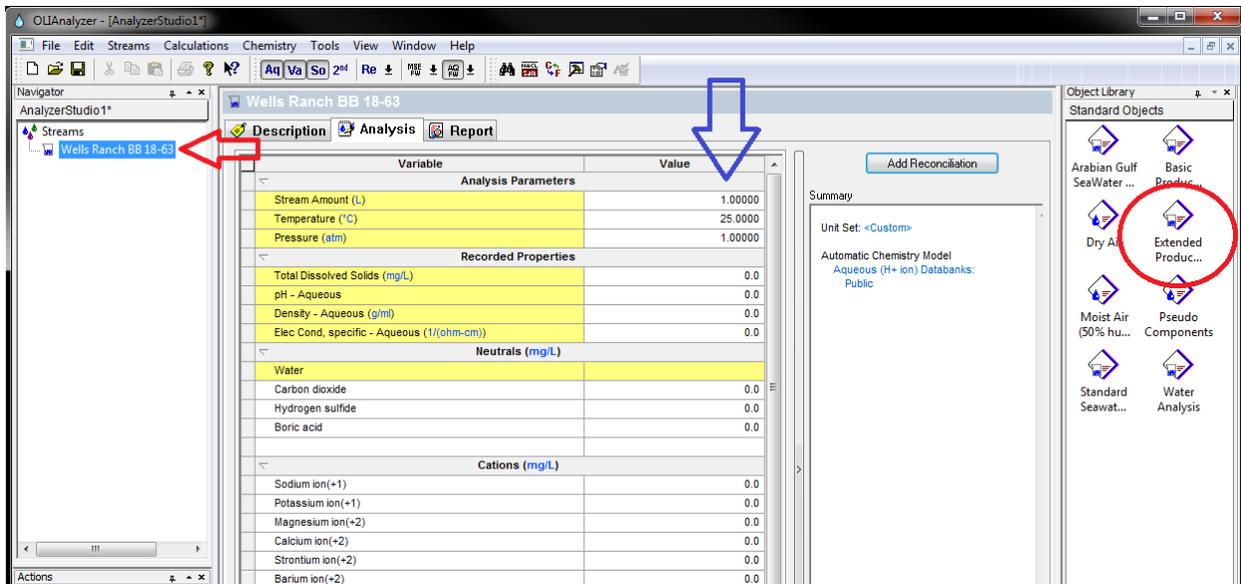
Figure 16. Screenshot of Water Quality input step

- Once you have input all the relevant water quality data, the stream has to be reconciled for estimating charge imbalance and what is required to bring it to equilibrium. This can be done clicking on the "Add Reconciliation" button as shown in Figure 16.
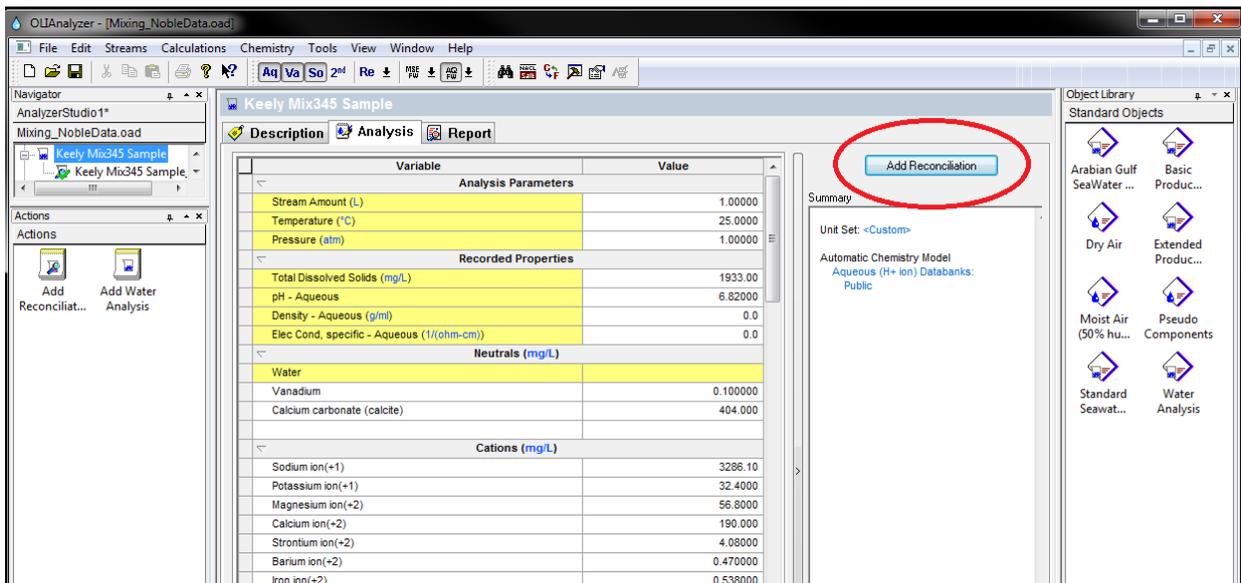
Figure 17. Screenshot of "Add Reconciliation" step

- After you click on Add Reconciliation, you get 3 options to choose from. We select the "No Reconcile" step, such that we just do a processed stream and calculate the charge imbalance and what is required to balance it, and click on "Calculate". The step is done as shown in Figure 17. Once this step is done, one can look at the reconciliation specifics in the Report tab.
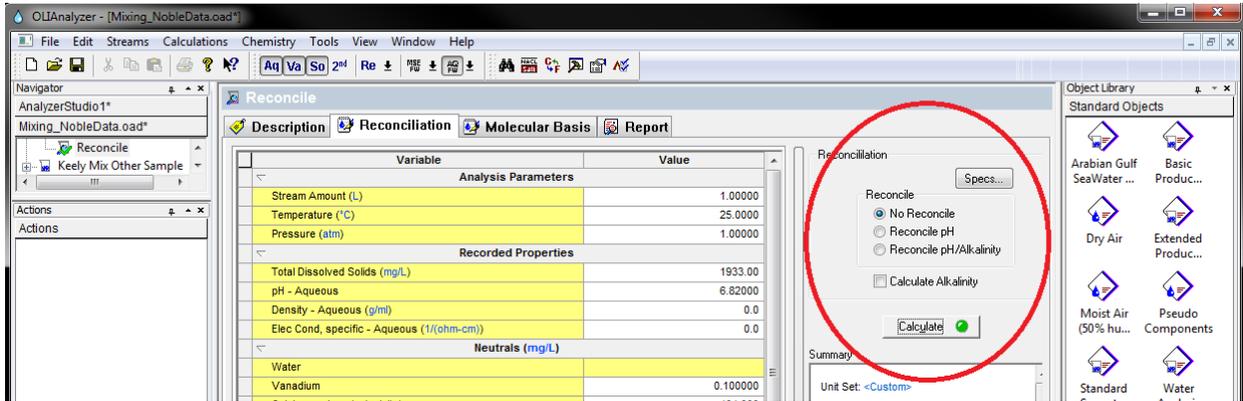
Figure 18. Screenshot of the Reconcile step

- The results overview of the calculation done is displayed below the "Calculate" button as shown in Figure 18. Rename the stream as [StreamName]_Rec as a processed stream as shown in Figure 18.
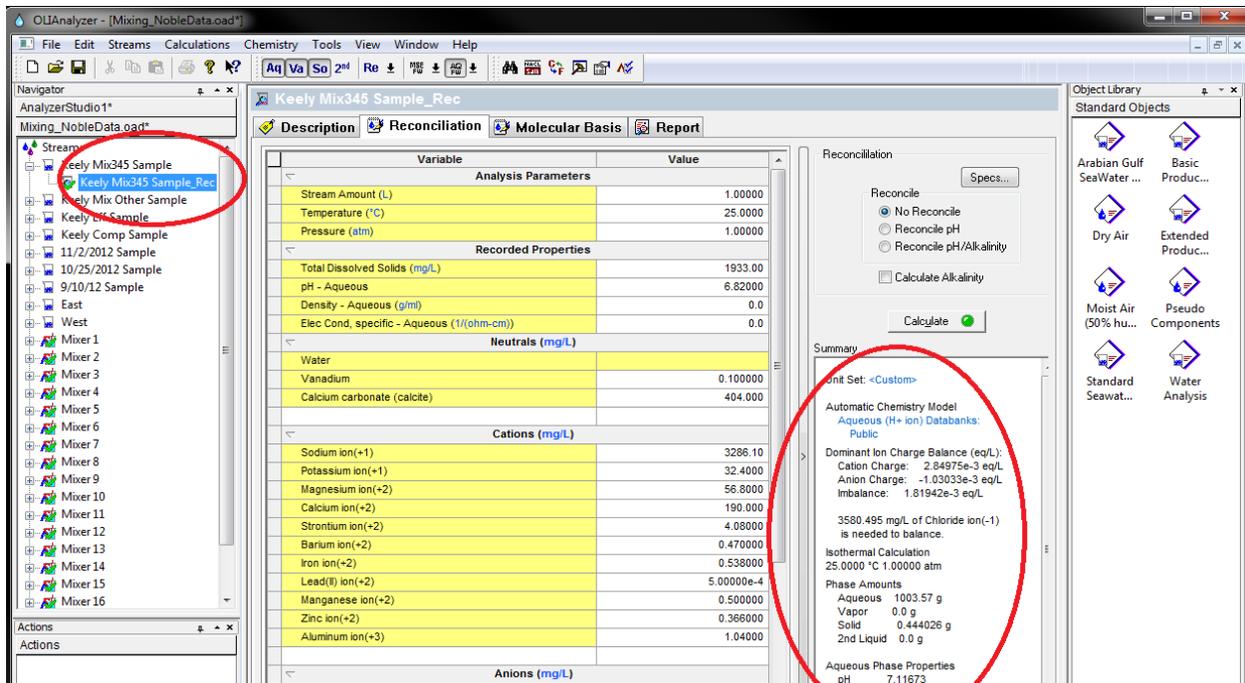
Figure 19. Screenshot of the calculation results window

- The steps were repeated and 18 samples were added to this, and each was reconciled separately to calculate charge imbalance and they were saved as separate streams.

- Once this was done, the "Streams" in the Studio was selected, and a mixer was added as shown in Figure 19.
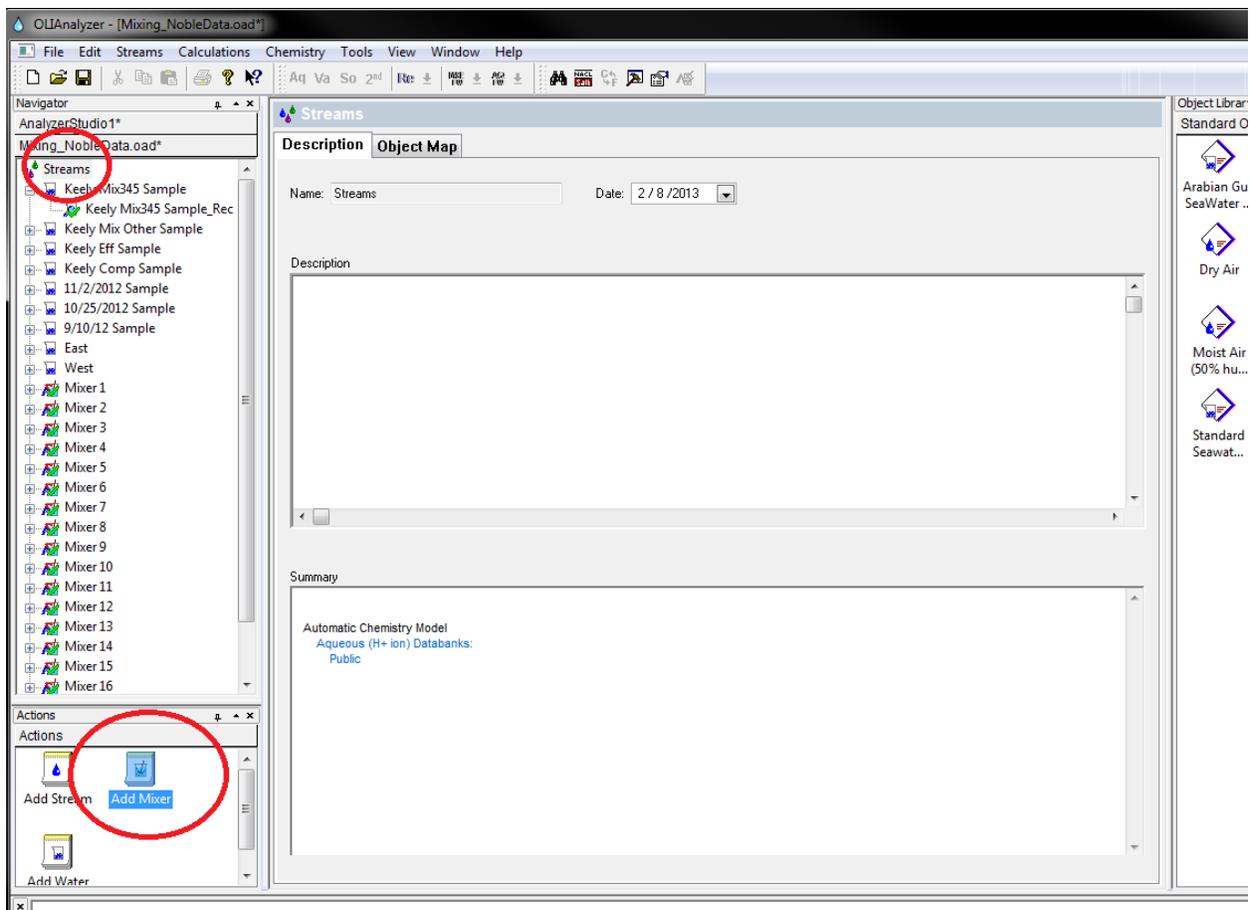
Figure 20. Screenshot of the "Add Mixer" step

- A new mixer stream is added to the list of streams. Click on it and choose parameters as shown in Figure 20. Lists of streams available in for mixing are shown. All these are processed streams from the reconciliations. You can select any number of streams. You can edit the multiplier values accordingly to the percentage mixture required. Once the parameters are selected, the calculate button is pressed to get the mixture specifics.
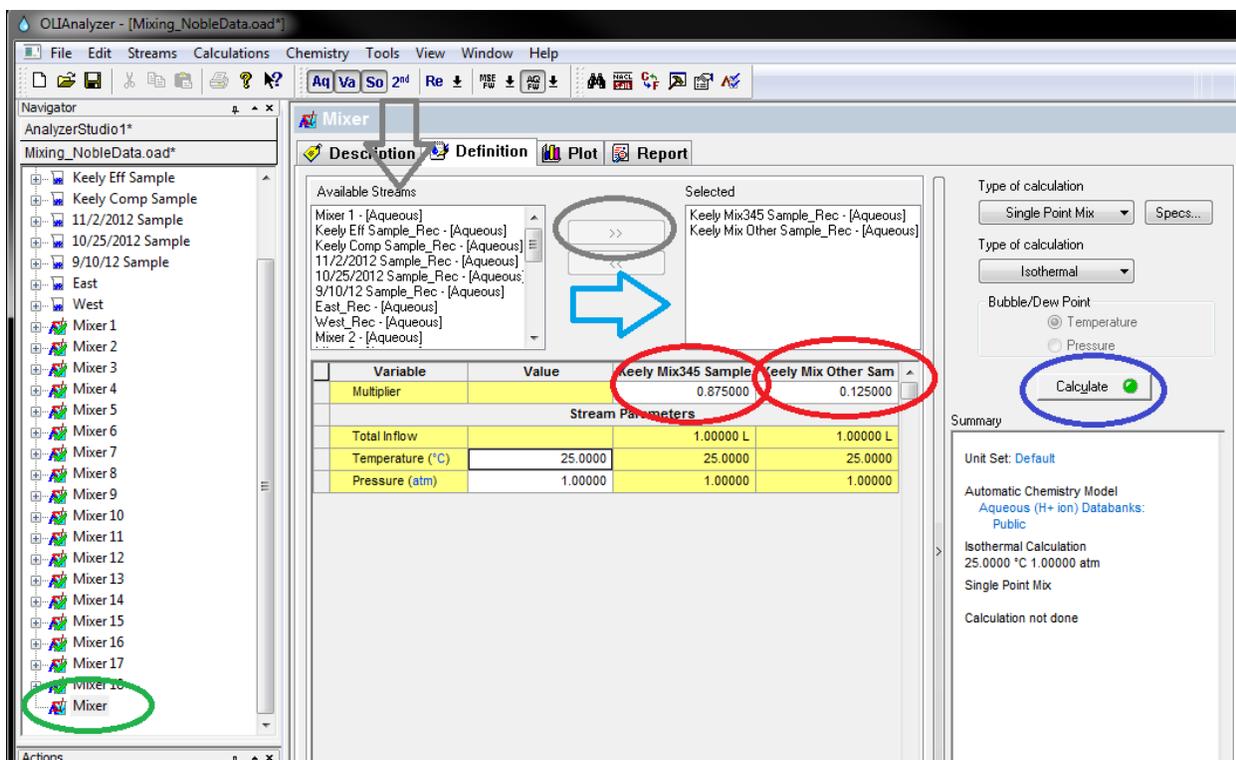
Figure 21. Screenshot of stream selection for mixing

- After this is done, the results of the mixing can be seen in the report tab. It can also be exported in a CSV format for further calculations as shown in Figure 21.
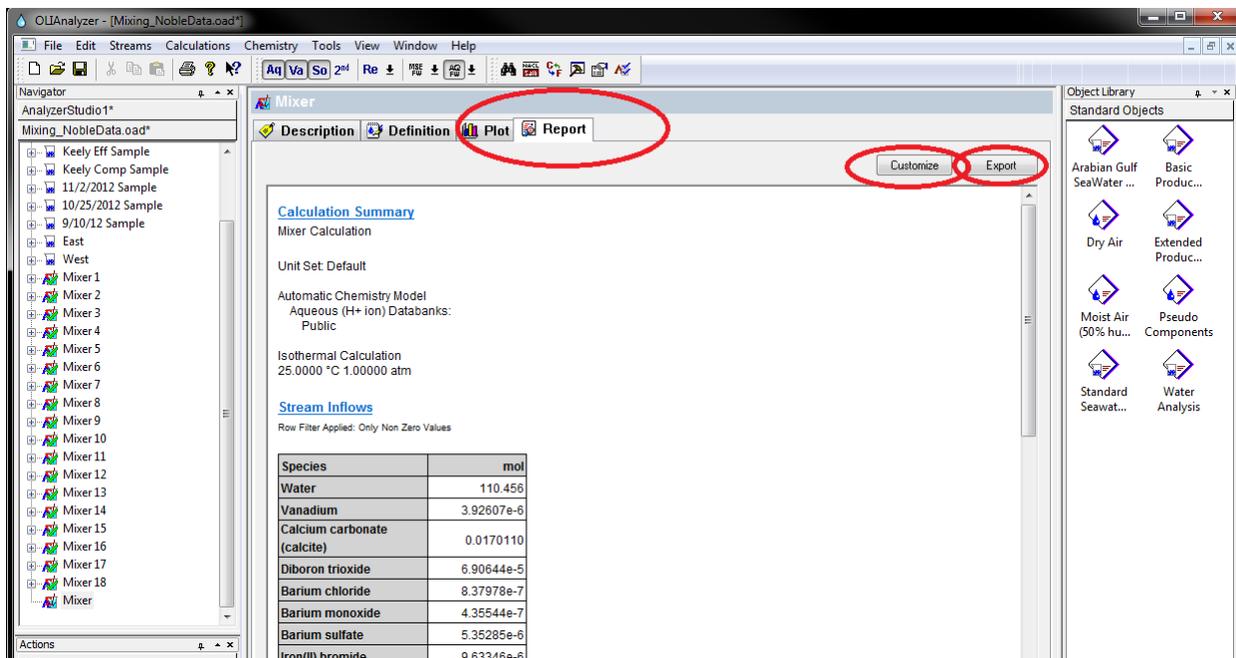
Figure 22. Screenshot of Report tab

- From the above case study we could derive characteristics such stream inflows specifics, pH levels for different mixtures, possible compounds formed or present in streams, solids formed, scaling tendency, and chemical complexes formed. There were valuable treatment specifics which could be used to optimize treatment and reduced use of unnecessary chemicals. The detailed reports from this case study are presented in the Appendix Section A2. This has been very useful optimize specific steps in treatment to optimize use of chemicals, conditions, etc.

- It was planned in such a way that these values would be used in a GIS application such that the spreadsheet containing all this data would be interlinked with a GIS web map, and as soon as the calculations were done using the analyzer would work their way to the application because of the live link, they could be used in custom GIS interpolation plots to give an idea of how treatment would vary spatially. This could be done if the

Analyzer's function could be programmed into a spreadsheet, and the spreadsheet could be connected to the GIS application using a FTP as shown in Figure 22.
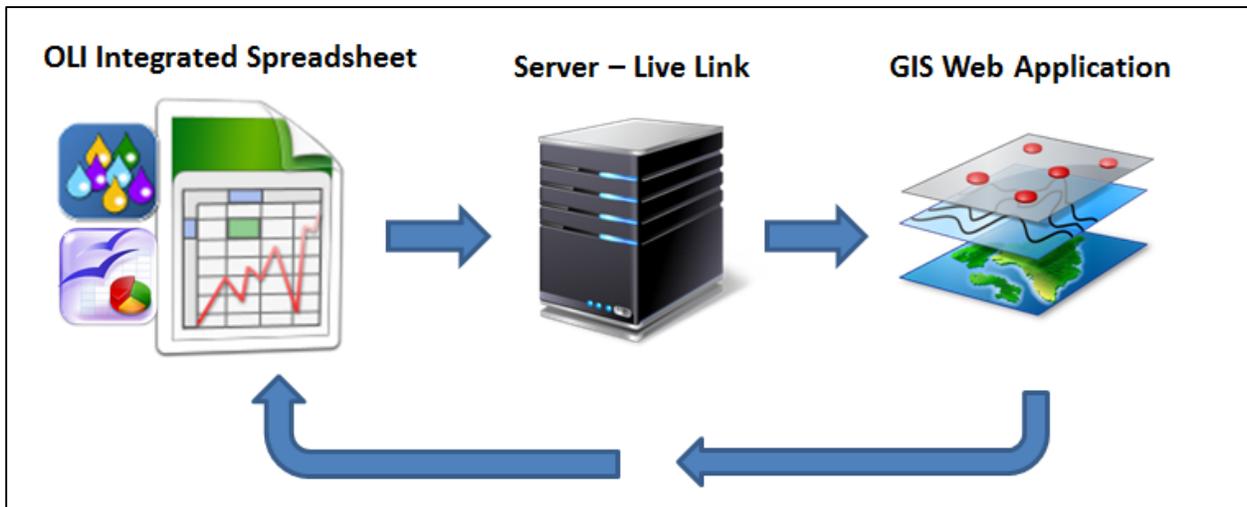
Figure 23. Initial idea schematic

Multiple steps were used in the OLI to CalcAQ integration process. These are documented as follows.

1. All of the calculations are then done with OLI functions, as called through CalcAQ.

2. With the given procedures for reconciling the analytical results with reality, we produce an output stream that can simulate the sample in other calculations and the corresponding deviations from the measured analytical data.

3. We take in the water data and then process it into the chemistry calculator.

4. After an initial charge balance, we calculate the pH and estimate the amount of carbonate from the reported alkalinity.

5. We then iterate on those until we get a match with the amount of acid required in the alkalinity titration and the sample pH. There will be errors and we report those.

6. We then use the OLI functions to give an equivalent stream of stable species and we calculate the measurable and important properties for processing the stream.

7. At present, we calculate only one sample at a time. We will implement mixing and in-line treatment later.

8. We also show the results of running the stream through the built-in choice of treatment process.

9. Where a special function was necessary, such as removing water to a precipitation point, we programmed a customized solver and combinations of CalcAq functions.

The chemistry tool reconciles the chemical and physical data and predicts the chemical and physical properties of the fluid. The chemistry tool uses these predictions, in turn, to predict the requirements for treatment of the fluid and its behavior under treatment or disposal. These calculations would normally be the responsibility of a field chemist or a field water manager for a production company operating wells in a particular field. The chemistry tool uses the best available software and database from OLI Systems Inc. and standardizes the calculations so that they can be used with confidence by a variety of organizations. In the future, the chemistry tool will also automate the calculations, so that they can be performed reproducibly for thousands of wells in a field or in multiple fields across the country. OLI Analyzer has a limitation on the amount of data it can process in a single set of calculation. Hence, we proposed the idea of running batch calculations in Microsoft Excel using the CalcAQ Plug-in which pulls the

calculation service from the OLI Engine and does the calculations for a huge set of data. This could essentially help us in the future to run multiple calculations in a single click. The fields generate a huge amount of data and it would be a necessity to have a batch calculator do the analysis that we program it to do.

3.4.4   Customization:

The particular goals were to validate the water analyses, recommend improvements to the analyses, predict the properties of the produced water, and predict the results of transportation, treatment, and disposal. The data were from new analyses by ACZ Laboratories of samples newly drawn from separator tanks at the well sites. The following data were available: Well location and operator; Ba, Ca, Fe, K, Mg, Na, Cl^-, PO_4^{3-}, SO_4^{2-}; pH; Alkalinity by titration; electrical conductivity; total dissolved solids (TDS) by evaporation.

The following parameters could be calculated by OLI software: equivalent composition, using stable species; pH; alkalinity; ORP; TDS; conductivity; scaling tendency and solids; viscosity; thermal conductivity; surface tension; vapor pressure and gases. The same computer programs allow the prediction of the results of treatment by processes like precipitation with base and reverse osmosis (RO).

There were three things that shaped our plans and progress on the tools for modeling the chemistry. First, water analyses are sparse to nonexistent. Sometimes the flows or truckloads go direct to disposal. When sampling and analyses were done, the conditions were seldom documented and only a few parameters were measured. The analyses on which we tested the chemistry tool were new and standardized. Second, we are still programming while sampling is in progress. The chemistry and the analytical procedures have been changing as we look at the

data. Third, there is the list, provided above, of the data to be reconciled by the first version of

the tool. Some of the species affect the other measurements strongly, so we are still working out

means to detect errors.
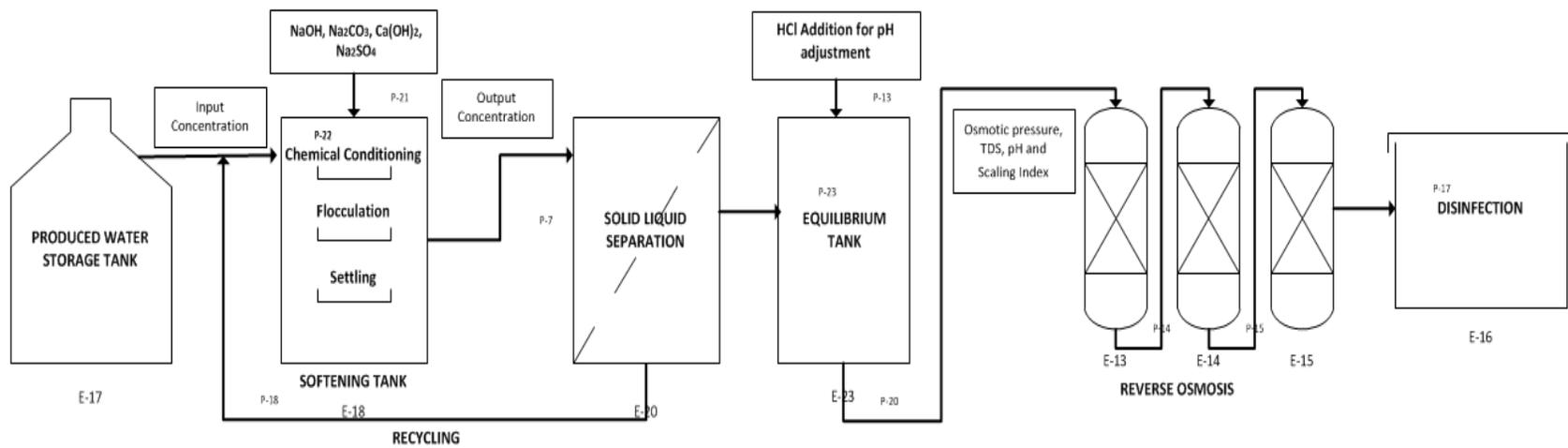
Figure 24. Schematic of the process train chosen for simulation in the first version of the chemistry tool.

3.4.5   Integration into Excel Database – CalcAQ Case Study:

The problem that needed to be solved here was the single stream restriction in OLI Analyzer. The water quality field data was going to be numerous and since OLI Analyzer only supports single stream data, the process of inputting each set of data and processing them individually was a time consuming process. Thus, integration to Microsoft Excel would have to be programmed to run batch calculations to help us integrate into a GIS tool in the future. This problem was solved by programming OLI Analyzers functions into Microsoft Excel. The process is described as follows. Figure 23 depicts the process train that was chosen for simulation in the first version of the chemistry tool. We built the model in our tool to simulate the steps in this particular train. As shown, we can easily modify the steps to represent the facilities available at a particular site.

Each unit operation was identified and a detailed flow chart that can be simulated by individual calculations in Excel. All of the calculations are then done with OLI functions, as called through CalcAQ.

The calculations projected to be done in CalcAQ are based on single steps such as calculating compound compositions of the input water quality and adding them into an excel sheet with CalcAQ Plug-in, then analyzing it for settling, softening, filtration and reverse osmosis. This will also include the periodic addition of chemicals to maintain specific characteristics such as pH and composition. The survey done with variation of temperature yielded plots which could be used to depict the changes in concentration of the ions during the analysis done by OLI Analyzer. CalcAQ could be used to get a working application based on Excel which could be used to illustratively describe an output when a prospective input within the limits of the processor is entered.

53
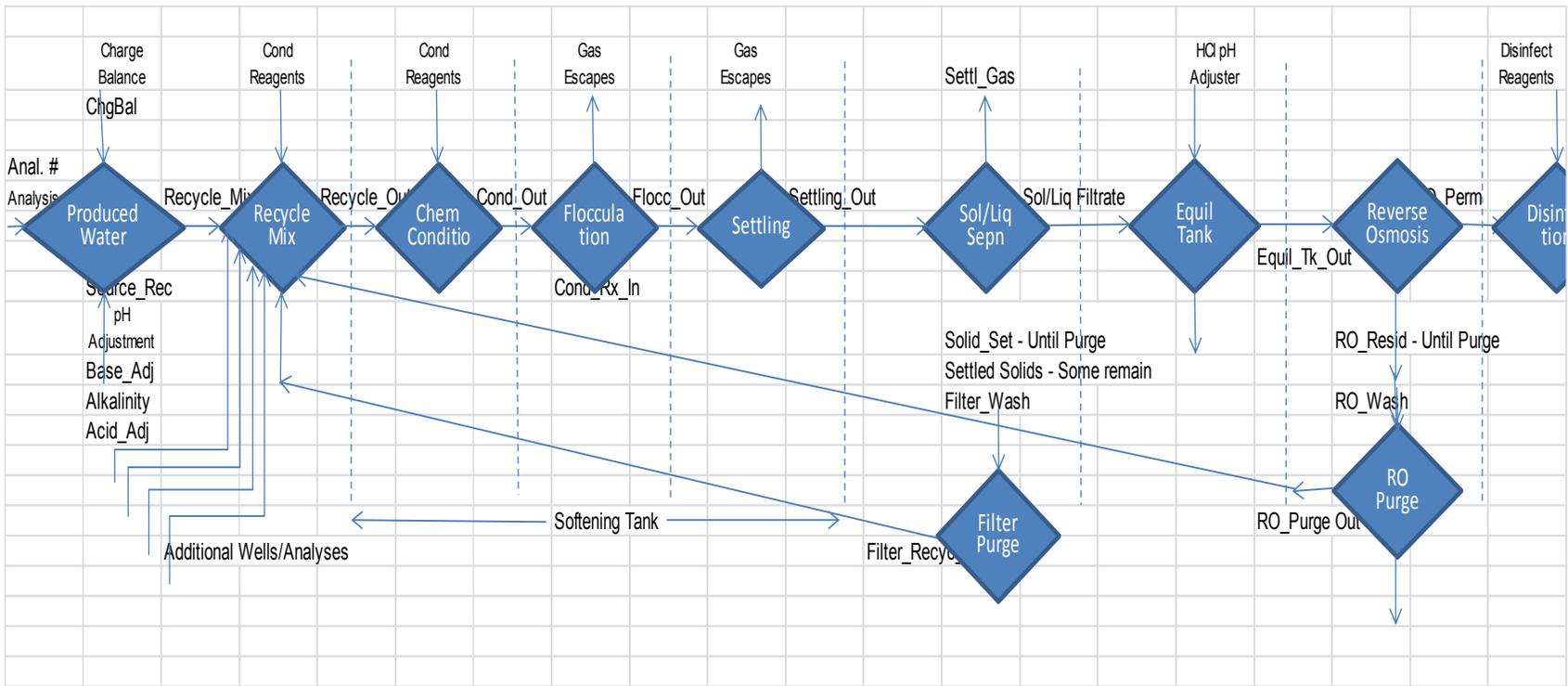
Figure 25. A Screenshot of the Process Schema used for the tool development

The schematic process was converted to a list of specific processes that we could model. Each step then became a page in an Excel workbook and we worked each like a process block in an ESP model (as shown in Figure 24). The Excel environment with the functions of CalcAq allows us to modify each block to reflect changing understanding or variable efficiencies. At this stage, evaluating the results still requires an expert to judge whether the analytical data are valid and the treatment processes are appropriate for the sample.

Date/Time	Well	Code #	Parameter mg/L Barium, di	mg/L Calcium, c	mg/L Chloride	mg/L Iron, disso	mg/L Magnesiur	mg/L Phospha
06/22/2012	WELLS RANCH 25-68-1HZ	L9530-01	4.54	163	8900	20.4	23	0.0
06/28/2012	HARRINGTON 2-30	L95930-02	4.51	200	3600	113	16	
06/29/2012	WALCKER VSX AB 1-7 1-8	L95930-03	9.11	604	23000	135	69	1.0
06/28/2012	FURROW 15-99HZ	L95930-04	52.3	1170	29000	45	140	
06/29/2012	JOHNSON 13-15 13-23	L95930-05	20.3	293	10000	39.7	31	0.6
06/29/2012	ROUSSE 05-05 05-06	L95930-06	19.6	338	11600	94.9	34	0.3
07/13/2012	NAT'L HOG FARMS 12-21	L95930-07	28.7	261	11600	280	31	0.3
07/31/2012	WELLS RANCH AE 32-03 32-04	L95930-08	27.7	426	18500	294	59	0.6
07/31/2012	WELLS RANCH USX BB1-11 2 7 8	L95930-09	15.5	284	13300	122	35	0.6
07/31/2012	WELLS RANCH USX HA 35-9 15 1(	L95930-10	4.23	188	9700	107	21	0.3

Figure 26. Screenshot of the input portion of the file of measured parameters from tabulated from the report of the analytical laboratory

56

Results from the analytical laboratory were converted into the table of measured parameters shown in Figure 25 and loaded as the corresponding comma-separated-values (.csv) file. This is a "flat" file, with no indexing, as distinct from a database. The program could more efficiently load and save to a database, such as a SQL or MS/Access file, but this would require new programming. In operation, the macro of the "Load Params" button reads the .csv file and loads the data into the locations on the "Well1" worksheet in the program workbook. The indicated cells are highlighted in yellow, as shown in Figure 26.

The "Summary" worksheet is shown Figure 27. It presents the same data alongside the parameters of the equivalent output stream obtained by reconciling all of the available data and the results of treating the equivalent stream in the process simulators. The deviations from measured values are displayed on the summary as well, so the operator can judge the validity of the simulations and modify the reconciliation or treatment processes as necessary. The operator can also examine and modify each process step by opening the corresponding worksheet. The "Summary" worksheet also contains the buttons that start the macros for loading the data, running any necessary solver, and saving the results. The loading macro turns off automatic calculation of cells, so that a calculation does not start with incomplete data. It runs calculations when necessary.

The program flow for sample reconciliation is visible in Figure 27, showing "Well1". After an initial charge balance, we calculate the pH and estimate the amount of carbonate from the reported alkalinity. We then iterate on those until we get a match with the amount of acid required in the alkalinity titration and the sample pH. There will be errors and we report those. We then use the OLI functions to give an equivalent stream of stable species and we calculate

57

Figure 27. Screenshot of the "Well1" worksheet in the chemistry tool workbook showing analytical data and the reconciliation process.
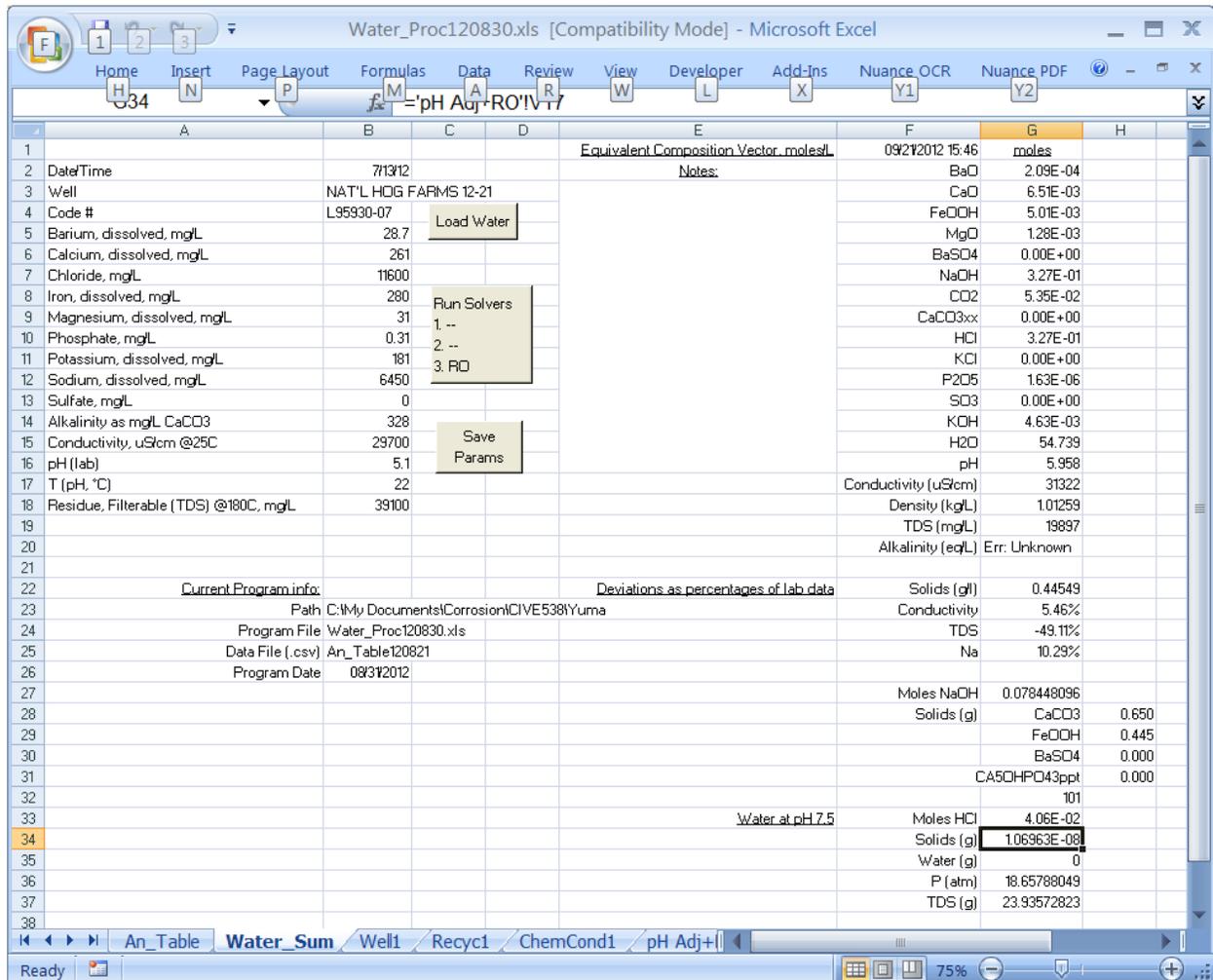
Figure 28. Screenshot of the summary worksheet, which provides the operator an overview of all data and predictions.

the measurable and important properties for processing the stream. At present, we calculate only one sample at a time. We expect to implement mixing and in-line treatment later, such as the injection of scale inhibitors into a pipeline or truckload. The "Recyc1" worksheet is configured to accommodate those enhancements, along with treating the byproduct streams from subsequent processes.

The calculations for "Well1" are fairly straightforward. All are done with the version of the OLI Engine and databank packaged with OLI Analyzer v. 3.2. First, we balance charge with Na+. We have other options, but all of our current samples are deficient in cations. Second, we use the reported alkalinity to estimate the amount of CO_2 present and adjust the pH to the measured value. The alkalinity was measured by titration, but we only have the number of equivalents, no pH for the end point, so we guess a pH of 4.1, based on a titration curve that we calculated for a single sample with OLI Water Analyzer v. 3.2. We then calculate the titration requirement and adjust the CO_2 and the pH again, repeating this process until the calculated pH and alkalinity match the measured values. So far, we have found convergence within 3 iterations, so we have not used a formal solver. We then calculate the molecular equivalent stream.

The calculations for "Recyc1" are even simpler. All of the species in the calculated molecular equivalent stream are tabulated and their amounts are passed to a summing table which adds (zero) flows from the other process wells and recycle streams. The resulting table is then available for further use.

From the output of "Recyc1", which, for now, is the same as "Well1", we calculate the results of running the stream through the built-in choice of treatment process. The first is the chemical conditioning ("ChemCond1" worksheet) with a simple "SetpH" function from the CalcAq library. We specify pH 10.4, based on some process experience, but the setpoint can be readily modified by the operator and the process repeated, recording the new results in the output table. By cataloging all of the solids from the calculated stream, we can remove them to produce a simulated "filtrate", which can be characterized with a new molecular equivalent stream.

60

The "filtrate" is then treated in the "RO1" worksheet. We neutralize in the same way, using the SetpH function as we did in the pH adjustments of "Well1" and the conditioning of "ChemCond1". Again, the pH can be adjusted by the operator, although the choice should be documented in the output file. Then, we see if we can remove water from the neutralized stream to simulate RO. Most samples, so far, allowed some water to be removed before we got to 1.E-7 M solids. The program could accommodate a more sophisticated model of RO, including better choices of how much solid the membrane could tolerate. In order to remove water to a precipitation point without forecasting the precipitating species, we programmed a customized solver and combinations of CalcAq functions.
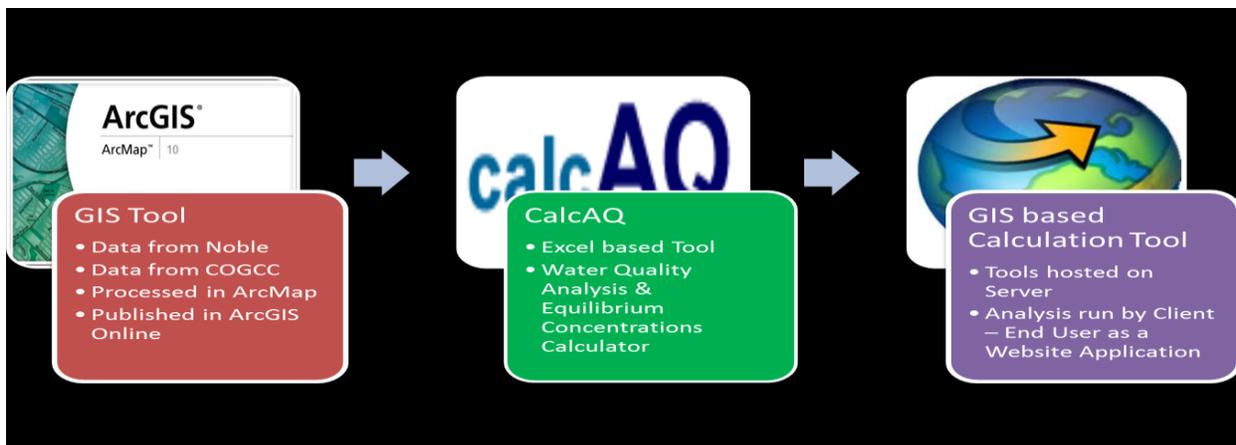
Figure 29. Schematic of the proposed plan

To summarize, an Excel based tool was developed to make the equilibrium concentration calculations for each water quality we had from the oil and gas wells. This tool utilized the CalcAQ add-in to calculate the formulas used for making the equilibrium calculations. The CalcAQ add-in uses the OLI Engine from the OLI Analyzer to run the calculations and estimations. The final tool was linked with an ArcGIS module for spatial analysis (as shown in Figure 28) which will be explained in detail further.

This tool was initially formulated to process 10 water quality values, since that was the only water quality data that was present at this time. These water quality values were taken from the initial database with all the location data i.e. co-ordinates. These values were then processed using the CalcAQ tool. The equilibrium concentrations were determined for further chemical addition. The concentration and quantity of chemical additives required to treat the water to a desired water quality were determined along with the most suitable chemical additives for each step in the treatment process. Various other conditions such as pH and osmotic pressure were also determined according to the water quality analysis done using this tool.

The chemistry behind the tool is as follows:

1. Balance charge with Na+. We have other options, but all of our current samples are deficient in cations.

2. Use the reported alkalinity to estimate the amount of CO_2 present and adjust the pH to the measured value. The alkalinity was measured by titration, but we only have the number of equivalents.

3. Calculate the titration requirement and adjust the CO_2 and the pH again, repeating this process until the calculated pH and alkalinity match the measured values. So far, we have found convergence within 3 iterations, so we have not used a formal solver. It takes about a minute on a 5-year old computer.

4. Calculate the molecular equivalent stream.

5. Run through the chemical conditioning with a simple "Set pH"
   After removing solids, neutralize the same way, and then we see if we can remove water to simulate RO. Most samples, so far, allowed some water to be removed before we got

62

to 1.E-7 M solids. The amount of solids is optimum at 1.E-7 M solids for maximum efficient removal of water.

3.4.6 Real-Time Integration:

Water sampling was conducted on site by Colorado State University with help from Noble Energy Inc. Thus, the water quality values for each specific well were obtained. Future work involves a real-time integration module that would enable the user to use real-time water quality values to predict equilibrium and scaling potential for a more accurate treatment prediction (Figure 29).

Figure 30. A schematic of the Water Analyzer Tool

The real-time data would be setup through telemetry systems connected to the water storage tanks that measure water quality on a real-time basis. This data would be transmitted via transmitters, nodes or satellites. The receiver would in turn process the data and send it to a cloud based server. This data could be linked to the analyzer program hosted on a server. The server would be accessible to users in the form of webpage or essentially a map based application. The

user would be able to select a specific area, obtain the water quality for that area and also be able to run simulations and analyses for that specific area with the real-time data.

3.5 User Application:

A framework was developed for the analysis to be integrated with a GIS database; in such a way that it can be hosted on a server and run from a browser by the client. Various interpolated maps of water quality were developed based on the water quality. These were instrumental in determining the best ways to sample according to the diverse water qualities.

The framework for the user application was developed in this process. The base was to develop a user friendly application where the user could access all data on a GIS interface, select any set of data points, in this case wells, analyze them cumulatively or individually and export results to any required format. The programming was to be done using JavaScript as it was the most popular and multi-feature compatible language and best suited for this purpose.

The initial maps were done using Microsoft Silverlight. The switch to JavaScript ensured the compatibility of any browser on a desktop, Apple Computers or mobile. This way the portability of the application was enhanced. The GIS part of the application was more of what the user would see first in the application, since the chemistry tool would be background processing and the calculation engine.

The target was to make the map visually appealing in a map friendly structure with multiple layers to choose from according to the user's requirements or interests. In this way, the user would be able to perform multiple tasks altogether in the same page.

All the map data were to be processed in the ArcMap Application individually. Then these would be sized and prepared as Shapefiles or datasets ready to be hosted on a server or a cloud from where they could be accessed in the pre-processed condition. All the layers were prepared according to the multiple functions deployable, converted into feature services in order to support queries and then hosted on ArcGIS Online through a paid subscription.

Once these files were hosted, they were tested in various web maps in ArcGIS Explorer Online in order to prove their analytical capabilities. After testing, they were securely stored in the server folder for the subscription, which would enable it to be shared only by a secure login. The application was then formulized according to requirements with a single basemap as a default layout and all the layers were then securely added from the server as clickable switch on/off layers. These layers could be turned on or off whenever required or not respectively. More details on the functionality is provided in the appendix.

The data sets for analysis were to be prepared in a server database file. These were processed, filtered according to our requirements for the default analysis tasks layout and securely stored in the server for direct dynamic access. This way any changes made to the database file linked to a real-time source would be reflected instantly on the map.

The chemistry tool part was the easier part of the two main phases. The chemistry tool was programmed in Microsoft Excel as mentioned in the previous sections. This enabled us to program it in an FTP on the server directly with input/output feeds setup. All the calculations were already done once on the base model. This was programmed for the demonstration in two parts. The first was to do the analysis using the map only on the given dataset. The next phase,

that is still underway, will allow a user to input his/her own data and perform analysis according to his requirements.

A live link would be setup from the chemistry tool dataset to the map using the ArcGIS Online link to CSV feed module. The chemistry tool as mentioned earlier, would be setup on the server from where it could be securely connected to the map application. This way the application would consist of a complex access to a web map and a chemistry tool with custom programmed functions. So fundamentally, a user would interact with a map, view data on a spatial scale, perform analysis and see the relativity on a map, which he could export or print according to his requirement. A conceptual schematic is shown in Figure 30.
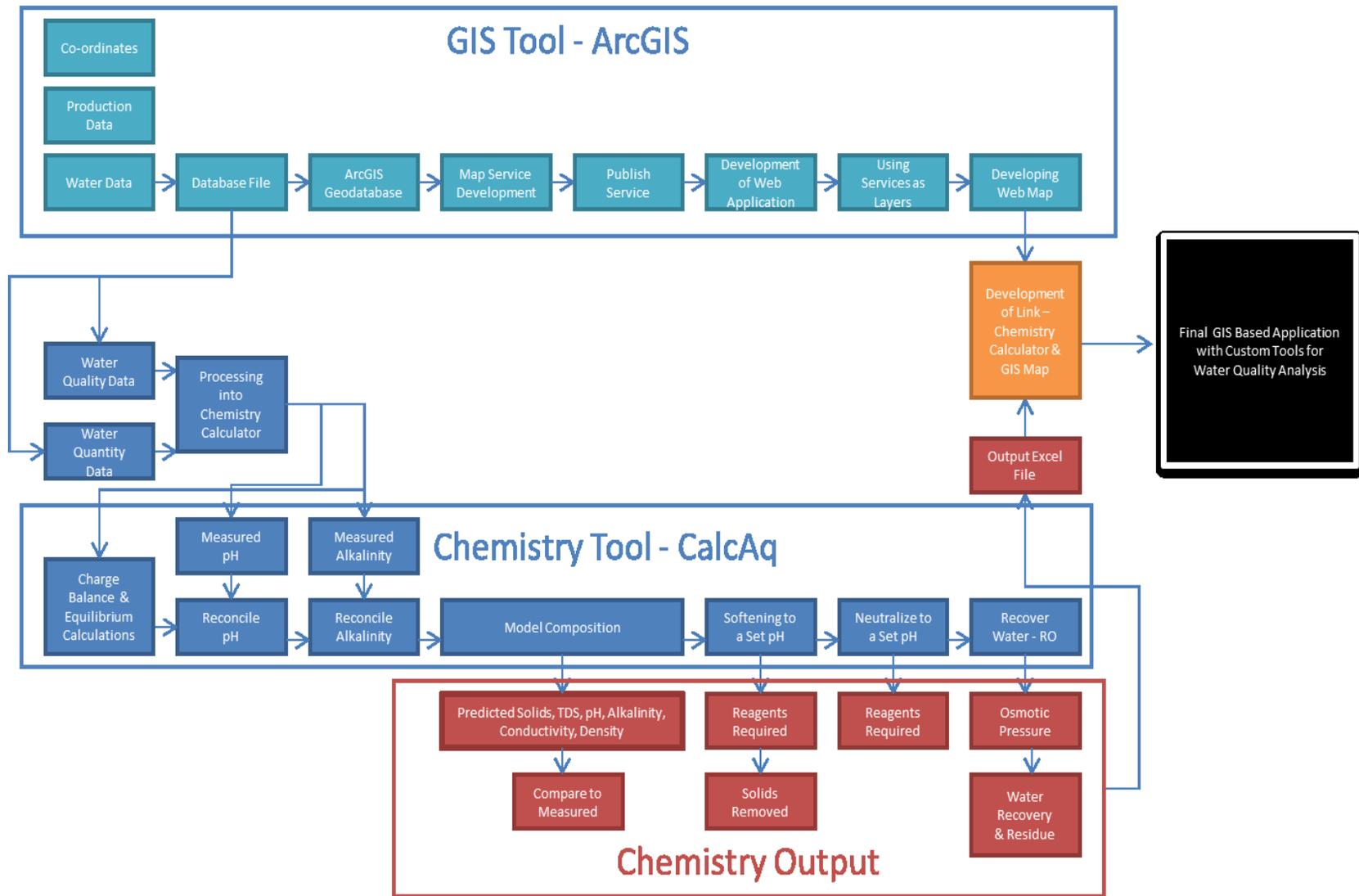
Figure 31. Schematic of the Final User Application Framework

4. CONCLUSION

The GIS aspect of the chemistry tool is a valuable asset to the oil and gas industry since we could analyze the water quality spatially and monitor it on a map. Analysis of the water quality for any specific set of data on any field which could also be viewed spatially. This helps in preparing the kind of treatment required for each specific field. The tool can also be used to mix water qualities before we send them to a centralized treatment facility. This would also help in effectively managing produced water for re-injection or groundwater discharge based on their water quality, instead of disposing them in disposal pits or evaporation ponds. This would also be influential in reduced truck traffic and air pollution caused by trucks. The future of this tool involves further fabrication with improved models for the treatment processes so that the operator will be more confident in the relevance of the results including real-time monitoring of water quality. Improved error handling would also be done, so that the operator can interpret problems in either the program or the chemical process. For easier use, Wizards would be programmed to solve chemistry problems so that the operator need not be an experience chemical engineer to manage routine streams. Work will also be done for improving the water analysis that we use as input, including oil carryover. That way, the full capability of OLI software and databases would be utilized. The final objective will be to develop a web based application for the public and the industry to use to know more about what is happening in their neighborhood, and what kinds of actions have to be taken accordingly.

Extensive analysis was done on the wells for which data was obtained from the Colorado Oil and Gas Conservation Commission. Based on this obtained data, the inputs for the OLI Analyzer were prepared. A template was prepared in the OLI Analyzer using standard water quality values obtained earlier from the USGS Database and the water quality values from the initial sampling

done by our research group. This template can be used for any set of water qualities from other sources. Documentation of steps used to run the analysis of water using OLI Analyzer has been provided. Once the analysis was done, the data was input and treatment specifics were derived using CalcAQ, an additional independent plug-in for Microsoft Excel using the databanks from OLI Analyzer. Once the analysis was done using CalcAQ, this data was relatively conveniently placed in the excel sheet which was linked back to the ArcGIS database. Hence, once the calculations and analysis were performed on this spreadsheet, this was to be directly updating the ArcGIS database. A proposed deliverable in the near future would be a tool which automates the whole process of organizing the database and analyzing it according to our requirements. This would be an excellent opportunity for Oil and Gas companies to be more environment-friendly should they decide to utilize this tool.

5. REFERENCES

Abbott, L. T. and C. D. Argentati (1995). "GIS: A New Component of Public Services." Journal of Academic Librarianship 21(4): 251-256.

Al-Deffeeri, N. S. (2008). "The release of CO_2 in MSF distillers and its use for the recarbonation plant: a case study." Desalination 222(1): 579-591.

Ali, M. G., K. Younes, et al. (2011). "Assessment of Geostatistical Methods for Spatial Analysis of SPI and EDI Drought Indices." World Applied Sciences Journal 15(4): 474-482.

Amiri, M. and J. Moghadasi (2010). "Prediction the amount of barium sulfate scale formation in Siri oilfield using OLI ScaleChem software." Asian Journal of Scientific Research 3(4): 230-239.

Amiri, M. and J. Moghadasi (2012). "The Effect of Temperature on Calcium Carbonate Scale Formation in Iranian Oil Reservoirs Using OLI ScaleChem Software." Petroleum Science and Technology 30(5): 453-466.

Amiri, M., J. Moghadasi, et al. (2013). "The Study of Calcium Sulfate Scale Formation during Water Injection in Iranian Oil Fields at Different Pressures." Energy Sources, Part A: Recovery, Utilization, and Environmental Effects 35(7): 648-658.

Anderson, S. (2002). An evaluation of spatial interpolation methods on air temperature in Phoenix, AZ. Department of Geography, Arizona State University.

Arthur, J. D., B. Bohm, et al. (2009). "Hydraulic fracturing considerations for natural gas wells of the Marcellus Shale."

Aspinall, R. and D. Pearson (2000). "Integrated geographical assessment of environmental condition in water catchments: Linking landscape ecology, environmental modelling and GIS." Journal of Environmental Management 59(4): 299-319.

Ayatollahi, S. and M. Zerafat (2012). Nanotechnology-Assisted EOR Techniques: New Solutions to Old Challenges. SPE International Oilfield Nanotechnology Conference.

Benko, K. L. and J. E. Drewes (2008). "Produced water in the western United States: Geographical distribution, occurrence, and composition." Environmental Engineering Science 25(2): 239-246.

Boulding, J. R. and J. S. Ginn (2003). Practical handbook of soil, vadose zone, and ground-water contamination: assessment, prevention, and remediation, CRC.

Boulos, M. N. (2004). "Towards evidence-based, GIS-driven national spatial health information infrastructure and surveillance services in the United Kingdom." International Journal of Health Geographics 3(1): 1.

Clark, M. J. (1998). "Putting water in its place: a perspective on GIS in hydrology and water management." Hydrological Processes 12(6): 823-834.

Crittenden, J. C., R. R. Trussell, et al. (2012). MWH's Water Treatment: Principles and Design, Wiley.

CSM Website, C. S. o. M. (2009, June 18, 2009). "Potential Gas Committee reports unprecedented increase in magnitude of U.S. natural gas resource base." from http://www.mines.edu/Potential-Gas-Committee-reports-unprecedented-increase-in-magnitude-of-U.S.-natural-gas-resource-base.

Curtis, J. B. (2002). "Fractured shale-gas systems." AAPG bulletin 86(11): 1921-1938.

Dmour, H. N. (2013). "Productivity Index Enhancement of Stimulated Gas Wells through Hydraulic Fracturing." Petroleum Science and Technology 31(3): 225-236.

DOE, U. (2009). "Modern shale gas development in the United States: a primer." Washington, DC: US DOE. DoE-FG26-04NT15455.

Goodwin, S., K. Carlson, et al. (2012). "Life cycle analysis of water use and intensity of oil and gas recovery in Wattenberg field, Colo." Oil and Gas Journal.

Halliburton, W. (2008). "U.S. Shale Gas -An Unconventional Resource. Unconventional Challenges."   from http://www.halliburton.com/public/solutions/contents/shale/related_docs/H063771.pdf.

Hatzenbuhler, H. and T. J. Centner (2012). "Regulation of Water Pollution from Hydraulic Fracturing in Horizontally-Drilled Wells in the Marcellus Shale Region, USA." Water 4(4): 983-994.

HCTI Website, H. (2008).   About Reverse Osmosis 2013,   from http://www.hcti.com/sm/aboutro/aboutro.html.

Helmenstine, A. M. "What Is Reverse Osmosis and How Does It Work?".

Jarvie, D. M., R. J. Hill, et al. (2007). "Unconventional shale-gas systems: The Mississippian Barnett Shale of north-central Texas as one model for thermogenic shale-gas assessment." AAPG bulletin 91(4): 475-499.

Kouli, M., N. Lydakis-Simantiris, et al. (2008). "GIS-based aquifer modeling and planning using integrated geoenvironmental and chemical approaches." Groundwater: modeling, management and contamination. Nova Publishers, USA (ISBN: 978-1-60456-832-5).

Kurihara, M., H. Yamamura, et al. (1999). "High recovery/high pressure membranes for brine conversion SWRO process development and its performance data." Desalination 125(1): 9-15.

Lauver, L. S. (2012). "Environmental Health Advocacy: An Overview of Natural Gas Drilling in Northeast Pennsylvania and Implications for Pediatric Nursing." Journal of Pediatric Nursing-Nursing Care of Children and Families 27(4): 383-389.

McFarlane, J., D. T. Bostick, et al. (2002). Characterization and modeling of produced water. Proceedings of the Groundwater Protection Council Produced Water Conference, Colorado Springs.

McKinney, D. C. and X. Cai (2002). "Linking GIS and water resources management models: an object-oriented method." Environmental Modelling and Software 17(5): 413-425.

Mollah, M. Y. A., R. Schennach, et al. (2001). "Electrocoagulation (EC)—science and applications." Journal of hazardous materials 84(1): 29-41.

Murray-Gulde, C., J. E. Heatley, et al. (2003). "Performance of a hybrid reverse osmosis-constructed wetland treatment system for brackish oil field produced water." Water Research 37(3): 705-713.

Nicot, J. P. and I. J. Duncan (2012). "Common attributes of hydraulically fractured oil and gas production and CO2 geological sequestration." Greenhouse Gases-Science and Technology 2(5): 352-368.

Nourani, V. and R. G. Ejlali "Quantity and Quality Modeling of Groundwater by Conjugation of ANN and Co-Kriging Approaches."

OLI Website, O. (2005). Analyzer 2.0. 2005. OLI Systems, Morris Plains, NJ.

Pan America Website, E. (2007). Dissolved Air Flotation Theory, from http://www.dissolved-air-flotation.com/dissolved-air-flotation-theory.html.

Rey, P., S. Rey, et al. (2010). Methods of Treating Flowback Water, Google Patents.

Robinson, T. and G. Metternicht (2006). "Testing the performance of spatial interpolation techniques for mapping soil properties." Computers and electronics in agriculture 50(2): 97-108.

Rogers, H. (2011). "Shale gas-the unfolding story." Oxford Review of Economic Policy 27(1): 117-143.

Sahebjalal, E. (2012). "Application of Geostatistical Analysis for Evaluating Variation in Groundwater Characteristics." World Applied Sciences Journal 18(1): 135-141.

Schmidt, C. W. (2011). "Blind rush? Shale gas boom proceeds amid human health questions." Environmental Health Perspectives 119(8): a348.

Siemek, J., S. Nagy, et al. (2013). "Challenges for Sustainable Development: The Case of Shale Gas Exploitation in Poland." Problemy Ekorozwoju 8(1): 91-104.

Singh, V. P. and R. N. Yadava (2003). Watershed Hydrology: Proceedings of the International Conference on Water and Environment (WE-2003), December 15-18, 2003, Bhopal, India, Allied Publishers.

Smith, M., G. Holman, et al. (1978). "The azimuth of deep, penetrating fractures in the Wattenberg field." Journal of Petroleum Technology 30(2): 185-193.

Sourirajan, S. (1970). Reverse osmosis, London, UK: Logos Press Ltd.

Stevenson, D. G. (1997). Water treatment unit processes, World Scientific.

Steyaert, L. T. and M. F. Goodchild (1994). "Integrating geographic information systems and environmental simulation models: a status review." Environmental information management and analysis: ecosystem to global scales: 333-355.

Tao, F., S. Curtice, et al. (1993). "Reverse osmosis process successfully converts oil field brine into freshwater." Oil and Gas Journal;(United States) 91(38).

Toray Industries Website, T. (2013). "Reverse Osmosis Basics." from http://www.toraywater.com/knowledge/kno_001_01.html.

Turner, H. (2012). "CalcAQ Website." from http://www.turnertechnologies.net/calcAQ/index.php.

Veil, J. A., M. G. Puder, et al. (2004). "A white paper describing produced water from production of crude oil, natural gas, and coal bed methane." prepared by Argonne National Laboratory for the US Department of Energy, National Energy Technology Laboratory, January. Available at http://www. ead. anl. gov/pub/dsp_detail. cfm.

Warlick, D. (2006). "Gas shale and CBM development in North America." Oil and Gas Financial Journal 3(11): 1-5.

Weltman-Fahs, M. and J. M. Taylor (2013). "Hydraulic Fracturing and Brook Trout Habitat in the Marcellus Shale Region: Potential Impacts and Research Needs." <u>Fisheries</u> 38(1): 4-15.

Wiedeman, A. (1996). Regulation of produced water by the US Environmental Protection Agency. <u>Produced Water 2</u>, Springer: 27-41.

Yeh, G. C. (1995). Apparatus for dissolved air floatation and similar gas-liquid contacting operations, Google Patents.

Zabel, T. (1985). "The advantages of dissolved-air flotation for water treatment." <u>Journal (American Water Works Association)</u>: 42-46.

Zangaeva, E. (2010). "Produced water challenges: influence of production chemicals on flocculation."

A. APPENDICES

A1. Documentation of steps in the GIS Tool Development

All the steps involved in the setting up of the GIS tool have been explained here in brief with screenshots to help with each step. The initial steps include how the data has been setup for importing to the GIS application. Further after, the steps for customizing operations with the tool have been explained.

(a) Data Preparation for Addition in ESRI Shapefile Format (.shp):

- Finalize the data you need to add to your map. Make a copy of the file. Create a MAP DATA folder in your Desktop. Copy the Excel file into this folder. The MAP DATA is placed in the Desktop for maximum performance.

- Open ESRI ArcMap 10. Click on the Add data icon (as shown in Figure 31).
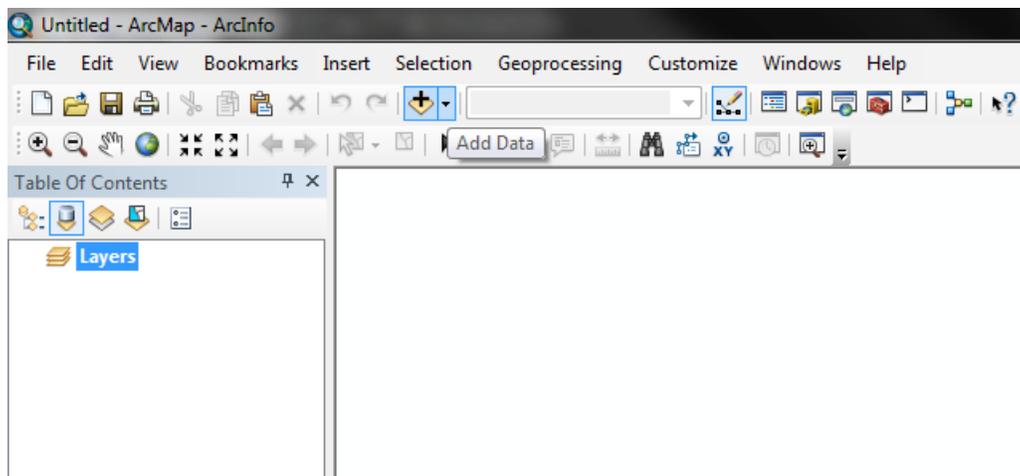
Figure 32. Screenshot of Add Data Tool

- A dialog box opens. Select the appropriate Excel File, corresponding Sheet and then click Add. (As shown in Figure 32).
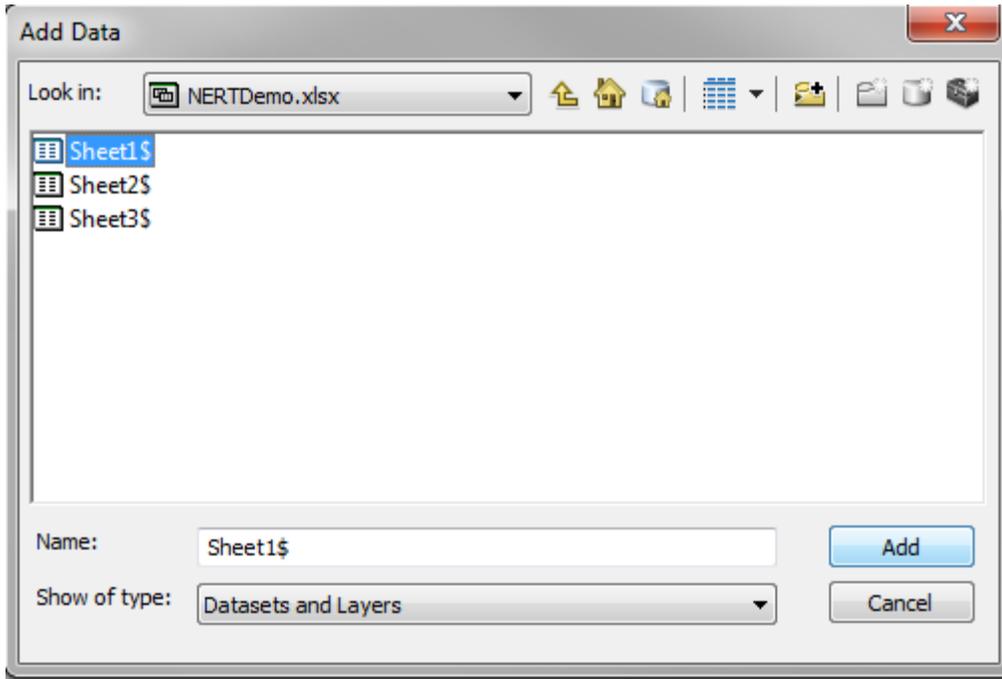
Figure 33. Screenshot of Add Data Dialog Box.

- Once the data is added from the Excel file to the map, you should be able to view it in the table of contents on the left toolbar. (Shown in Figure 33)
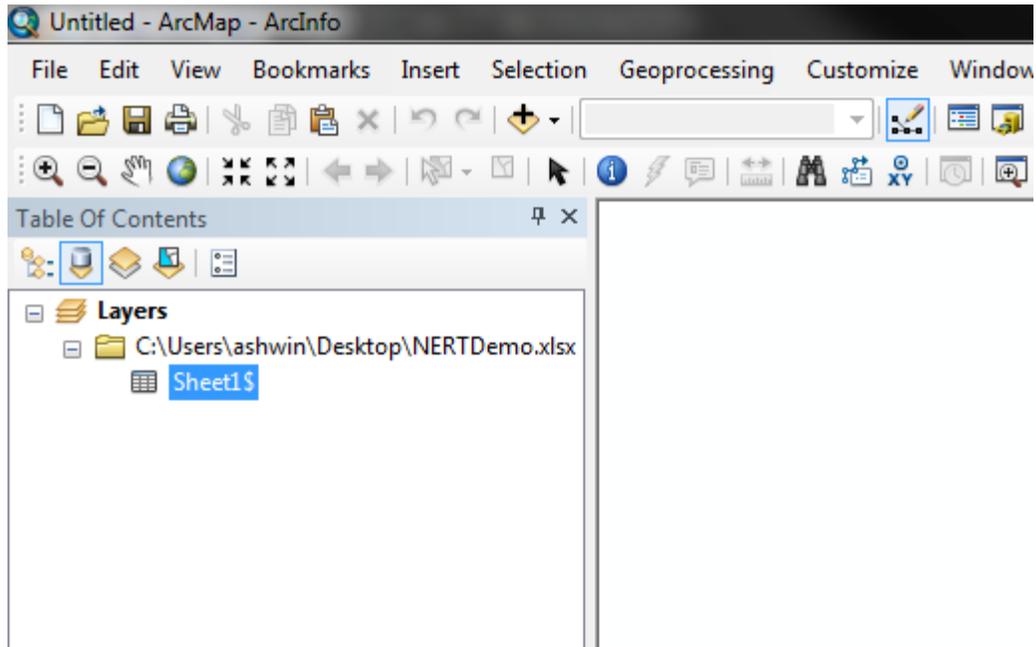
Figure 34. Screenshot of Table of Contents

- Right Click on Sheet 1$ in the Table of Contents and Select "Display XY Data" (As shown in Figure 34).
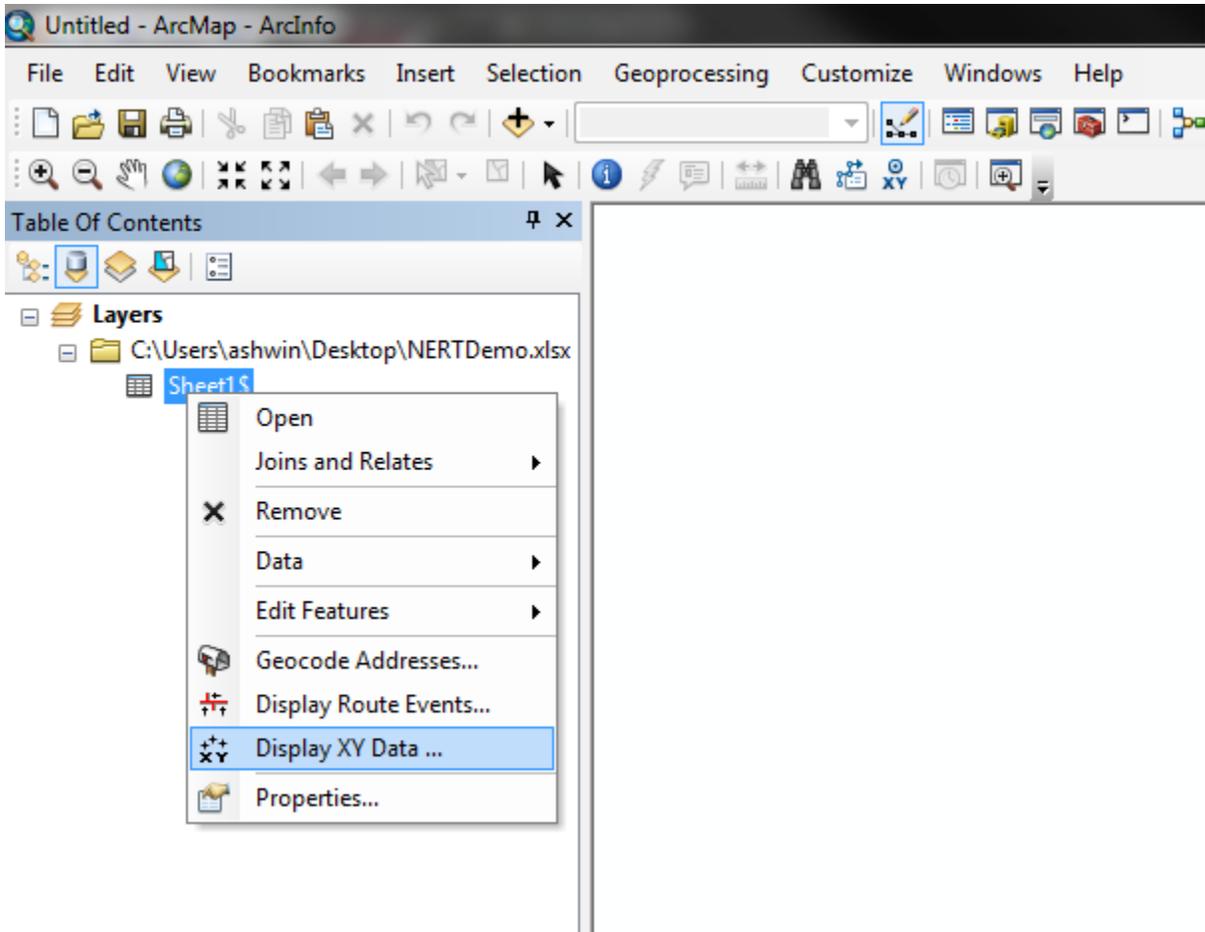
Figure 35. Screenshot of Right Click Window

- A dialog box should open up. Click on Edit (As shown in Figure 35).
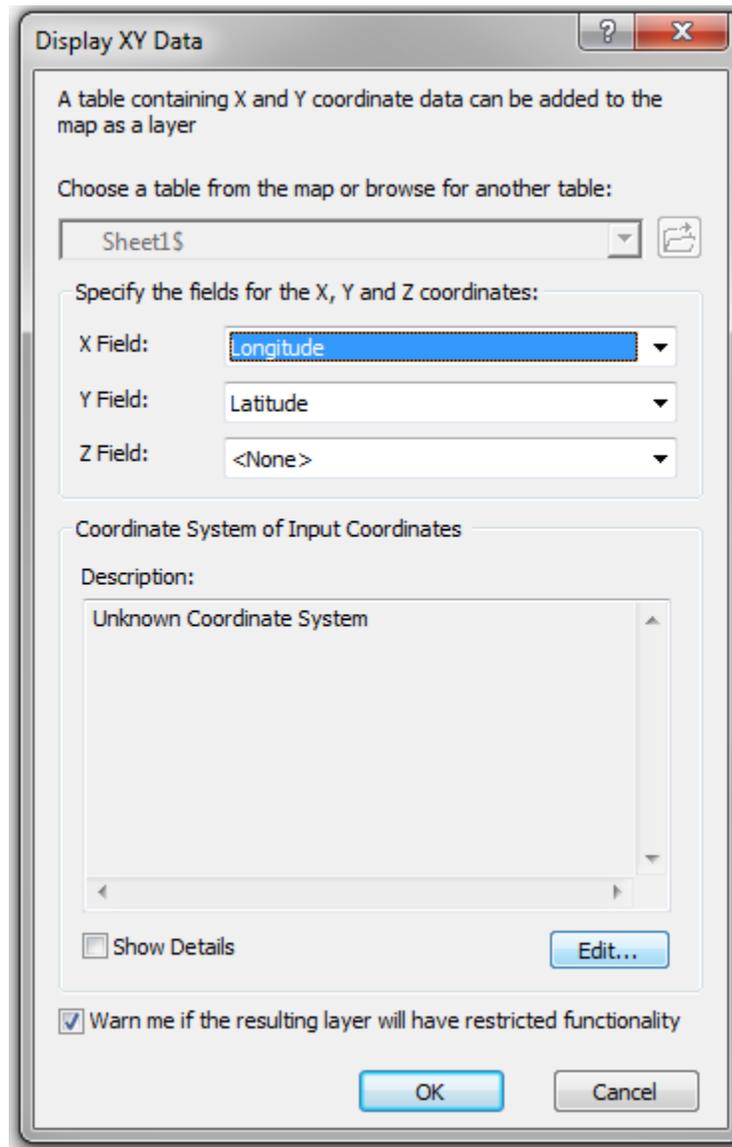
Figure 36. Screenshot of Dialog Box for Display XY Data

- After you click on Edit, another dialog box opens up. Click on Select to "choose a predefined co-ordinate system". Choose "Geographic Coordinate System/World/WGS 1984.prj" and Click "Add". (As shown in Figure 36)
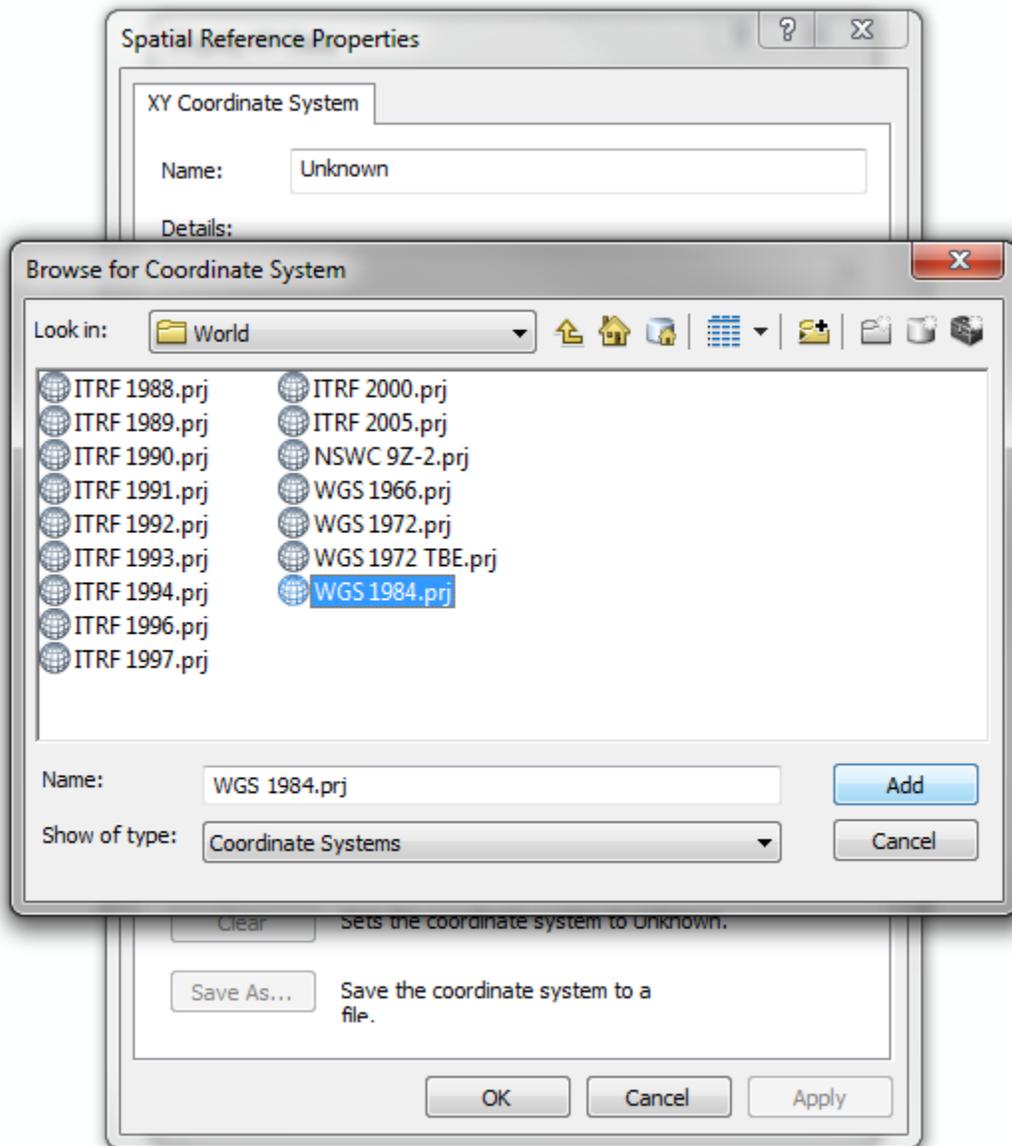
Figure 37. Screenshot of the Co-ordinate system selection Dialog box

- Click on Apply changes and then click OK. Another dialog box will open as follows.

Click OK and proceed. (As shown in Figure 37)

Table Does Not Have Object-ID Field

The table you specified does not have an Object-ID field so you will not be able to select, query, or edit the features in the resulting layer, or define relates for them.

After you create this layer, you can export it to a shapefile or feature class if you need these functions. To export a layer, right-click it in the Table Of Contents and choose Data>Export Data. Add the exported data to the map as a new layer.

OK   Cancel

Figure 38. Screenshot of Dialog Box

• You should now be able to see the points on the screen. (As shown in Figure 38)
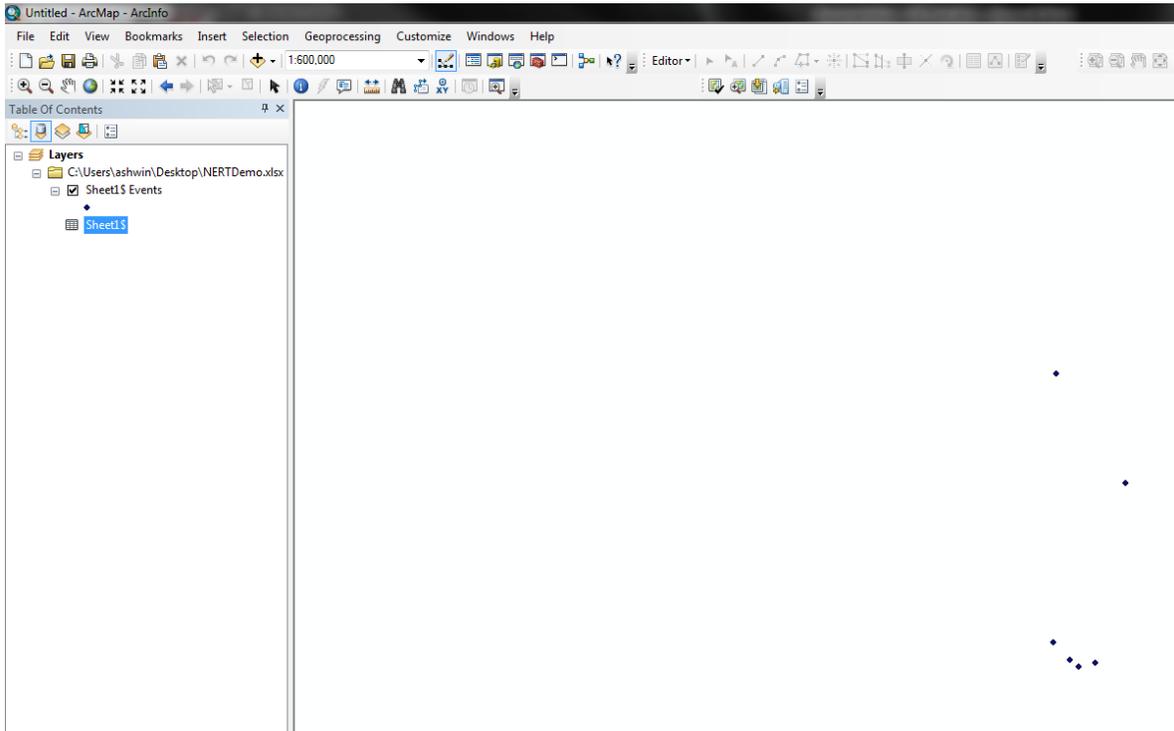
Figure 39. Screenshot of Display Screen

- Right Click on the Layer "Sheet 1$ Events" in the Table of Contents and Select "Export Data" from the Data tab as shown in Figure 39.
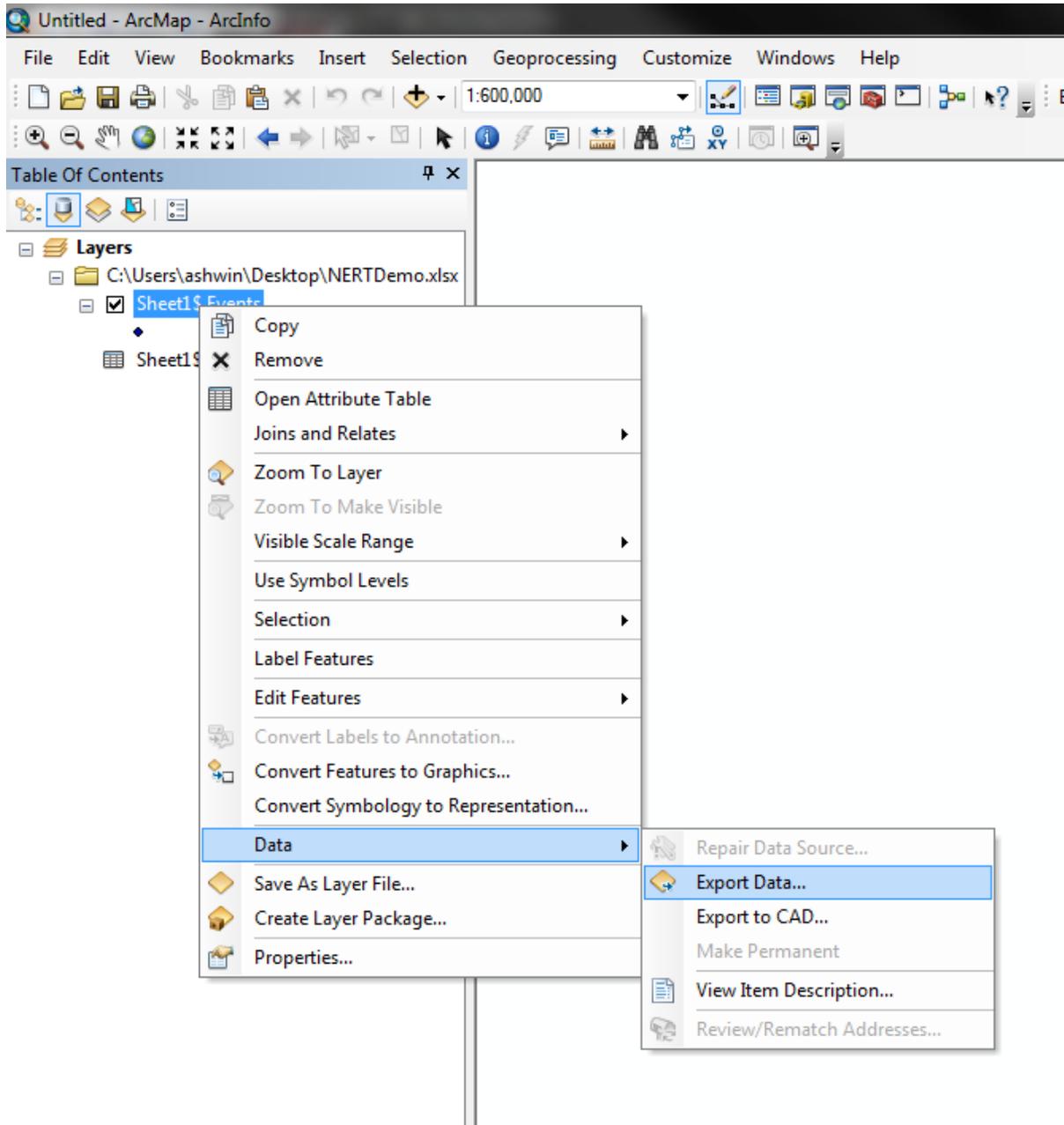
Figure 40. Screenshot of Export Data Process

- Now Type in your layer name, choose "this layer's source data" as the co-ordinate system choice and export all features to your corresponding Map Data folder located in your Desktop. (As shown in Figure 40)
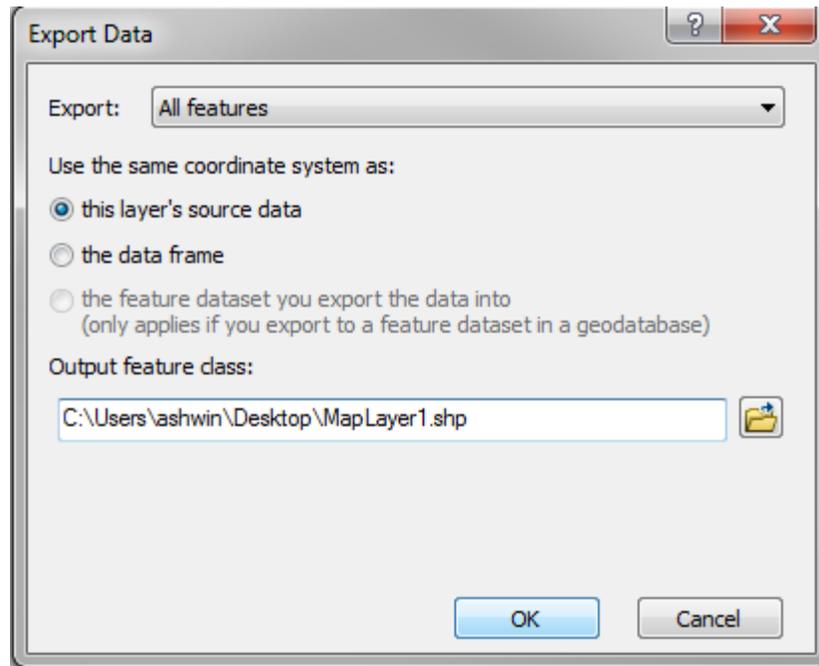
Figure 41. Screenshot of Exporting Data

- Now your shape file is ready for exporting to ArcGIS Explorer Online. Compress all the contents of your shape file (.dbf, .prj, etc) to a single zip file.

(b) Display Functionality - Adding Layers:

- Open your browser, go to http://www.arcgis.com/explorer/ and click on the "New Map" button. (As shown in Figure 41)
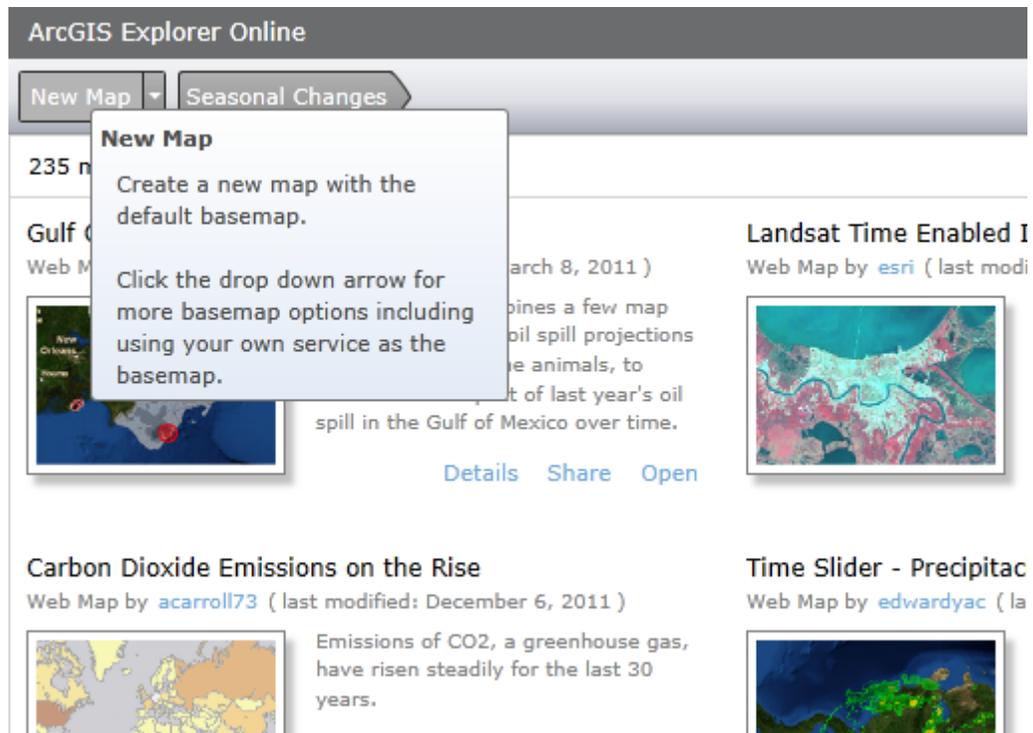
Figure 42. Screenshot of the New Map button

- After the New Map opens with a default basemap. The first step would be to add some data to it. Click on the Add Content button as shown in Figure 42.
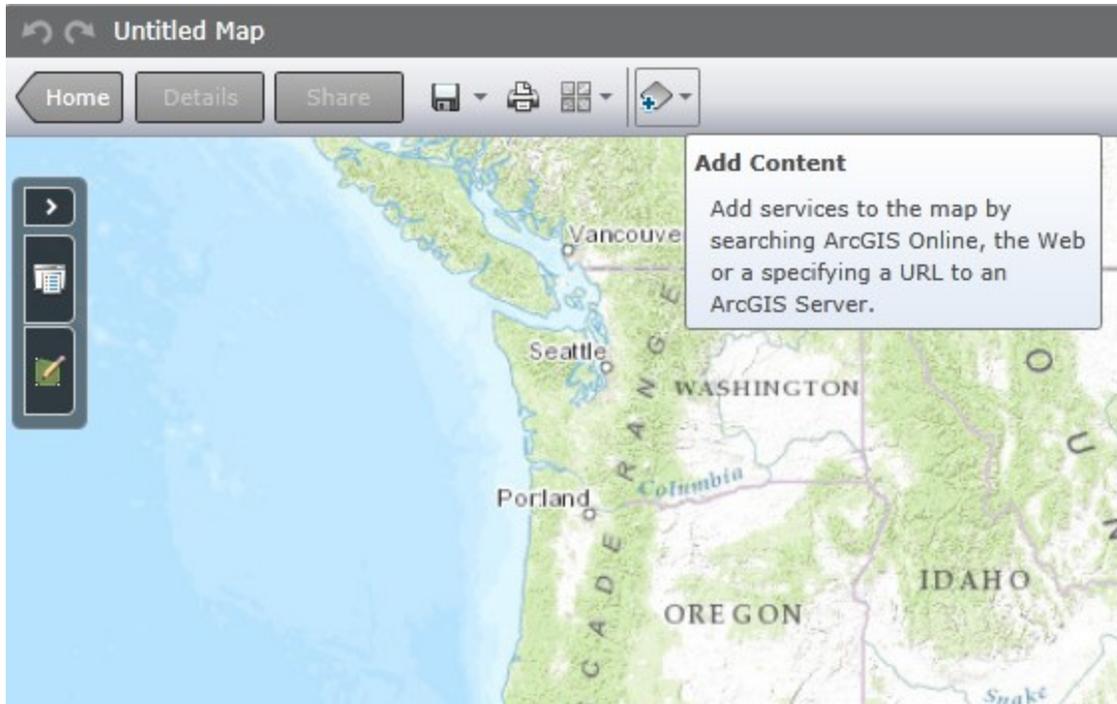
Figure 43. Screenshot of the Add Content Step

• After you click on Add Content, you will have options such as searching for layers, services on ArcGIS online or adding content with which you have worked with earlier or importing files like shapefiles, .gpx files or .csv files. Select the Shapefile option. (As shown in Figure 43)
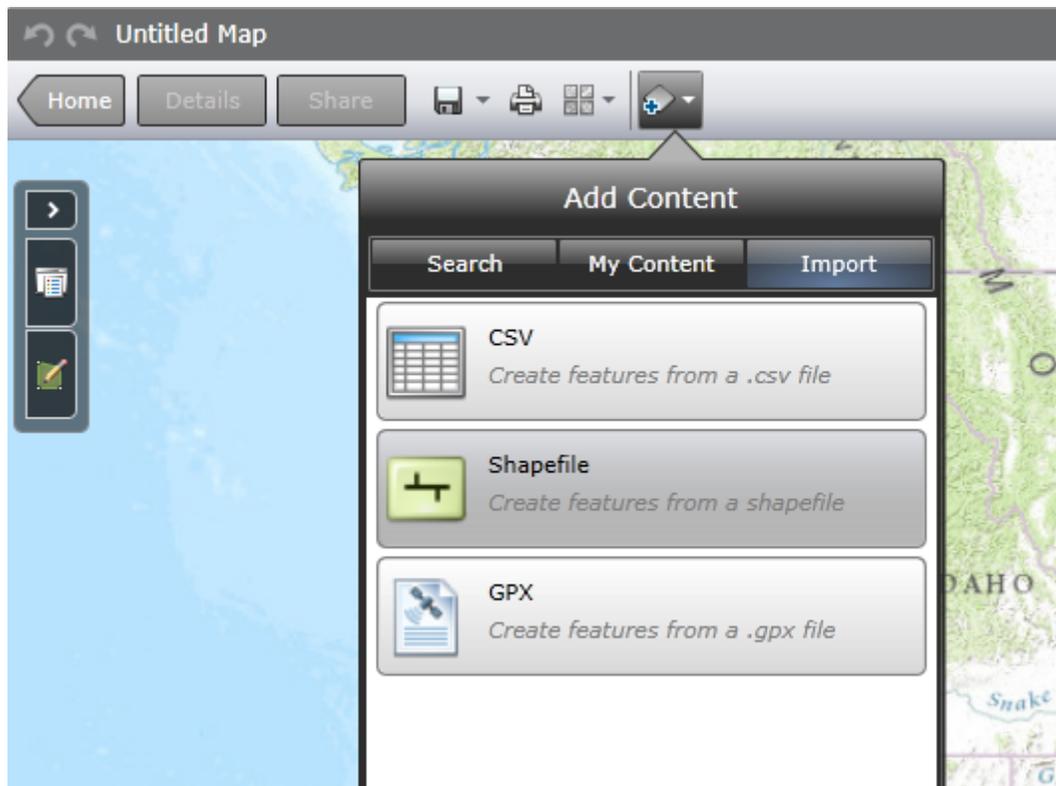
Figure 44. Screenshot of Import Shapefile Step

- A dialog box opens asking you to select the compressed zip file containing the Shapefile. Select the Zip File from your Map Data folder placed on the Desktop. (As shown in Figrue 44)
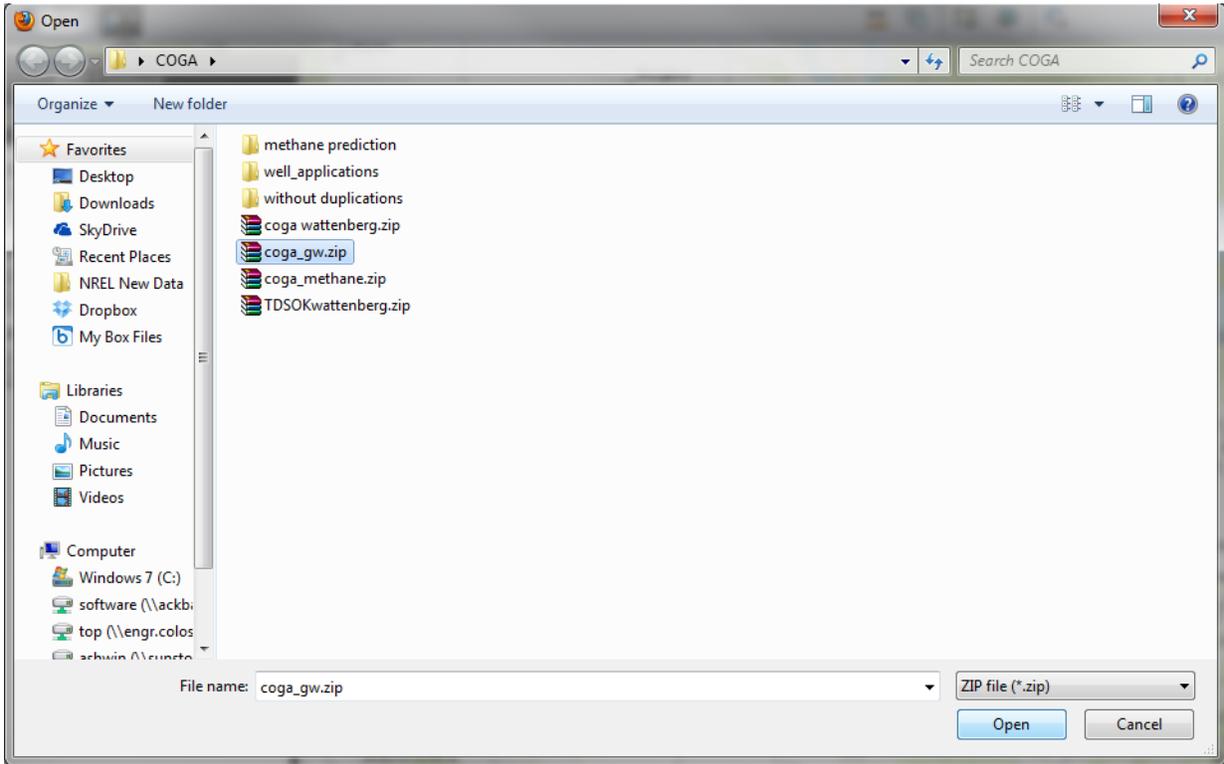
Figure 45. Screenshot of the Dialog box

- Once you select the file and click OK, the import shape file dialog box opens and gives you options to choose from. Select options as shown in the screenshot. The data has to be stored as a feature service for queries to be executed. If you want the map to more illustrative and if you don't need queries setup, then you can go ahead and the store features in map option as shown in Figure 45.
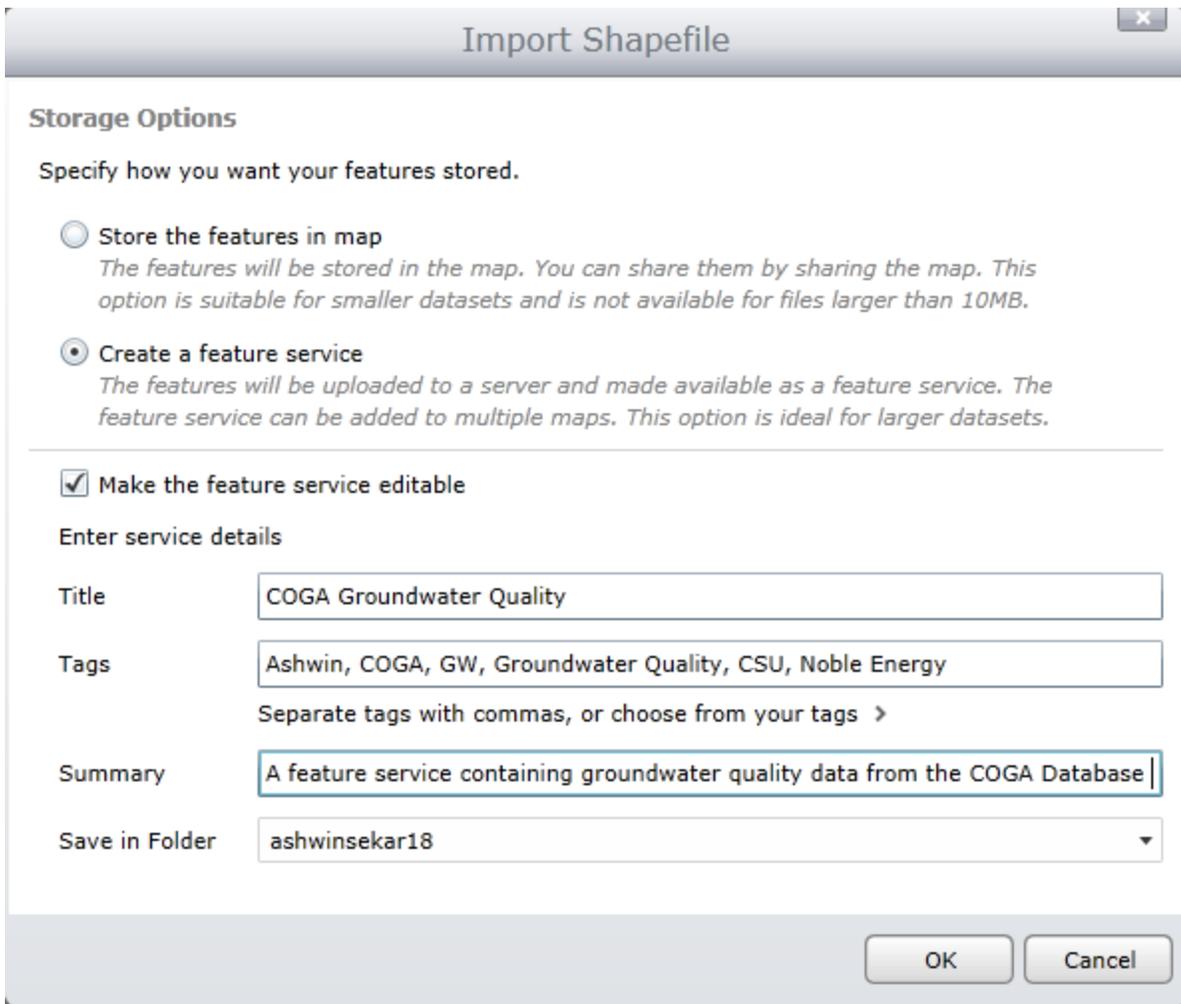
Figure 46. Screenshot of the import Shapefile dialog box.

- The feature service is now created and it's available in the "Layers" section for customization. Click on the arrow next to the layer to open its properties for editing. (As shown in Figure 46)
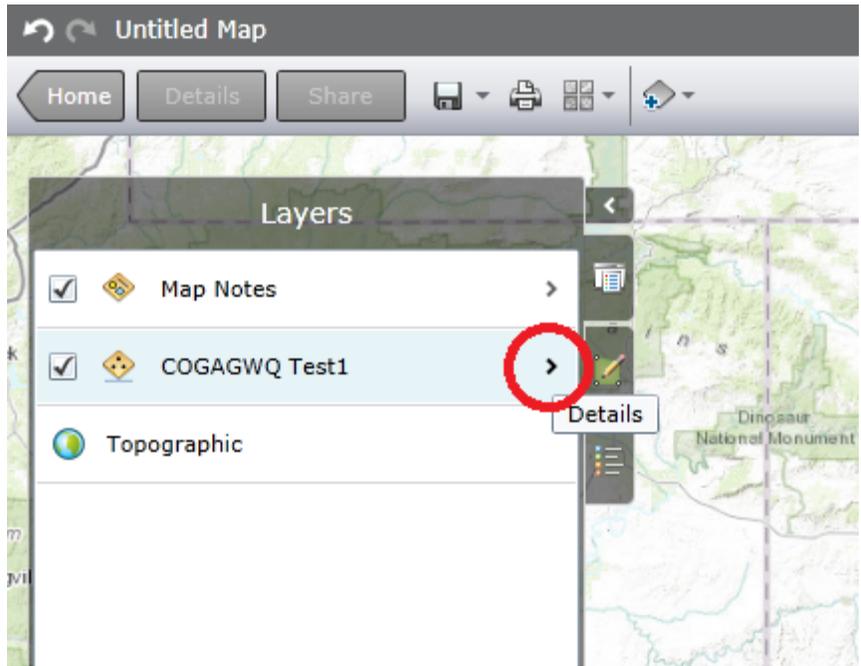
Figure 47. Screenshot of Layers section

(c) Changing Display Properties or Setting Symbology:

- To change the symbology of the datapoints in this layer, click on the configure button in the display section as shown in Figure 47.
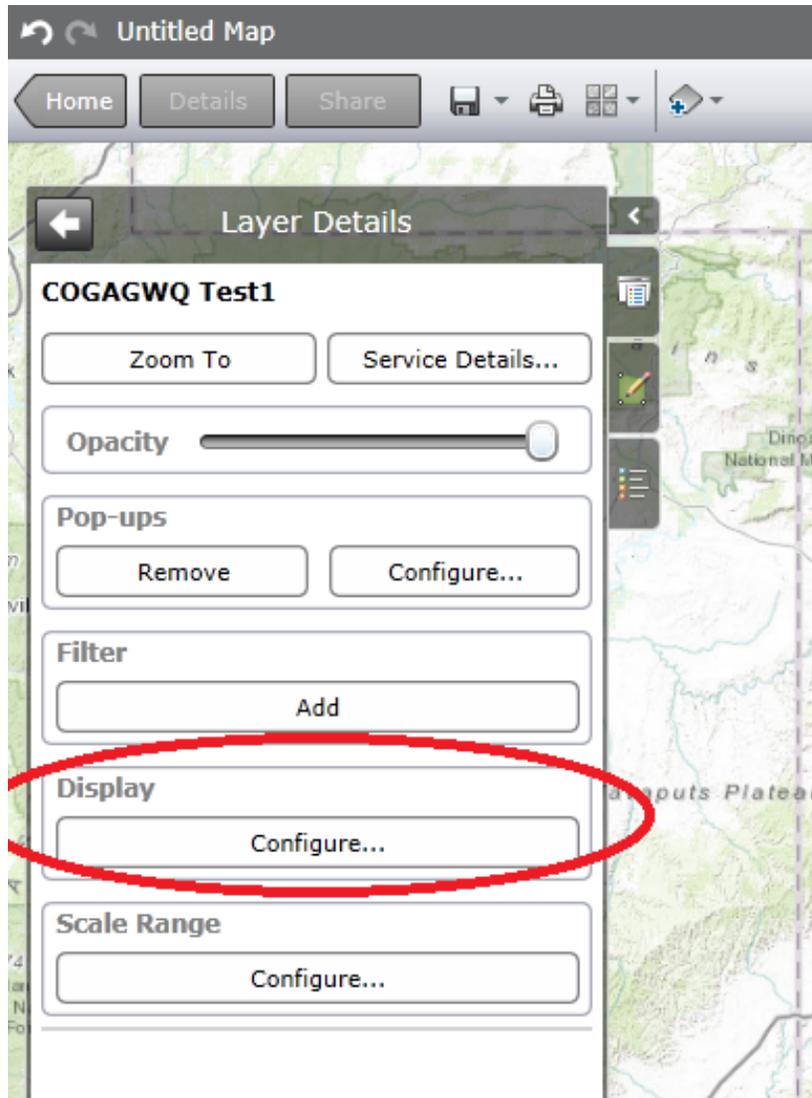
Figure 48. Screenshot of the Layer Details Section

- To change the symbology of the points from a single symbol to unique symbol colors, click on the dropdown menu in the "Configure Display Section". You will now see 4 options for setting styles. (as shown in Figure 48)
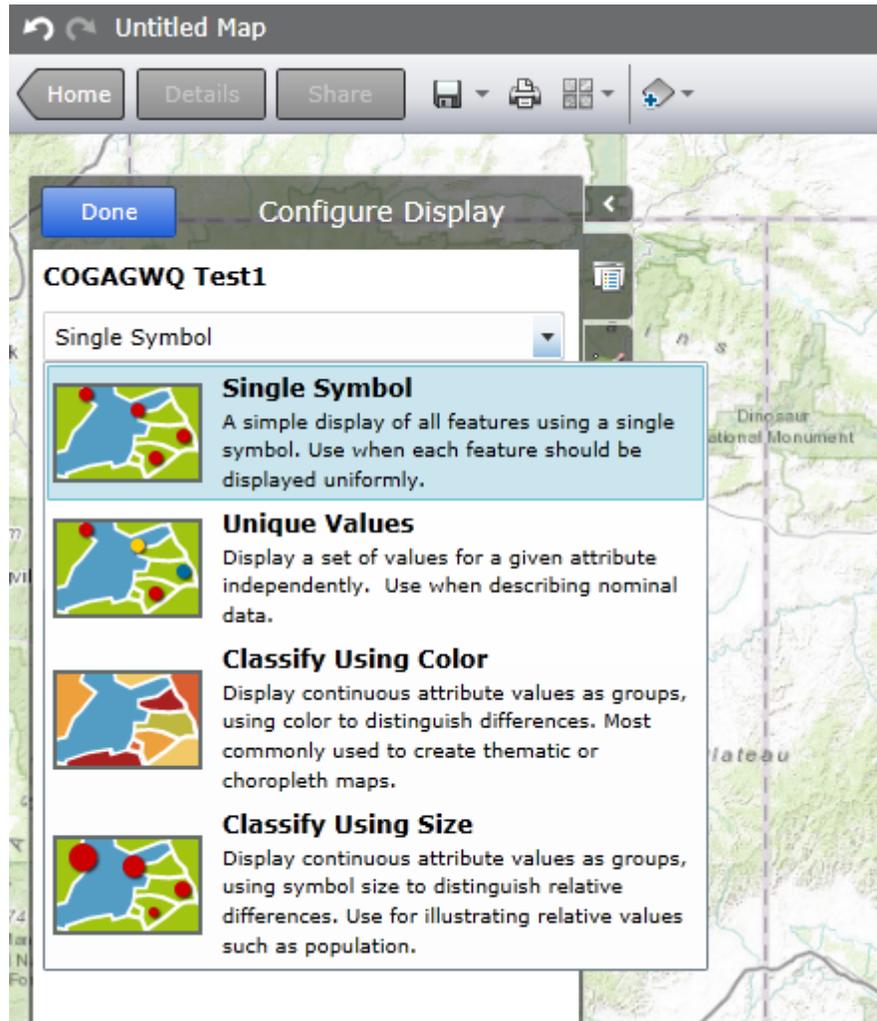
Figure 49. Screenshot of the Configure Display Window

- Each feature is unique in its own way and used for demonstrative purposes. The Single Symbol option can be used to show similar datapoints in a field. The Unique Values option can be used for displaying points in terms of a single attributes (as shown in Figure 49). It classifies the colors of the points based on a single attribute. The "Classify using Colors" option helps display continuous attribute values as groups. The "Classify Using Size" option uses different sizes for each point to distinguish the values. For this case, we are going to use the Unique Values and set the "Attribute" tab to Aquifer Name "AQFR_NAME1". We get the corresponding classes as shown in Figure. The colors can be changed by using the Color Ramp menu. Once finished, click "Done" and "Upload Properties to the Service" by clicking on the tab.
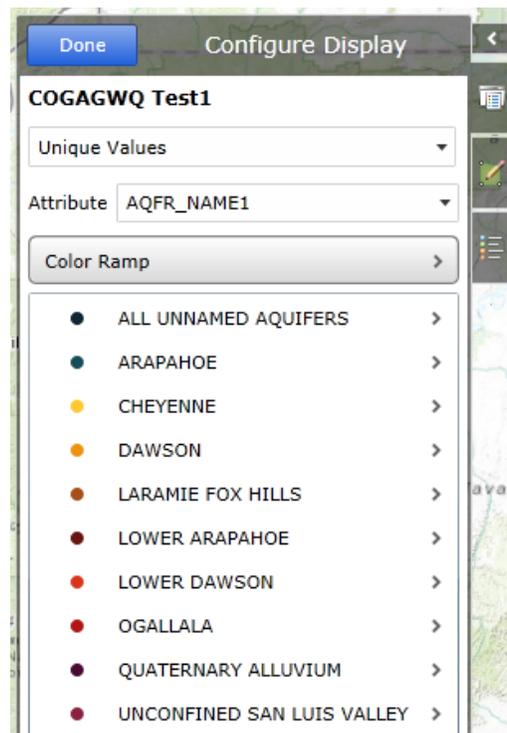
Figure 50. Screenshot of Classify using Unique Values

- When you click on each point, a pop-up opens displaying the attributes of that specific point. To change the contents displayed in this pop-up, you will need to click on the "Configure" tab on the Layer Details Section as shown in Figure 50 and choose what data you want it to display in the pop-up.
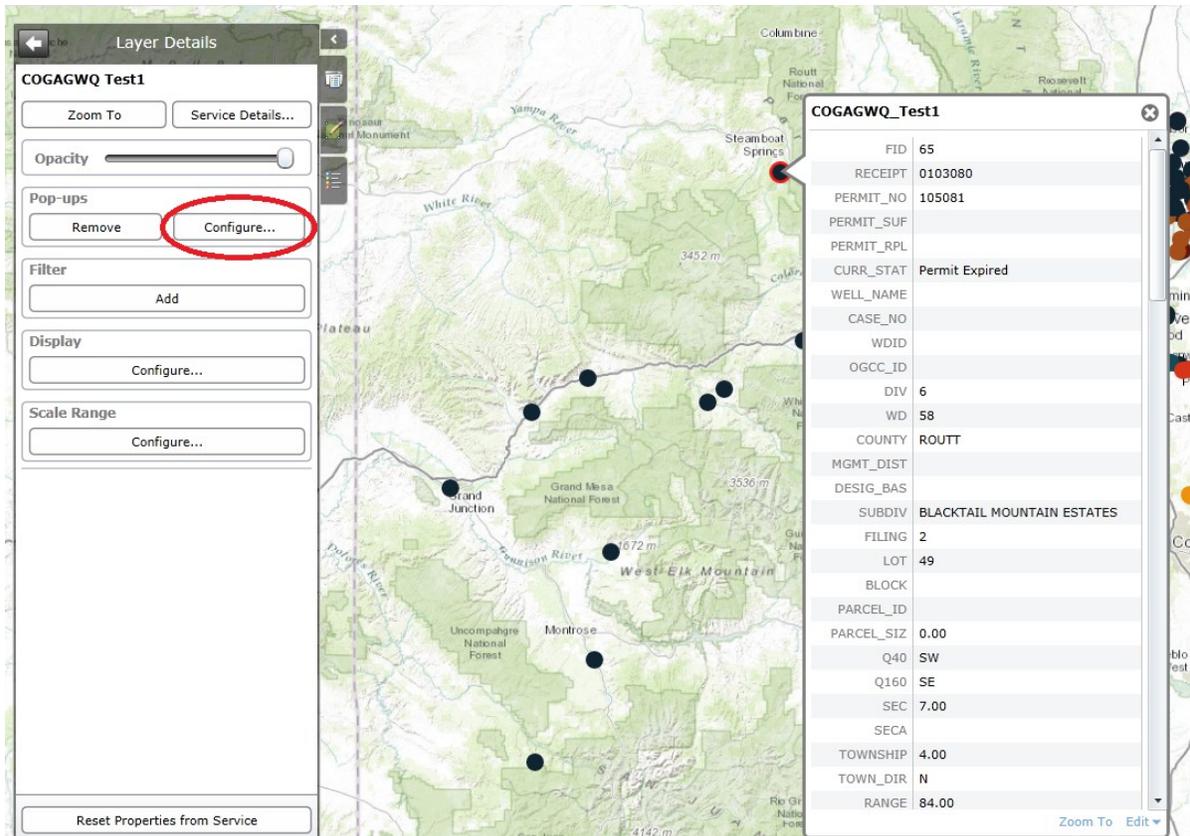
Figure 51. Screenshot of the Pop-Up editing Step

- In the Title and Description section of the Configure Pop-ups dialog box, you will be able to edit the title of the Layer, Select Pop-ups for display and or select a single field or a custom description instead of displaying the set of attributes. (As shown in Figure 51)
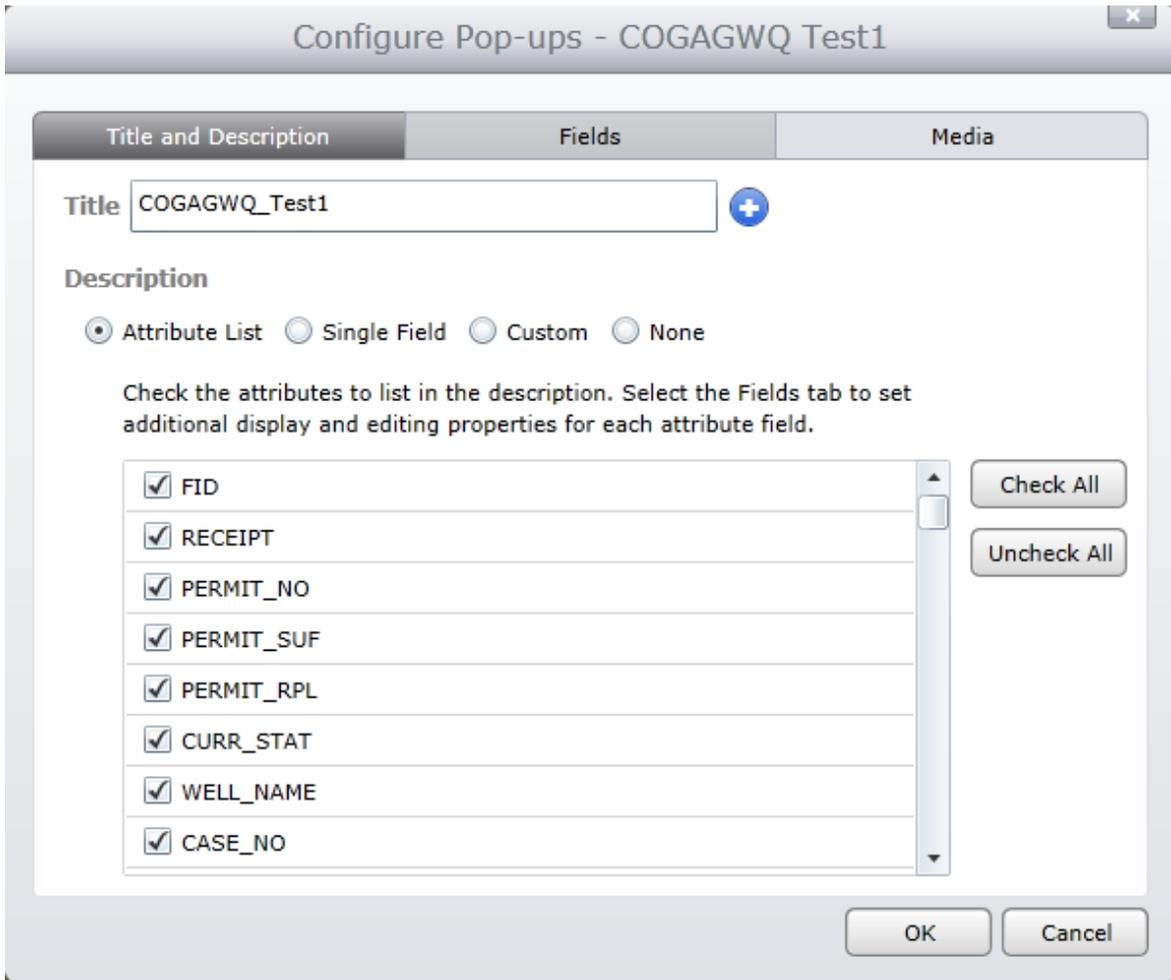
Figure 52. Screenshot of Title and Description Section of Configure Pop-ups

- In the Fields section, you will be able to choose custom names for each attributes to explain them better. (Shown in Figure 52) You can also customize the viewing of data types by adjusting their display properties. And the media tab allows you to add custom links, graphs, or images to your pop-up.
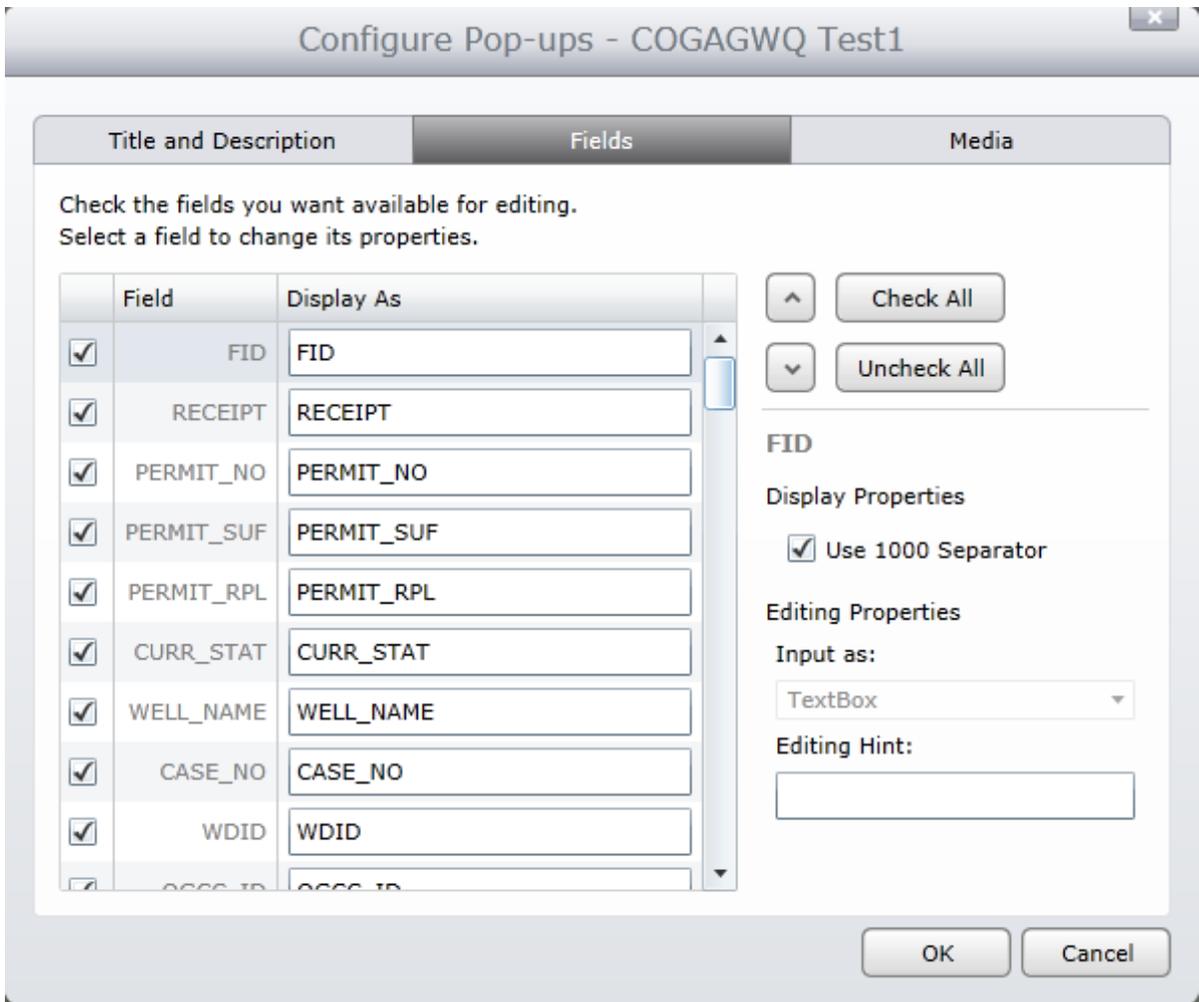
Figure 53. Screenshot of the Fields Section of Configure Pop-ups.

(d) Queries:

• Click on the "Queries" tab on the Top Middle Menu (As shown in Figure 53) to initiate

queries.
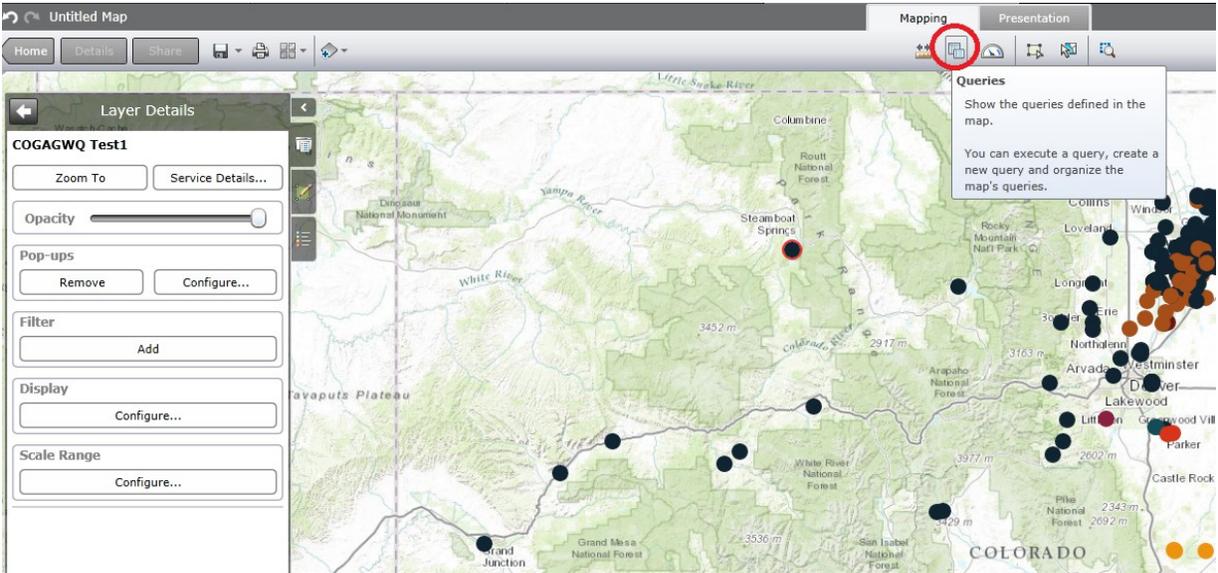
Figure 54. Screenshot of the Queries Button

• A tab opens up on the left asking if you want to create a new query. Click on the "New Query" option as shown in Figure 54.
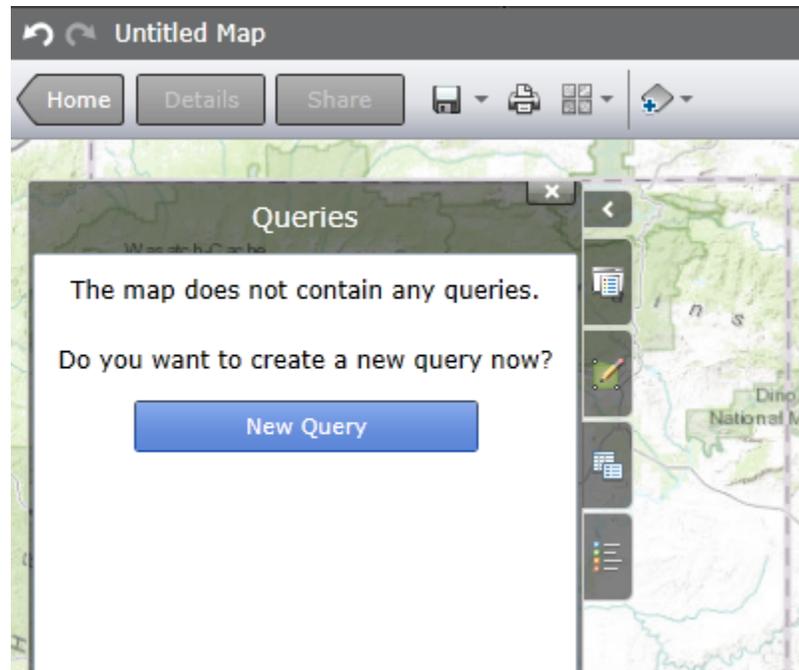
Figure 55. Screenshot of New Query

- Once you click on New Query, a dialog box opens up with your feature services (layers) in the map available for queries. Select the appropriate one, and click OK. (As shown in Figure 55)
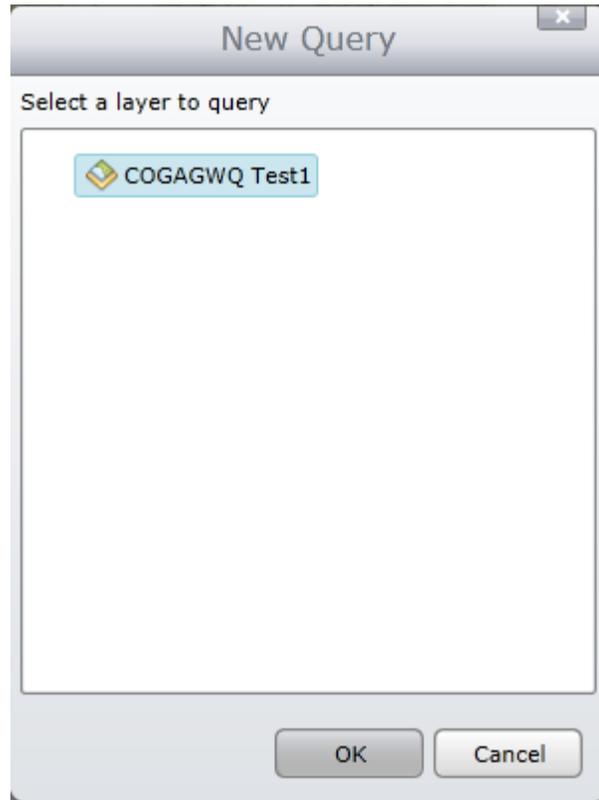
Figure 56. Screenshot of Feature Service Selection for Query

101

- A query definition window opens up now in order for you to define a query. Type in the definitions accordingly, add the query and click OK. (As shown in Figure 56). You can choose what fields to display by selecting the "Display Fields" tab. You can also choose what kind of data should be specified in your query results by selecting the "Data" tab.
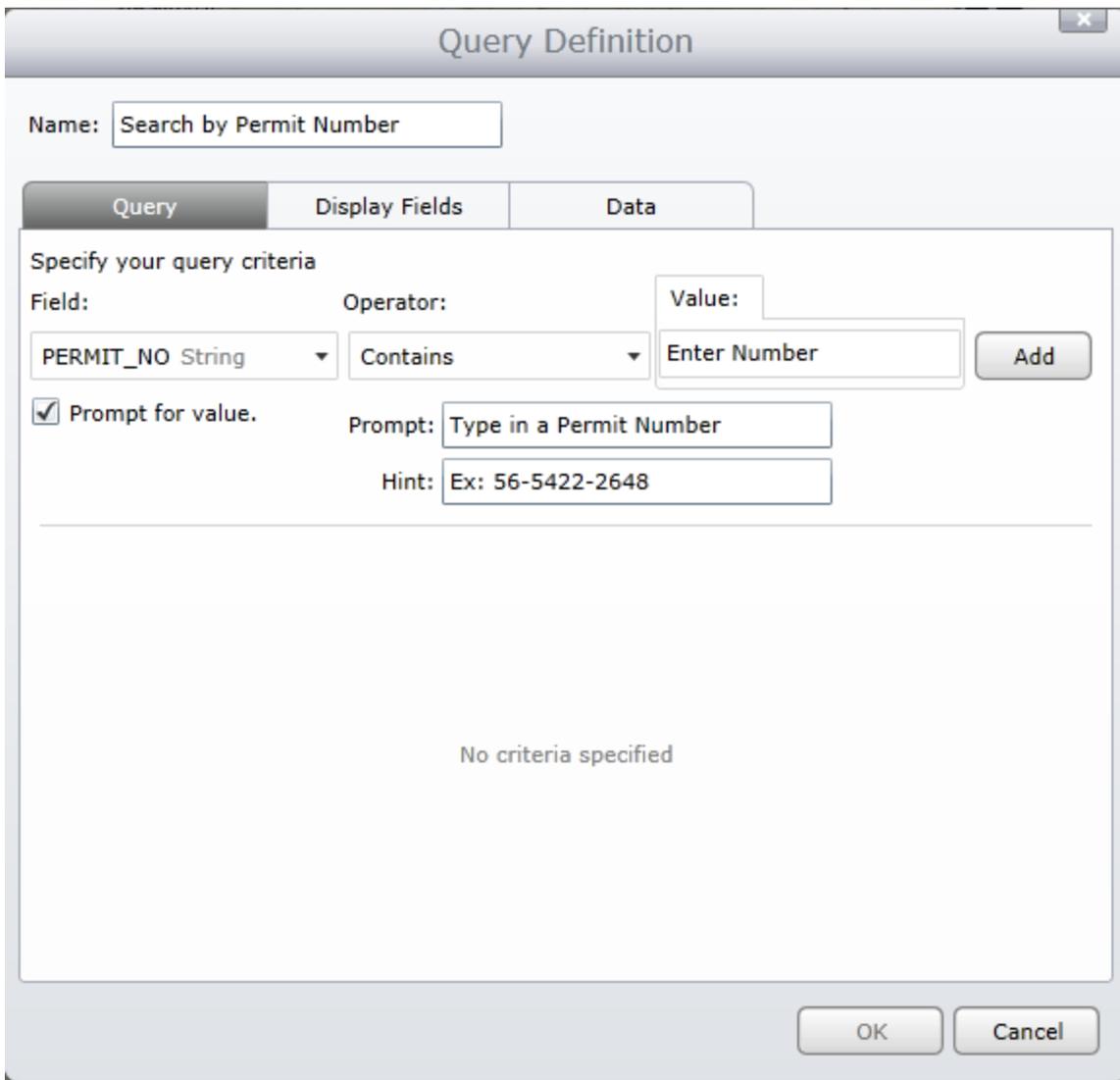
Figure 57. Screenshot of Query Definition

- Now you can see the query functioning as a pop-up window (shown below in Figure 57) asks you to enter the number.
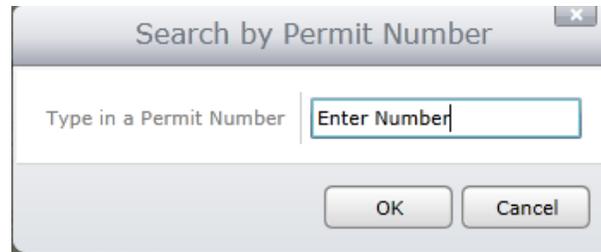
Figure 58. Screenshot of Query Pop-Up

- Type in the value and click OK, and you should be able to see the results on a dashboard (shown below in Figure 58) to the right. You can select the point and see the corresponding point highlighted in the map.
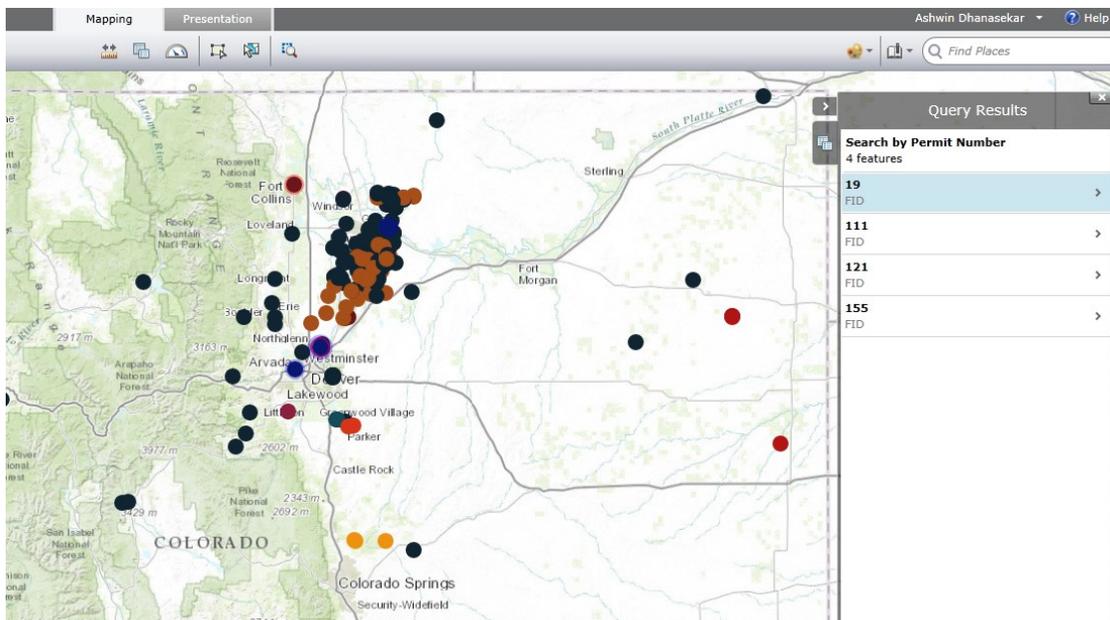
Figure 59. Screenshot of Query Results

(e) Dashboard:

The dashboard is a complex interactive feature in a map which gives you the freedom to display a few of the unique characteristics from your data points in an illustrative fashion. It is a console on the right side of a map where you can display pie charts, histograms, colorful descriptions, status bars, etc. An example is shown below in Figure 59.
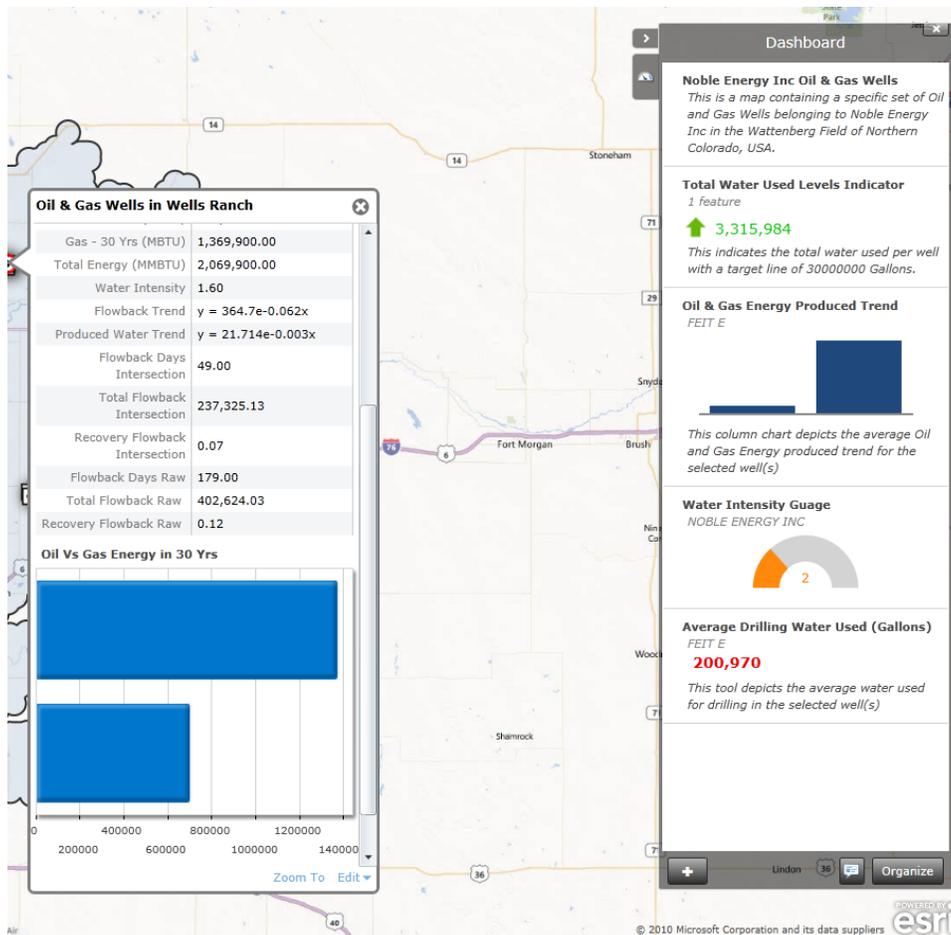
Figure 60. Screenshot of the Dashboard

- Setting up a dashboard is an easy process. All you need to do is click on the Dashboard icon on the top console toolbar (as shown in Figure 60). A dashboard opens up your right. To add specific gadgets, simply click on the "Add New Gadget" button.
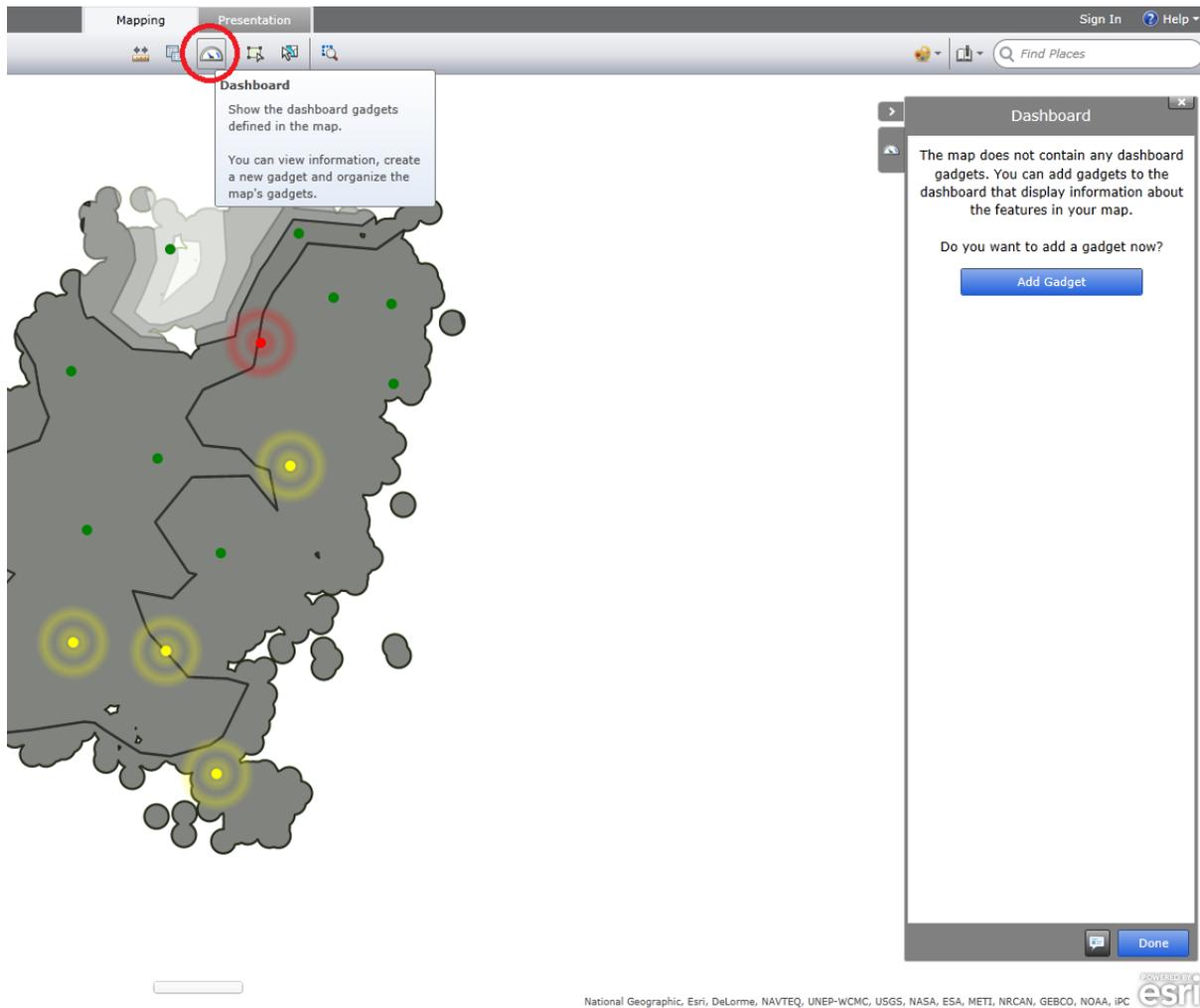
Figure 61. Screenshot of the Dashboard Setup

- After you click on Add New Gadget, a dialog box opens up with options like what kind of display type do you need to use and on what specific layer is it based on. (As shown in Figure 61)
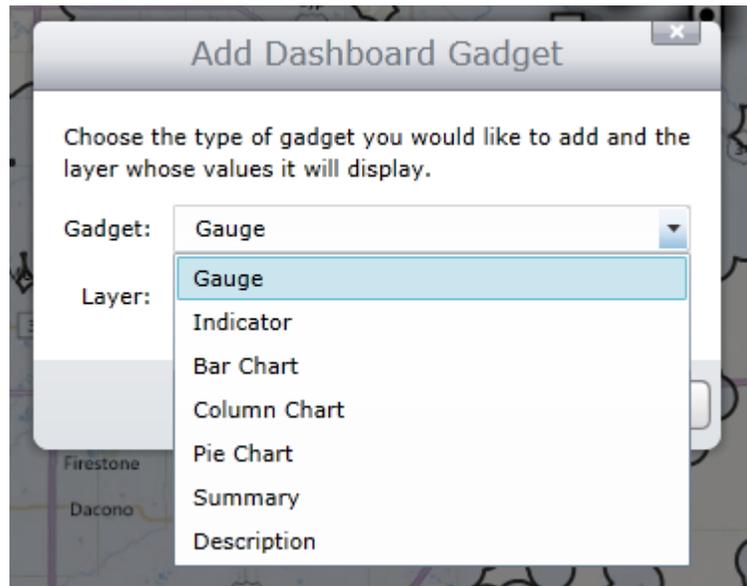
Figure 62. Screenshot of Add Dashboard Gadget

- All these gadgets can be used either in single display or in a comparative mode.

   I. Gauge: The Gauge can be used to show a measurement of any specific attribute in the form of a half-donut, horizontal bar or a vertical bar. It can either show the exact value or the percentage if you set a target value. This can also be programmed to calculate the sum or average of multiple selected points.

   II. Indicator: The indicator is merely an illustrative description display. It can be programmed in easy steps to show values for each point or cumulatively for

multiple selected points in the map. It can also work with arrows or other similar indicators if set a target value.

III. Bar Chart: The Bar Chart is the easiest way to include a bar chart with characteristic attributes from the layer. This can be made dynamic if the layer had continuous attributes data. The bar chart can also be programmed to be normalized on the basis of a single attribute.

IV. Column Chart: The Column Chart is similar to the Bar Chart in all functions and can be used for the same functions like it. It can also be programmed to display the average, sum of different selected data points and its values.

V. Pie Chart: The Pie Chart is a more illustrative way of presenting data from the map. You can use multiple colors to show the difference in attributes or differences in a single attribute over different selected points in a map. All the charts can be drawn in a comparative format as well.

VI. Summary: The Summary Gadget is a simple yet strong tool to compare cumulative statistics of multiple selected datapoints over any specific area chosen with the capacity to use multiple functions like summing up or giving an average value for a specific attribute.

VII. Description: The Description gadget is a simple text box in your dashboard. You can type in any description or relevant explanation in this space.

- Once you click and select your chosen gadget, you can now the select the layer which you need available for setting up for your gadget. Each gadget can be set for only one specific layer and its attributes as shown in Figure 62.
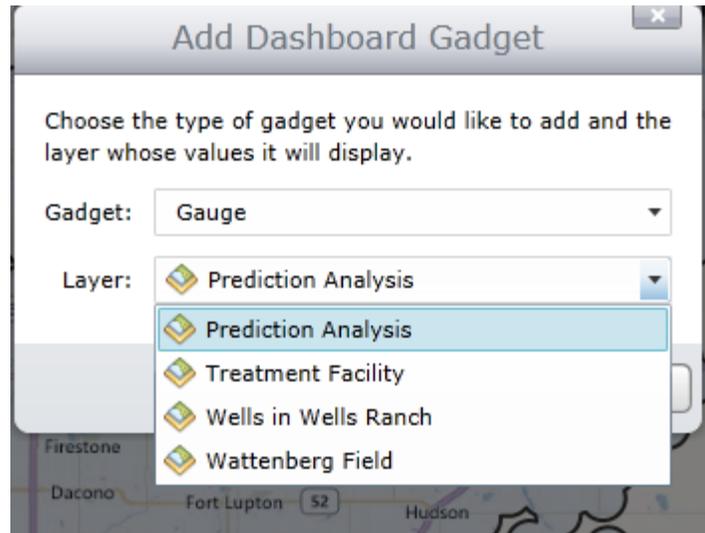
Figure 63. Screenshot of Layer Selection Tool

- After selecting your gadget and layer, click OK and now you will see a gadget editor window where you can customize how you want your gadget to work. Once you are done setting up, click OK. Now you will able to view the functioning gadget in the dashboard. Open the dashboard by clicking on the dashboard icon if it's not open by default. Click on some points and see the dashboard work according to how you set it up.

(f) Basemaps:

There are 9 basic basemaps that you could use as the background in ArcGIS explorer online. You can access each of them by clicking on the basemap button and selecting one. (As shown in Figure 63).
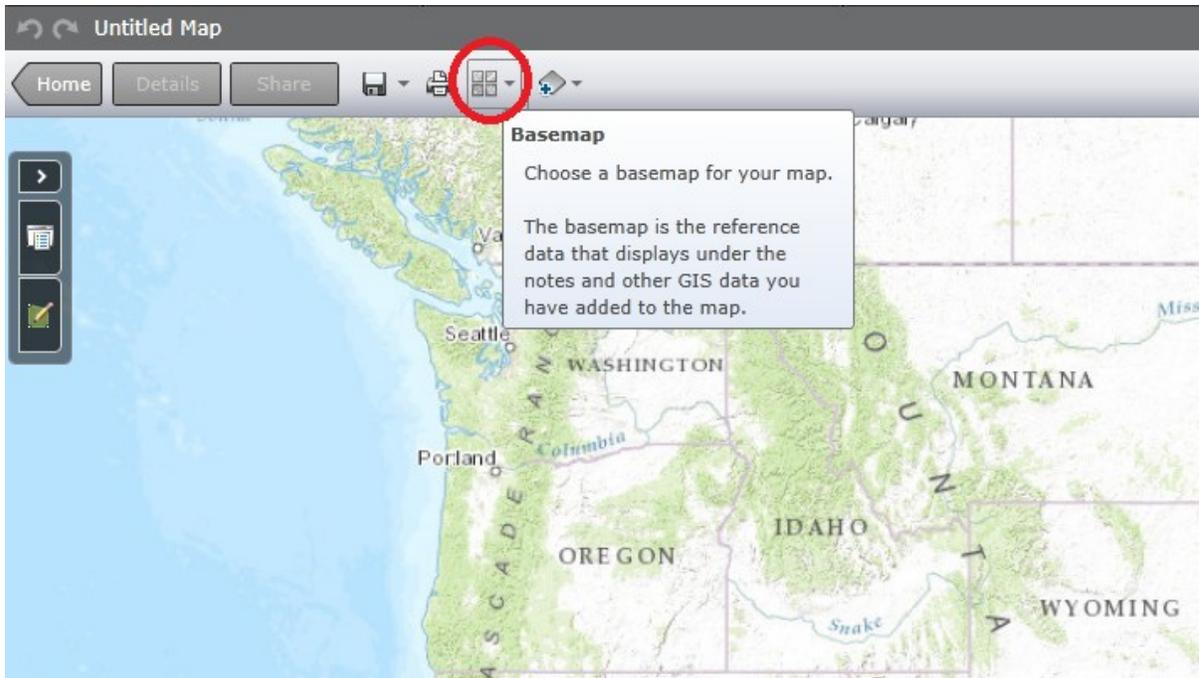
Figure 64. Screenshot of the Basemap Tool

- After you click on the icon, a basemap panel opens up letting you choose one of the 9 basemaps.

    1. Imagery

    2. Imagery with Labels

    3. Streets

    4. Topographic

    5. Terrain with Labels

    6. Light Gray Canvas

    7. National Geographic

    8. Oceans

    9. Open Street Map

    10. Bing Maps Aerial

    11. Bing Maps Hybrid

    12. Bing Maps Road

    (As shown in Figure 64)
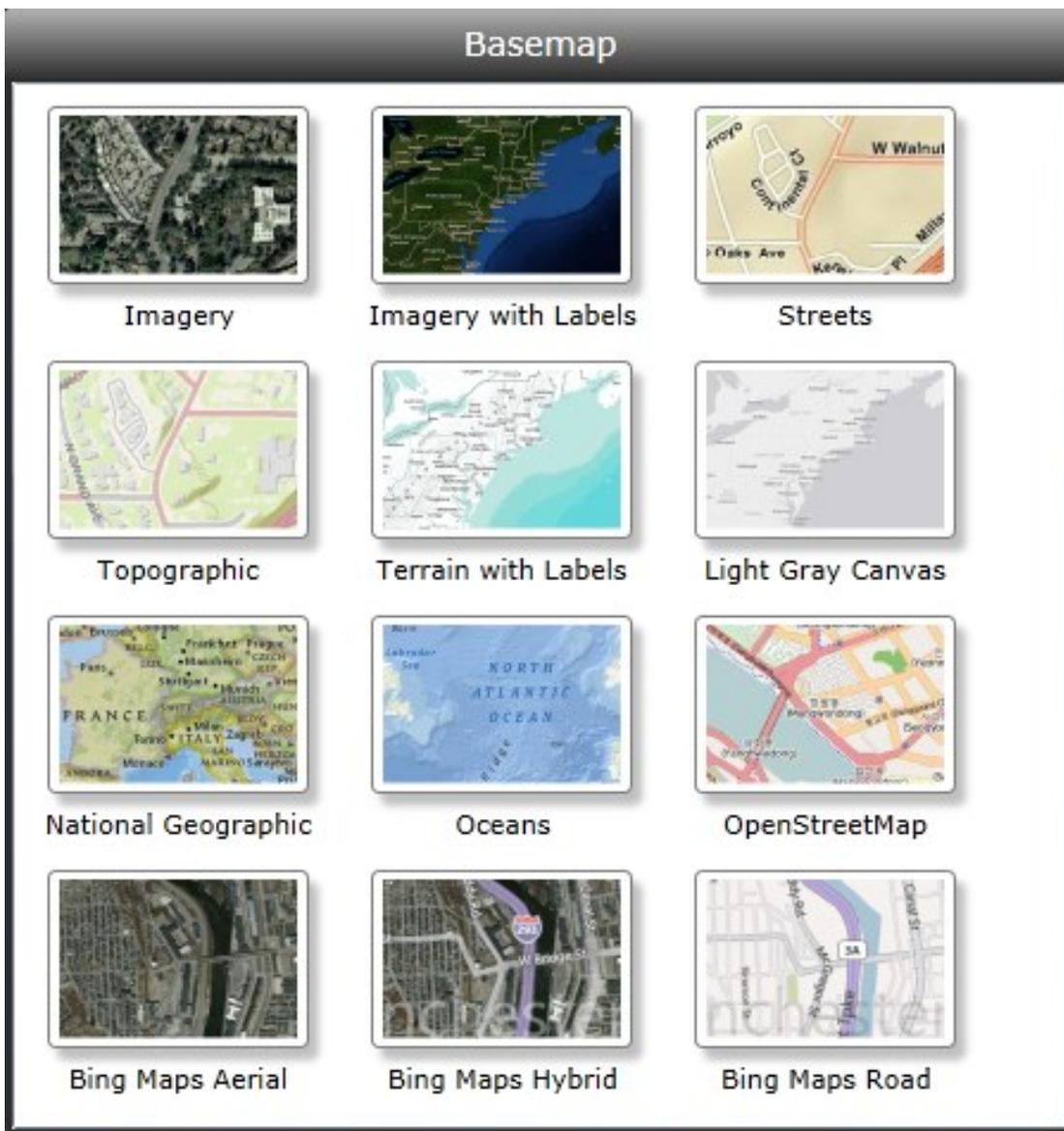
Figure 65. Screenshot of the Basemap Panel

A2. Documentation of steps in OLI Analyzer 3.2:

1. The first step is to start the Analyzer program by clicking on the OLI Analyzer 3.2 Icon which is placed conveniently on your desktop after you install the program as shown below in Figure 65.
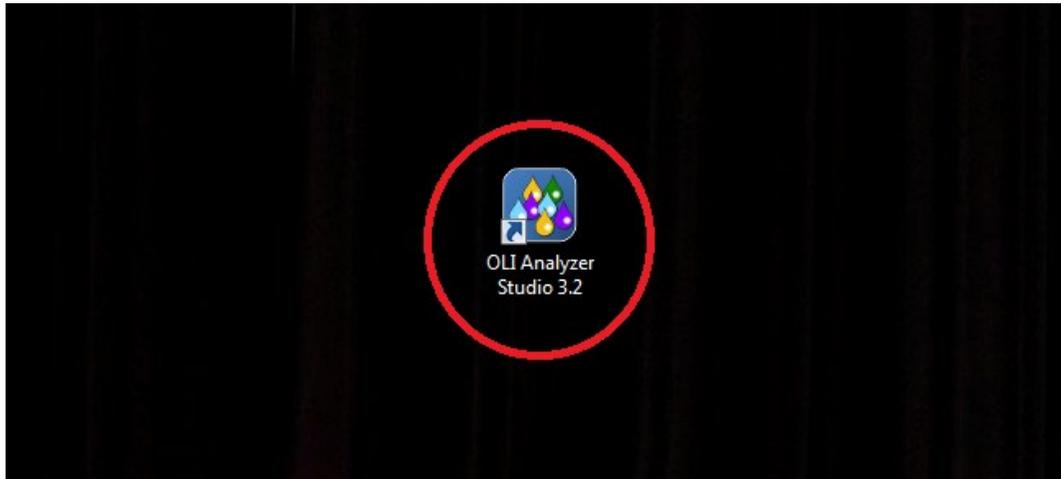
Figure 66. A screenshot of the OLI Analyzer Studio Icon.

2. The analyzer now opens with a default new Analyzer studio format. The next step is to double click on the Add Water Analysis Icon placed on lower left of the analyzer window as shown in Figure 66.
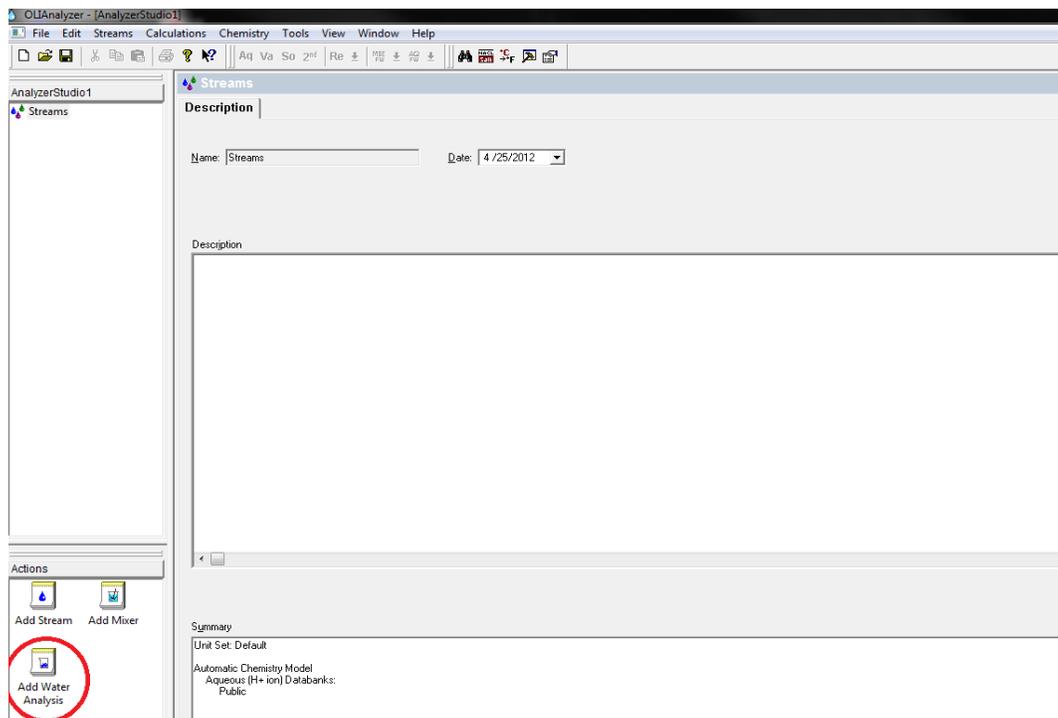
Figure 67. Screenshot of the OLI Analyzer new studio window

3.   Now, a Water Analysis window opens up in your main description window in the main

part of the console as shown below in Figure 67.
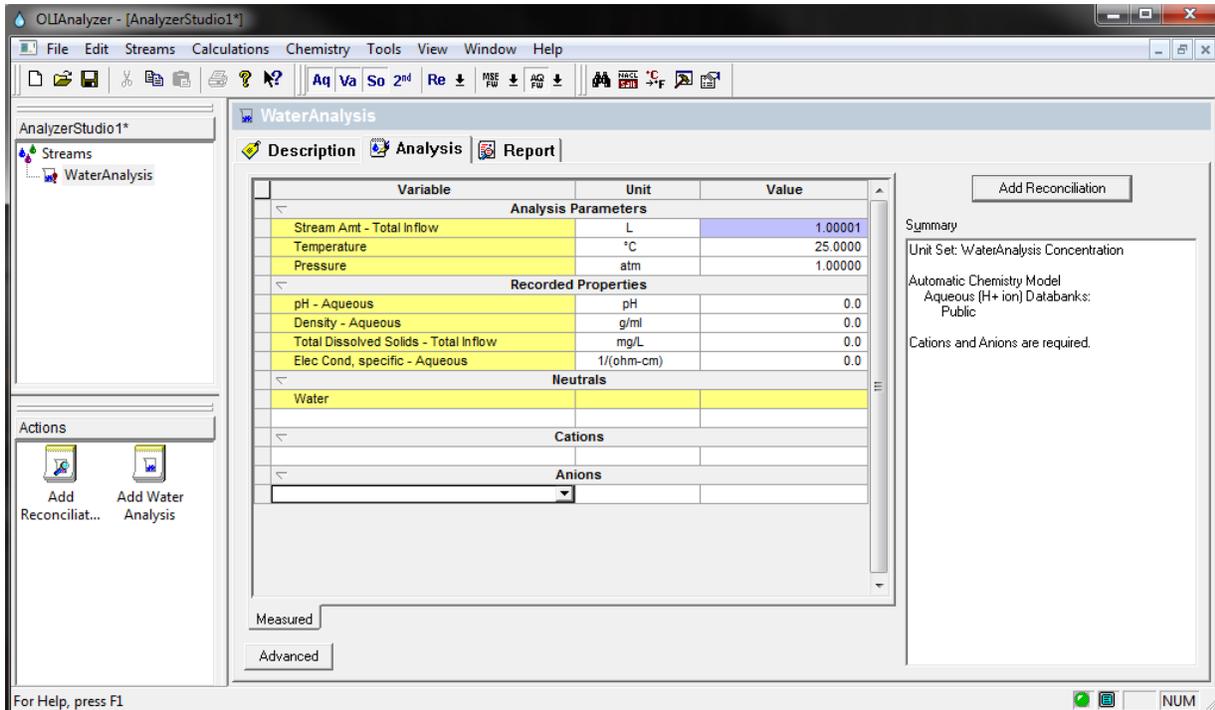
Figure 68. Screenshot of the basic water analysis window

4.   The water analyzer window opens up with entries possible for the input water quality.

The water quality with the characteristics such as Pressure, pH, Temperature and Electrical

Conductivity can be added to this now. Once this is done, the next part would be to click on Add

Reconciliation as shown below in Figure 68.
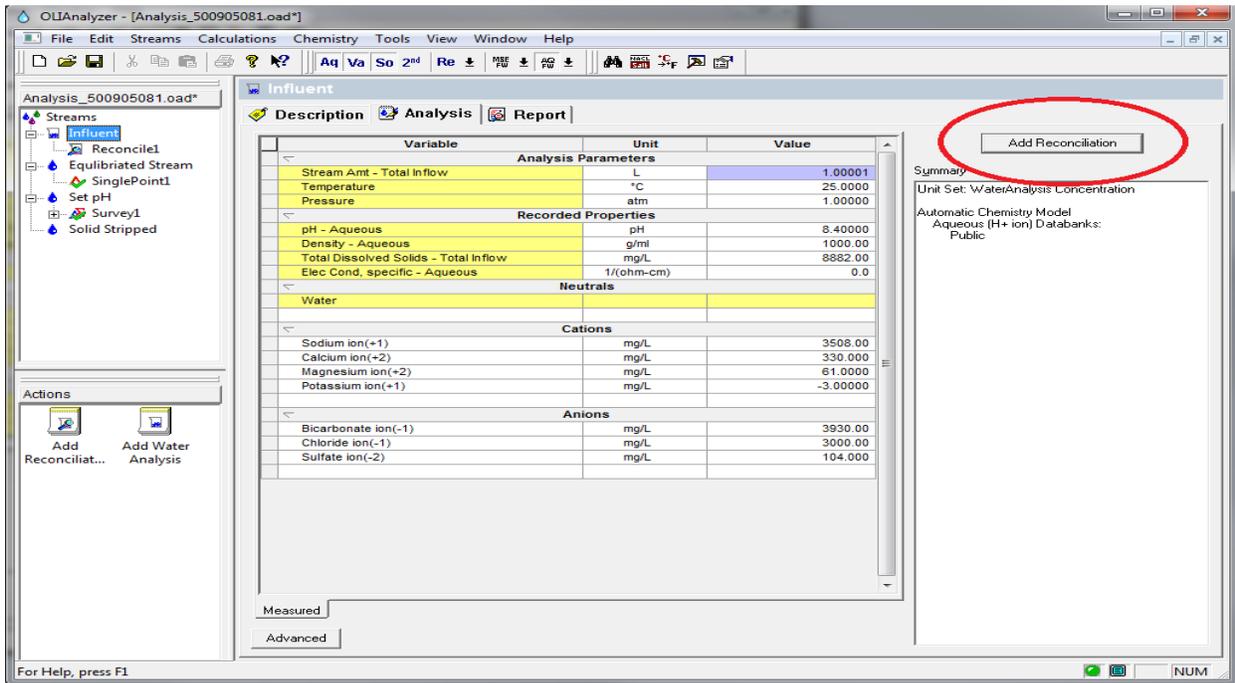
Figure 69. Screenshot of the Reconciliation step

5. Once you click on it you can see an additional sub-tab under the influent tab to as Reconcile1. Click on this new sub tab and select No Reconcile or according to your requirement pick one among the 3 options and click on the Calculate Button as shown below in Figure 69.
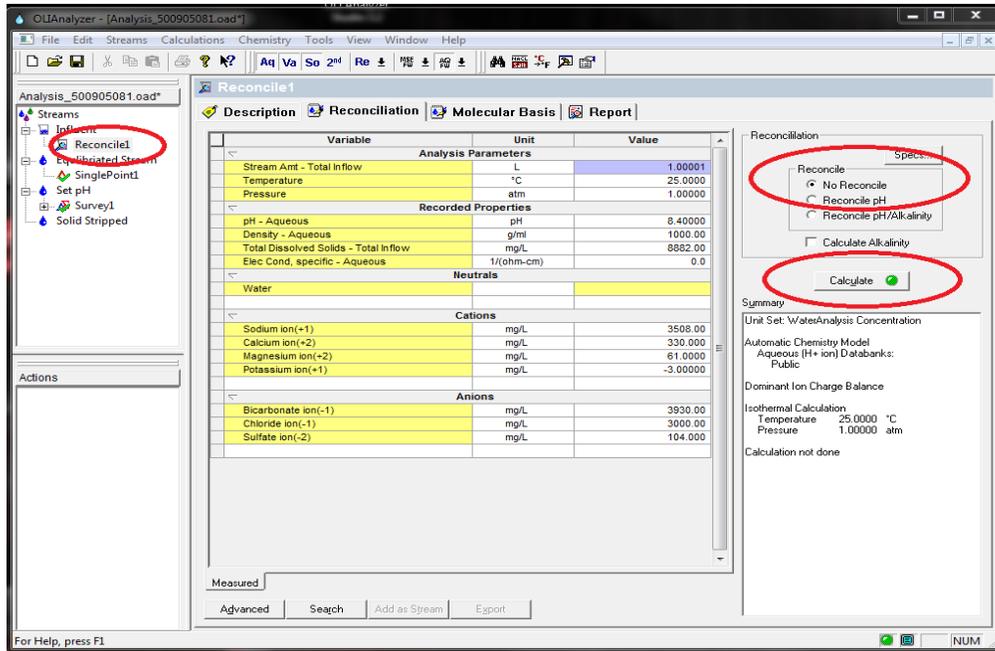
Figure 70. Screenshot of the reconciliation calculation step

6. After the calculation is complete, click on the Report Tab on the main console to get a detailed description of what output has been obtained from the given inputs and how to calculation works. You can also customize the details you need in the report by selecting so as shown below and this report can also be exported using the tool specified in figure 70.
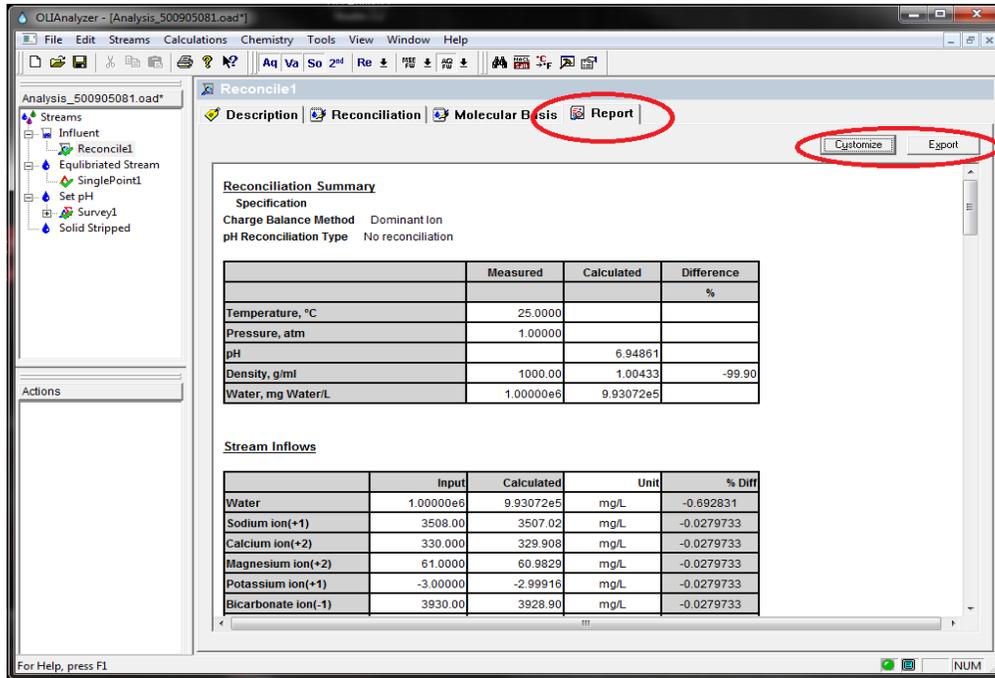
Figure 71. Screenshot of the report window

7. After this is done. You can add the processed calculation as an additional stream by right clicking in on the tab in the index section on the left and selecting the option "Add as Stream" as shown in Figure 71.
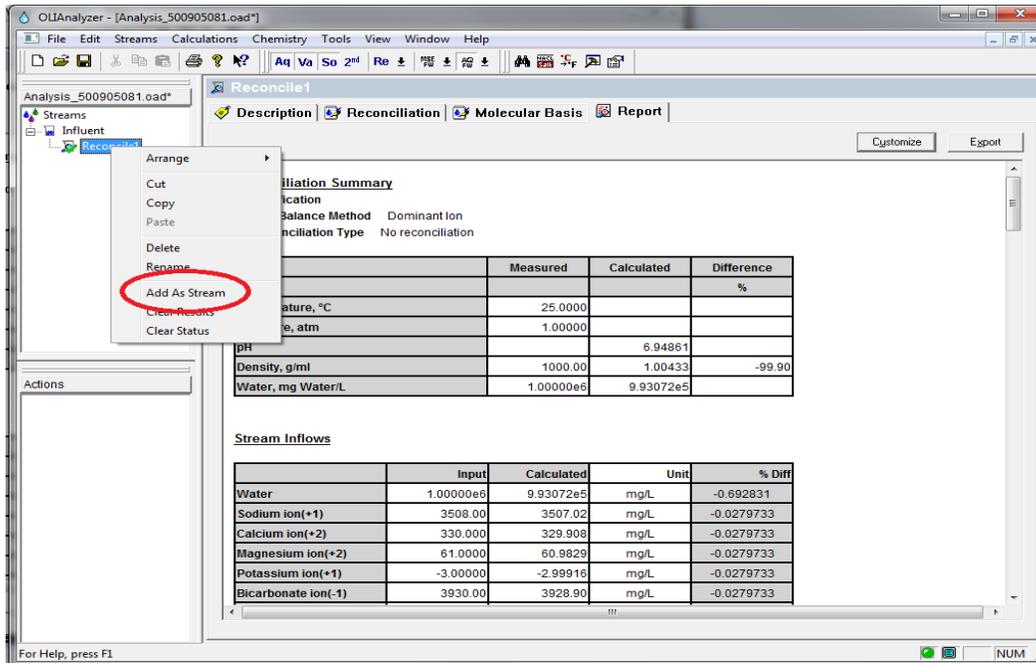
Figure 72. Screenshot of the "Add as Stream Step"

8. Now an additional stream with the outputs from this calculation will be added under the index tab as shown in Figure 72.

Figure 73. Screenshot of the stream addition step

9. The next step will be adjusting the pH of this stream. This can be done by clicking on the "Add Calculation" tab as shown below in Figure 73 and selecting "Single Point".
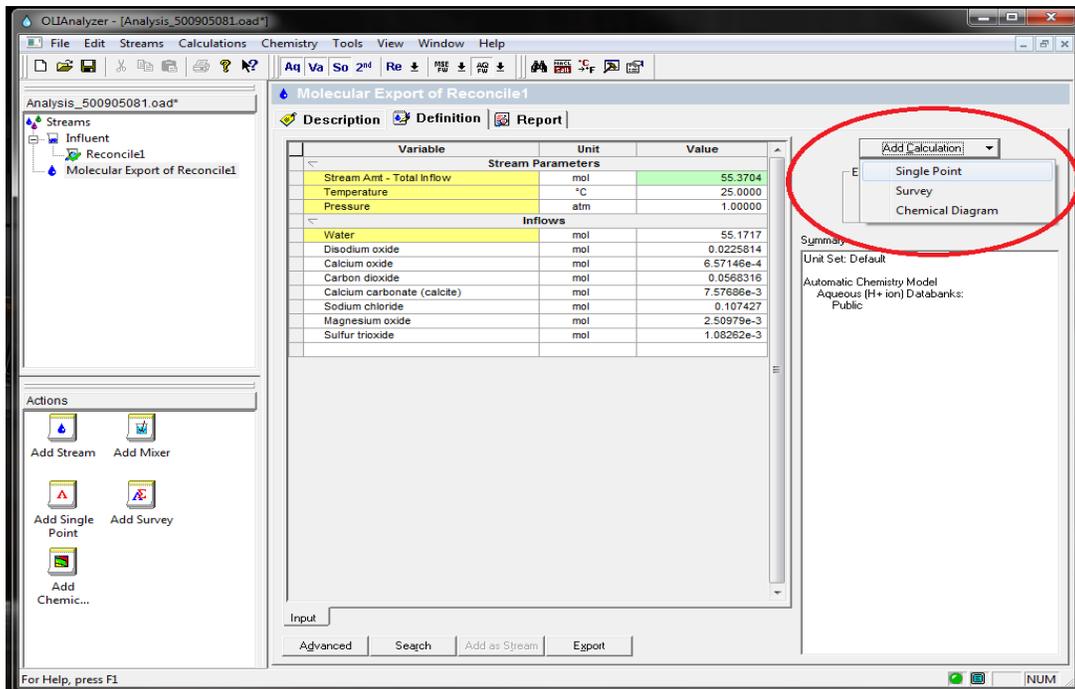
Figure 74. Screenshot of the add calculation step

10. Now a new tab will be added to the index with the name "SinglePoint1". All the tab names are customizable, so once the calculation is done, appropriate naming can be done. The next step will be clicking on "Add Calculation" and selecting "Set pH" as shown below in Figure 74.
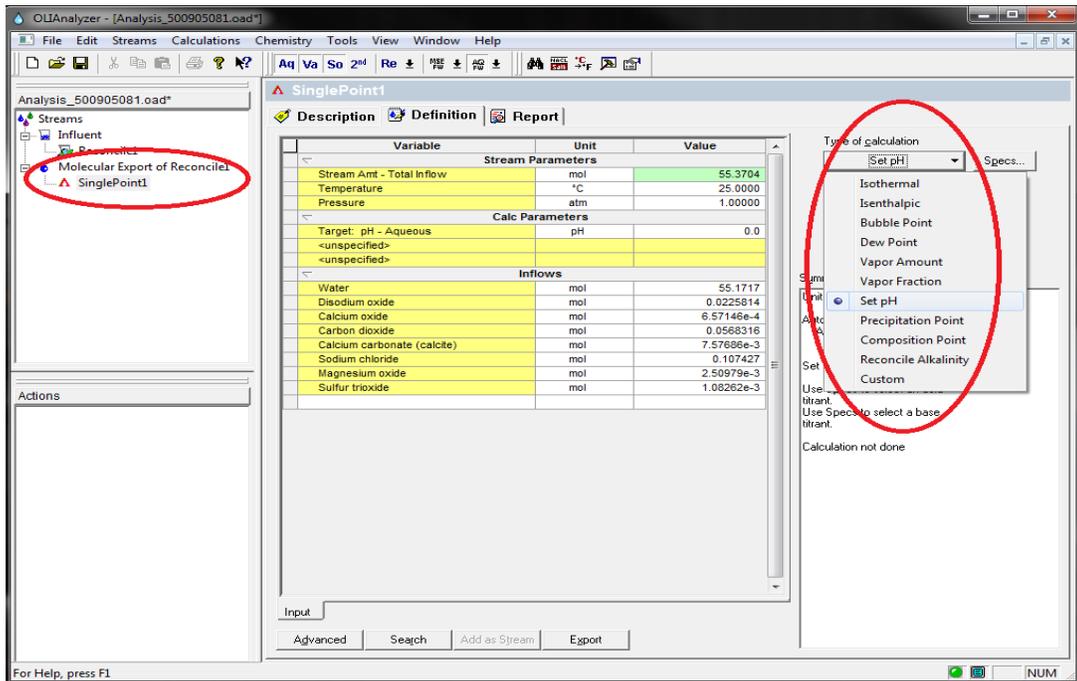
Figure 75. Screenshot of the Set pH step

11. When you click on "Set pH", you will notice that there are two new fields in the main
console. These are for adding titrants. The calculation cannot be done until you can
select the titrants. After typing in the target pH, the next step would be click on Specs in
the right side of the window, and selecting you r corresponding titrants from your inflows
as shown below in Figure 75.
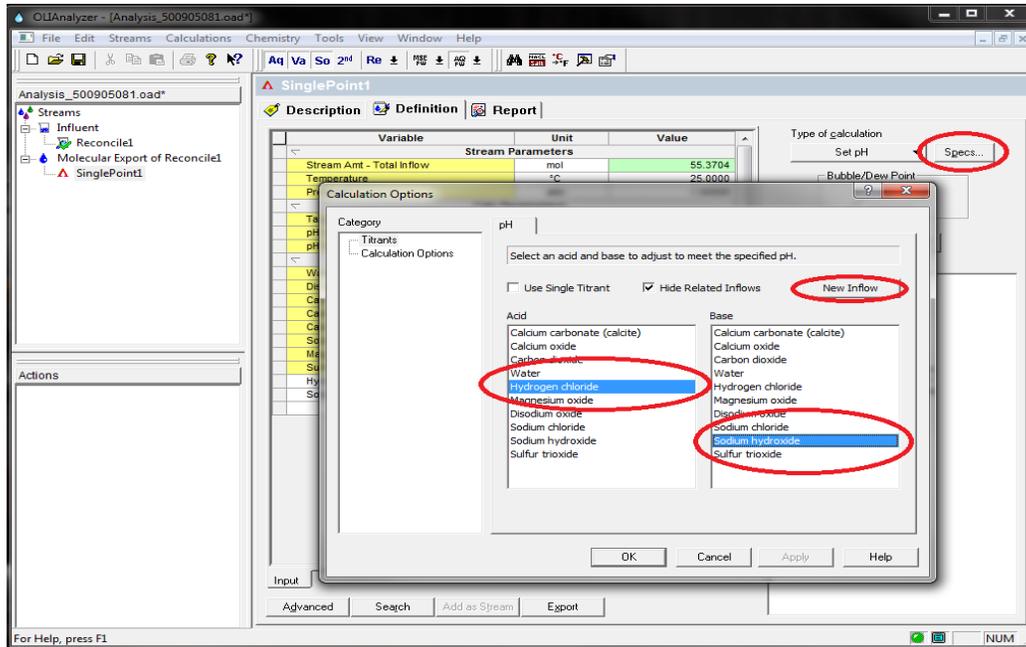
Figure 76. Screenshot of the adding titrants step

12. You can also use a single titrant by using the "Use Single Titrant" option in the

Calculation Options. If you don't find the titrants, or you need an additional or specific

titrant, you can always add it to your stream by clicking on the New Inflow button shown

in the above Figure 75. When you click on it, a component search window as shown

below opens up where you can type in and add to your existing stream as shown in

Figure 76.
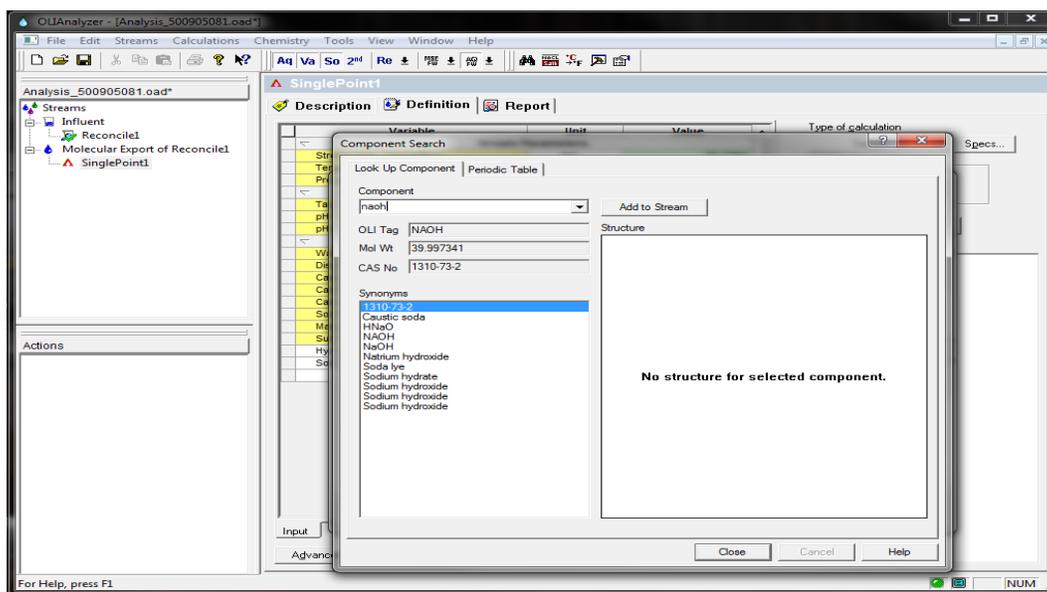
Figure 77. Screenshot of the single titrant selection step

13. After adding the required titrants, click on the calculate button. Get an output, view

specifics in the report tab similar to Step 5. Add this as a separate stream similar to step 7.

But now, you will be able to separate the streams accordingly to get a separate solid

stream and a solids free stream for further processing. When you try to add this

calculation as a stream, you will see a window as shown below to pick which stream you

need as a separate one as shown in Figure 77.
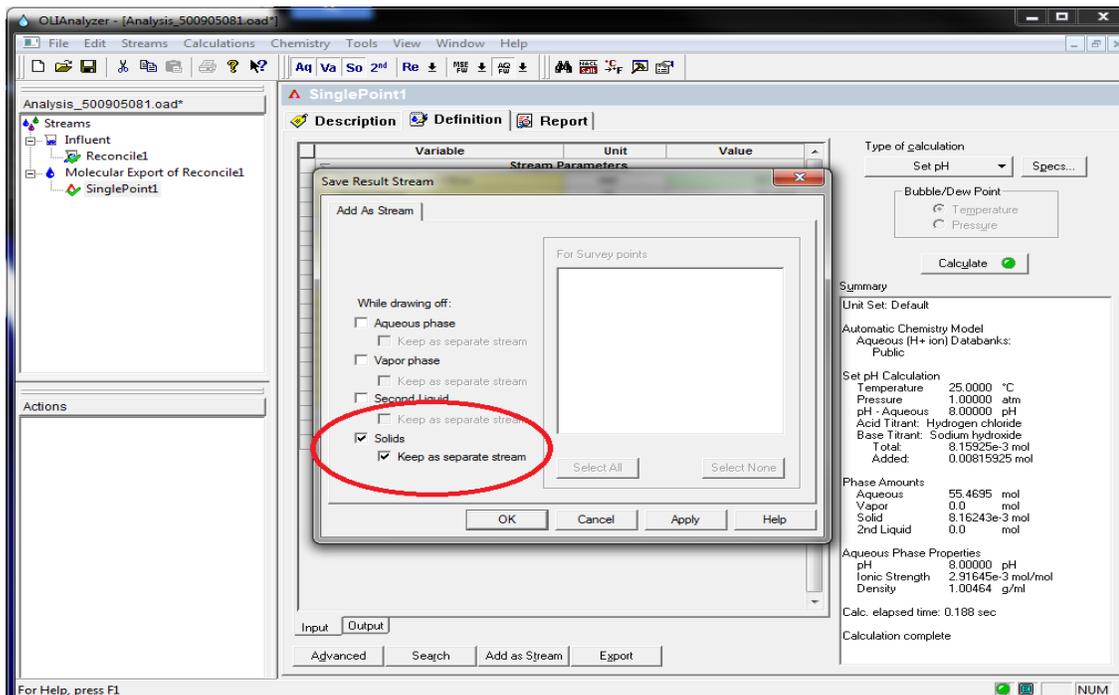
Figure 78. Screenshot of the solids separation step

14. In order to proceed, the next step would be to select the Solids Free Stream, click on

"Add Calculation" and select "Survey" as shown below in Figure 78. This is an

illustrative tool which can be used to calculate how the constituents react to a change in

temperature, pressure, pH or composition.
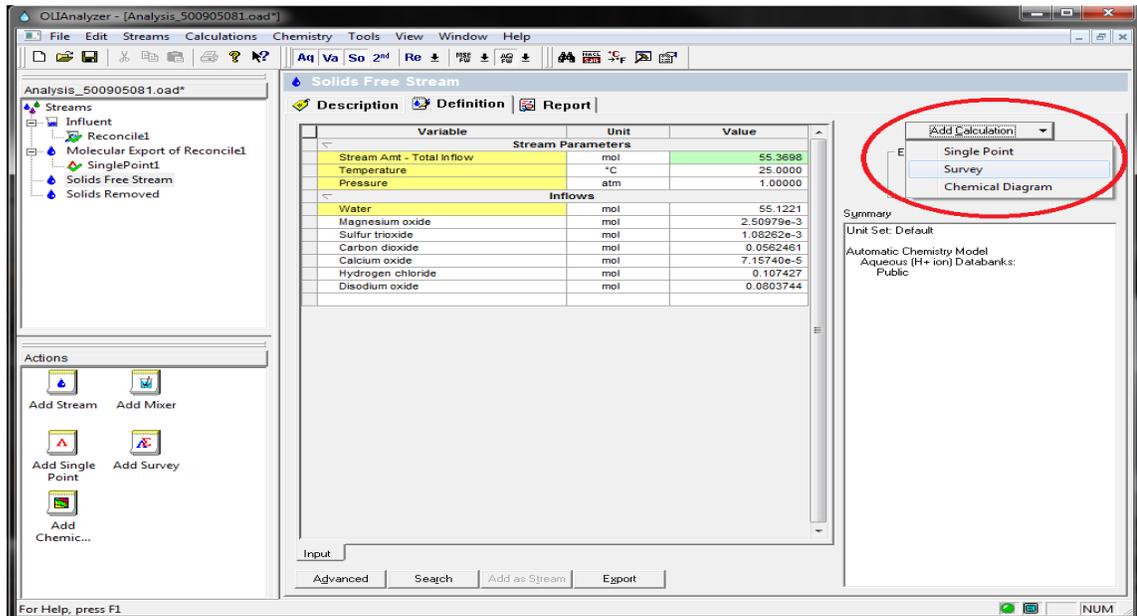
Figure 79. Screenshot of the add calculation step

15. After you click on Survey, you get a sub-tab which says "Survey1". You can select the more convenient option for you among the 4 options, which in our case we might select Temperature as shown in Figure 79.
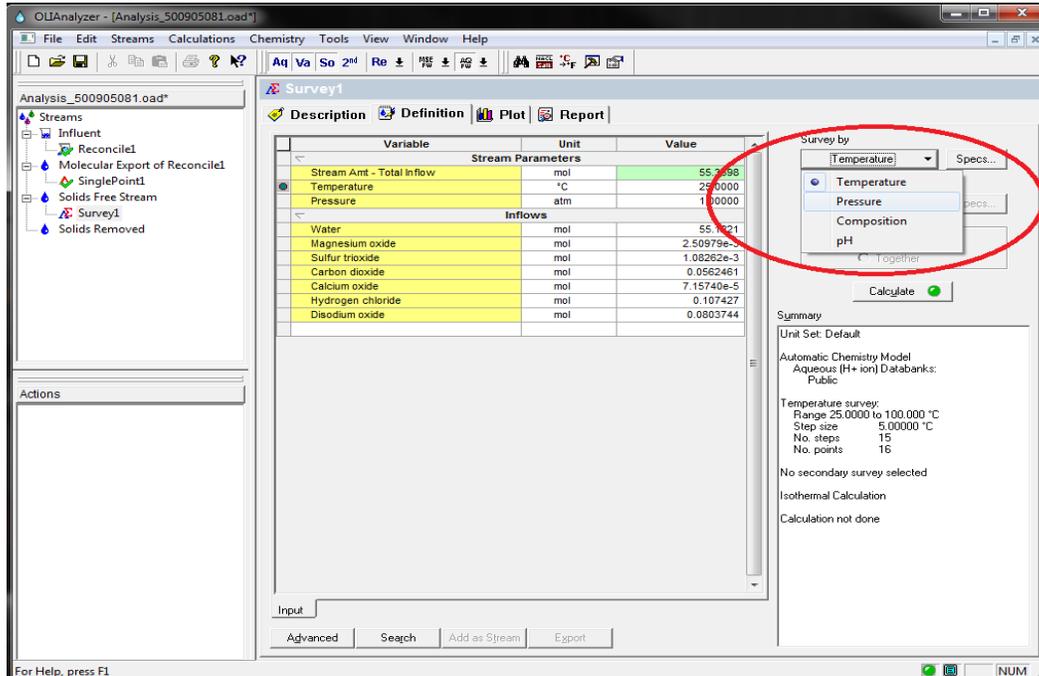
Figure 80. Screenshot of the survey choice step

16. You can pick your survey options such as range of temperature in this case by clicking on

"Specs" and entering your Start and End Variable Values as shown in Figure 80.
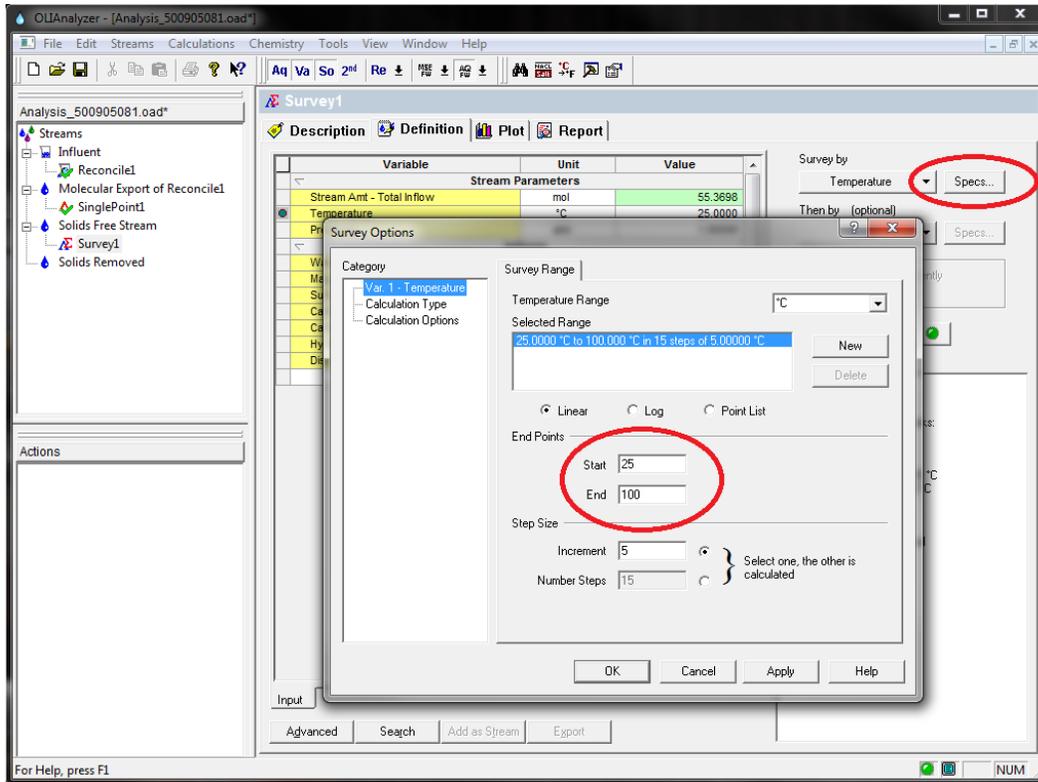
Figure 81. Screenshot of the survey range selection step

17. Once this is done, click on calculate. After the calculation is complete, you can click on the "Plot" tab in the main console to check on the plot which depicts the composition of the ions which vary according to the changes in temperature as shown below in Figure 81. This can also be customized by selecting what you need as your axis and constituents by clicking on the "Curves" option.
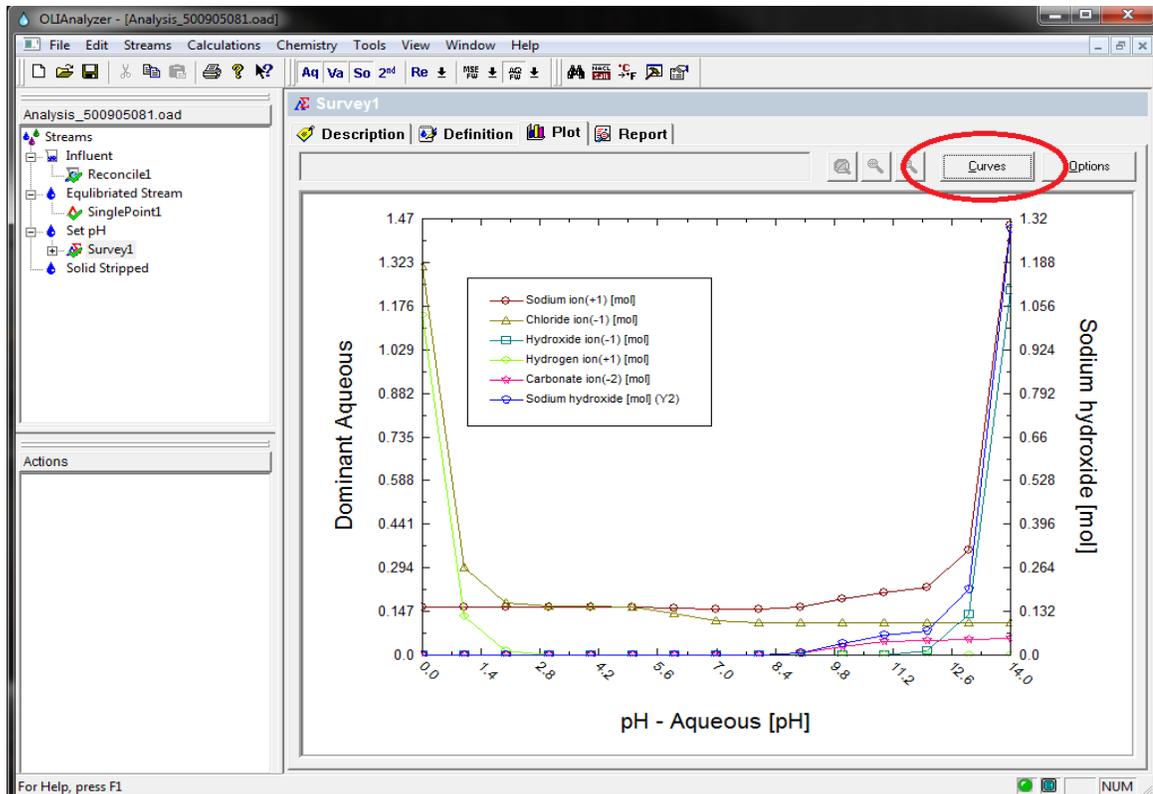
Figure 82. Screenshot of the plot generation step

All these steps will help you analyze your Input Water Quality successfully and calculate characteristics for each step in the complete treatment process train involving Settling, Softening, pH Adjustment, Filtration and Osmosis. The features which can be monitored like pH, Pressure, Temperature, Chemical Additions and Osmotic Pressure are also visible in the reports of this analyzer.

A3. Documentation of Chemistry Tool:

The chemistry tool was developed as a part of a complex GIS Application which would help spatially analyze oil and gas wells in a specific field and derive treatment specifics based on a detailed water quality analysis. The programming consisted of developing a sample model based on initial tested water quality. This base model would then be fixed free of errors in all aspects and developed as an integral part of the main program. This processed model would then be modified in order to be used with an active or current database in a universally accepted format. Once the model was planned and programmed with limit parameters, this would be then further integrated with a GIS map to work on a real-time and dynamic scenario.

Some of the Key Points, which formed the basis:

- The chemistry tool was designed to reconcile all of the chemical and physical data on produced water and predict the corresponding properties of the fluid.

- Water Analyses were close to non-existent, hence sampling was done by us and since it was seldom documented, only a few parameters were tested.

- Programming is being done, when the sampling is still in progress.

- The tool was also made to use the above mentioned predictions to correlate the requirements of treatment of the fluid and simultaneously monitoring its behavior under treatment or disposal.

- All the functions in this tool are from the OLI engine. All these functions are called from the engine using the CalcAq program.

- As explained earlier, the tool was based on a sample process train chosen for simulation in initial version.

- The chemistry and analytical procedures have been changing throughout the process.

- The measurements are contradicted constantly by the new additions of samples, so work is still being done to detect errors.

- The data were from analyses done by ACZ Laboratories of samples drawn newly drawn from the separator tanks at the Well Sites.

The steps involved are as follows:

1. A sample process train was chosen for simulation in the first version of the tool. All the steps were modeled for this particular setup.

2. Each unit operation was identified and a detailed flow chart which would be used in such a way that they could be simulated by individual calculations in Microsoft Excel.

3. All the calculations from then on were done with OLI Functions from the OLI Engine by using a plug-in in Excel called CalcAq.

4. The table of results obtained from the analytical laboratory, i.e. the water quality values were converted into measured parameters for our tool.

5. A macro called "Load Params" was programmed in such a way that it would read the .csv file and load the data into the locations on the "Well 1" worksheet in the program workbook.

6. The next step was reconciliation of all the available data and summarizing them as a result of treating the equivalent stream in the process separators.

7. The deviations of the measured values from the reconciled values would be displayed alongside in such a way that the operator would be able to verify the validity of the simulations and modify reconciliation or treatment if necessary.

8. The operator will also be able to modify or examine each process individually by opening the corresponding worksheet.

9. The "Summary" worksheet has been programmed in such a way that it has buttons which allow the macros for loading the data, running any necessary solver and saving the results for future analysis.

10. It has also been modified that the calculation is run only when necessary, and it doesn't start with incomplete data and give irrelevant results.

11. The program flow starts with an initial charge balance, calculation of pH and the estimation of the amount of carbonate from the reported alkalinity.

12. Iterations are done until a match is found with the amount of acid required in the alkalinity titration and the sample pH.

13. The OLI Functions are then used to give an equivalent stream of stable species and we calculate the measurable and important properties for processing the stream.

14. The functionality is limited at this point enabling us to calculate only one sample at a time.

15. Plans are to implement mixing and in-line treatment later on in the development of this tool like the injection of scale inhibitors into a pipeline or truckload.

Summary:

All calculations are done with the version of the OLI Engine and databank packaged with OLI Analyzer v 3.2. Initially, charge balance is done with Na+. Other options can be used but since all our current samples are deficient in cations, this would be the optimal one. We then use the reported alkalinity to estimate the amount of CO_2 present and adjust the pH to the measure value. The alkalinity was measured by titration, but we only have the number of equivalents and no pH for the end point. We approximate a guess of 4.1 based on a titration curve that we calculated for a single sample with OLI Analyzer v 3.2. We calculate the titration requirements after that and adjust the CO2 and the pH again repeatedly till the calculated pH and the alkalinity match the measured values. Since we found the convergence within 3 iterations, we abstained from using a formal solver. The molecular equivalent stream was calculated.

All of the characteristics in the calculated molecular equivalent stream are tabulated and their values are summed up in a table where flows from other processes and recycle streams are added. The final table is used for further use. Results are calculated by running the stream through the built-in choice of treatment processes. Initially the chemical conditioning is added with a simple Set pH function from the CalcAq library. A pH of 10.4 is specified based on some process experience, but the operator can easily modify it and the process repeated, simultaneously recording the new results in the output table. By cataloging all of the solids from the calculated stream, a filtrate can be simulated by removing the solids and it can be characterized with a new molecular equivalent stream.

Next, we move the processing to the "RO1" worksheet where the filtrate is then treated. We repeat essential functions like "Set pH" in the previous step as we did in the pH adjustments in the previous step. Again, the operator can modify the pH according to requirements. We try to remove the water from the neutralized stream to simulate RO. In order to remove water to a precipitation point without forecasting the precipitating species, we programmed a customized solver with CalcAq functions. Thereby simulating all the steps in a treatment process involved with Produced Water.

A4. Produced Water Quality Analysis:

Sampling was done for Water Qualities used in this project. Safeland Trained Student Researchers did them in accordance with OSHA Regulations with the help of people from the industry such as Noble Energy. The samples were prepared at the University Lab including preliminary analysis and then shipped to certified labs for further analyses. The analyses were done by EPA suggested methods as shown below in Table.

Table 8.   Laboratory Analyses Methods suggested by EPA

Analyst	USEPA Methods	Standard Methods	Method detection limit
Major cations: Dissolved sodium, calcium, magnesium, potassium, iron	EPA Method 6010		
Major anion: Chloride, sulfate, carbonate, bicarbonate, nitrate, nitrite	EPA 300/SM2320B EPA 353		
Dissolved metals: Arsenic, barium, cadmium, chromium, lead, selenium, manganese	EPA Method 6010		
Fluoride	EPA 300		
Bromide	EPA 300		
Chloride		4500- Cl⁻ -B; HACH titration method	10-10,000 mg/L 500-100,000 mg/L
Ammonia		4500-NH$_3$ D	0.03 mg/L
Sulfate		4500- SO$_4^{-2}$	0.1 mg/L
pH	EPA 150.1	4500-H* B	0.01 SU
Total dissolved solids (TDS)	EPA 160.1	2540 B	0.1 mg/L
Total suspended solids (TSS)		2540 B	0.1 mg/L
Alkalinity		2320 B	2 mg/L as CaCO3
Dissolved methane	RSK 175		
Benzene, toluene, ethybenzene, xylenens (BTEX)	SW846 8260B		
Conductivity	SM2510B	2510 B	0.1 μS/cm
Oil and Grease	1664 A		-5 mg/L

The results from the certified lab are shown below.

Table 9.   Sample of Analysis Results from ACZ Laboratories:

LABID	CLIENTID	ANALYTE	METHOD	RESULT	QUAL	UNITS	ANALYST
L95930-01	WELLS RANCH 25-68-1HZ	Barium, dissolved	M200.7 ICP	4.54		mg/L	jjc
L95930-01	WELLS RANCH 25-68-1HZ	Calcium, dissolved	M200.7 ICP	163		mg/L	jjc
L95930-01	WELLS RANCH 25-68-1HZ	Iron, dissolved	M200.7 ICP	20.4		mg/L	jjc
L95930-01	WELLS RANCH 25-68-1HZ	Magnesium, dissolved	M200.7 ICP	23		mg/L	jjc
L95930-01	WELLS RANCH 25-68-1HZ	Potassium, dissolved	M200.7 ICP	361		mg/L	jjc
L95930-01	WELLS RANCH 25-68-1HZ	Sodium, dissolved	M200.7 ICP	5140		mg/L	jjc
L95930-01	WELLS RANCH 25-68-1HZ	Bicarbonate as CaCO3	SM2320B - Titration	990	H	mg/L	jad
L95930-01	WELLS RANCH 25-68-1HZ	Carbonate as CaCO3	SM2320B - Titration		UH	mg/L	jad
L95930-01	WELLS RANCH 25-68-1HZ	Cation-Anion Balance	Calculation	-4.8		%	calc
L95930-01	WELLS RANCH 25-68-1HZ	Chloride	SM4500Cl-E	8900	H	mg/L	lhb
L95930-01	WELLS RANCH 25-68-1HZ	Conductivity @25C	SM2510B	23700	H	umhos/cm	las
L95930-01	WELLS RANCH 25-68-1HZ	Hydroxide as CaCO3	SM2320B - Titration		UH	mg/L	jad
L95930-01	WELLS RANCH 25-68-1HZ	pH	SM4500H+ B	8.1	H	units	jad
L95930-01	WELLS RANCH 25-68-1HZ	pH measured at	SM4500H+ B	22		C	jad
L95930-01	WELLS RANCH 25-68-1HZ	Phosphate	Calculation based on	0.09	B	mg/L	calc
L95930-01	WELLS RANCH 25-68-1HZ	Phosphorus, ortho	M365.1 - Automated	0.03	BH	mg/L	pjb

		dissolved	A				
L95930-01	WELLS RANCH 25-68-1HZ	Residue, Filterable (TDS) @180C	SM2540C	17300	H	mg/L	ljr
L95930-01	WELLS RANCH 25-68-1HZ	Sulfate	D516-02 - Turbidimet	130	H	mg/L	tcd
L95930-01	WELLS RANCH 25-68-1HZ	Sum of Anions	Calculation	272		meq/L	calc
L95930-01	WELLS RANCH 25-68-1HZ	Sum of Cations	Calculation	247		meq/L	calc
L95930-01	WELLS RANCH 25-68-1HZ	TDS (calculated)	Calculation	15300		mg/L	calc
L95930-01	WELLS RANCH 25-68-1HZ	TDS (ratio - measured/calculated)	Calculation	1.13			calc
L95930-01	WELLS RANCH 25-68-1HZ	Total Alkalinity	SM2320B - Titration	990	H	mg/L	jad

A5. Detailed Report from OLI Analyzer – Mixing Case Study:

(a) Mixture 1: (9/10/12 Sample 50% + East 50%)

Calculation		Summary
Mixer		Calculation
Unit	Set:	Default
Automatic	Chemistry	Model
Aqueous	(H+ | ion)	Databanks:
Public		
Isothermal		Calculation
25.0000	°C	1.00000	atm
Stream		Inflows

Row Filter Applied: Only Non Zero Values

Species	mol
Water	54.5562
Vanadium	9.81518e-7
Calcium carbonate (calcite)	1.14999e-3
Diboron trioxide	2.47338e-5
Barium monoxide	7.52887e-7
Barium sulfate	3.50438e-6
Iron(II) carbonate	2.46749e-6
Iron(II) oxide	4.89190e-6
Potassium chloride	0.0134494
Magnesium oxide	4.26497e-4
Disodium oxide	1.64461e-3
Sodium bromide	2.94375e-4
Sodium chloride	0.0685117
Sulfur trioxide	8.52751e-4
Strontium monoxide	4.29982e-5
Lead(II) oxide yellow	1.20656e-9
Manganese(II) bromide	6.17059e-7
Carbon dioxide	3.37030e-3
Zinc bromide	9.17572e-8

Aluminum oxide	7.12128e-9
Sodium aluminum dihydroxide carbonate	4.43324e-6

Mixture Properties

StrAmt	54.6460	mol
Temp	25.0000	°C
Pres	1.00000	atm

Aqueous Properties

pH	7.76995	---
Ionic Strength	1.63447e-3	mol/mol
Osmotic Pressure	4.24549	atm
Elec Cond, specific	9.65525e-3	mho/cm
Elec Cond, molar	106.198	cm2/ohm-mol
Viscosity, absolute	0.899090	cP
Viscosity, relative	1.00940	---
Standard Liquid Volume	0.989043	L

Solid Properties

Standard Liquid Volume	1.71028e-5	L

	Unit	Total	Aqueous	Solid
Density	g/ml	1.00079	1.00077	2.73144
Enthalpy	cal	-3.73614e6	-3.73603e6	-109.344

Total and Phase Flows (Amounts)
column Filter Applied: Only Non Zero Values

	Total	Aqueous	Solid
	mol	mol	mol
Mole (True)	54.7282	54.7278	3.79600e-4
Mole (App)	54.6468	54.6464	3.79600e-4
	g	g	g
Mass	988.345	988.306	0.0382606
	L	L	cm3
Volume	0.987560	0.987546	0.0140075

Row Filter Applied: Values > 1.0e-4

Solids	Tendency
Calcium carbonate (calcite)	1.00000
Barium sulfate	1.00000
Aluminum hydroxide	1.00000
Strontium carbonate	0.465391
Iron(II) carbonate	0.427179
Sodium aluminum dihydroxide carbonate	0.348483
Manganese(II) carbonate	0.0524381
Strontium sulfate	0.0187448
Calcium sulfate dihydrate	2.36881e-3
Zinc carbonate	1.74449e-3
Calcium sulfate	1.73383e-3
Lead(II) carbonate (cerussite)	1.60997e-3
Sodium bicarbonate	6.26898e-4
Iron(II) hydroxide	3.11883e-4
Magnesium carbonate trihydrate	2.85398e-4
Magnesium carbonate	2.69530e-4
Barium carbonate	1.46838e-4

Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

	Total	Aqueous	Solid
	mol	mol	mol
Water	54.5541	54.5541	0.0
Hydrogen ion(+1)	2.08161e-8	2.08161e-8	0.0
Hydroxide ion(-1)	7.37411e-7	7.37411e-7	0.0
Aluminum ion(+3)	3.62764e-16	3.62764e-16	0.0
Aluminum chloride dihydroxide	1.23234e-28	1.23234e-28	0.0
Aluminum dihydroxide ion(+1)	9.41407e-12	9.41407e-12	0.0
Aluminum hydroxide	4.40261e-6	2.32474e-9	4.40029e-6
Aluminum tetrahydroxide ion(-1)	4.48649e-8	4.48649e-8	0.0
Aluminum chloride hydroxide ion(+1)	7.67151e-15	7.67151e-15	0.0

Aluminum monohydroxide ion(+2)	6.93412e-14	6.93412e-14	0.0
Aluminum disulfate ion(-1)	3.15804e-19	3.15804e-19	0.0
Aluminum monosulfate ion(+1)	1.59383e-17	1.59383e-17	0.0
Diboron oxide pentahydroxide ion(-1)	1.45835e-10	1.45835e-10	0.0
Triboron trioxide tetrahydroxide ion(-1)	8.26433e-13	8.26433e-13	0.0
Tetraboron pentaoxide tetrahydroxide ion(-2)	3.95275e-17	3.95275e-17	0.0
Barium chloride ion (+1)	7.75527e-8	7.75527e-8	0.0
Barium carbonate	1.43273e-9	1.43273e-9	0.0
Barium bicarbonate ion(+1)	1.63013e-8	1.63013e-8	0.0
Barium ion(+2)	1.06501e-6	1.06501e-6	0.0
Barium hydroxide ion(+1)	1.79461e-13	1.79461e-13	0.0
Boric acid	4.72965e-5	4.72965e-5	0.0
Boron tetrahydroxide ion(-1)	2.07537e-6	2.07537e-6	0.0
Bromide ion (-1)	2.95222e-4	2.95222e-4	0.0
Calcium chloride	1.16431e-24	1.16431e-24	0.0
Calcium monochloride ion(+1)	4.78835e-10	4.78835e-10	0.0
Calcium carbonate (calcite)	3.89803e-4	1.86817e-5	3.71121e-4
Calcium dihydrogen borate ion(+1)	3.63554e-8	3.63554e-8	0.0
Calcium bicarbonate ion(+1)	1.28592e-5	1.28592e-5	0.0
Calcium ion(+2)	7.44494e-4	7.44494e-4	0.0
Calcium hydroxide ion(+1)	3.85182e-9	3.85182e-9	0.0
Calcium sulfate	2.79522e-6	2.79522e-6	0.0
Chloride ion(-1)	0.0819554	0.0819554	0.0
Carbon dioxide	1.05508e-4	1.05508e-4	0.0
Carbonate ion(-2)	2.33906e-5	2.33906e-5	0.0
Iron(II) chloride	4.32299e-14	4.32299e-14	0.0
Iron(II) monochloride ion(+1)	2.33455e-10	2.33455e-10	0.0
Iron(II) dicarbonate ion(-2)	1.6246e-9	1.6246e-9	0.0
Iron(II) carbonate	2.11676e-6	2.11676e-6	0.0
Iron(II) bicarbonate ion(+1)	1.10909e-9	1.10909e-9	0.0
Iron ion(+2)	5.1653e-6	5.1653e-6	0.0
Iron(II) monohydroxide ion(+1)	7.43299e-8	7.43299e-8	0.0
Iron(II) oxide	2.73568e-11	2.73568e-11	0.0
Sulfuric(VI) acid	2.59834e-28	2.59834e-28	0.0
Hydrogen bromide	3.84207e-20	3.84207e-20	0.0
Hydrogen chloride	6.35659e-16	6.35659e-16	0.0

Bicarbonate ion(-1)	3.73511e-3	3.73511e-3	0.0
Hydrogen dioxyiron ion(-1)	3.41811e-15	3.41811e-15	0.0
Hydrogen dioxylead ion(-1)	2.54808e-16	2.54808e-16	0.0
Bisulfate(VI) ion (-1)	5.09804e-10	5.09804e-10	0.0
Potassium chloride	5.53897e-6	5.53897e-6	0.0
Potassium bisulfate(VI)	8.00162e-14	8.00162e-14	0.0
Potassium ion(+1)	0.013418	0.013418	0.0
Potassium sulfate(VI) ion(-1)	2.58629e-5	2.58629e-5	0.0
Magnesium carbonate	1.2274e-6	1.2274e-6	0.0
Magnesium bicarbonate ion(+1)	2.28876e-5	2.28876e-5	0.0
Magnesium ion(+2)	3.99696e-4	3.99696e-4	0.0
Magnesium hydroxide ion(+1)	2.01594e-8	2.01594e-8	0.0
Magnesium sulfate	2.66503e-6	2.66503e-6	0.0
Manganese(II) bromide	4.79153e-13	4.79153e-13	0.0
Manganese(II) monobromide ion(+1)	2.03779e-9	2.03779e-9	0.0
Manganese(II) monochloride ion(+1)	6.56719e-8	6.56719e-8	0.0
Manganese ion(+2)	5.37793e-7	5.37793e-7	0.0
Manganese(II) hydroxide	4.21796e-14	4.21796e-14	0.0
Manganese(II) trihydroxide ion(-1)	8.48799e-19	8.48799e-19	0.0
Manganese(II) tetrahydroxide ion(-2)	3.57495e-24	3.57495e-24	0.0
Manganese(II) monohydroxide ion (+1)	8.34494e-10	8.34494e-10	0.0
Manganese(II) sulfate	1.07218e-8	1.07218e-8	0.0
Sodium boron hydroxide	5.90461e-8	5.90461e-8	0.0
Sodium bromide	5.68157e-7	5.68157e-7	0.0
Sodium carbonate ion(-1)	2.09249e-6	2.09249e-6	0.0
Sodium bicarbonate	2.32179e-4	2.32179e-4	0.0
Sodium ion(+1)	0.0717184	0.0717184	0.0
Sodium sulfate ion(-1)	1.46353e-4	1.46353e-4	0.0
Lead(II) bromide	1.90742e-17	1.90742e-17	0.0
Lead(II) tribromide ion(-1)	2.33486e-19	2.33486e-19	0.0
Lead(II) monobromide ion(+1)	1.56449e-13	1.56449e-13	0.0
Lead(II) chloride	3.34761e-12	3.34761e-12	0.0
Lead(II) trichloride ion(-1)	1.38195e-13	1.38195e-13	0.0
Lead(II) tetrachloride ion(-2)	1.41072e-14	1.41072e-14	0.0
Lead(II) monochloride ion(+1)	1.81569e-11	1.81569e-11	0.0
Lead(II) carbonate ion (-2)	5.74815e-11	5.74815e-11	0.0
Lead(II) carbonate (cerussite)	5.00271e-10	5.00271e-10	0.0

Lead(II) ion(+2)	2.03583e-11	2.03583e-11	0.0
Lead(II) oxide yellow	1.04781e-13	1.04781e-13	0.0
Lead(II) monohydroxide ion(+1)	6.05618e-10	6.05618e-10	0.0
Lead(II) sulfate	9.16947e-13	9.16947e-13	0.0
Sulfur trioxide	3.37341e-32	3.37341e-32	0.0
Sulfate ion(-2)	6.74785e-4	6.74785e-4	0.0
Strontium ion(+2)	4.23126e-5	4.23126e-5	0.0
Strontium monohydroxide ion(+1)	7.95061e-11	7.95061e-11	0.0
Strontium sulfate	6.85536e-7	6.85536e-7	0.0
Zinc bromide	6.01203e-17	6.01203e-17	0.0
Zinc tribromide ion(-1)	6.48696e-20	6.48696e-20	0.0
Zinc bromide ion(+1)	2.45745e-12	2.45745e-12	0.0
Zinc chloride	2.16581e-10	2.16581e-10	0.0
Zinc trichloride ion(-1)	6.24531e-12	6.24531e-12	0.0
Zinc chloride ion(+1)	3.85171e-9	3.85171e-9	0.0
Zinc bicarbonate ion(+1)	2.42927e-9	2.42927e-9	0.0
Zinc ion(+2)	8.202e-8	8.202e-8	0.0
Zinc hydroxide, amorphous	4.92079e-10	4.92079e-10	0.0
Zinc trihydroxide ion(-1)	3.69868e-13	3.69868e-13	0.0
Zinc tetrahydroxide ion(-2)	6.2635e-18	6.2635e-18	0.0
Zinc monohydroxide ion(+1)	2.73841e-9	2.73841e-9	0.0
Barium sulfate	3.09696e-6	0.0	3.09696e-6
Vanadium	9.81518e-7	0.0	9.81518e-7
Total (by phase)	54.7282	54.7278	3.796e-4

Element   Balance
Row   Filter   Applied: Only   Non   Zero   Values
column Filter Applied: Only Non Zero Values

	Total	Aqueous	Solid
	mol	mol	mol
H(+1)	109.112	109.112	1.32009e-5
K(+1)	0.0134494	0.0134494	0.0
Na(+1)	0.0720997	0.0720997	0.0
Ba(+2)	4.25726e-6	1.1603e-6	3.09696e-6
Ca(+2)	1.14999e-3	7.7887e-4	3.71121e-4
Zn(+2)	9.17572e-8	9.17572e-8	0.0
Fe(+2)	7.35939e-6	7.35939e-6	0.0

Mg(+2)	4.26497e-4	4.26497e-4	0.0
Pb(+2)	1.20656e-9	1.20656e-9	0.0
Al(+3)	4.44749e-6	4.71991e-8	4.40029e-6
Mn(+2)	6.17059e-7	6.17059e-7	0.0
O(-2)	54.5712	54.5701	1.13895e-3
Cl(-1)	0.0819611	0.0819611	0.0
Br(-1)	2.95792e-4	2.95792e-4	0.0
C(+4)	4.5272e-3	4.15608e-3	3.71121e-4
S(+6)	8.56256e-4	8.53159e-4	3.09696e-6
Sr(+2)	4.29982e-5	4.29982e-5	0.0
B(+3)	4.94676e-5	4.94676e-5	0.0
V(0)	9.81518e-7	0.0	9.81518e-7

(b) Mixture 2: (9/10/12 Sample 50% + West 50%):

Calculation	Summary
Mixer	Calculation
Unit	Set:	Default
Automatic	Chemistry	Model
Aqueous	(H+	ion)	Databanks:
Public		
Isothermal		Calculation
25.0000	°C	1.00000	atm
Stream		Inflows

Row Filter Applied: Only Non Zero Values

Species	mol
Water	54.5710
Vanadium	9.81518e-7
Calcium carbonate (calcite)	2.81053e-3
Diboron trioxide	2.47338e-5
Barium monoxide	7.52887e-7
Barium sulfate	3.50438e-6
Iron(II) carbonate	1.40286e-6
Iron(II) oxide	7.74714e-6
Potassium chloride	0.0134494
Magnesium oxide	8.06418e-4
Disodium oxide	3.32465e-3
Sodium bromide	2.94375e-4
Sodium chloride	0.0687937
Sulfur trioxide	3.19495e-3
Strontium monoxide	4.29982e-5
Lead(II) oxide yellow	1.20656e-9
Manganese(II) bromide	6.17059e-7
Carbon dioxide	3.45081e-3
Zinc bromide	9.17572e-8

Aluminum oxide	7.12128e-9	
Sodium aluminum dihydroxide carbonate	4.43324e-6	

Row column	Filter Filter	Applied: Applied:	Only Only	Non Non	Zero Zero	Values Values

Mixture Properties

StrAmt	54.6672	mol
Temp	25.0000	°C
Pres	1.00000	atm

Aqueous Properties

pH	7.51611	---
Ionic Strength	1.77133e-3	mol/mol
Osmotic Pressure	4.51120	atm
Elec Cond, specific	0.0100521	mho/cm
Elec Cond, molar	103.209	cm2/ohm-mol
Viscosity, absolute	0.900384	cP
Viscosity, relative	1.01085	---
Standard Liquid Volume	0.989466	L

Solid Properties

Standard Liquid Volume	6.93314e-5	L

	Unit	Total	Aqueous	Solid
Density	g/ml	1.00121	1.00111	2.71687
Enthalpy	cal	-3.73839e6	-3.73795e6	-436.596

Total   and   Phase   Flows   (Amounts)
column Filter Applied: Only Non Zero Values

	Total	Aqueous	Solid
	mol	mol	mol
Mole (True)	54.7510	54.7495	1.51561e-3
Mole (App)	54.6685	54.6670	1.51561e-3
	g	g	g
Mass	989.104	988.951	0.152070

	L	L	cm3
Volume	0.987907	0.987851	0.0559726

<u>Scaling</u> <u>Tendencies</u>
Row Filter Applied: Values > 1.0e-4

Solids	Tendency
Calcium carbonate (calcite)	1.00000
Barium sulfate	1.00000
Aluminum hydroxide	1.00000
Sodium aluminum dihydroxide carbonate	0.400808
Iron(II) carbonate	0.361239
Strontium carbonate	0.267840
Strontium sulfate	0.0629253
Manganese(II) carbonate	0.0301837
Calcium sulfate dihydrate	0.0138117
Calcium sulfate	0.0101133
Lead(II) carbonate (cerussite)	1.67111e-3
Zinc carbonate	1.06240e-3
Sodium bicarbonate	7.20885e-4
Magnesium carbonate trihydrate	3.17451e-4
Magnesium carbonate	2.99977e-4
Iron(II) hydroxide	1.32493e-4
Sodium chloride	1.01120e-4

<u>Species</u> <u>Output</u> <u>(True</u> <u>Species)</u>
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

	Total	Aqueous	Solid
	mol	mol	mol
Water	54.5686	54.5686	0.0
Hydrogen ion(+1)	3.76832e-8	3.76832e-8	0.0
Hydroxide ion(-1)	4.13944e-7	4.13944e-7	0.0
Aluminum ion(+3)	2.24761e-15	2.24761e-15	0.0
Aluminum chloride dihydroxide	2.20556e-28	2.20556e-28	0.0
Aluminum dihydroxide ion(+1)	1.70309e-11	1.70309e-11	0.0

Aluminum hydroxide	4.42225e-6	2.32323e-9	4.41993e-6
Aluminum tetrahydroxide ion(-1)	2.52158e-8	2.52158e-8	0.0
Aluminum chloride hydroxide ion(+1)	2.4871e-14	2.4871e-14	0.0
Aluminum monohydroxide ion(+2)	2.30223e-13	2.30223e-13	0.0
Aluminum disulfate ion(-1)	2.39379e-17	2.39379e-17	0.0
Aluminum monosulfate ion(+1)	3.34719e-16	3.34719e-16	0.0
Diboron oxide pentahydroxide ion(-1)	8.53182e-11	8.53182e-11	0.0
Triboron trioxide tetrahydroxide ion(-1)	4.93349e-13	4.93349e-13	0.0
Tetraboron pentaoxide tetrahydroxide ion(-2)	1.3766e-17	1.3766e-17	0.0
Barium chloride ion (+1)	2.16605e-8	2.16605e-8	0.0
Barium carbonate	2.45469e-10	2.45469e-10	0.0
Barium bicarbonate ion(+1)	5.05752e-9	5.05752e-9	0.0
Barium ion(+2)	3.04675e-7	3.04675e-7	0.0
Barium hydroxide ion(+1)	2.7958e-14	2.7958e-14	0.0
Boric acid	4.82107e-5	4.82107e-5	0.0
Boron tetrahydroxide ion(-1)	1.18816e-6	1.18816e-6	0.0
Bromide ion (-1)	2.95205e-4	2.95205e-4	0.0
Calcium chloride	1.87475e-24	1.87475e-24	0.0
Calcium monochloride ion(+1)	7.73535e-10	7.73535e-10	0.0
Calcium carbonate (calcite)	1.52495e-3	1.86695e-5	1.50628e-3
Calcium dihydrogen borate ion(+1)	3.37295e-8	3.37295e-8	0.0
Calcium bicarbonate ion(+1)	2.32457e-5	2.32457e-5	0.0
Calcium ion(+2)	1.24601e-3	1.24601e-3	0.0
Calcium hydroxide ion(+1)	3.50024e-9	3.50024e-9	0.0
Calcium sulfate	1.62937e-5	1.62937e-5	0.0
Chloride ion(-1)	0.0822376	0.0822376	0.0
Carbon dioxide	2.09845e-4	2.09845e-4	0.0
Carbonate ion(-2)	1.50042e-5	1.50042e-5	0.0
Iron(II) chloride	5.88631e-14	5.88631e-14	0.0
Iron(II) monochloride ion(+1)	3.21594e-10	3.21594e-10	0.0
Iron(II) dicarbonate ion(-2)	8.78097e-10	8.78097e-10	0.0
Iron(II) carbonate	1.78885e-6	1.78885e-6	0.0
Iron(II) bicarbonate ion(+1)	1.69784e-9	1.69784e-9	0.0
Iron ion(+2)	7.30111e-6	7.30111e-6	0.0
Iron(II) monohydroxide ion(+1)	5.71261e-8	5.71261e-8	0.0

Iron(II) oxide	1.16163e-11	1.16163e-11	0.0
Sulfuric(VI) acid	3.01379e-27	3.01379e-27	0.0
Hydrogen bromide	6.84615e-20	6.84615e-20	0.0
Hydrogen chloride	1.13743e-15	1.13743e-15	0.0
Bicarbonate ion(-1)	4.17674e-3	4.17674e-3	0.0
Hydrogen dioxyiron ion(-1)	8.16532e-16	8.16532e-16	0.0
Hydrogen dioxylead ion(-1)	7.46555e-17	7.46555e-17	0.0
Bisulfate(VI) ion (-1)	3.31959e-9	3.31959e-9	0.0
Potassium chloride	5.4508e-6	5.4508e-6	0.0
Potassium bisulfate(VI)	5.10416e-13	5.10416e-13	0.0
Potassium ion(+1)	0.0133511	0.0133511	0.0
Potassium sulfate(VI) ion(-1)	9.28375e-5	9.28375e-5	0.0
Magnesium carbonate	1.36516e-6	1.36516e-6	0.0
Magnesium bicarbonate ion(+1)	4.60699e-5	4.60699e-5	0.0
Magnesium ion(+2)	7.41673e-4	7.41673e-4	0.0
Magnesium hydroxide ion(+1)	2.03913e-8	2.03913e-8	0.0
Magnesium sulfate	1.72897e-5	1.72897e-5	0.0
Manganese(II) bromide	4.40383e-13	4.40383e-13	0.0
Manganese(II) monobromide ion(+1)	1.90236e-9	1.90236e-9	0.0
Manganese(II) monochloride ion(+1)	6.15778e-8	6.15778e-8	0.0
Manganese ion(+2)	5.17167e-7	5.17167e-7	0.0
Manganese(II) hydroxide	1.21888e-14	1.21888e-14	0.0
Manganese(II) trihydroxide ion(-1)	1.3799e-19	1.3799e-19	0.0
Manganese(II) tetrahydroxide ion(-2)	3.32283e-25	3.32283e-25	0.0
Manganese(II) monohydroxide ion (+1)	4.36494e-10	4.36494e-10	0.0
Manganese(II) sulfate	3.59748e-8	3.59748e-8	0.0
Sodium boron hydroxide	3.47758e-8	3.47758e-8	0.0
Sodium bromide	5.85067e-7	5.85067e-7	0.0
Sodium carbonate ion(-1)	1.35171e-6	1.35171e-6	0.0
Sodium bicarbonate	2.66815e-4	2.66815e-4	0.0
Sodium ion(+1)	0.0749206	0.0749206	0.0
Sodium sulfate ion(-1)	5.52428e-4	5.52428e-4	0.0
Lead(II) bromide	3.16129e-17	3.16129e-17	0.0
Lead(II) tribromide ion(-1)	3.88248e-19	3.88248e-19	0.0
Lead(II) monobromide ion(+1)	2.63371e-13	2.63371e-13	0.0
Lead(II) chloride	5.59494e-12	5.59494e-12	0.0
Lead(II) trichloride ion(-1)	2.32523e-13	2.32523e-13	0.0

Lead(II) tetrachloride ion(-2)	2.42018e-14	2.42018e-14	0.0
Lead(II) monochloride ion(+1)	3.07006e-11	3.07006e-11	0.0
Lead(II) carbonate ion (-2)	3.81762e-11	3.81762e-11	0.0
Lead(II) carbonate (cerussite)	5.1893e-10	5.1893e-10	0.0
Lead(II) ion(+2)	3.53179e-11	3.53179e-11	0.0
Lead(II) oxide yellow	5.4612e-14	5.4612e-14	0.0
Lead(II) monohydroxide ion(+1)	5.71715e-10	5.71715e-10	0.0
Lead(II) sulfate	5.55371e-12	5.55371e-12	0.0
Sulfur trioxide	3.91355e-31	3.91355e-31	0.0
Sulfate ion(-2)	2.51334e-3	2.51334e-3	0.0
Strontium ion(+2)	4.06983e-5	4.06983e-5	0.0
Strontium monohydroxide ion(+1)	4.16111e-11	4.16111e-11	0.0
Strontium sulfate	2.29981e-6	2.29981e-6	0.0
Zinc bromide	5.84619e-17	5.84619e-17	0.0
Zinc tribromide ion(-1)	6.32884e-20	6.32884e-20	0.0
Zinc bromide ion(+1)	2.42725e-12	2.42725e-12	0.0
Zinc chloride	2.1238e-10	2.1238e-10	0.0
Zinc trichloride ion(-1)	6.1654e-12	6.1654e-12	0.0
Zinc chloride ion(+1)	3.82114e-9	3.82114e-9	0.0
Zinc bicarbonate ion(+1)	2.67764e-9	2.67764e-9	0.0
Zinc ion(+2)	8.33703e-8	8.33703e-8	0.0
Zinc hydroxide, amorphous	1.50449e-10	1.50449e-10	0.0
Zinc trihydroxide ion(-1)	6.35734e-14	6.35734e-14	0.0
Zinc tetrahydroxide ion(-2)	6.15361e-19	6.15361e-19	0.0
Zinc monohydroxide ion(+1)	1.51663e-9	1.51663e-9	0.0
Barium sulfate	3.92562e-6	0.0	3.92562e-6
Vanadium	9.81518e-7	0.0	9.81518e-7
Total (by phase)	54.751	54.7495	1.51561e-3

Element   Balance
Row   Filter   Applied: Only   Non   Zero   Values
column Filter Applied: Only Non Zero Values

	Total	Aqueous	Solid
	mol	mol	mol
H(+1)	109.142	109.142	1.32598e-5
K(+1)	0.0134494	0.0134494	0.0
Na(+1)	0.0757418	0.0757418	0.0

Ba(+2)	4.25726e-6	3.31639e-7	3.92562e-6
Ca(+2)	2.81053e-3	1.30426e-3	1.50628e-3
Zn(+2)	9.17572e-8	9.17572e-8	0.0
Fe(+2)	9.15e-6	9.15e-6	0.0
Mg(+2)	8.06418e-4	8.06418e-4	0.0
Pb(+2)	1.20656e-9	1.20656e-9	0.0
Al(+3)	4.44749e-6	2.75563e-8	4.41993e-6
Mn(+2)	6.17059e-7	6.17059e-7	0.0
O(-2)	54.6002	54.5956	4.5478e-3
Cl(-1)	0.0822432	0.0822432	0.0
Br(-1)	2.95792e-4	2.95792e-4	0.0
C(+4)	6.26718e-3	4.76091e-3	1.50628e-3
S(+6)	3.19845e-3	3.19453e-3	3.92562e-6
Sr(+2)	4.29982e-5	4.29982e-5	0.0
B(+3)	4.94676e-5	4.94676e-5	0.0
V(0)	9.81518e-7	0.0	9.81518e-7

(c) Mixture 3: (9/10/12 Sample 75% + East 25%):

Calculation		Summary
Mixer	3	Calculation
Unit	Set:	Default
Automatic	Chemistry	Model
Aqueous	(H+ | ion)	Databanks:
Public		
Isothermal		Calculation
25.0000	°C	1.00000	atm
Stream		Inflows

Row Filter Applied: Only Non Zero Values

Species	mol
Water	54.8559
Vanadium	1.47228e-6
Calcium carbonate (calcite)	1.28486e-3
Diboron trioxide	3.71007e-5
Barium monoxide	1.12933e-6
Barium sulfate	5.25656e-6
Iron(II) carbonate	1.23374e-6
Iron(II) oxide	4.43353e-6
Potassium chloride	0.0201742
Magnesium oxide	5.19770e-4
Disodium oxide	2.29217e-3
Sodium bromide	4.41562e-4
Sodium chloride	0.102485
Sulfur trioxide	1.01888e-3
Strontium monoxide	6.44973e-5
Lead(II) oxide yellow	1.80985e-9
Manganese(II) bromide	9.25589e-7
Carbon dioxide	4.81812e-3
Zinc bromide	1.37636e-7
Aluminum oxide	1.06819e-8
Sodium aluminum dihydroxide carbonate	6.64986e-6

152

Row	Filter	Applied:	Only	Non	Zero	Values
column	Filter	Applied:	Only	Non	Zero	Values

Mixture Properties

StrAmt	54.9891	mol
Temp	25.0000	°C
Pres	1.00000	atm

Aqueous Properties

pH	7.61725	---
Ionic Strength	2.39917e-3	mol/mol
Osmotic Pressure	6.21281	atm
Elec Cond, specific	0.0139345	mho/cm
Elec Cond, molar	103.994	cm2/ohm-mol
Viscosity, absolute	0.902424	cP
Viscosity, relative	1.01314	---
Standard Liquid Volume	0.996074	L

Solid Properties

Standard Liquid Volume	1.54668e-5	L

	Unit	Total	Aqueous	Solid
Density	g/ml	1.00262	1.00260	2.74765
Enthalpy	cal	-3.76096e6	-3.76086e6	-100.330

Total	and	Phase	Flows	(Amounts)

column Filter Applied: Only Non Zero Values

	Total	Aqueous	Solid
	mol	mol	mol
Mole (True)	55.1118	55.1115	3.48199e-4
Mole (App)	54.9900	54.9897	3.48199e-4
	g	g	g
Mass	996.384	996.349	0.0353015
	L	L	cm3
Volume	0.993781	0.993768	0.0128479

Row Filter Applied: Values > 1.0e-4

Solids	Tendency
Calcium carbonate (calcite)	1.00000
Barium sulfate	1.00000
Aluminum hydroxide	1.00000
Sodium aluminum dihydroxide carbonate	0.646292
Strontium carbonate	0.560740
Iron(II) carbonate	0.284767
Manganese(II) carbonate	0.0598585
Strontium sulfate	0.0244578
Lead(II) carbonate (cerussite)	2.61975e-3
Calcium sulfate dihydrate	2.55780e-3
Zinc carbonate	2.02877e-3
Calcium sulfate	1.87758e-3
Sodium bicarbonate	1.16095e-3
Magnesium carbonate trihydrate	2.82863e-4
Magnesium carbonate	2.68299e-4
Potassium chloride	2.05605e-4
Sodium chloride	2.02389e-4
Barium carbonate	1.35596e-4
Iron(II) hydroxide	1.13112e-4

Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

	Total	Aqueous	Solid
	mol	mol	mol
Water	54.853	54.853	0.0
Hydrogen ion(+1)	3.03751e-8	3.03751e-8	0.0
Hydroxide ion(-1)	5.34163e-7	5.34163e-7	0.0
Aluminum ion(+3)	1.29271e-15	1.29271e-15	0.0
Aluminum chloride dihydroxide	2.52358e-28	2.52358e-28	0.0
Aluminum dihydroxide ion(+1)	1.39045e-11	1.39045e-11	0.0
Aluminum hydroxide	6.63836e-6	2.31928e-9	6.63604e-6
Aluminum tetrahydroxide ion(-1)	3.28497e-8	3.28497e-8	0.0

Aluminum chloride hydroxide ion(+1)	2.35139e-14	2.35139e-14	0.0
Aluminum monohydroxide ion(+2)	1.56352e-13	1.56352e-13	0.0
Aluminum disulfate ion(-1)	9.20502e-19	9.20502e-19	0.0
Aluminum monosulfate ion(+1)	4.73725e-17	4.73725e-17	0.0
Diboron oxide pentahydroxide ion(-1)	2.48992e-10	2.48992e-10	0.0
Triboron trioxide tetrahydroxide ion(-1)	2.15226e-12	2.15226e-12	0.0
Tetraboron pentaoxide tetrahydroxide ion(-2)	1.25293e-16	1.25293e-16	0.0
Barium chloride ion (+1)	1.16277e-7	1.16277e-7	0.0
Barium carbonate	1.31993e-9	1.31993e-9	0.0
Barium bicarbonate ion(+1)	2.24385e-8	2.24385e-8	0.0
Barium ion(+2)	1.21903e-6	1.21903e-6	0.0
Barium hydroxide ion(+1)	1.33122e-13	1.33122e-13	0.0
Boric acid	7.17656e-5	7.17656e-5	0.0
Boron tetrahydroxide ion(-1)	2.29993e-6	2.29993e-6	0.0
Bromide ion (-1)	4.42508e-4	4.42508e-4	0.0
Calcium chloride	2.66255e-24	2.66255e-24	0.0
Calcium monochloride ion(+1)	7.20436e-10	7.20436e-10	0.0
Calcium carbonate (calcite)	3.53702e-4	1.86378e-5	3.35064e-4
Calcium dihydrogen borate ion(+1)	4.49863e-8	4.49863e-8	0.0
Calcium bicarbonate ion(+1)	1.87813e-5	1.87813e-5	0.0
Calcium ion(+2)	9.0931e-4	9.0931e-4	0.0
Calcium hydroxide ion(+1)	3.09414e-9	3.09414e-9	0.0
Calcium sulfate	3.01987e-6	3.01987e-6	0.0
Chloride ion(-1)	0.122648	0.122648	0.0
Carbon dioxide	1.93196e-4	1.93196e-4	0.0
Carbonate ion(-2)	2.51748e-5	2.51748e-5	0.0
Iron(II) chloride	6.5901e-14	6.5901e-14	0.0
Iron(II) monochloride ion(+1)	2.56703e-10	2.56703e-10	0.0
Iron(II) dicarbonate ion(-2)	1.15565e-9	1.15565e-9	0.0
Iron(II) carbonate	1.40777e-6	1.40777e-6	0.0
Iron(II) bicarbonate ion(+1)	1.09049e-9	1.09049e-9	0.0
Iron ion(+2)	4.21717e-6	4.21717e-6	0.0
Iron(II) monohydroxide ion(+1)	3.98162e-8	3.98162e-8	0.0
Iron(II) oxide	9.91266e-12	9.91266e-12	0.0
Sulfuric(VI) acid	5.14486e-28	5.14486e-28	0.0

Hydrogen bromide	7.87844e-20	7.87844e-20	0.0
Hydrogen chloride	1.29981e-15	1.29981e-15	0.0
Bicarbonate ion(-1)	5.05194e-3	5.05194e-3	0.0
Hydrogen dioxyiron ion(-1)	9.14977e-16	9.14977e-16	0.0
Hydrogen dioxylead ion(-1)	1.64936e-16	1.64936e-16	0.0
Bisulfate(VI) ion (-1)	7.38203e-10	7.38203e-10	0.0
Potassium chloride	1.14623e-5	1.14623e-5	0.0
Potassium bisulfate(VI)	1.60339e-13	1.60339e-13	0.0
Potassium ion(+1)	0.0201244	0.0201244	0.0
Potassium sulfate(VI) ion(-1)	3.8271e-5	3.8271e-5	0.0
Magnesium carbonate	1.21893e-6	1.21893e-6	0.0
Magnesium bicarbonate ion(+1)	3.3592e-5	3.3592e-5	0.0
Magnesium ion(+2)	4.82076e-4	4.82076e-4	0.0
Magnesium hydroxide ion(+1)	1.61252e-8	1.61252e-8	0.0
Magnesium sulfate	2.86606e-6	2.86606e-6	0.0
Manganese(II) bromide	1.25782e-12	1.25782e-12	0.0
Manganese(II) monobromide ion(+1)	3.88973e-9	3.88973e-9	0.0
Manganese(II) monochloride ion(+1)	1.23653e-7	1.23653e-7	0.0
Manganese ion(+2)	7.84057e-7	7.84057e-7	0.0
Manganese(II) hydroxide	2.61335e-14	2.61335e-14	0.0
Manganese(II) trihydroxide ion(-1)	3.88507e-19	3.88507e-19	0.0
Manganese(II) tetrahydroxide ion(-2)	1.30569e-24	1.30569e-24	0.0
Manganese(II) monohydroxide ion (+1)	7.65201e-10	7.65201e-10	0.0
Manganese(II) sulfate	1.32227e-8	1.32227e-8	0.0
Sodium boron hydroxide	9.03988e-8	9.03988e-8	0.0
Sodium bromide	1.17722e-6	1.17722e-6	0.0
Sodium carbonate ion(-1)	2.85975e-6	2.85975e-6	0.0
Sodium bicarbonate	4.28964e-4	4.28964e-4	0.0
Sodium ion(+1)	0.106873	0.106873	0.0
Sodium sulfate ion(-1)	2.1169e-4	2.1169e-4	0.0
Lead(II) bromide	7.13763e-17	7.13763e-17	0.0
Lead(II) tribromide ion(-1)	1.32859e-18	1.32859e-18	0.0
Lead(II) monobromide ion(+1)	4.25694e-13	4.25694e-13	0.0
Lead(II) chloride	1.24567e-11	1.24567e-11	0.0
Lead(II) trichloride ion(-1)	7.72476e-13	7.72476e-13	0.0
Lead(II) tetrachloride ion(-2)	1.23081e-13	1.23081e-13	0.0
Lead(II) monochloride ion(+1)	4.87338e-11	4.87338e-11	0.0

Lead(II) carbonate ion (-2)	1.01108e-10	1.01108e-10	0.0
Lead(II) carbonate (cerussite)	8.1213e-10	8.1213e-10	0.0
Lead(II) ion(+2)	4.07649e-11	4.07649e-11	0.0
Lead(II) oxide yellow	9.26764e-14	9.26764e-14	0.0
Lead(II) monohydroxide ion(+1)	7.91626e-10	7.91626e-10	0.0
Lead(II) sulfate	1.61229e-12	1.61229e-12	0.0
Sulfur trioxide	6.68921e-32	6.68921e-32	0.0
Sulfate ion(-2)	7.62359e-4	7.62359e-4	0.0
Strontium ion(+2)	6.36048e-5	6.36048e-5	0.0
Strontium monohydroxide ion(+1)	7.78217e-11	7.78217e-11	0.0
Strontium sulfate	8.92371e-7	8.92371e-7	0.0
Zinc bromide	1.60788e-16	1.60788e-16	0.0
Zinc tribromide ion(-1)	2.63813e-19	2.63813e-19	0.0
Zinc bromide ion(+1)	4.77896e-12	4.77896e-12	0.0
Zinc chloride	5.75988e-10	5.75988e-10	0.0
Zinc trichloride ion(-1)	2.495e-11	2.495e-11	0.0
Zinc chloride ion(+1)	7.38867e-9	7.38867e-9	0.0
Zinc bicarbonate ion(+1)	4.21259e-9	4.21259e-9	0.0
Zinc ion(+2)	1.22531e-7	1.22531e-7	0.0
Zinc hydroxide, amorphous	3.10611e-10	3.10611e-10	0.0
Zinc trihydroxide ion(-1)	1.70555e-13	1.70555e-13	0.0
Zinc tetrahydroxide ion(-2)	2.29499e-18	2.29499e-18	0.0
Zinc monohydroxide ion(+1)	2.58715e-9	2.58715e-9	0.0
Barium sulfate	5.02683e-6	0.0	5.02683e-6
Vanadium	1.47228e-6	0.0	1.47228e-6
Total (by phase)	55.1118	55.1115	3.48199e-4

Element   Balance
Row   Filter   Applied: Only   Non   Zero   Values
column Filter Applied: Only Non Zero Values

	Total	Aqueous	Solid
	mol	mol	mol
H(+1)	109.712	109.712	1.99081e-5
K(+1)	0.0201742	0.0201742	0.0
Na(+1)	0.107518	0.107518	0.0
Ba(+2)	6.3859e-6	1.35907e-6	5.02683e-6
Ca(+2)	1.28486e-3	9.49797e-4	3.35064e-4

Zn(+2)	1.37636e-7	1.37636e-7	0.0
Fe(+2)	5.66727e-6	5.66727e-6	0.0
Mg(+2)	5.1977e-4	5.1977e-4	0.0
Pb(+2)	1.80985e-9	1.80985e-9	0.0
Al(+3)	6.67123e-6	3.5183e-8	6.63604e-6
Mn(+2)	9.25589e-7	9.25589e-7	0.0
O(-2)	54.8755	54.8745	1.04521e-3
Cl(-1)	0.12266	0.12266	0.0
Br(-1)	4.43689e-4	4.43689e-4	0.0
C(+4)	6.11087e-3	5.77581e-3	3.35064e-4
S(+6)	1.02414e-3	1.01911e-3	5.02683e-6
Sr(+2)	6.44973e-5	6.44973e-5	0.0
B(+3)	7.42014e-5	7.42014e-5	0.0
V(0)	1.47228e-6	0.0	1.47228e-6

(d) Mixture 4: (9/10/12 Sample + West 25%):

Calculation		Summary
Mixer	4	Calculation
Unit	Set:	Default
Automatic	Chemistry	Model
Aqueous	(H+ ion)	Databanks:
Public		
Isothermal		Calculation
25.0000	°C 1.00000	atm
Stream		Inflows

Row Filter Applied: Only Non Zero Values

Species	mol
Water	54.8633
Vanadium	1.47228e-6
Calcium carbonate (calcite)	2.11513e-3
Diboron trioxide	3.71007e-5
Barium monoxide	1.12933e-6
Barium sulfate	5.25656e-6
Iron(II) carbonate	7.01430e-7
Iron(II) oxide	5.86114e-6
Potassium chloride	0.0201742
Magnesium oxide	7.09731e-4
Disodium oxide	3.13219e-3
Sodium bromide	4.41562e-4
Sodium chloride	0.102626
Sulfur trioxide	2.18998e-3
Strontium monoxide	6.44973e-5
Lead(II) oxide yellow	1.80985e-9
Manganese(II) bromide	9.25589e-7
Carbon dioxide	4.85838e-3
Zinc bromide	1.37636e-7
Aluminum oxide	1.06819e-8
Sodium aluminum dihydroxide carbonate	6.64986e-6

159

Mixture Properties

StrAmt	54.9997	mol
Temp	25.0000	°C
Pres	1.00000	atm

Aqueous Properties

pH	7.50656	---
Ionic Strength	2.46458e-3	mol/mol
Osmotic Pressure	6.34352	atm
Elec Cond, specific	0.0141137	mho/cm
Elec Cond, molar	102.865	cm2/ohm-mol
Viscosity, absolute	0.903046	cP
Viscosity, relative	1.01384	---
Standard Liquid Volume	0.996285	L

Solid Properties

Standard Liquid Volume	4.21861e-5	L

	Unit	Total	Aqueous	Solid
Density	g/ml	1.00282	1.00276	2.72612
Enthalpy	cal	-3.76208e6	-3.76181e6	-267.820

	Total	Aqueous	Solid
	mol	mol	mol
Mole (True)	55.1232	55.1222	9.29553e-4
Mole (App)	55.0009	54.9999	9.29553e-4
	g	g	g
Mass	996.764	996.670	0.0935823
	L	L	cm3
Volume	0.993956	0.993922	0.0343281

Row Filter Applied: Values > 1.0e-4

Solids	Tendency
Calcium carbonate (calcite)	1.00000
Barium sulfate	1.00000
Aluminum hydroxide	1.00000
Sodium aluminum dihydroxide carbonate	0.676681
Strontium carbonate	0.437686
Iron(II) carbonate	0.275973
Strontium sulfate	0.0504511
Manganese(II) carbonate	0.0467749
Calcium sulfate dihydrate	6.75827e-3
Calcium sulfate	4.96195e-3
Lead(II) carbonate (cerussite)	2.64075e-3
Zinc carbonate	1.61659e-3
Sodium bicarbonate	1.21543e-3
Magnesium carbonate trihydrate	3.04058e-4
Magnesium carbonate	2.88486e-4
Sodium chloride	2.04661e-4
Potassium chloride	2.04414e-4

Species   Output   (True   Species)
Row   Filter   Applied: Only   Non   Zero   Values
column Filter Applied: Only Non Zero Values

	Total	Aqueous	Solid
	mol	mol	mol
Water	54.8603	54.8603	0.0
Hydrogen ion(+1)	3.93269e-8	3.93269e-8	0.0
Hydroxide ion(-1)	4.15032e-7	4.15032e-7	0.0
Aluminum ion(+3)	2.8488e-15	2.8488e-15	0.0
Aluminum chloride dihydroxide	3.25364e-28	3.25364e-28	0.0
Aluminum dihydroxide ion(+1)	1.79965e-11	1.79965e-11	0.0
Aluminum hydroxide	6.64567e-6	2.31857e-9	6.64335e-6
Aluminum tetrahydroxide ion(-1)	2.55373e-8	2.55373e-8	0.0
Aluminum chloride hydroxide ion(+1)	3.92601e-14	3.92601e-14	0.0

Aluminum monohydroxide ion(+2)	2.63254e-13	2.63254e-13	0.0
Aluminum disulfate ion(-1)	8.91294e-18	8.91294e-18	0.0
Aluminum monosulfate ion(+1)	2.16344e-16	2.16344e-16	0.0
Diboron oxide pentahydroxide ion(-1)	1.96539e-10	1.96539e-10	0.0
Triboron trioxide tetrahydroxide ion(-1)	1.71203e-12	1.71203e-12	0.0
Tetraboron pentaoxide tetrahydroxide ion(-2)	7.8566e-17	7.8566e-17	0.0
Barium chloride ion (+1)	5.50256e-8	5.50256e-8	0.0
Barium carbonate	4.99303e-10	4.99303e-10	0.0
Barium bicarbonate ion(+1)	1.09905e-8	1.09905e-8	0.0
Barium ion(+2)	5.81783e-7	5.81783e-7	0.0
Barium hydroxide ion(+1)	4.88221e-14	4.88221e-14	0.0
Boric acid	7.22853e-5	7.22853e-5	0.0
Boron tetrahydroxide ion(-1)	1.80037e-6	1.80037e-6	0.0
Bromide ion (-1)	4.42497e-4	4.42497e-4	0.0
Calcium chloride	3.31547e-24	3.31547e-24	0.0
Calcium monochloride ion(+1)	8.97681e-10	8.97681e-10	0.0
Calcium carbonate (calcite)	9.34332e-4	1.8632e-5	9.157e-4
Calcium dihydrogen borate ion(+1)	4.39479e-8	4.39479e-8	0.0
Calcium bicarbonate ion(+1)	2.43004e-5	2.43004e-5	0.0
Calcium ion(+2)	1.14847e-3	1.14847e-3	0.0
Calcium hydroxide ion(+1)	2.99892e-9	2.99892e-9	0.0
Calcium sulfate	7.97823e-6	7.97823e-6	0.0
Chloride ion(-1)	0.122789	0.122789	0.0
Carbon dioxide	2.57879e-4	2.57879e-4	0.0
Carbonate ion(-2)	2.04682e-5	2.04682e-5	0.0
Iron(II) chloride	7.95273e-14	7.95273e-14	0.0
Iron(II) monochloride ion(+1)	3.11102e-10	3.11102e-10	0.0
Iron(II) dicarbonate ion(-2)	9.09165e-10	9.09165e-10	0.0
Iron(II) carbonate	1.36387e-6	1.36387e-6	0.0
Iron(II) bicarbonate ion(+1)	1.36822e-9	1.36822e-9	0.0
Iron ion(+2)	5.1587e-6	5.1587e-6	0.0
Iron(II) monohydroxide ion(+1)	3.7401e-8	3.7401e-8	0.0
Iron(II) oxide	7.19253e-12	7.19253e-12	0.0
Sulfuric(VI) acid	1.81468e-27	1.81468e-27	0.0
Hydrogen bromide	1.01412e-19	1.01412e-19	0.0
Hydrogen chloride	1.67568e-15	1.67568e-15	0.0

Bicarbonate ion(-1)	5.24317e-3	5.24317e-3	0.0
Hydrogen dioxyiron ion(-1)	5.16324e-16	5.16324e-16	0.0
Hydrogen dioxylead ion(-1)	9.67791e-17	9.67791e-17	0.0
Bisulfate(VI) ion (-1)	2.02312e-9	2.02312e-9	0.0
Potassium chloride	1.13923e-5	1.13923e-5	0.0
Potassium bisulfate(VI)	4.36013e-13	4.36013e-13	0.0
Potassium ion(+1)	0.0200818	0.0200818	0.0
Potassium sulfate(VI) ion(-1)	8.09492e-5	8.09492e-5	0.0
Magnesium carbonate	1.31023e-6	1.31023e-6	0.0
Magnesium bicarbonate ion(+1)	4.67435e-5	4.67435e-5	0.0
Magnesium ion(+2)	6.53518e-4	6.53518e-4	0.0
Magnesium hydroxide ion(+1)	1.68058e-8	1.68058e-8	0.0
Magnesium sulfate	8.14161e-6	8.14161e-6	0.0
Manganese(II) bromide	1.22021e-12	1.22021e-12	0.0
Manganese(II) monobromide ion(+1)	3.79474e-9	3.79474e-9	0.0
Manganese(II) monochloride ion(+1)	1.20834e-7	1.20834e-7	0.0
Manganese ion(+2)	7.73082e-7	7.73082e-7	0.0
Manganese(II) hydroxide	1.52883e-14	1.52883e-14	0.0
Manganese(II) trihydroxide ion(-1)	1.76758e-19	1.76758e-19	0.0
Manganese(II) tetrahydroxide ion(-2)	4.64687e-25	4.64687e-25	0.0
Manganese(II) monohydroxide ion (+1)	5.79545e-10	5.79545e-10	0.0
Manganese(II) sulfate	2.72977e-8	2.72977e-8	0.0
Sodium boron hydroxide	7.13936e-8	7.13936e-8	0.0
Sodium bromide	1.18826e-6	1.18826e-6	0.0
Sodium carbonate ion(-1)	2.32659e-6	2.32659e-6	0.0
Sodium bicarbonate	4.48952e-4	4.48952e-4	0.0
Sodium ion(+1)	0.108431	0.108431	0.0
Sodium sulfate ion(-1)	4.55602e-4	4.55602e-4	0.0
Lead(II) bromide	8.93199e-17	8.93199e-17	0.0
Lead(II) tribromide ion(-1)	1.66507e-18	1.66507e-18	0.0
Lead(II) monobromide ion(+1)	5.35723e-13	5.35723e-13	0.0
Lead(II) chloride	1.56358e-11	1.56358e-11	0.0
Lead(II) trichloride ion(-1)	9.72229e-13	9.72229e-13	0.0
Lead(II) tetrachloride ion(-2)	1.55995e-13	1.55995e-13	0.0
Lead(II) monochloride ion(+1)	6.14317e-11	6.14317e-11	0.0
Lead(II) carbonate ion (-2)	8.27696e-11	8.27696e-11	0.0
Lead(II) carbonate (cerussite)	8.18388e-10	8.18388e-10	0.0

Lead(II) ion(+2)	5.18861e-11	5.18861e-11	0.0
Lead(II) oxide yellow	6.99442e-14	6.99442e-14	0.0
Lead(II) monohydroxide ion(+1)	7.73704e-10	7.73704e-10	0.0
Lead(II) sulfate	4.29652e-12	4.29652e-12	0.0
Sulfur trioxide	2.35963e-31	2.35963e-31	0.0
Sulfate ion(-2)	1.63496e-3	1.63496e-3	0.0
Strontium ion(+2)	6.2657e-5	6.2657e-5	0.0
Strontium monohydroxide ion(+1)	5.88903e-11	5.88903e-11	0.0
Strontium sulfate	1.8402e-6	1.8402e-6	0.0
Zinc bromide	1.59054e-16	1.59054e-16	0.0
Zinc tribromide ion(-1)	2.61359e-19	2.61359e-19	0.0
Zinc bromide ion(+1)	4.75416e-12	4.75416e-12	0.0
Zinc chloride	5.71513e-10	5.71513e-10	0.0
Zinc trichloride ion(-1)	2.48229e-11	2.48229e-11	0.0
Zinc chloride ion(+1)	7.36253e-9	7.36253e-9	0.0
Zinc bicarbonate ion(+1)	4.34524e-9	4.34524e-9	0.0
Zinc ion(+2)	1.23143e-7	1.23143e-7	0.0
Zinc hydroxide, amorphous	1.85292e-10	1.85292e-10	0.0
Zinc trihydroxide ion(-1)	7.91053e-14	7.91053e-14	0.0
Zinc tetrahydroxide ion(-2)	8.32591e-19	8.32591e-19	0.0
Zinc monohydroxide ion(+1)	1.99865e-9	1.99865e-9	0.0
Barium sulfate	5.7376e-6	0.0	5.7376e-6
Vanadium	1.47228e-6	0.0	1.47228e-6
Total (by phase)	55.1232	55.1222	9.29553e-4

Element   Balance
Row   Filter   Applied: Only   Non   Zero   Values
column Filter Applied: Only Non Zero Values

	Total	Aqueous	Solid
	mol	mol	mol
H(+1)	109.727	109.727	1.99301e-5
K(+1)	0.0201742	0.0201742	0.0
Na(+1)	0.109339	0.109339	0.0
Ba(+2)	6.3859e-6	6.48298e-7	5.7376e-6
Ca(+2)	2.11513e-3	1.19943e-3	9.157e-4
Zn(+2)	1.37636e-7	1.37636e-7	0.0
Fe(+2)	6.56257e-6	6.56257e-6	0.0

Mg(+2)	7.09731e-4	7.09731e-4	0.0
Pb(+2)	1.80985e-9	1.80985e-9	0.0
Al(+3)	6.67123e-6	2.78742e-8	6.64335e-6
Mn(+2)	9.25589e-7	9.25589e-7	0.0
O(-2)	54.89	54.8872	2.78998e-3
Cl(-1)	0.122801	0.122801	0.0
Br(-1)	4.43689e-4	4.43689e-4	0.0
C(+4)	6.98086e-3	6.06516e-3	9.157e-4
S(+6)	2.19524e-3	2.1895e-3	5.7376e-6
Sr(+2)	6.44973e-5	6.44973e-5	0.0
B(+3)	7.42014e-5	7.42014e-5	0.0
V(0)	1.47228e-6	0.0	1.47228e-6

(e) Mixture 5: (9/10/12 Sample 87.5% + East 12.5%):

Calculation		Summary
Mixer	5	Calculation
Unit	Set:	Default
Automatic	Chemistry	Model
Aqueous	(H+ ion)	Databanks:
Public		
Isothermal		Calculation
25.0000	°C	1.00000 atm
Stream		Inflows

Row Filter Applied: Only Non Zero Values

Species	mol
Water	55.0058
Vanadium	1.71766e-6
Calcium carbonate (calcite)	1.35230e-3
Diboron trioxide	4.32841e-5
Barium monoxide	1.31755e-6
Barium sulfate	6.13266e-6
Iron(II) carbonate	6.16872e-7
Iron(II) oxide	4.20434e-6
Potassium chloride	0.0235365
Magnesium oxide	5.66406e-4
Disodium oxide	2.61595e-3
Sodium bromide	5.15156e-4
Sodium chloride	0.119472
Sulfur trioxide	1.10195e-3
Strontium monoxide	7.52468e-5
Lead(II) oxide yellow	2.11149e-9
Manganese(II) bromide	1.07985e-6
Carbon dioxide	5.54203e-3
Zinc bromide	1.60575e-7
Aluminum oxide	1.24622e-8
Sodium aluminum dihydroxide carbonate	7.75817e-6

Row column	Filter Filter	Applied: Applied:	Only Only	Non Non	Zero Zero	Values Values

Mixture Properties

StrAmt	55.1606	mol
Temp	25.0000	°C
Pres	1.00000	atm

Aqueous Properties

pH	7.55721	---
Ionic Strength	2.77682e-3	mol/mol
Osmotic Pressure	7.18501	atm
Elec Cond, specific	0.0160089	mho/cm
Elec Cond, molar	103.065	cm2/ohm-mol
Viscosity, absolute	0.904062	cP
Viscosity, relative	1.01498	---
Standard Liquid Volume	0.999589	L

Solid Properties

Standard Liquid Volume	1.49896e-5	L

	Unit	Total	Aqueous	Solid
Density	g/ml	1.00352	1.00350	2.75604
Enthalpy	cal	-3.77336e6	-3.77326e6	-97.9615

Total   and   Phase   Flows   (Amounts)
column Filter Applied: Only Non Zero Values

	Total	Aqueous	Solid
	mol	mol	mol
Mole (True)	55.3036	55.3033	3.39921e-4
Mole (App)	55.1616	55.1613	3.39921e-4
	g	g	g
Mass	1000.40	1000.37	0.0345677
	L	L	cm3
Volume	0.996896	0.996883	0.0125425

Row Filter Applied: Values > 1.0e-4

Solids	Tendency
Calcium carbonate (calcite)	1.00000
Barium sulfate	1.00000
Aluminum hydroxide	1.00000
Sodium aluminum dihydroxide carbonate	0.817508
Strontium carbonate	0.598959
Iron(II) carbonate	0.228259
Manganese(II) carbonate	0.0623932
Strontium sulfate	0.0271992
Lead(II) carbonate (cerussite)	3.12812e-3
Calcium sulfate dihydrate	2.65919e-3
Zinc carbonate	2.12665e-3
Calcium sulfate	1.95481e-3
Sodium bicarbonate	1.46746e-3
Magnesium carbonate trihydrate	2.83970e-4
Potassium chloride	2.70760e-4
Magnesium carbonate	2.69927e-4
Sodium chloride	2.66630e-4
Barium carbonate	1.30239e-4

Species   Output   (True   Species)
Row   Filter   Applied: Only   Non   Zero   Values
column Filter Applied: Only Non Zero Values

	Total	Aqueous	Solid
	mol	mol	mol
Water	55.0025	55.0025	0.0
Hydrogen ion(+1)	3.52248e-8	3.52248e-8	0.0
Hydroxide ion(-1)	4.70445e-7	4.70445e-7	0.0
Aluminum ion(+3)	2.11301e-15	2.11301e-15	0.0
Aluminum chloride dihydroxide	3.32656e-28	3.32656e-28	0.0
Aluminum dihydroxide ion(+1)	1.62178e-11	1.62178e-11	0.0
Aluminum hydroxide	7.754e-6	2.31662e-9	7.75169e-6
Aluminum tetrahydroxide ion(-1)	2.90787e-8	2.90787e-8	0.0
Aluminum chloride hydroxide	3.63768e-14	3.63768e-14	0.0

ion(+1)			
Aluminum monohydroxide ion(+2)	2.14798e-13	2.14798e-13	0.0
Aluminum disulfate ion(-1)	1.42113e-18	1.42113e-18	0.0
Aluminum monosulfate ion(+1)	7.32601e-17	7.32601e-17	0.0
Diboron oxide pentahydroxide ion(-1)	3.03999e-10	3.03999e-10	0.0
Triboron trioxide tetrahydroxide ion(-1)	3.08483e-12	3.08483e-12	0.0
Tetraboron pentaoxide tetrahydroxide ion(-2)	1.93211e-16	1.93211e-16	0.0
Barium chloride ion (+1)	1.34652e-7	1.34652e-7	0.0
Barium carbonate	1.26633e-9	1.26633e-9	0.0
Barium bicarbonate ion(+1)	2.52429e-8	2.52429e-8	0.0
Barium ion(+2)	1.27627e-6	1.27627e-6	0.0
Barium hydroxide ion(+1)	1.1768e-13	1.1768e-13	0.0
Boric acid	8.4032e-5	8.4032e-5	0.0
Boron tetrahydroxide ion(-1)	2.38117e-6	2.38117e-6	0.0
Bromide ion (-1)	5.16081e-4	5.16081e-4	0.0
Calcium chloride	3.65541e-24	3.65541e-24	0.0
Calcium monochloride ion(+1)	8.38324e-10	8.38324e-10	0.0
Calcium carbonate (calcite)	3.43055e-4	1.86164e-5	3.24439e-4
Calcium dihydrogen borate ion(+1)	4.88227e-8	4.88227e-8	0.0
Calcium bicarbonate ion(+1)	2.17886e-5	2.17886e-5	0.0
Calcium ion(+2)	9.8426e-4	9.8426e-4	0.0
Calcium hydroxide ion(+1)	2.84772e-9	2.84772e-9	0.0
Calcium sulfate	3.14046e-6	3.14046e-6	0.0
Chloride ion(-1)	0.142993	0.142993	0.0
Carbon dioxide	2.44348e-4	2.44348e-4	0.0
Carbonate ion(-2)	2.59025e-5	2.59025e-5	0.0
Iron(II) chloride	7.25217e-14	7.25217e-14	0.0
Iron(II) monochloride ion(+1)	2.49964e-10	2.49964e-10	0.0
Iron(II) dicarbonate ion(-2)	9.49545e-10	9.49545e-10	0.0
Iron(II) carbonate	1.12712e-6	1.12712e-6	0.0
Iron(II) bicarbonate ion(+1)	1.01882e-9	1.01882e-9	0.0
Iron ion(+2)	3.66249e-6	3.66249e-6	0.0
Iron(II) monohydroxide ion(+1)	2.93778e-8	2.93778e-8	0.0
Iron(II) oxide	6.26788e-12	6.26788e-12	0.0
Sulfuric(VI) acid	6.76981e-28	6.76981e-28	0.0
Hydrogen bromide	1.03873e-19	1.03873e-19	0.0

Hydrogen chloride	1.71218e-15	1.71218e-15	0.0
Bicarbonate ion(-1)	5.68103e-3	5.68103e-3	0.0
Hydrogen dioxyiron ion(-1)	5.14235e-16	5.14235e-16	0.0
Hydrogen dioxylead ion(-1)	1.37494e-16	1.37494e-16	0.0
Bisulfate(VI) ion (-1)	8.59422e-10	8.59422e-10	0.0
Potassium chloride	1.50772e-5	1.50772e-5	0.0
Potassium bisulfate(VI)	2.10681e-13	2.10681e-13	0.0
Potassium ion(+1)	0.0234767	0.0234767	0.0
Potassium sulfate(VI) ion(-1)	4.46911e-5	4.46911e-5	0.0
Magnesium carbonate	1.22492e-6	1.22492e-6	0.0
Magnesium bicarbonate ion(+1)	3.93857e-5	3.93857e-5	0.0
Magnesium ion(+2)	5.22782e-4	5.22782e-4	0.0
Magnesium hydroxide ion(+1)	1.49332e-8	1.49332e-8	0.0
Magnesium sulfate	2.9986e-6	2.9986e-6	0.0
Manganese(II) bromide	1.80326e-12	1.80326e-12	0.0
Manganese(II) monobromide ion(+1)	4.9545e-9	4.9545e-9	0.0
Manganese(II) monochloride ion(+1)	1.56576e-7	1.56576e-7	0.0
Manganese ion(+2)	9.03254e-7	9.03254e-7	0.0
Manganese(II) hydroxide	2.1473e-14	2.1473e-14	0.0
Manganese(II) trihydroxide ion(-1)	2.83735e-19	2.83735e-19	0.0
Manganese(II) tetrahydroxide ion(-2)	8.73924e-25	8.73924e-25	0.0
Manganese(II) monohydroxide ion (+1)	7.34082e-10	7.34082e-10	0.0
Manganese(II) sulfate	1.4333e-8	1.4333e-8	0.0
Sodium boron hydroxide	1.05666e-7	1.05666e-7	0.0
Sodium bromide	1.55051e-6	1.55051e-6	0.0
Sodium carbonate ion(-1)	3.21132e-6	3.21132e-6	0.0
Sodium bicarbonate	5.41595e-4	5.41595e-4	0.0
Sodium ion(+1)	0.124436	0.124436	0.0
Sodium sulfate ion(-1)	2.44866e-4	2.44866e-4	0.0
Lead(II) bromide	1.17221e-16	1.17221e-16	0.0
Lead(II) tribromide ion(-1)	2.56174e-18	2.56174e-18	0.0
Lead(II) monobromide ion(+1)	6.2114e-13	6.2114e-13	0.0
Lead(II) chloride	2.04205e-11	2.04205e-11	0.0
Lead(II) trichloride ion(-1)	1.47902e-12	1.47902e-12	0.0
Lead(II) tetrachloride ion(-2)	2.7865e-13	2.7865e-13	0.0
Lead(II) monochloride ion(+1)	7.06907e-11	7.06907e-11	0.0
Lead(II) carbonate ion (-2)	1.24471e-10	1.24471e-10	0.0

Lead(II) carbonate (cerussite)	9.68613e-10	9.68613e-10	0.0
Lead(II) ion(+2)	5.28524e-11	5.28524e-11	0.0
Lead(II) oxide yellow	8.72942e-14	8.72942e-14	0.0
Lead(II) monohydroxide ion(+1)	8.69971e-10	8.69971e-10	0.0
Lead(II) sulfate	2.00224e-12	2.00224e-12	0.0
Sulfur trioxide	8.80822e-32	8.80822e-32	0.0
Sulfate ion(-2)	8.05365e-4	8.05365e-4	0.0
Strontium ion(+2)	7.42555e-5	7.42555e-5	0.0
Strontium monohydroxide ion(+1)	7.69009e-11	7.69009e-11	0.0
Strontium sulfate	9.91257e-7	9.91257e-7	0.0
Zinc bromide	2.31816e-16	2.31816e-16	0.0
Zinc tribromide ion(-1)	4.46561e-19	4.46561e-19	0.0
Zinc bromide ion(+1)	6.12161e-12	6.12161e-12	0.0
Zinc chloride	8.28924e-10	8.28924e-10	0.0
Zinc trichloride ion(-1)	4.19372e-11	4.19372e-11	0.0
Zinc chloride ion(+1)	9.40889e-9	9.40889e-9	0.0
Zinc bicarbonate ion(+1)	5.17279e-9	5.17279e-9	0.0
Zinc ion(+2)	1.42351e-7	1.42351e-7	0.0
Zinc hydroxide, amorphous	2.56663e-10	2.56663e-10	0.0
Zinc trihydroxide ion(-1)	1.24624e-13	1.24624e-13	0.0
Zinc tetrahydroxide ion(-2)	1.53418e-18	1.53418e-18	0.0
Zinc monohydroxide ion(+1)	2.50889e-9	2.50889e-9	0.0
Barium sulfate	6.01278e-6	0.0	6.01278e-6
Vanadium	1.71766e-6	0.0	1.71766e-6
Total (by phase)	55.3036	55.3033	3.39921e-4

Element Balance
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

	Total	Aqueous	Solid
	mol	mol	mol
H(+1)	110.012	110.012	2.32551e-5
K(+1)	0.0235365	0.0235365	0.0
Na(+1)	0.125227	0.125227	0.0
Ba(+2)	7.45021e-6	1.43743e-6	6.01278e-6
Ca(+2)	1.3523e-3	1.02786e-3	3.24439e-4
Zn(+2)	1.60575e-7	1.60575e-7	0.0

Fe(+2)	4.82121e-6	4.82121e-6	0.0
Mg(+2)	5.66406e-4	5.66406e-4	0.0
Pb(+2)	2.11149e-9	2.11149e-9	0.0
Al(+3)	7.7831e-6	3.14118e-8	7.75169e-6
Mn(+2)	1.07985e-6	1.07985e-6	0.0
O(-2)	55.0277	55.0266	1.02062e-3
Cl(-1)	0.143009	0.143009	0.0
Br(-1)	5.17637e-4	5.17637e-4	0.0
C(+4)	6.90271e-3	6.57827e-3	3.24439e-4
S(+6)	1.10808e-3	1.10207e-3	6.01278e-6
Sr(+2)	7.52468e-5	7.52468e-5	0.0
B(+3)	8.65683e-5	8.65683e-5	0.0
V(0)	1.71766e-6	0.0	1.71766e-6

(f) Mixture 6: (9/10/12 87.5% + West 12.5%):

Calculation		Summary
Mixer	6	Calculation
Unit	Set:	Default
Automatic	Chemistry	Model
Aqueous	(H+ ion)	Databanks:
Public		
Isothermal		Calculation
25.0000	°C	1.00000	atm
Stream		Inflows

Row Filter Applied: Only Non Zero Values

Species	mol
Water	55.0094
Vanadium	1.71766e-6
Calcium carbonate (calcite)	1.76743e-3
Diboron trioxide	4.32841e-5
Barium monoxide	1.31755e-6
Barium sulfate	6.13266e-6
Iron(II) carbonate	3.50715e-7
Iron(II) oxide	4.91814e-6
Potassium chloride	0.0235365
Magnesium oxide	6.61387e-4
Disodium oxide	3.03595e-3
Sodium bromide	5.15156e-4
Sodium chloride	0.119543
Sulfur trioxide	1.68750e-3
Strontium monoxide	7.52468e-5
Lead(II) oxide yellow	2.11149e-9
Manganese(II) bromide	1.07985e-6
Carbon dioxide	5.56216e-3
Zinc bromide	1.60575e-7
Aluminum oxide	1.24622e-8
Sodium aluminum dihydroxide carbonate	7.75817e-6

173

Row	Filter	Applied:	Only	Non	Zero	Values
column	Filter	Applied:	Only	Non	Zero	Values

Mixture Properties

StrAmt	55.1659	mol
Temp	25.0000	°C
Pres	1.00000	atm

Aqueous Properties

pH	7.50482	---
Ionic Strength	2.80886e-3	mol/mol
Osmotic Pressure	7.24963	atm
Elec Cond, specific	0.0160946	mho/cm
Elec Cond, molar	102.560	cm2/ohm-mol
Viscosity, absolute	0.904368	cP
Viscosity, relative	1.01532	---
Standard Liquid Volume	0.999694	L

Solid Properties

Standard Liquid Volume	2.84908e-5	L

	Unit	Total	Aqueous	Solid
Density	g/ml	1.00362	1.00358	2.73669
Enthalpy	cal	-3.77393e6	-3.77374e6	-182.628

Total	and	Phase	Flows	(Amounts)

column Filter Applied: Only Non Zero Values

	Total	Aqueous	Solid
	mol	mol	mol
Mole (True)	55.3093	55.3086	6.33765e-4
Mole (App)	55.1670	55.1664	6.33765e-4
	g	g	g
Mass	1000.59	1000.53	0.0640428
	L	L	cm3
Volume	0.996984	0.996960	0.0234016

Row Filter Applied: Values > 1.0e-4

Solids	Tendency
Calcium carbonate (calcite)	1.00000
Barium sulfate	1.00000
Aluminum hydroxide	1.00000
Sodium aluminum dihydroxide carbonate	0.833364
Strontium carbonate	0.532039
Iron(II) carbonate	0.228902
Manganese(II) carbonate	0.0554616
Strontium sulfate	0.0408936
Calcium sulfate dihydrate	4.50050e-3
Calcium sulfate	3.30869e-3
Lead(II) carbonate (cerussite)	3.13536e-3
Zinc carbonate	1.90638e-3
Sodium bicarbonate	1.49586e-3
Magnesium carbonate trihydrate	2.95674e-4
Magnesium carbonate	2.81092e-4
Potassium chloride	2.70060e-4
Sodium chloride	2.67901e-4

Species   Output   (True   Species)
Row   Filter   Applied: Only   Non   Zero   Values
column Filter Applied: Only Non Zero Values

	Total	Aqueous	Solid
	mol	mol	mol
Water	55.0061	55.0061	0.0
Hydrogen ion(+1)	3.98019e-8	3.98019e-8	0.0
Hydroxide ion(-1)	4.17443e-7	4.17443e-7	0.0
Aluminum ion(+3)	3.06866e-15	3.06866e-15	0.0
Aluminum chloride dihydroxide	3.75189e-28	3.75189e-28	0.0
Aluminum dihydroxide ion(+1)	1.83223e-11	1.83223e-11	0.0
Aluminum hydroxide	7.75727e-6	2.31627e-9	7.75495e-6
Aluminum tetrahydroxide ion(-1)	2.58092e-8	2.58092e-8	0.0
Aluminum chloride hydroxide ion(+1)	4.63637e-14	4.63637e-14	0.0

Aluminum monohydroxide ion(+2)	2.74766e-13	2.74766e-13	0.0
Aluminum disulfate ion(-1)	4.73327e-18	4.73327e-18	0.0
Aluminum monosulfate ion(+1)	1.60314e-16	1.60314e-16	0.0
Diboron oxide pentahydroxide ion(-1)	2.7168e-10	2.7168e-10	0.0
Triboron trioxide tetrahydroxide ion(-1)	2.76651e-12	2.76651e-12	0.0
Tetraboron pentaoxide tetrahydroxide ion(-2)	1.5475e-16	1.5475e-16	0.0
Barium chloride ion (+1)	8.86066e-8	8.86066e-8	0.0
Barium carbonate	7.48049e-10	7.48049e-10	0.0
Barium bicarbonate ion(+1)	1.68496e-8	1.68496e-8	0.0
Barium ion(+2)	8.42927e-7	8.42927e-7	0.0
Barium hydroxide ion(+1)	6.86326e-14	6.86326e-14	0.0
Boric acid	8.43049e-5	8.43049e-5	0.0
Boron tetrahydroxide ion(-1)	2.12001e-6	2.12001e-6	0.0
Bromide ion (-1)	5.16075e-4	5.16075e-4	0.0
Calcium chloride	4.06363e-24	4.06363e-24	0.0
Calcium monochloride ion(+1)	9.32107e-10	9.32107e-10	0.0
Calcium carbonate (calcite)	6.36405e-4	1.86136e-5	6.17791e-4
Calcium dihydrogen borate ion(+1)	4.83674e-8	4.83674e-8	0.0
Calcium bicarbonate ion(+1)	2.46122e-5	2.46122e-5	0.0
Calcium ion(+2)	1.10105e-3	1.10105e-3	0.0
Calcium hydroxide ion(+1)	2.81113e-9	2.81113e-9	0.0
Calcium sulfate	5.31471e-6	5.31471e-6	0.0
Chloride ion(-1)	0.143064	0.143064	0.0
Carbon dioxide	2.79589e-4	2.79589e-4	0.0
Carbonate ion(-2)	2.34301e-5	2.34301e-5	0.0
Iron(II) chloride	8.08476e-14	8.08476e-14	0.0
Iron(II) monochloride ion(+1)	2.79182e-10	2.79182e-10	0.0
Iron(II) dicarbonate ion(-2)	8.60705e-10	8.60705e-10	0.0
Iron(II) carbonate	1.13012e-6	1.13012e-6	0.0
Iron(II) bicarbonate ion(+1)	1.15442e-9	1.15442e-9	0.0
Iron ion(+2)	4.10735e-6	4.10735e-6	0.0
Iron(II) monohydroxide ion(+1)	2.90825e-8	2.90825e-8	0.0
Iron(II) oxide	5.4916e-12	5.4916e-12	0.0
Sulfuric(VI) acid	1.31105e-27	1.31105e-27	0.0
Hydrogen bromide	1.1707e-19	1.1707e-19	0.0
Hydrogen chloride	1.931e-15	1.931e-15	0.0

Bicarbonate ion(-1)	5.77001e-3	5.77001e-3	0.0
Hydrogen dioxyiron ion(-1)	3.99966e-16	3.99966e-16	0.0
Hydrogen dioxylead ion(-1)	1.06872e-16	1.06872e-16	0.0
Bisulfate(VI) ion (-1)	1.47687e-9	1.47687e-9	0.0
Potassium chloride	1.5036e-5	1.5036e-5	0.0
Potassium bisulfate(VI)	3.60783e-13	3.60783e-13	0.0
Potassium ion(+1)	0.0234535	0.0234535	0.0
Potassium sulfate(VI) ion(-1)	6.79447e-5	6.79447e-5	0.0
Magnesium carbonate	1.27539e-6	1.27539e-6	0.0
Magnesium bicarbonate ion(+1)	4.63342e-5	4.63342e-5	0.0
Magnesium ion(+2)	6.08477e-4	6.08477e-4	0.0
Magnesium hydroxide ion(+1)	1.53514e-8	1.53514e-8	0.0
Magnesium sulfate	5.28454e-6	5.28454e-6	0.0
Manganese(II) bromide	1.77952e-12	1.77952e-12	0.0
Manganese(II) monobromide ion(+1)	4.90138e-9	4.90138e-9	0.0
Manganese(II) monochloride ion(+1)	1.55014e-7	1.55014e-7	0.0
Manganese ion(+2)	8.97731e-7	8.97731e-7	0.0
Manganese(II) hydroxide	1.66757e-14	1.66757e-14	0.0
Manganese(II) trihydroxide ion(-1)	1.95609e-19	1.95609e-19	0.0
Manganese(II) tetrahydroxide ion(-2)	5.36204e-25	5.36204e-25	0.0
Manganese(II) monohydroxide ion (+1)	6.44144e-10	6.44144e-10	0.0
Manganese(II) sulfate	2.15615e-8	2.15615e-8	0.0
Sodium boron hydroxide	9.44255e-8	9.44255e-8	0.0
Sodium bromide	1.55661e-6	1.55661e-6	0.0
Sodium carbonate ion(-1)	2.90477e-6	2.90477e-6	0.0
Sodium bicarbonate	5.51989e-4	5.51989e-4	0.0
Sodium ion(+1)	0.125206	0.125206	0.0
Sodium sulfate ion(-1)	3.75094e-4	3.75094e-4	0.0
Lead(II) bromide	1.30437e-16	1.30437e-16	0.0
Lead(II) tribromide ion(-1)	2.8526e-18	2.8526e-18	0.0
Lead(II) monobromide ion(+1)	6.9288e-13	6.9288e-13	0.0
Lead(II) chloride	2.27535e-11	2.27535e-11	0.0
Lead(II) trichloride ion(-1)	1.65004e-12	1.65004e-12	0.0
Lead(II) tetrachloride ion(-2)	3.11828e-13	3.11828e-13	0.0
Lead(II) monochloride ion(+1)	7.89145e-11	7.89145e-11	0.0
Lead(II) carbonate ion (-2)	1.1279e-10	1.1279e-10	0.0
Lead(II) carbonate (cerussite)	9.70709e-10	9.70709e-10	0.0

Lead(II) ion(+2)	5.92577e-11	5.92577e-11	0.0
Lead(II) oxide yellow	7.64447e-14	7.64447e-14	0.0
Lead(II) monohydroxide ion(+1)	8.60933e-10	8.60933e-10	0.0
Lead(II) sulfate	3.39753e-12	3.39753e-12	0.0
Sulfur trioxide	1.7059e-31	1.7059e-31	0.0
Sulfate ion(-2)	1.23198e-3	1.23198e-3	0.0
Strontium ion(+2)	7.37566e-5	7.37566e-5	0.0
Strontium monohydroxide ion(+1)	6.7439e-11	6.7439e-11	0.0
Strontium sulfate	1.49011e-6	1.49011e-6	0.0
Zinc bromide	2.307e-16	2.307e-16	0.0
Zinc tribromide ion(-1)	4.44728e-19	4.44728e-19	0.0
Zinc bromide ion(+1)	6.10721e-12	6.10721e-12	0.0
Zinc chloride	8.2605e-10	8.2605e-10	0.0
Zinc trichloride ion(-1)	4.18437e-11	4.18437e-11	0.0
Zinc chloride ion(+1)	9.39381e-9	9.39381e-9	0.0
Zinc bicarbonate ion(+1)	5.23904e-9	5.23904e-9	0.0
Zinc ion(+2)	1.42647e-7	1.42647e-7	0.0
Zinc hydroxide, amorphous	2.01008e-10	2.01008e-10	0.0
Zinc trihydroxide ion(-1)	8.66327e-14	8.66327e-14	0.0
Zinc tetrahydroxide ion(-2)	9.49139e-19	9.49139e-19	0.0
Zinc monohydroxide ion(+1)	2.2204e-9	2.2204e-9	0.0
Barium sulfate	6.50108e-6	0.0	6.50108e-6
Vanadium	1.71766e-6	0.0	1.71766e-6
Total (by phase)	55.3093	55.3086	6.33765e-4

Element _____ Balance
Row   Filter   Applied: Only   Non   Zero   Values
column Filter Applied: Only Non Zero Values

	Total	Aqueous	Solid
	mol	mol	mol
H(+1)	110.019	110.019	2.32649e-5
K(+1)	0.0235365	0.0235365	0.0
Na(+1)	0.126138	0.126138	0.0
Ba(+2)	7.45021e-6	9.49131e-7	6.50108e-6
Ca(+2)	1.76743e-3	1.14964e-3	6.17791e-4
Zn(+2)	1.60575e-7	1.60575e-7	0.0
Fe(+2)	5.26886e-6	5.26886e-6	0.0

Mg(+2)	6.61387e-4	6.61387e-4	0.0
Pb(+2)	2.11149e-9	2.11149e-9	0.0
Al(+3)	7.7831e-6	2.81442e-8	7.75495e-6
Mn(+2)	1.07985e-6	1.07985e-6	0.0
O(-2)	55.0349	55.033	1.90264e-3
Cl(-1)	0.143079	0.143079	0.0
Br(-1)	5.17637e-4	5.17637e-4	0.0
C(+4)	7.3377e-3	6.71991e-3	6.17791e-4
S(+6)	1.69363e-3	1.68713e-3	6.50108e-6
Sr(+2)	7.52468e-5	7.52468e-5	0.0
B(+3)	8.65683e-5	8.65683e-5	0.0
V(0)	1.71766e-6	0.0	1.71766e-6

(g) Mixture 7: (10/25/12 Sample 12.5% + East 87.5%):

Calculation		Summary
Mixer	7	Calculation
Unit	Set:	Default
Automatic	Chemistry	Model
Aqueous	(H+ ion)	Databanks:
Public		
Isothermal		Calculation
25.0000	°C 1.00000	atm
Stream		Inflows

Row Filter Applied: Only Non Zero Values

Species	mol
Water	54.1023
Vanadium	2.45379e-7
Calcium carbonate (calcite)	1.55777e-3
Diboron trioxide	2.40996e-5
Barium monoxide	2.22853e-7
Barium sulfate	1.02442e-6
Iron(II) carbonate	4.31811e-6
Iron(II) oxide	6.03608e-6
Potassium chloride	7.87758e-4
Magnesium oxide	3.85847e-4
Disodium oxide	3.93676e-4
Sodium bromide	1.10603e-4
Sodium chloride	0.0262319
Sulfur trioxide	6.10862e-4
Strontium monoxide	2.04163e-5
Lead(II) oxide yellow	4.22297e-10
Manganese(II) bromide	5.04660e-7
Carbon dioxide	9.33828e-4
Zinc bromide	3.44089e-8
Aluminum oxide	1.40993e-9
Sodium aluminum dihydroxide carbonate	3.02945e-7

Mixture Properties

StrAmt	54.1334	mol
Temp	25.0000	°C
Pres	1.00000	atm

Aqueous Properties

pH	8.17166	---
Ionic Strength	5.76236e-4	mol/mol
Osmotic Pressure	1.48585	atm
Elec Cond, specific	3.39627e-3	mho/cm
Elec Cond, molar	106.932	cm2/ohm-mol
Viscosity, absolute	0.894543	cP
Viscosity, relative	1.00429	---
Standard Liquid Volume	0.978581	L

Solid Properties

Standard Liquid Volume	4.54265e-5	L

	Unit	Total	Aqueous	Solid
Density	g/ml	0.998261	0.998197	2.71176
Enthalpy	cal	-3.69933e6	-3.69905e6	-284.808

Total	and	Phase	Flows	(Amounts)

column Filter Applied: Only Non Zero Values

	Total	Aqueous	Solid
	mol	mol	mol
Mole (True)	54.1605	54.1595	9.88948e-4
Mole (App)	54.1339	54.1329	9.88948e-4
	g	g	g
Mass	976.565	976.466	0.0990319
	L	L	cm3
Volume	0.978266	0.978230	0.0365194

Scaling				Tendencies

Row Filter Applied: Values > 1.0e-4

Solids	Tendency
Calcium carbonate (calcite)	1.00000
Barium sulfate	1.00000
Aluminum hydroxide	1.00000
Iron(II) carbonate	0.731970
Strontium carbonate	0.310108
Manganese(II) carbonate	0.0658009
Sodium aluminum dihydroxide carbonate	0.0589175
Strontium sulfate	0.0133502
Iron(II) hydroxide	3.27745e-3
Calcium sulfate dihydrate	2.54219e-3
Calcium sulfate	1.85318e-3
Zinc carbonate	8.99718e-4
Magnesium carbonate trihydrate	3.60362e-4
Lead(II) carbonate (cerussite)	3.54980e-4
Magnesium carbonate	3.38255e-4
Zinc hydroxide, amorphous	1.98328e-4
Barium carbonate	1.37382e-4
Sodium bicarbonate	1.06204e-4
Magnesium hydroxide	1.02007e-4

Species Output (True Species)
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

	Total	Aqueous	Solid
	mol	mol	mol
Water	54.1015	54.1015	0.0
Hydrogen ion(+1)	7.7029e-9	7.7029e-9	0.0
Hydroxide ion(-1)	1.72733e-6	1.72733e-6	0.0
Aluminum ion(+3)	1.23722e-17	1.23722e-17	0.0
Aluminum chloride dihydroxide	1.75576e-29	1.75576e-29	0.0
Aluminum dihydroxide ion(+1)	3.42108e-12	3.42108e-12	0.0
Aluminum hydroxide	2.02252e-7	2.3299e-9	1.99922e-7
Aluminum tetrahydroxide ion(-1)	1.03509e-7	1.03509e-7	0.0
Aluminum chloride hydroxide ion(+1)	3.89531e-16	3.89531e-16	0.0

Aluminum monohydroxide ion(+2)	8.18657e-15	8.18657e-15	0.0
Aluminum disulfate ion(-1)	2.19682e-20	2.19682e-20	0.0
Aluminum monosulfate ion(+1)	9.92207e-19	9.92207e-19	0.0
Diboron oxide pentahydroxide ion(-1)	2.81244e-10	2.81244e-10	0.0
Triboron trioxide tetrahydroxide ion(-1)	1.46107e-12	1.46107e-12	0.0
Tetraboron pentaoxide tetrahydroxide ion(-2)	1.22045e-16	1.22045e-16	0.0
Barium chloride ion (+1)	2.35238e-8	2.35238e-8	0.0
Barium carbonate	1.34344e-9	1.34344e-9	0.0
Barium bicarbonate ion(+1)	5.46262e-9	5.46262e-9	0.0
Barium ion(+2)	7.12703e-7	7.12703e-7	0.0
Barium hydroxide ion(+1)	3.74475e-13	3.74475e-13	0.0
Boric acid	4.36318e-5	4.36318e-5	0.0
Boron tetrahydroxide ion(-1)	4.43719e-6	4.43719e-6	0.0
Bromide ion (-1)	1.11584e-4	1.11584e-4	0.0
Calcium chloride	1.44622e-25	1.44622e-25	0.0
Calcium monochloride ion(+1)	1.72167e-10	1.72167e-10	0.0
Calcium carbonate (calcite)	1.00672e-3	1.87231e-5	9.87998e-4
Calcium dihydrogen borate ion(+1)	7.31557e-8	7.31557e-8	0.0
Calcium bicarbonate ion(+1)	4.74995e-6	4.74995e-6	0.0
Calcium ion(+2)	5.43218e-4	5.43218e-4	0.0
Calcium hydroxide ion(+1)	8.59063e-9	8.59063e-9	0.0
Calcium sulfate	2.99426e-6	2.99426e-6	0.0
Chloride ion(-1)	0.0270195	0.0270195	0.0
Carbon dioxide	1.72769e-5	1.72769e-5	0.0
Carbonate ion(-2)	1.67435e-5	1.67435e-5	0.0
Iron(II) chloride	9.20093e-15	9.20093e-15	0.0
Iron(II) monochloride ion(+1)	1.26725e-10	1.26725e-10	0.0
Iron(II) dicarbonate ion(-2)	2.01086e-9	2.01086e-9	0.0
Iron(II) carbonate	3.63512e-6	3.63512e-6	0.0
Iron(II) bicarbonate ion(+1)	6.9195e-10	6.9195e-10	0.0
Iron ion(+2)	6.4321e-6	6.4321e-6	0.0
Iron(II) monohydroxide ion(+1)	2.83851e-7	2.83851e-7	0.0
Iron(II) oxide	2.87534e-10	2.87534e-10	0.0
Sulfuric(VI) acid	4.55697e-29	4.55697e-29	0.0
Hydrogen bromide	6.27754e-21	6.27754e-21	0.0
Hydrogen chloride	9.07487e-17	9.07487e-17	0.0

Bicarbonate ion(-1)	1.39484e-3	1.39484e-3	0.0
Hydrogen dioxyiron ion(-1)	8.17578e-14	8.17578e-14	0.0
Hydrogen dioxylead ion(-1)	7.95141e-16	7.95141e-16	0.0
Bisulfate(VI) ion (-1)	2.06803e-10	2.06803e-10	0.0
Potassium chloride	1.28102e-7	1.28102e-7	0.0
Potassium bisulfate(VI)	2.27337e-15	2.27337e-15	0.0
Potassium ion(+1)	7.85954e-4	7.85954e-4	0.0
Potassium sulfate(VI) ion(-1)	1.67578e-6	1.67578e-6	0.0
Magnesium carbonate	1.54379e-6	1.54379e-6	0.0
Magnesium bicarbonate ion(+1)	1.04665e-5	1.04665e-5	0.0
Magnesium ion(+2)	3.70197e-4	3.70197e-4	0.0
Magnesium hydroxide ion(+1)	5.63844e-8	5.63844e-8	0.0
Magnesium sulfate	3.58273e-6	3.58273e-6	0.0
Manganese(II) bromide	9.78225e-14	9.78225e-14	0.0
Manganese(II) monobromide ion(+1)	9.11379e-10	9.11379e-10	0.0
Manganese(II) monochloride ion(+1)	2.61059e-8	2.61059e-8	0.0
Manganese ion(+2)	4.60895e-7	4.60895e-7	0.0
Manganese(II) hydroxide	3.25321e-13	3.25321e-13	0.0
Manganese(II) trihydroxide ion(-1)	1.48982e-17	1.48982e-17	0.0
Manganese(II) tetrahydroxide ion(-2)	1.19539e-22	1.19539e-22	0.0
Manganese(II) monohydroxide ion (+1)	2.33543e-9	2.33543e-9	0.0
Manganese(II) sulfate	1.44122e-8	1.44122e-8	0.0
Sodium boron hydroxide	5.64793e-8	5.64793e-8	0.0
Sodium bromide	9.60579e-8	9.60579e-8	0.0
Sodium carbonate ion(-1)	8.07028e-7	8.07028e-7	0.0
Sodium bicarbonate	3.94215e-5	3.94215e-5	0.0
Sodium ion(+1)	0.0270273	0.0270273	0.0
Sodium sulfate ion(-1)	6.25311e-5	6.25311e-5	0.0
Lead(II) bromide	6.84246e-19	6.84246e-19	0.0
Lead(II) tribromide ion(-1)	3.10115e-21	3.10115e-21	0.0
Lead(II) monobromide ion(+1)	1.22946e-14	1.22946e-14	0.0
Lead(II) chloride	9.16822e-14	9.16822e-14	0.0
Lead(II) trichloride ion(-1)	1.24142e-15	1.24142e-15	0.0
Lead(II) tetrachloride ion(-2)	3.67091e-17	3.67091e-17	0.0
Lead(II) monochloride ion(+1)	1.26824e-12	1.26824e-12	0.0
Lead(II) carbonate ion (-2)	8.97937e-12	8.97937e-12	0.0
Lead(II) carbonate (cerussite)	1.10549e-10	1.10549e-10	0.0

Lead(II) ion(+2)	3.2347e-12	3.2347e-12	0.0
Lead(II) oxide yellow	1.41713e-13	1.41713e-13	0.0
Lead(II) monohydroxide ion(+1)	2.97802e-10	2.97802e-10	0.0
Lead(II) sulfate	2.16518e-13	2.16518e-13	0.0
Sulfur trioxide	5.90426e-33	5.90426e-33	0.0
Sulfate ion(-2)	5.40094e-4	5.40094e-4	0.0
Strontium ion(+2)	1.99268e-5	1.99268e-5	0.0
Strontium monohydroxide ion(+1)	1.16058e-10	1.16058e-10	0.0
Strontium sulfate	4.89327e-7	4.89327e-7	0.0
Zinc bromide	5.04475e-18	5.04475e-18	0.0
Zinc tribromide ion(-1)	2.01538e-21	2.01538e-21	0.0
Zinc bromide ion(+1)	4.5173e-13	4.5173e-13	0.0
Zinc chloride	1.38747e-11	1.38747e-11	0.0
Zinc trichloride ion(-1)	1.3123e-13	1.3123e-13	0.0
Zinc chloride ion(+1)	6.29313e-10	6.29313e-10	0.0
Zinc bicarbonate ion(+1)	4.48424e-10	4.48424e-10	0.0
Zinc ion(+2)	2.86602e-8	2.86602e-8	0.0
Zinc hydroxide, amorphous	1.5599e-9	1.5599e-9	0.0
Zinc trihydroxide ion(-1)	2.7165e-12	2.7165e-12	0.0
Zinc tetrahydroxide ion(-2)	8.82792e-17	8.82792e-17	0.0
Zinc monohydroxide ion(+1)	3.09396e-9	3.09396e-9	0.0
Barium sulfate	5.04236e-7	0.0	5.04236e-7
Vanadium	2.45379e-7	0.0	2.45379e-7
Total (by phase)	54.1605	54.1595	9.88948e-4

Element   Balance
Row   Filter   Applied: Only   Non   Zero   Values
column Filter Applied: Only Non Zero Values

	Total	Aqueous	Solid
	mol	mol	mol
H(+1)	108.205	108.205	5.99767e-7
K(+1)	7.87758e-4	7.87758e-4	0.0
Na(+1)	0.0271302	0.0271302	0.0
Ba(+2)	1.24727e-6	7.43033e-7	5.04236e-7
Ca(+2)	1.55777e-3	5.69767e-4	9.87998e-4
Zn(+2)	3.44089e-8	3.44089e-8	0.0
Fe(+2)	1.03542e-5	1.03542e-5	0.0

Mg(+2)	3.85847e-4	3.85847e-4	0.0
Pb(+2)	4.22297e-10	4.22297e-10	0.0
Al(+3)	3.05765e-7	1.05842e-7	1.99922e-7
Mn(+2)	5.0466e-7	5.0466e-7	0.0
O(-2)	54.1116	54.1086	2.96661e-3
Cl(-1)	0.0270197	0.0270197	0.0
Br(-1)	1.11681e-4	1.11681e-4	0.0
C(+4)	2.49621e-3	1.50822e-3	9.87998e-4
S(+6)	6.11886e-4	6.11382e-4	5.04236e-7
Sr(+2)	2.04163e-5	2.04163e-5	0.0
B(+3)	4.81992e-5	4.81992e-5	0.0
V(0)	2.45379e-7	0.0	2.45379e-7

A6. Documentation of steps for Initial GIS Tool (ArcGIS Explorer Online) use:

- Once you click on the link to the Larger Map, select the "Open this map in ArcGIS Explorer Online" Link on the left side of the map, below the description. (As shown below)

Figure 83. Screenshot of open Explorer step

- Now this map opens in the Explorer page. You have a set of tools which you can use to compare and view various characteristics as shown on the dashboard to your left.
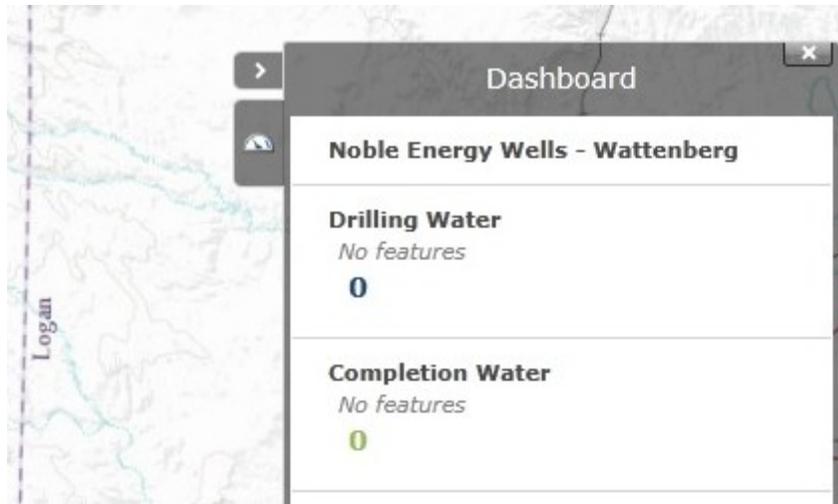
Figure 84. Screenshot of Dashboard Window

- To use these tools more specifically and effectively, click on the "Select Features" button in your Mapping Tab.
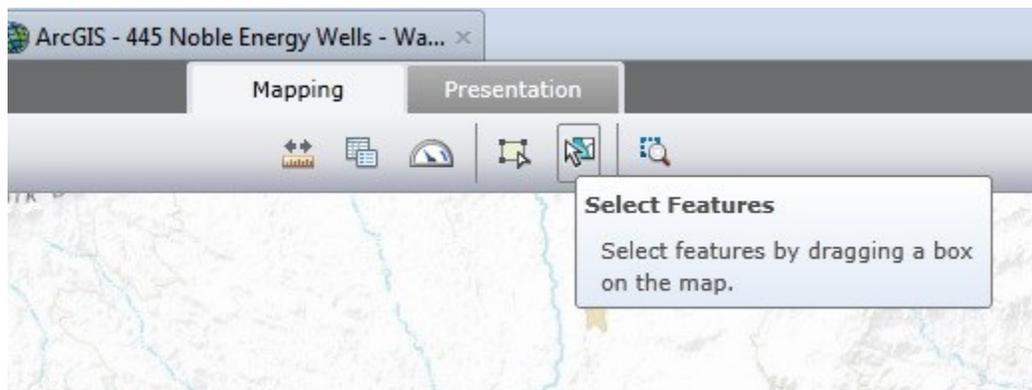
Figure 85. Screenshot of Select Features tool

- Once you click on the "Select Features" button, you will be able to select more than one well to view their characteristics and compare with the other wells. You can drag the cursor and choose any area desired.
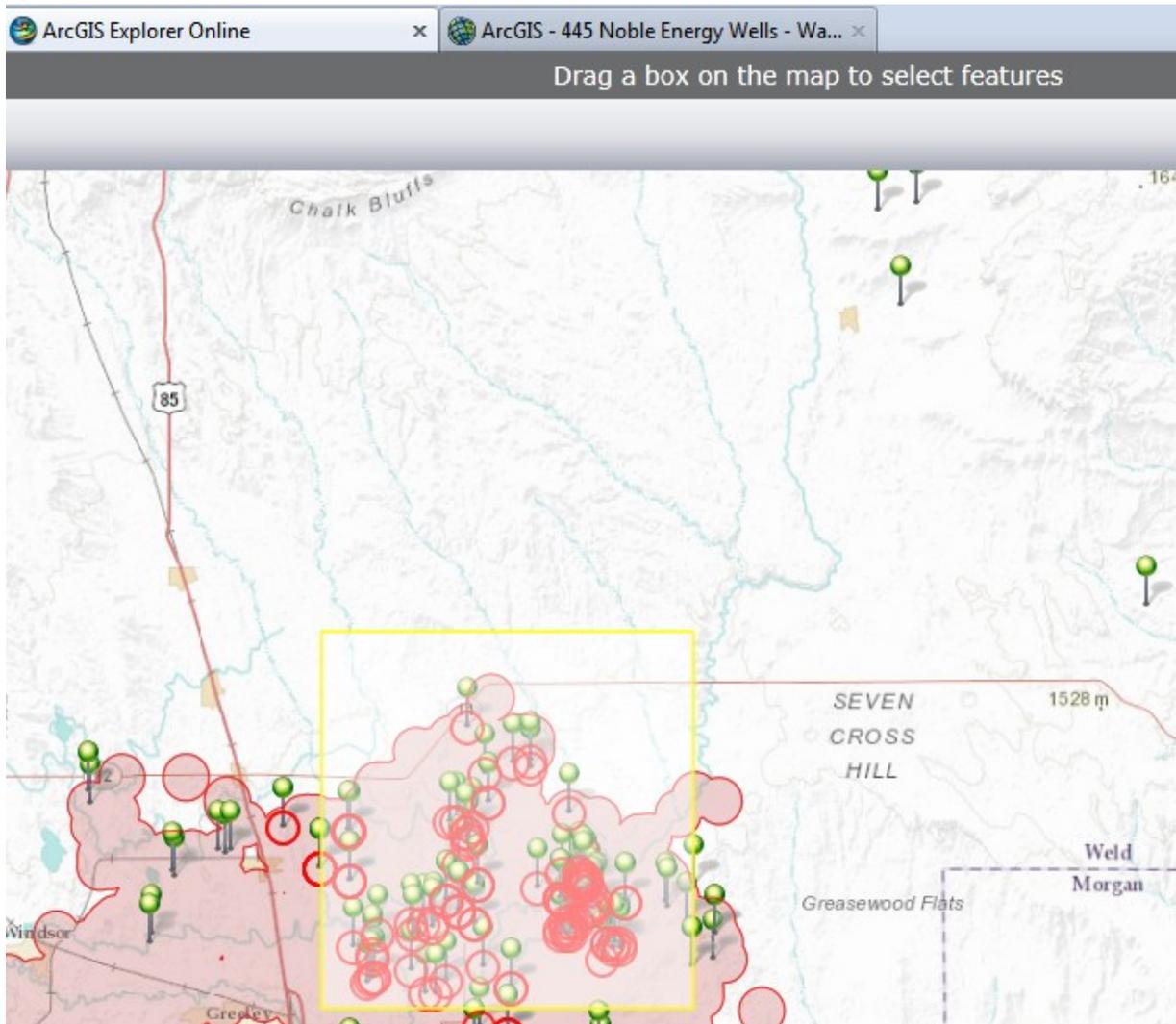
Figure 86. Screenshot of Selection step